SC-Database
Software version = 5.81 Data version = 4.62
Experiment list contains 3276 experiments for
 (no ligands specified)
 5 metals : Fe(0), Fe(IV), Fe+, Fe++, Fe+++
 (no references specified)
 (no experimental details specified)

****
CO L Carbon monoxide CAS 630-08-0 (551)
Carbon monoxide;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe(0) cal non-aq 25°C 100% U HM 1993NBa (2788) 1
Medium:Cyclohexane. K:FeL3A+L=FeL4A, A=PMe3 DH=-171.1 kJ mol-1. For A=PEt3
DH=-158.6. Data also for other phosphines

Fe(0) cal non-aq 25°C 100% U HM 1993NBa (2789) 2
Medium:Cyclohexane. K:FeL2A2+L=FeL3A2. A=PMe3. DH=-124.7 kJ mol-1.
For A=1,2-bis(dimethylphosphino)ethane DH=-151.0 Data for other phosphines
---
Fe(0) gl none 0°C 0.0 U M 1952HHb (2790) 3
K(HFeL4+H)=4.44
K(FeL4+H)=14.0
K(H2FeL4(s)=H2FeL4)=-2.96

Fe(0) gl oth/un 18°C var U M 1949KSa (2791) 4
K(HFeL4+H)=4.4
K(FeL4+H)=13.4
K(H2FeL4(s)=H2FeL4)=-2.74
****
CHO3F3S HL CAS 1493-13-6 (6755)
Trifluoromethanesulfonic acid; CF3SO3H

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe(0) cal non-aq 25°C 100% U HM 1992SZa (17462) 5
Medium: CH2Cl2. DH(Fe(CO)3A+HL=(Fe(CO)3AH)L(ion pair))=-100 kJ mol-1.
A=Ph2P(CH2)PPh2. DH values also for many other A ligands
****
C6H6 L Benzene CAS 71-43-2 (2143)
Benzene, cyclohexatriene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe(0) kin non-aq rt 100% U M 1993WMa (43166) 6
K(FeA2B+L=FeA2L+B)=0.677
Medium:Cyclohexane. A:Me2PCH2CH2PMe2. B:C6H12. For L=toluene K=0.52
****

OH- HL Hydroxide (57)
Hydroxide;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe(IV) sp NaCl 25°C 0.0 C T H 2001SBd (11316) 7
*K(HFeO4)=-7.227
Medium: 0.1-2.5 m NaCl containing 0.005 M Na2HPO4/0.001 M borate, pH 9.0.
Data extrapolated to I = 0.0. Metal ion is Fe(VI). DH(*K)=17.0 kJ mol-1.
****
C52H46N4O12S4 H4L (6861)
5,10,15,20-Tetrakis(2,6-dimethyl-3-sulfonatophenyl)porphin;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe(IV) vlt NaNO3 ? 0.20M C 1991KZa (107475) 8
*K(FeL)=-5.7
*K(FeL(OH))=-9.0
****
e- HL Electron (442)
Electron;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+ EMF none 20°C 0.0 U 1957HCa (469) 9
K=-25.4(-740 mV)
K: 1/3Fe3(CO)12(s)+2e=Fe(-II)(CO)4--
****
CO L Carbon monoxide CAS 630-08-0 (551)
Carbon monoxide;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+ vlt non-aq 25°C 100% U M 1987SKa (2792) 10
K(FeP+2L)=6.29
K(FePCl+L)=4.85
P=tetraphenylporphyrin; Medium: CH2Cl2, 0.1 M Bu4NClO4
Constants determined by cyclic voltammetry
****
C4H6N2 L 2-Me-Imidazole CAS 693-98-1 (122)
2-Methyl-1,3-diazole; C3H3N2.CH3

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+ vlt non-aq 20°C 100% U 1978KBb (29480) 11
K(Fe(phthalocyanine)+L)=1.08
Medium: DMSO
****
C5H5N L Pyridine CAS 110-86-1 (31)
Pyridine, Azine;

```
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe+        vlt non-aq 20°C 100%  U                         1978KBb (36623)  12
                                        K(Fe(phthalocyanine)+L)=1.16
Medium: DMSO
*******************************************************************************
C5H8N2                  L                      CAS 1759-84-0  (173)
1,2-Dimethylimidazole; C3H2N2(CH3)2
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe+        vlt non-aq 20°C 100%  U                         1978KBb (37624)  13
                                        K(Fe(phthalocyanine)+L)=0.90
Medium: DMSO
*******************************************************************************
C6H7N                   L    beta-Picoline    CAS 108-99-6  (324)
3-Methylpyridine; C5H4N.CH3
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe+        vlt non-aq 20°C 100%  U                         1978KBb (44698)  14
                                        K(Fe(phthalocyanine)+L)=1.08
Medium: DMSO
*******************************************************************************
e-                     HL    Electron           (442)
Electron;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe++       vlt non-aq 20°C 100%  U                         1993BGa   (470)  15
E(2e + FeC10H10-x(Cl)x+)=1.246, 0.774, 0.315 and 0.168V (vs ferrocenium/
ferrocene) for x=10, 5, 2 and 1 respectively.  Medium: MeCN, 0.1 M Bu4NBF4.
-------------------------------------------------------------------------------
Fe++       sol NaClO4 50°C 1.00M U                         1982GRd   (471)  16
                                        E(Fe+2e=Fe(s))=-425.6 mV
From the reaction Fe(s)+2Tl(I)=Fe(II)+2Tl(s).
-------------------------------------------------------------------------------
Fe++       oth none   50°C 0.00  U T                      1972LEc   (472)  17
                                        K=-13.04(-418mV,50C)
K: Fe++ + 2e=Fe(s). K=-8.41(-353mV,150 C), -6.26(-325mV,250 C),        -5.44
(-336mV,350 C). Method: combination of thermodynamic data
-------------------------------------------------------------------------------
Fe++       oth none   50°C 0.00  U T                      1972LEc   (473)  18
                                        K=16.00(513mV,50 C)
K: HFeO2- +3H + 2e=Fe(s)+2H2O. K=14.20(596mV,150 C), 12.99(674mV,250 C),
11.99(741mV,350 C). Method: combination of thermodynamic data
-------------------------------------------------------------------------------
Fe++       oth none   50°C 0.00  U T                      1972LEc   (474)  19
                                        K=-0.97(-31mV,50 C)
```

K:Fe(OH)2(s)+2H + 2e=Fe(s)+2H2O. K=0.48(20mV,150 C), 0.92(48mV,250 C), 0.79 (49mV,350 C). Method: combination of thermodynamic data

---

Fe++ cal none 25°C 0.00 U H 1970IWa (475) 20
DH(Fe++ + Fe(CN)6--- = Turnbull's blue)=-63.6 kJ mol-1. (Fe+++ + Fe(CN)6---- = Prussian blue)=2.9

Fe++ oth none 25°C 0.0 M H 1968LCd (476) 21
K(Fe+2e=Fe(s))=-15.99(-473 mV)
DH=92.3 kJ mol-1

Fe++ cal none 25°C 0.0 M H 1968SCd (477) 22
DH(2Fe + H2O2 + 2H = 2Fe+++ + 2H20) = -291.8 KJ mol-1

Fe++ oth none 25°C 0.0 U 1966SIa (478) 23
K=33.21 ?
K: Fe3O4 + 8H + 2e = 3Fe + 4H2O. By potential measurements, K=40.77, 1206 mV or 41.58, 1230 mV

Fe++ cal none 25°C 0.0 U H 1960HSb (479) 24
DH(Fe(CN)6+0.5Br2(l)=Fe(III)(CN)6+Br)=-17.6 kJ mol-1

Fe++ EMF none 20°C 0.0 U 1960HUa (480) 25
K(Fe+2e=Fe(s))=-16.06(-467 mV)

Fe++ EMF none 25°C 0.0 U 1932RFa (481) 26
K(Fe+2e=Fe(s))=-14.89(-440.2mV

Fe++ EMF none 25°C 0.0 U 1932RFa (482) 27
K=-29.6(-973 + 98 mV)
K: Fe(OH)2(s)+2e=Fe(s)+2OH

Fe++ EMF oth/un 30°C 40% U T 1920GGa (483) 28
K=-28.4(-855 mV)
Medium:40% w/w NaOH. K: Fe+2e=Fe(s). At 80 C: K=-24.4(-855 mV)

****

AsO2- HL Arsenite CAS 14102-45-5 (2616)
Arsenite; As(OH)4- or AsO2-

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	kin	oth/un	25°C	?	U	HM	K(FeA+L=FeAL)=-0.05	1994LCa (1083)	29

A=Desulfoviridin. DH(FeA+L)=-50.6 kJ mol-1, DS(FeA+L)=-113 J K-1 mol-1

****

AsO4--- H3L Arsenate CAS 7778-39-4 (1557)
Arsenate;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo

```
Fe++       oth none   25°C  0.0  M                        1997SAb  (1140)  30
Ks(Fe3(AsO4)2(s)+2H=3Fe+2HAsO4)=-18.  Calculated from thermodynamic data.
--------------------------------------------------------------------------
Fe++       oth oth/un 25°C  0.0  U                        1990SAa  (1141)  31
                                        *K(Fe3L2(s)+2H=3Fe+2HL)=-11.41
Calculated from thermodynamic data.
--------------------------------------------------------------------------
Fe++       sp  oth/un 25°C  1.0M U                        1966WOa  (1142)  32
                                        K1eff=0.28 in 1 M H2SO4
**************************************************************************
AsW11O39-------       H7L                        (2468)
alpha-Heteromonoarseno-polytungstate;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe++       gl  NaNO3  25°C 1.00M U        K1=3.62        1984COa  (1177)  33
**************************************************************************
As2W17H2O61--------   H8L                        (2469)
alpha-Heteropolydiarseno-polytungstate;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe++       gl  NaNO3  25°C 1.00M U        K1=8.20        1984COa  (1187)  34
                                        K1=5.00 (alpha2 isomer)
**************************************************************************
BO4H4-                 HL    Borate           CAS 10043-35-3  (991)
Borate; B(OH)4-
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe++       kin NaCl   25°C  1.0M C        K1=3.2         1989MIb  (1306)  35
Medium: 1.0 M NaCl/NaB(OH)4.
**************************************************************************
Br-                    HL    Bromide          CAS 10035-10-6  (19)
Bromide;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe++       sp  non-aq 25°C 100%  U    M                   1991STa  (1923)  36
                                        K(FeA2B2+L=FeA2BL+B)=-1.0
Medium: MeCN(B). A=dimethylglyoximedifluoroborate
--------------------------------------------------------------------------
Fe++       cal KNO3   25°C 0.50M U   H                   1985BPb  (1924)  37
                                        B4=-8.6
DH(B4)=47.7 kJ mol-1; TDS(B4)=-1.7 kJ mol-1
--------------------------------------------------------------------------
Fe++       sol NaCl   25°C 0.50M U    M                  1980PGa  (1925)  38
                                        Kout(FeA3+Br=FeA3Br)=0.62
                                        Kout(FeA3Br+Br=FeA3Br2)=0.42
                                        Kout(FeA3Br2+Br=FeA3Br3)=0.43
```

A:2,2'-dipyridyl. Medium: 0.5 M NaClO4/NaCl

Fe++ sp non-aq 25°C 100% U K1=5.5 1970KLb (1926) 39

Medium: MeCN, 0.01 M Bu4NClO4

****

CN- HL Cyanide CAS 74-90-8 (230)

Cyanide;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	sp	non-aq	25°C	100%	U			1998BEa (2661)	40
							K(FeP(dmso)2+L=FeP(dmso)L)=3.6		
							K(FeP(dmso)+L=FePL+dmso)=2.83		

Medium: dmso. FeP: phthalocyaninatoiron(II)

Fe++	kin	oth/un	25°C	?	U	HM		1994LCa (2662)	41
							K(FeA+L=FeAL)=-0.59		

A=Desulfoviridin. DH(FeA+L)=-48.1 kJ mol-1, DS(FeA+L)=-92.0 J K-1 mol-1

Fe++	sp	non-aq	25°C	100%	U			1993NYa (2663)	42
							K(FeP(S)2+L=FePSL+S)=3.48		
							K(FePSL+L=FePL2+S)=2.76		

Medium(S):dimethylsulfoxide. P:phthalocyanine.

Fe++	sp	non-aq	25°C	100%	U	M		1991STa (2664)	43
							K(FeA2B2+L=FeA2BL+B) > 5		

Medium: MeCN(B). A=dimethylglyoximedifluoroborate

Fe++	EMF	oth/un	25°C	0.0	U			1972SPa (2665)	44
							B6=32.5		

Solubility also used

Fe++	sp	oth/un	0°C	var	U			1970EJb (2666)	45
							K(Fe2(CN)10+Fe2L10=2Fe2L10)=5		

Fe++	cal	oth/un	25°C	0.0	U	H		1965WCa (2667)	46
							B6=35.4		

DH(B6)=-358.5 kJ mol-1. B6 also given as 36.9 by thermoduynamic calculations

---

Fe++	vlt	oth/un	10°C	dil	U			1964EMa (2668)	47
							K(2FeL5H2O=Fe2L10+2H2O)=2		

Fe++	cal	oth/un	25°C	var	U	H		1964GHc (2669)	48

DH(B6)=-308.1 kJ mol-1

Fe++	cal	oth/un	25°C	?	U	H		1961GUa (2670)	49

DH(B6)=-321.7 kJ mol-1

Fe++	oth	none	25°C	0.0	U			1956SMa (2671)	50
							B6=24		

Method: combination of thermodynamic data

Fe++ kin oth/un 20°C var U 1955ELa (2672) 51
K6=8.30

Fe++ kin oth/un ??? ? U 1953EMa (2673) 52
K6=ca.9

Fe++ cal oth/un ??? ? U H 1951YAa (2674) 53
DH(B6)=-281.2 kJ mol-1

****

CO L Carbon monoxide CAS 630-08-0 (551)
Carbon monoxide;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	sp	non-aq	25°C	100%	U		1998BEa (2793)	54	
							K(FeP(dmso)2+CO)=4.04		

Medium: dmso. FeP: phthalocyaninatoiron(II)

Fe++ kin non-aq 25°C 100% U T HM 1994BGb (2794) 55
K(FeAB+L)=2.62
Medium:Toluene. T:-20 to 25C. A:(OC2O)-linked capped porphyrin
B:1-Methylimidazole. DH=-24.3 kJ mol-1; DS=-121

Fe++ sp non-aq 20°C 100% U T HM 1994DJa (2795) 56
Medium: Toluene. K: FeAB+L(g). H2A: (1,4-dibutyldurene)-capped porphyrin.
B: Dicyclohexylimidazole. Data for T=0-30 C. DH=-39.3 kJ mol-1; DS=48.5

Fe++ sp non-aq 20°C 100% U T HM 1994DJa (2796) 57
Medium: Toluene. K: FeAB+L(g). H2A: (1,4-dibutyldurene)-capped porphyrin.
B: 1,2-Dimethylimidazole. T: 0-30 C. DH=-57.3 kJ mol-1; DS=-135.6

Fe++ sp non-aq 20°C 100% U M 1994TLb (2797) 58
K(FeAB+L)=10.63
Additional method:kinetics. Medium:Toluene. A:heme model (hybrid model TPP
derivative, n=10). B:1,2-Dimethylimidazole. Also models with n=6, 7 and 8.

Fe++ sp non-aq 20°C 100% U M 1993PMa (2798) 59
K(FeACD+L=FeACL+D)=-0.19
K(FeBCD+L=FeBCL+D)=-1.36
K(FeADE+L=FeAEL+D)=-0.55
K(FeBDE+L=FeBEL+D)=-1.48
In toluene. A=Tetramesitylporphine, B=Tetraphenylporphine, C=Methylimidazole
D=Tosylmethylisocyanide. Data also for other substituted A and B.

Fe++ EMF non-aq 22°C 100% U 1992PMa (2799) 60
K((FeL2A)2=2FeL2A)=-18.40
Metal:Fe+. Medium: MeCN, 0.1 M Bu4NPF6. A=C5H5. Dimer-monomer equilibrium

---

```
Fe++       sp  non-aq 25°C 100%  U                        1991KHb  (2800)  61
                                      K(FeP+CO)=6.8
FeP=5,10,15,20-tetrakis(2,6-di-tert-butylacetoxyphenyl)porphyrinatoiron(II)
-------------------------------------------------------------------------------
Fe++       oth non-aq 25°C 100%  U    M                   1989UKa  (2801)  62
                                      K(FeAB+L)=1.08
A=5,15-Diphenyl-10a,20a-bis(nonanediamidodi-o-phenylene)porphyrin
B=1,2-Dimethylimidazole. Medium: toluene. Data for other similar porphyrins
-------------------------------------------------------------------------------
Fe++       sp  oth/un 25°C    ?  U                        1987NHa  (2802)  63
At pH 7.4. Keff(Porphyrinatoiron+L)=5.70, Keff(red blood cell+L)=5.57
-------------------------------------------------------------------------------
Fe++       sp  non-aq 20°C 100%  U                        1985PEb  (2803)  64
                                      K(FeABS+L=FeABL+S)=4.96
Medium (S): DMSO. A=phthalocyanin. B=Pyridine
-------------------------------------------------------------------------------
Fe++       kin mixed  25°C  50%  U                        1984TNa  (2804)  65
                                      K(FeAB+L)=4.40
Medium:50% ethylene glycol/H2O,pH10.A=heme;B=poly(2-methyl-1-vinylimidazole)
-------------------------------------------------------------------------------
Fe++       sp  non-aq 20°C 100%  U T  M                   1981EMa  (2805)  66
                                      K(FeA+CO=Fe(CO)A)=4.013
A=Phthalocyanin. Temperature range: 20-53.5 C
-------------------------------------------------------------------------------
Fe++       sp  non-aq 23°C 100%  U    M                   1977JRa  (2806)  67
                                      K(X2FeA+L=XFeAL+X)=3.37
Medium: Toluene. A=Octamethyltetrabenzoporphyrin, X= Piperidine.
For X=pyridine, K=2.32
-------------------------------------------------------------------------------
Fe++       sp  non-aq 23°C 100%  U    M                   1977JRa  (2807)  68
                                      K(X2FeA+L=XFeAL+X)=2.41
Medium: Toluene. A=Octamethyltetrabenzoporphyrin, X=1-Methyl-imidazole.
-------------------------------------------------------------------------------
Fe++       EMF NaClO4 20°C  1.0M U                       1971GKc  (2808)  69
                                      K(H+Fe(CO)4)=12.68
                                      K(H+HFe(CO)4)=4.00
-------------------------------------------------------------------------------
Fe++       con non-aq   ?  100%  U                       1971JGa  (2809)  70
                                      K((SiCl3)2Fe(CO)C5H5+H)=2.6
Medium: MeCN. Method: NMR also used
*******************************************************************************
CO3--                  H2L    Carbonate        CAS 465-79-6  (268)
Carbonate;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe++       oth none   25°C  0.0  M                       2002PGa  (3218)  71
                                      Kso(FeCO3)=-10.59
                                      *Kso(FeCO3)=7.56
Method:evaluation of published solubility data by application of Davies
```

equation. K1=5.3, B2=7.1 assumed. FeCO3 is siderite.

Fe++	sol	NaCl	25°C	0.10M	C	K1=5.41 Kso(FeCO3)=-10.22 Ks(FeCO3+2H=Fe+CO2(g))=-7.26	2002SLa	(3219) 72

Method: solubility of siderite (FeCO3) in 0.1-5.5 m NaCl at constant p(CO2). At I=0, K1=6.30, Kso=-10.9.

Fe++	oth	oth/un	25°C	0.72M	C	K1=3.65 B2= 5.19 K(Fe+HCO3)=0.58	1995MYa	(3220) 73

By extrapolation of literature data using Pitzer equations.

Fe++	sol	NaClO4	25°C	1.00M	C	K1=4.13 B2=5.73 K(FeL(s)=Fe+L)=-9.45	1992BWa	(3221) 74

Solubility study of siderite (FeCO3)suspensions. Constants at I=0 also given

---

Fe++	oth	oth/un	25°C	0.0	C H	K1=4.73 K(Fe+HCO3)=2.17	1984FCa	(3222) 75

K(Fe+HCO3) calc using electrostatic model. K1 from oxalate correlation. DH(K1)=-0.3 kJ mol-1, DH(Fe+HCO3)=4.4 (from DS calc by electrostat model)

Fe++	EMF	none	25°C	0.0	U	K1=<5 Kso=-10.24	1970SSc	(3223) 76

Fe++	oth	none	50°C	0.0	U T	Kso=-11.04	1969HEa	(3224) 77

Method: Estimated data. Temp. range 50-300 C,(siderite). Kso=-11.21(60C); -11.95(100 C); -12.86(150 C); -14.05(200 C); -15.32(250 C); -16.67(300 C)

Fe++	sol	none	30°C	0.0	U	Kso(FeCO3(s))=-10.50	1935KAa	(3225) 78

I=0 corr. From thermodynamic data, 25 C: Kso=-10.68, K(FeCO3(s)+CO2(g)+H2O= Fe+2HCO3)=-8.19

Fe++	sol	none	30°C	0.0	U	Kso(FeCO3(s))=-10.46 +Kso=-6.58	1918SMa	(3226) 79

I=0 corr. +Kso: FeCO3(s)+H2CO3=Fe+2HCO3

****

CS3-- H2L CAS 549-08-1 (936)
Trithiocarbonate;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	sp	oth/un	?	?	U		B2=9.3	1957BIa (3466)	80

****

C6N6Fe---- H4L (2191)
Hexacyanoferrate (II); Fe(II)(CN)6----

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo

```
--------------------------------------------------------------------------------
Fe++       sol none   25°C 0.00  U                        1972SPa  (3566)  81
                                        Kso=-14.14
********************************************************************************
Cl-                    HL    Chloride         CAS 7647-01-0  (50)
Chloride;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       sol NaCl   250°C 0.10M M TI     K1=1.2    B2=1.6    1994OHa  (4825)  82
Constants at I=0. Pyrite and pyrrotite solubility measurements.
I=0-4 M NaCl and 250-350 C
--------------------------------------------------------------------------------
Fe++       sol NaCl   400°C  var  C TI     K1=4.6    B2=7.51   1992DSa  (4826)  83
I=0.03 to 1.24 M Cl-. 200-450 C, P=300-500 bar. Constants at I=0
--------------------------------------------------------------------------------
Fe++       sol KCl    300°C  var  U TI     K1=2.02   B2=3.75   1992FHa  (4827)  84
I=0.01-2.0 M KCl, 0.5-2.0 kbar, 300-600 C. Constants at I=0
--------------------------------------------------------------------------------
Fe++       sp  non-aq 25°C 100%  U    M                1991STa  (4828)  85
                                        K(FeA2B2+L=FeA2BL+B)=1.0
Medium: MeCN(B). A=dimethylglyoximedifluoroborate
--------------------------------------------------------------------------------
Fe++       sp  oth/un 25°C  var  U TI     K1=-0.16       1990HSa  (4829)  86
25-200 C, I=0.01 to 3.4 M Cl-. Constants at I=0
--------------------------------------------------------------------------------
Fe++       kin NaCl   25°C  5.0M C        K1=0.08        1989MIb  (4830)  87
--------------------------------------------------------------------------------
Fe++       sol NaCl   25°C 0.50M U    M                1980PGa  (4831)  88
                                        Kout(FeA3+Cl=FeA3Cl)=0.4
A:2,2'-dipyridyl;  Medium: 0.5 M NaClO4/NaCl
--------------------------------------------------------------------------------
Fe++       kin non-aq 25°C 100%  U        K1=1.3         1973UWa  (4832)  89
                                        K(FeCl(DMSO)+H)=0.7
Medium: DMSO, 0.2 M HClO4
--------------------------------------------------------------------------------
Fe++       vlt non-aq 99°C 100%  U                       1971TEb  (4833)  90
                                        K(FeL2(s)=FeL+L)=-9.5
Medium: SbCl3. method: current-voltage studies
--------------------------------------------------------------------------------
Fe++       sp  non-aq 25°C 100%  U        K1=5.8         1970KLb  (4834)  91
Medium: MeCN, 0.01 M (C4H9)4NClO4
--------------------------------------------------------------------------------
Fe++       kin NaClO4 25°C  1.0M U        K1=0.78        1969WEb  (4835)  92
--------------------------------------------------------------------------------
Fe++       sp  NaClO4       1.0M U        K1=<-0.3       1968PSd  (4836)  93
--------------------------------------------------------------------------------
Fe++       EMF NaClO4 20°C  2.0M U        K1=0.36   B2=0.40   1943OLa  (4837)  94
********************************************************************************
ClO4-                  HL    Perchlorate      CAS 7001-90-3  (287)
```

Perchlorate;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ dis oth/un 25°C 0.25M C H 1984PSc (6235) 95
Kout(Fe(phen)3+L)=2.73
Medium: 0.25 M NaF;Also Kout=2.95 in 0.5 M NaF, 3.18 in 0.75 M NaF;
Phen: phenantroline; for 0.25 M Na2SO4 Kout=3.00, for 0.5 M 2.36;

Fe++ con non-aq 25°C 100% U I 1983IMa (6236) 96
K1out(Fe(phen)3+L)=3.95
K2out(Fe(phen)3L+L)=2.18
Medium: 50% w/w CCl4/nitrobenz. Data for 0 - 55%

Fe++ sol NaCl 25°C 0.50M U M 1980PGa (6237) 97
Kout(FeA3+L=FeA3L)=1.18
Kout(FeA3L+L=FeA3L2)=0.89
A:2,2'-dipyridyl; Medium: 0.5 M NaClO4/NaCl

Fe++ ISE none 25°C 0.0 U T 1968HRb (6238) 98
Kso(FeA3L2(s)=FeA3+2L)=-7.65
A=1,10-phenantroline. Kso=-7.76(15 C), -7.40(35 C). Method: ClO4 ISE

Fe++ ix oth/un ? var U K1=-0.9? 1960BHc (6239) 99
****
F- HL Fluoride CAS 7644-39-3 (201)
Fluoride;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ ISE R4N.X 25°C 0.05M U I K1=1.45 1983SBa (6866) 100
Medium: 0.05 M Et4NF. In MeOH, 0.05 Et4NF, K1=3.79

Fe++ ISE NaClO4 25°C 1.0M U K1=0.83 1972BHc (6867) 101
****
GeW11O39-------- H8L CAS 37369-86-1 (2466)
alpha-Heteromonogermanium-polytungstate;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl NaNO3 25°C 1.00M U K1=6.12 1984COa (7469) 102
****
I- HL Iodide CAS 10034-85-2 (20)
Iodide;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ sol NaCl 25°C 0.50M U M 1980PGa (8023) 103
Kout(FeA3+I=FeA3I)=0.95
Kout(FeA3I+I=FeA3I2)=0.77

A:2,2'-dipyridyl; Medium: 0.5 M NaClO4/NaCl

Fe++ sp non-aq 25°C 100% U K1=4.3 1970KLb (8024) 104

Medium: MeCN, 0.01 M Bu4NClO4

****

NH3 L Ammonia CAS 7664-41-7 (414)

Ammonia

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	sol	none	25°C	0.0	C				1998ZJa (9147)	105
							K(Fe(OH)+L)=3.44			
Fe++	gl	alc/w	25°C	2.0M	U	I	K1=1.82	B2= 3.10	1992MPb (9148)	106
							K3=0.87			
							for 100% H2O K1=1.53			
							for 100% H2O K2=0.98			
							for 100% H2O K3=0.56			

Medium: 2.0 M NH4NO3 in 50% v/v EtOH in H2O

Fe++	cal	oth/un	25°C	2.0M	C		K1=1.6	B2= 2.60	1992MPc (9149)	107
							K3=0.5			
							K4=0.2			

Medium: 2.0 M NH4NO3;

Corresponding DH: -8.1; -7.9; -8.0; -7.5 kJ mol-1

Fe++	gl	diox/w	25°C	2.0M	U		K1=1.85	B2= 3.15	1992MSc (9150)	108
							K3=0.89			
							K1=1.53 (100%H2O)			
							K2=0.98 (100% H2O)			
							K3=0.56 (100%H2O)			

Medium: NH4NO3 in 50% v/v dioxane/H2O; for 20% K1=1.69; K2=1.16, K3=0.66

For 2 M NH4NO3 in50%v/v acetone/H2O K1=1.83; K2=1.31; K3=0.85

Fe++ gl R4N.X 25°C 5.00M U K1=1.4 1985MMa (9151) 109

Fe++	sol	none	25°C	0.0	U				1953LKa (9152)	110
							B4=ca.3.7			

I=0 corr.

****

NH3O L Hydroxylamine; CAS 5470-11-1 (1808)

Hydroxylamine; NH2.OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	kin	oth/un	25°C	?	U	HM			1994LCa (9263)	111
							K(FeA+HL=FeAHL)=1.77			

A=Desulfoviridin. DH(FeA+HL)=39.7 kJ mol-1, DS(FeA+HL)=156.9 J K-1 mol-1

****

NO L Nitric oxide CAS 10102-43-9 (850)

Nitric oxide;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	ISE	NaClO4	25°C	0.50M	C	M	K1=3.06 K(Fe(edta)+L)=6.31 K(Fe(hpdta)+L)=5.0 K(Fe(egta)+L)=3.89 K(Fe(edda)+L)=5.52	2001SFa	(9294) 112
Method: NO membrane electrode. Medium pH 5.0. K(Fe(edtp)+L)=3.15. Data for many related complexones.									
Fe++	ISE	NaClO4	25°C	0.50M	C	M	K(Fe(dtpa)+L)=6.48 K(Fe(ida)+L)=4.08 K(Fe(mida)+L)=3.98 K(Fe(nta)+L)=6.24	2001SFa	(9295) 113
Method: NO membrane electrode. Medium pH 5.0. Data for many related complexones.									
Fe++	ISE	NaClO4	23°C	0.50M	C	M	K(FeA+L)=3.04 K(FeB+L)=4.04 K(FeC+L)=3.11 K(FeD+L)=4.32	2001SFa	(9296) 114
Method: NO membrane electrode. Medium pH 5.0. H2A is glutaric acid, H2B is dipicolinic acid, H2C is L-tartaric acid, H3D is citric acid.									
Fe++	sp	non-aq	20°C	100%	U		K1=6.041	1987ABa	(9297) 115
Metal = phthalocyanatoiron(II), solvent = DMSO									
Fe++	sol	oth/un	25°C	aq	U		K1=2.67	1982LCa	(9298) 116
Fe++	kin	oth/un	25°C	0.50M	U		K1=2.65	1966KTb	(9299) 117
Fe++	nmr	oth/un	25°C	var	U	M	K(Fe2L4(HPO4)2+2HPO4)=0.15	1965MPa	(9300) 118
Fe++	oth	oth/un	25°C	0.0	U		Kp(Fe+NO(g))=-0.18	1961TAb	(9301) 119
Method: Chemical analysis									
Fe++	sol	alc/w	25°C	100%	U	T H	Kp(Fe+NO(g))=0.40	1958GLa	(9302) 120
Medium: EtOH. Kp=1.24(9.4 C), 0.59(21.4 C). DH=-85.4 kJ mol-1									
Fe++	sol	oth/un	25°C	0.03M	U	T H	Kp(Fe+NO(g))=-0.18	1924MHa	(9303) 121
Medium:Fe(NH4)2(SO4)2. Kp=0.61(0 C), 0.20(13 C); DH=-48 kJ mol-1									

****

NO2- HL Nitrite CAS 7782-77-6 (635)
Nitrite;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ kin oth/un 25°C ? U HM 1994LCa (9368) 122
K(FeA+L=FeAL)=-1.80
A=Desulfoviridin. DH(FeA+L)=9.2 kJ mol-1, DS(FeA+L)=108.8 J K-1 mol-1
****
N2H4 L Hydrazine CAS 302-01-2 (2117)
Hydrazine; H2N.NH2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ EMF oth/un 25°C var U K1=3.62 B2=6.47 1972AKb (10080) 123
K3=1.71
****
N3- HL Azide CAS 7782-79-8 (441)
Azide;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ kin oth/un 25°C ? U HM 1994LCa (10207) 124
K(FeA+L=FeAL)=1.49
A=Desulfoviridin. DH(FeA+L)=29.3 kJ mol-1, DS(FeA+L)=107.1 J K-1 mol-1

Fe++ oth none 25°C 0.0 U K1=0.69 1980GAa (10208) 125
K1 from the plot logK1 vs atomic no. for first transition series
****
OH- HL Hydroxide (57)
Hydroxide;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ oth oth/un 25°C 0.72M C 1995MYa (11317) 126
*K1=-9.88
*B2=-21.26
By extrapolation of literature data using Pitzer equations.

Fe++ con none 25°C 0.0 C 1988BOa (11318) 127
*K1=-9.63
Kso(Fe(OH)2)=-14.62
Ks(Fe(OH)2(s)=FeOH+OH)=-10.31
*Ks(Fe(OH)2+H=Fe(OH))=-3.75
Method: solubility of Fe in O2-free H2O.

Fe++ sol none 100°C 0.0 C T 1980TLa (11319) 128
*K1=-8.78
*B2=-17.15
*B3=-28.11

Method: solubility of magnetite under H2. Data for 100-300 C.

Fe++ gl none 25°C 0.0 M T 1978JBb (11320) 129
*K1=-9.23
Kso(Fe(OH)2)=-14.39
At 1 C: *K1=-9.75; 40 C: -8.87

Fe++ ix NaClO4 18°C 0.10M U K1=7.3 B2=13.3 1975IKa (11321) 130
B3=16.9

Fe++ oth none 50°C 0.00 U T 1972LEc (11322) 131
*K1=-7.97
*Kso=12.1
*K1=-4.67, *Kso=8.9(150 C). *K1=-2.79, *Kso=7.2(250 C).
*K1=-1.61, *Kso=6.2(350 C). Method: combination of thermodynamic data

---

Fe++ EMF none 25°C 0.00 U 1971MEa (11323) 132
*K1=-9.49

Fe++ kin NaClO4 25°C 0.50M U T 1970BSc (11324) 133
K(FeSO4+H2O=Fe(OH)SO4+H)=-1.4
15 C, K=-1.3; 35 C, K=-1.5

Fe++ sp R4N.X ? 2.00M U I 1970ELc (11325) 134
*K1=-8.30
Medium: (NH4)2SO4. For 2 M NaClO4, *K1=-8.07. K(FeOH+H2O=FeO(OH)+2H)=-25.7
at pH=ca.13

Fe++ EMF oth/un 25°C U 1970MEa (11326) 135
*K1=-9.58

Fe++ sol oth/un 25°C U 1970SBb (11327) 136
*K1=-9.3

Fe++ gl NaClO4 0°C 0.01M U TI 1968WSe (11328) 137
*K1=-4.6
*K1=-3..8(15 C), -3.3(25 C), -2.0?(35 C). By kinetics, 25 C: *B2=-7.96(I=4),
-6.35(I=1), -5.85(I=0)

Fe++ EMF oth/un 25°C U 1967MPa (11329) 138
*K1=-9.5

Fe++ kin NaClO4 25°C 1.00M U 1965WSb (11330) 139
*K1=-3.32 ?

Fe++ gl NaClO4 25°C 0.50M U T 1963BAc (11331) 140
*K1=-6.74
Medium: 0.5 to 2.2 M NaClO4; *K1=-6.93(20 C), -6.49(35 C), -6.34(40 C)

Fe++ gl none 20°C 0.0 M 1963DDa (11332) 141

```
                                        Kso=-15.82
                                        K(FeL2(s)=FeL+L)=-9.43
-------------------------------------------------------------------------------
Fe++       gl  NaClO4 25°C 1.00M U                    1963KOb (11333) 142
                                        *K1=-6.51
                                        *B2=-11.5
-------------------------------------------------------------------------------
Fe++       gl  NaClO4 12°C 1.00M U T                  1961BLa (11334) 143
                                        *K1=-8.50
*K1=-8.03(15 C), -7.15(20 C), -6.8(25 C), -5.95?(30 C)
-------------------------------------------------------------------------------
Fe++       gl  NaClO4 25°C  1.0M U T                  1961BOb (11335) 144
                                        *K1=-6.8(?)
*K1=-7.15(20 C)
-------------------------------------------------------------------------------
Fe++       gl  oth/un 25°C  dil  U  I                 1956GWa (11336) 145
                                        *K1=-7.92
Medium: FeCl2. In 0.5 M KCl *K1=-7.17
-------------------------------------------------------------------------------
Fe++       sol none   25°C  0.0  U                   1956GWb (11337) 146
                                        K(Fe(OH)2(s)+OH=Fe(OH)3)=-5.08
                                        K(Fe(OH)2(s)+2OH)=-5.54
-------------------------------------------------------------------------------
Fe++       gl  NaClO4 25°C  1.0M U                   1953HEa (11338) 147
                                        *K1=-9.5
-------------------------------------------------------------------------------
Fe++       sol none   25°C  0.0  U       K1=5.7      1953LKa (11339) 148
                                        Kso(Fe(OH)2)=-15.1
                                        K(Fe(OH)2(s)=FeOH+OH)=-9.4
                                        *K1=-8.3
-------------------------------------------------------------------------------
Fe++       EMF oth/un 20°C  var  U                    1951QUa (11340) 149
                                        Kso(Fe(OH)2)=-14.78
-------------------------------------------------------------------------------
Fe++       EMF none   18°C  0.0  U                   1950AFa (11341) 150
                                        Kso(Fe(OH)2)=-15.02
-------------------------------------------------------------------------------
Fe++       gl  oth/un 20°C  var  U                    1950ARa (11342) 151
                                        Kso(Fe(OH)2)=-13.62
                                        K=-17.2
K: K(Fe3(OH)8(s)=2Fe(OH)3(s)+Fe+2OH)
-------------------------------------------------------------------------------
Fe++       gl  oth/un 25°C  dil  U                    1938OKa (11343) 152
                                        Kso(Fe(OH)2)=-14.01
-------------------------------------------------------------------------------
Fe++       dis oth/un 20°C  var  U       K1=6.10      1933JEa (11344) 153
-------------------------------------------------------------------------------
Fe++       con oth/un 25°C  dil  U                    1932MUa (11345) 154
                                        Kso=-14.54 (conductivity)
                                        Kso=-14.81 (solubility)
```

```
                                        Kso=-14.67 (colorimetry)
-------------------------------------------------------------------------------
Fe++       con oth/un 25°C  dil  U                      1932RFa (11346) 155
                                        Kso(Fe(OH)2)=-14.01
-------------------------------------------------------------------------------
Fe++       EMF none   25°C  0.0  U                      1932RFa (11347) 156
                                        Kso(Fe(OH)2)=-14.84
-------------------------------------------------------------------------------
Fe++       gl  none     ?   0.0  U                      1930ELa (11348) 157
                                        Kso(Fe(OH)2)=-15.32
-------------------------------------------------------------------------------
Fe++       vlt oth/un   ?  1.37M U                      1929SCa (11349) 158
                                        Kso(Fe(OH)2)=-12.15
                                        K(Fe(OH)2(s)+OH=Fe(OH)3)=-4.3
                                        B3=7.85
-------------------------------------------------------------------------------
Fe++       EMF oth/un 17°C  var  C                      1925BRa (11350) 159
                                        Kso(Fe(OH)2)=-20.35
Method: H electrode
-------------------------------------------------------------------------------
Fe++       sol oth/un 25°C  dil  U       B2=9.17        1925WRa (11351) 160
                                        Kso(Fe(OH)2)=-13.50
                                        K(Fe(OH)2(s)=Fe(OH)2)=-4.33
-------------------------------------------------------------------------------
Fe++       EMF oth/un  rt   var  U                      1909KRa (11352) 161
                                        Kso(Fe(OH)2)=-13.06
-------------------------------------------------------------------------------
Fe++       oth oth/un 18°C  dil  U                      1908MUa (11353) 162
                                        Kso(Fe(OH)2)=-13.79
method:combination of thermodynamic data
*******************************************************************************
O2                      L    Oxygen           CAS 7782-44-7  (83)
Dioxygen, also oxide; O--, and superoxide, O2-
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe++       sp  non-aq -45°C 100%  C T HM                 1998SSe (12618) 163
                                        K(FeA+O2)=-1.08
Medium: CH2Cl2. HA is N,N,N',N'-Tetrakis[(1-methyl-4,5-diphenyl-
2-imidazolyl)methyl]-1,3-diamino-2-propanol. DH=-55 kJ mol-1, DS=-263.
-------------------------------------------------------------------------------
Fe++       sp  non-aq  0°C 100%  U T HM                 1994DJa (12619) 164
Medium: Toluene.  K: FeAB+L(g). H2A: (1,4-dibutyldurene)-capped porphyrin
B: 1,2-Dimethylimidazole. T: -50 to 0 C. DH=-54.8 kJ mol-1; DS=-190.4
-------------------------------------------------------------------------------
Fe++       sp  non-aq  0°C 100%  U T HM                 1994DJa (12620) 165
Medium: Toluene.  K: FeAB+L(g). H2A: (1,4-dibutyldurene)-capped porphyrin.
B: 1,2-Dicyclohexylimidazole. T: -50 to 0 C. DH=-64.0 kJ mol-1; DS=-207.1
-------------------------------------------------------------------------------
Fe++       kin non-aq 20°C 100%  U    M                 1994TLb (12621) 166
```

```
                                        K(FeAB+L)=4.72
Medium:Toluene. A:Heme Model (hybrid model of TPP derivative, n=10)
B:1,2-Dimethylimidazole. Also data for other heme models (n=6, 7 and 8)
-------------------------------------------------------------------------------
Fe++       oth non-aq 20°C 100%  U                      1993ETa (12622) 167
                                        K(FeBP+L)=3.26
P is a strapped ('encumbered') porphyrin; B: 1-Methylimidazole.  Data for a
series of related porphyrins with various adducts B.
-------------------------------------------------------------------------------
Fe++       sp  non-aq 25°C 100%  U                      1991KHb (12623) 168
                                        K(FeP+O2)=2.80
FeP=5,10,15,20-tetrakis(2,6-di-tert-butylacetoxyphenyl)porphyrinatoiron(II)
-------------------------------------------------------------------------------
Fe++       sp  mixed  -45°C    ?  U T HM               1991PJa (12624) 169
                                        K(FeA+L=FeAL)=-1.8
3:1:1 acetone:pyridine:H2O.A=3,11-Dibz-14,20,24,24-tetraMe-2,12-diPh-3,11,15
19,22,26-hexaazatricycloctacosa-1,5,7,9,12,14,19 etc. At -20 C, K=-0.68
-------------------------------------------------------------------------------
Fe++       oth non-aq 25°C 100%  U    M                 1989UKa (12625) 170
                                        K(FeAB+L)=-1.43
A=5,15-Diphenyl-10a,20a-bis(nonanediamidodi-o-phenylene)porphyrin
B=1,2-Dimethylimidazole. Medium: toluene. Data for other similar porphyrins
-------------------------------------------------------------------------------
Fe++       sp  oth/un 25°C    ?  U                    1987NHa (12626) 171
At pH 7.4. Keff(Porphyrinatoiron+L)=3.50, Keff(red blood cell+L)=4.83
-------------------------------------------------------------------------------
Fe++       kin mixed  25°C  50%  U                    1984TNa (12627) 172
                                        K(FeAB+L)=2.79
Medium:50% ethylene glycol/H2O,pH10.A=heme;B=poly(2-methyl-1-vinylimidazole)
*******************************************************************************
PO4---                H3L    Phosphate        CAS 7664-38-2  (176)
Phosphate;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe++       gl  NaClO4 25°C  3.0M C  I                   1992CIa (13170) 173
                                        K(Fe+H2L)=0.55
                                        K(Fe+2H2L)=1.82
                                        K(Fe+2H2L=FeHL+H3L)=-1.94
                                        K(Fe+3H2L=FeH3L2+H3L)=-1.61
At I=0 (using SIT): K(Fe+H2L)=1.01, K(Fe+2H2L)=2.71, K(Fe+HL)=4.08
K(Fe+HL+H2L)=4.38
-------------------------------------------------------------------------------
Fe++       sol none   25°C  0.0  U                    1972NRb (13171) 174
                                        K(Fe+H2L)=2.7
                                        K(Fe+HL)=3.6
Kso(Fe3L2(H2O)8)=-36.0(vivianite)
-------------------------------------------------------------------------------
Fe++       EMF oth/un 30°C  0.0  U T                  1964LAc (13172) 175
                                        K(Fe+HL)=7.34
```

Medium: 0 corr. K=7.03(20 C)
****
PW11O39------- H7L (2467)
alpha-Heteromonophospho-polytungstate;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference ExptNo
Fe++	gl	NaNO3	25°C	1.00M	U		K1=4.81	1984COa (13403) 176

****
P2O7---- H4L Pyrophosphate CAS 2466-09-3 (198)
Diphosphate; from (HO)2PO.O.PO(OH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference ExptNo
Fe++	vlt	oth/un	?	var	U			1963RKa (13585) 177

K(Fe(H2L)3+Fe=Fe(H2L)2+H2L+Fe)=-12.54
****
P2W17O61---------- Polytungstate (2102)
alpha-Heterodiphospho-polytungstate (usually alpha1 isomer)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference ExptNo
Fe++	gl	NaNO3	25°C	1.00M	U		K1=8.13	1984COa (13719) 178
							K1=5.30 (alpha2 isomer)	

****
P3O10----- H5L CAS 10380-08-2 (1001)
Tripolyphosphate; from (HO)2PO.O.PO(OH).O.PO(OH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference ExptNo
Fe++	kin	NaClO4	25°C	1.0M	U		K1=2.54	1968WSf (13857) 179
							K(Fe+H2L)=2.38	
							K(Fe+H3L)=2.12	

****
P3O9--- H3L CAS 13566-25-1 (235)
Cyclotrimetaphosphate;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference ExptNo
Fe++	kin	NaClO4	25°C	1.0M	U	TI	K1=1.15	1968WSf (13960) 180

K1=1.72(0 C),1.43(10 C); at I=1.8: K1=0.76(35 C)
At I=4: K(Fe+HL)=1.79(0 C),1.02(25 C),0.81(35 C),0.49(45 C)
****
P6O12------ H6L CAS 25268-83-1 (6590)
Dodecaoxohexaphosphate(III); anion of (PO.OH)6

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference ExptNo
Fe++	sp	KCl	25°C	0.50M	U	I	K1=5.13	1990NTa (14059) 181

Data also at I=1.0 M KCl: B1=5.11; 1.5 5.06; 2.0 5.07; 2.5 5.09; 3.0 4.97

****

S-- H2L Sulfide CAS 7783-06-4 (705)
Sulfide;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	kin	non-aq	25°C	100%	C			2001DEa (14350)	182
							*K(Fe4S4(u-HS)A)=-8.5		
Medium: methanol. HA is HS.CH2.(OH)CH3.									
Fe++	vlt	oth/un	25°C	0.72M	C	I		1999AVb (14351)	183
							K(Fe+HL)=6.1		
Method: determination of free S-- by cathodic stripping voltammetry. Medium: seawater, pH 8.0, S=35. Also data for S=21 and 10.5.									
Fe++	vlt	NaClO4	24°C	0.50M	C	I	K1=5.60	1999CRb (14352)	184
							B(Fe2(S5))=11.39		
Ligand is S5--. Method: polarography. Also data for 0.55 M NaCl.									
Fe++	gl	NaClO4	20°C	0.0	M			1999DPa (14353)	185
							K(Fe+HS)=3.76		
							K(Fe+2HS)=6.46		
Calculated from data at I=0.10 M NaClO4. K(FeS(s)+H=Fe+HS)=-3.00									
Fe++	vlt	oth/un	25°C	0.70M	C	I		1996LRb (14354)	186
							K(Fe+HS)=5.07		
							K(2Fe+HS)=10.07		
							K(3Fe+HS)=16.15		
Method: voltammetry at Hg/HgS electrode. Medium: seawater. Also data for 0.1 and 0.5 strength seawater									
Fe++	kin	oth/un	25°C	?	U	HM		1994LCa (14355)	187
							K(FeA+HL=FeAHL)=1.32		
A=Desulfoviridin. DH(FeA+HL)=-0.4 kJ mol-1, DS(FeA+HL)=30.5 J K-1 mol-1									
Fe++	sol	NaCl	250°C	0.10M	M	TI		1994OHa (14356)	188
							K(FeS2(s)+2H=Fe+H2S)=3.7		
							K(FeS(s)+2H=Fe+H2S)=2.9		
Constants at I=0. Pyrite and pyrrotite solubility measurements. I=0-4 M NaCl and 250-350 C									
Fe++	vlt	NaCl	25°C	?	U			1994ZMa (14357)	189
							K1eff=5.3		
Medium: sea water, pH=8. Method: cathodic stripping square wave voltammetry									
Fe++	vlt	oth/un	?	0.70M	C			1993LFa (14358)	190
							K(Fe+HS)=5.50		
							K(2Fe+HS)=11.08		
							K(FeHS+H)=5.14		
Method: voltammetry at Hg/HgS electrode. Medium: seawater. Also K(H+HS)=6.70									

```
--------------------------------------------------------------------------------
Fe++       oth none   25°C    0  U                        1991DAa (14359) 191
                                        *Ks(FeS(am))=-2.95
                                        *Ks(mackinawite,FeS)=-3.6
                                        *Ks(greigite,Fe3S4)=-4.4
                                        *Ks(pyrrhotite,FeS)=-5.1
Eval. lit data. *Ks(FeS):FeS(s)+H=Fe+HS. *K(Fe3S4): Fe3S4(s)+3H=3Fe+3HS+S(0)
*Ks(troilite)=-5.25, K(pyrite+H=Fe+HS+S(0))=-16.4. K(H+S=HS)=17.3 assumed
--------------------------------------------------------------------------------
Fe++       oth none     ?     0  U                        1990DKa (14360) 192
                                        *Ks(FeS+H=Fe+HS)=-4.16
                                        *Ks(FeS+HS=FeHS2)=-0.97
From recalculation of literature data.
--------------------------------------------------------------------------------
Fe++       oth none   25°C  0.0  C                        1989DYa (14361) 193
                                        K(Fe+HS=FeS+H)=-0.2
                                        *Kso(FeS)=-7.9
                                        Kso(FeS)=-8.1
Calculated from literature data, based on K(H+S)=17.0.
FeS is troilite.
--------------------------------------------------------------------------------
Fe++       oth none   25°C    0  U                        1988LIa (14362) 194
                                        Kso(FeS)=-21.0
                                        *Kso(FeS)=-3.7
                                        Kso(FeS2,pyrite)=-51.0
                                        *Kso(FeS2,pyrite)=-16.3
Derived from thermodynamic data and K(H+S=HS)=17.3.
Kso(FeS2,marcasite)=-50.3, *Kso(FeS2,marcasite)=-15.6.
--------------------------------------------------------------------------------
Fe++       oth none   25°C    0  U                        1988SBc (14363) 195
                                        Kso(FeS,troilite)=-26.01
Method: recalc. from literature data using K(H+S=HS)=18.57 and K(H+HS)=6.99.
--------------------------------------------------------------------------------
Fe++       dis oth/un 25°C 0.69M U                        1985DYa (14364) 196
                                        K(Fe+2H2S=FeHS2+3H)=-10.91
                                        K(Fe+2H2S=Fe(HS)2+2H)=-4.63
--------------------------------------------------------------------------------
Fe++       sol NaClO4 50°C 1.00M U   H                    1982GRd (14365) 197
                                        *Ks(troilite,FeS)=-3.66
                                        *Ks(pyrrhotite,hex)=-3.67
                                        *Ks(pyrrhotite,mono)=-3.65
*Ks: 1/(1-x)Fe(1-x)S(s)+2H=Fe+H2S(g)+x/(1-x)S(s). Hexagonal pyrrhotite:
FeS1.11. Monoclinic pyrrhotite: FeS1.14
--------------------------------------------------------------------------------
Fe++       gl  NaClO4 51°C  1.0M C                        1977HGc (14366) 198
                                        K(FeS(s)+2H=Fe+H2S(g))=3.80
Solid phase is Fe0.88S (monoclinic pyrrotite).
Reaction is: 1.14Fe0.88S(s)+2H=Fe+H2S(g)+0.14S(s)
--------------------------------------------------------------------------------
Fe++       oth none   25°C  0.0  U                        1964PCa (14367) 199
```

```
                                        K(FeL(s)+2H=Fe+H2L(g))=3.50
From thermodynamic data. Alternative value 3.90
-------------------------------------------------------------------------
Fe++       oth none   25°C  0.0  U T                    1959CZa (14368) 200
                                        Kso(FeL)=-17.29
From thermodynamic data. Kso=-15.90(100 C), -14.70(200 C), -13.42(400 C),
-12.70(600 C)
-------------------------------------------------------------------------
Fe++       oth none   25°C  0.0  U                      1957BAa (14369) 201
                                        Kso(FeL2)=-30.25
From thermodynamic data.
-------------------------------------------------------------------------
Fe++       oth none   25°C  0.0  U                      1952GGc (14370) 202
                                        Kso(FeL)=-17.3
From thermodynamic data
-------------------------------------------------------------------------
Fe++       sol oth/un 25°C  dil  U T                    1941TGa (14371) 203
                                        K(FeL(s)+2H=Fe+H2L(g))=4.44
At 14 C: K=3.96. From thermodynamic data K=2.99(25 C)
-------------------------------------------------------------------------
Fe++       oth none   25°C  0.0  U                      1940KAa (14372) 204
                                        Kso(FeL)=-19.42
From thermodynamic data
-------------------------------------------------------------------------
Fe++       sol oth/un 20°C  dil  U                      1931KOa (14373) 205
                                        Kso(FeL)=-21.85
                                        K(FeL(s)+2H=Fe+H2L(g))=1.4
-------------------------------------------------------------------------
Fe++       sol oth/un 25?°C  var  U                     1909BZa (14374) 206
                                        Kso(FeL)=-18.43
                                        K(FeL(s)+2H=Fe+H2L(g))=4.54
*************************************************************************
SCN-                    HL    Thiocyanate      CAS 463-56-9  (106)
Thiocyanate;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe++       sp  non-aq 25°C 100%  U    M                   1991STa (14946) 207
                                        K(FeA2B2+L=FeA2BL+B)=2.7
Medium: MeCN(B). A=dimethylglyoximedifluoroborate
-------------------------------------------------------------------------
Fe++       sp  non-aq 130°C 100%  U                      1974HNa (14947) 208
                                        B6=12.3
Medium: dimethylsulfone
-------------------------------------------------------------------------
Fe++       sp  NaClO4 25°C  1.0M U T H    K1=2.41        1972EWa (14948) 209
DH(K1)=-36.8 kJ mol-1, DS=-78.2 J K-1 mol-1; K1=2.54(18.3 C), 2.19(34.6 C).
By a combination of thermodynamic data; B[Fe(CN)5OH+L=Fe(CN)5L+OH]=-3.04
-------------------------------------------------------------------------
Fe++       sp  non-aq 25°C 100%  U        K1=5.5    B2=9.20   1970KLb (14949) 210
```

Medium: acetonitrile, 0.01 M Bu4NClO4

Fe++ sp oth/un ? var U M 1967BPc (14950) 211
K(FeA2+L)=0.35
K(FeA2+2L)=0.95

Medium: KL. HA=dimethylglyoxime

Fe++ sp NaClO4 25°C 3.0M U T K1=0.81 1967CSa (14951) 212

Medium: 3(Mg,ClO4),1.8 H+. By kinetics: K1=0.85

Fe++ sp none 23°C 0.0 U K1=1.31 1958YKa (14952) 213

Fe++ sp oth/un 25°C var U K1=0.95 B2=0.07 1937MOa (14953) 214

****

SO3-- H2L Sulfite CAS 7782-99-2 (801)

Sulfite;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo

---

Fe++ kin oth/un 25°C ? U HM 1994LCa (15450) 215
K(FeA+HL=FeAHL)=-1.22

A=Desulfoviridin. DH(FeA+HL)=-33.1 kJ mol-1, DS(FeA+HL)=-41.8 J K-1 mol-1

Fe++ sp oth/un ? var U M 1965MCd (15451) 216
K(Fe(CN)5NO+L)=-1.96
K(Na+Fe(CN)5NO+L)=-0.89
K(K+Fe(CN)5NO+L)=-0.41
K(K+Fe(CN)5NOL)=1.56

****

SO4-- H2L Sulfate CAS 7664-93-9 (15)

Sulfate;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo

---

Fe++ gl NaClO4 25°C 3.0M C I K1=0.60 B2= 0.87 2002CTa (16179) 217

At I=0, extrapolation using SIT: K1=2.1, B2=2.5

Fe++ kin NaCl 25°C 1.0M C K1=1.8 1989MIb (16180) 218

Medium: 1.0 M NaCl/Na2SO4.

Fe++ con none 25°C 0.0 C T H K1=2.39 1988KMb (16181) 219

Data for 10-35 C. DH(K1)=9.72 kJ mol-1, DS(K1)=78.5 J K-1 mol-1.

Fe++ vlt NaClO4 25°C 0.06M U K1=2.72 1972MAd (16182) 220

Medium: HClO4

Fe++ cal none 25°C 0.0 U H K1=2.20 1969IEa (16183) 221

DH(K1)=2.3 kJ mol-1, DS(K1)=50.2 J K-1 mol-1

Fe++ kin NaClO4 35°C 1.0M U TI K1=0.76 1968WSf (16184) 222

K1=1.74(0 C),1.0(25 C); When I=4: K1=0.40(45 C).
At I=4: K(Fe+HL)=0.66(0 C), 0.57(5 C), 0.48(10 C), 0.29(25 C)

Fe++ ix oth/un ? var U K1=0.23 1960BHc (16185) 223
K(Fe+HL)=-0.21

Fe++ kin NaClO4 30°C 1.10M U K1=0.04 1956HDb (16186) 224

****

S2O3-- H2L Thiosulfate CAS 73686-28-7 (177)
Thiosulfate;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	sp	KNO3	6.1°C	0.48M	U	I	K1=0.92	1954PAb (16843)	225

At I=0 corr. K1=2.17

****

Se-- H2L Selenide (6335)
Selenide;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	oth	oth/un	25°C	0.0	U			1964BUe (16939)	226
							Kso=-26.0		

Estimated from thermodynamic data

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	oth	oth/un	25°C	0.0	U			1952LAa (16940)	227
							Kso=-26		

Estimated from thermodynamic data

****

SeCN- HL Selenocyanate CAS 73102-11-2 (440)
Selenocyanate;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	sp	oth/un	?	var	U	M		1967BPd (16983)	228
							K(FeA2+2L)=3.43		

A=dimethylglyoxime. Medium: KL

****

SeO4-- H2L Selenate CAS 7783-08-6 (459)
Selenate;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	kin	NaClO4	25°C	4.0M	U	TI	K1=1.08	1968WSf (17101)	229
							K(Fe+HL)=0.23		

K1=0.71(35 C); K(Fe+HL)=0.68(0 C), 0.64(5 C), 0.54(10 C).
At I=1: K1=1.73(0 C), 1.40(10 C)

****

SiO3-- H2L Silicate CAS 7699-41-4 (747)
Silicate; SiO2(OH)2--

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	oth	none	60°C	0.0	U	T			1969HEa (17208)	230
							*Ks(Fe2SiO4(s)+4H)=14.43			

Method: estimated data.(Fe2SiO4)
*Kso=11.96(100 C); 9.50(150 C); 7.67(200 C); 6.25(250 C); 5.05(300 C)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	oth	none	25°C	0.0	U				1957BAa (17209)	231

From thermodynamic data. Ks(FeSiO3(s)+H2O=SiO2(s)+Fe+2OH)=-18.92

****

SiW11O39-------- H8L (2464)

alpha-Heterosilicon-polytungstate;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	NaNO3	25°C	1.00M	U		K1=7.30		1984COa (17235)	232
							K(beta1 isomer)=6.87			
							K(beta2 isomer)=6.86			
							K(beta3 isomer)=6.90			

****

CH3NO HL Formaldoxime CAS 62479-75-2 (4206)

Formaldoxime; CH2:N.OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	oth	oth/un	20°C	0.10M	U		K1=22.9		1971BJa (17669)	233

Paper electrophoresis, acetate-veronal buffer

****

CH4N2O L Urea CAS 57-13-6 (2018)

Carbamide, Urea; (H2N)2CO

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	vlt	NaClO4	25°C	0.20M	U		K1=0.41	B2=0.90	1985MCc (17715)	234
							K3=-0.046			
							K4=0.32			
							K5-0.52			
							K6=-0.40			

****

CH5N L Methylamine CAS 74-89-5 (155)

Methylamine; CH3.NH2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	none	25°C	0.0	C	H			1998DFd (18015)	235
							K(Fe(CN)6+HL)=2.66			
							K(Fe(CN)6+2HL)=4.64			
							K(Fe(CN)6HL+HL)=1.98			

Constants are for ion pair formation. DH(Fe(CN)6+HL)=-5.8 kJ mol-1;

DH(Fe(CN)6+2HL)=8.8; DH(Fe(CN)6HL+HL)=14.6.

****

CH5NO L CAS 593-56-6 (4208)
O-Methylhydroxylamine; H2N.O.CH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	kin	oth/un	25°C	?	U	HM		1994LCa	(18038)	236
							K(FeA+L=FeAL)=2.28			

A=Desulfoviridin. DH(FeA+L)=-23.0 kJ mol-1, DS(FeA+L)=-52.3 J K-1 mol-1

****

CH6O6P2 H4L Medronic acid CAS 1984-15-2 (2384)
Methanediphosphonic acid; CH2(PO3H2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	KCl	25°C	0.10M	U		K1=12.6	B2=18.8	1967KLa (18281)	237
							K(Fe+HL)=6.6			
							K(Fe+2HL)=11.9			
							K(2Fe+L)=15.4			
							K(2Fe+HL)=9.1			

****

C2H2O4 H2L Oxalic acid CAS 144-62-7 (24)
Ethanedioic acid; (COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	KCl	25°C	1.0M	C		K1=3.05	B2= 5.01	1987MIa (18879)	238
Fe++	dis	NaClO4	20°C	0.10M	U		K1=2.30	B2=1.88	1969MBe (18880)	239
Fe++	gl	NaClO4	25°C	1.0M	U		K1=3.05	B2=5.15	1965BCb (18881)	240
Fe++	vlt	NaClO4	25°C	0.50M	U		B2=4.52		1954SLb (18882)	241
							B3=5.22			
Fe++	vlt	oth/un	?	?	U		B2=9.57		1941TOa (18883)	242
Fe++	con	oth/un	18°C	0.0	U		K1=>4.7		1932MDa (18884)	243
Fe++	sol	oth/un	25°C	>1.0	U		K2=>2.85		1905SAb (18885)	244

****

C2H3O2Cl HL Chloroacetic CAS 79-11-8 (34)
Chloroethanoic acid; ClCH2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	EMF	NaClO4	20°C	1.00M	U		K1=1.9	B2=3.7	1969PJc (19361)	245

****

C2H4OS HL Thioacetic acid CAS 507-09-5 (4223)

Thiolethanoic acid; CH3.CO.SH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	diox/w	30°C	60%	U		K1=4.2	B2=8.00	1972OTc (19507)	246

Medium: 60% dioxan, 1 M (K,Na)NO3

****

C2H4O2 HL Acetic acid CAS 64-19-7 (36)

Ethanoic acid; CH3.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	dis	NaClO4	20°C	0.10M	U		K1=1.90		1969MBe (19956)	247
Fe++	gl	NaClO4	25°C	3.00M	U		K1=0.54		1968OVa (19957)	248
Fe++	EMF	KCl	25°C	0.50M	U		K1=1.82		1961NPa (19958)	249

Medium: HCl

Fe++	oth	oth/un	?	0.0	U		K1=1.40		1956YFa (19959)	250

****

C2H4O2S H2L Thioglycolic CAS 68-11-1 (596)

Mercaptoethanoic acid; HS.CH2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	NaClO4	30°C	0.10M	U		K1=5.32	B2= 9.40	1988NDa (20318)	251
Fe++	sol	none	25°C	0.0	U		B2=10.92		1953LKb (20319)	252
							K(Fe(OH)L+H=Fe+L)=1.62			

****

C2H5NO2 HL Glycine CAS 56-40-6 (85)

2-Aminoethanoic acid; H2N.CH2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	KCl	25°C	1.0M	C		K1=3.73	B2= 6.65	1987MIa (21544)	253
							B3=8.87			
Fe++	EMF	NaClO4	25°C	3.0M	C		K1=4.20		1982BPc (21545)	254

Method: Pt/H2 electrode.

Fe++	kin	oth/un	25°C	0.10M	U	H			1978TMa (21546)	255
							K(Fe(CN)5+L)=4.02			

Medium: LiClO4. DH1=-35.5 kJ mol-1, DS1=-42 J K-1 mol-1

Fe++	gl	none	25°C	0.00	U	T	K1=4.31		1972IJb (21547)	256

10 C: K1=4.36; 40 C: K1=4.28

Fe++	gl	KNO3	25°C	0.10M	U	T	K1=4.13	B2=7.65	1969GEb (21548)	257

```
--------------------------------------------------------------------------------
Fe++       gl  KCl    20°C  1.0M U      T K1=3.83        1959PEc (21549) 258
--------------------------------------------------------------------------------
Fe++       gl  oth/un 20°C 0.01M U        K1=4.3    B2=7.8    1953ALa (21550) 259
********************************************************************************
C2H6N2O                 L    Methylurea       CAS 598-50-5  (2019)
N-Methylurea; CH3.NH.CO.NH2
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       vlt NaClO4 25°C 0.20M U        K1=0.26   B2=0.52   1985MCc (21967) 260
                                         K3=0.20
                                         K4=0.56
                                         K5=0.15
                                         K6=0.079
********************************************************************************
C2H6O                   L    Ethanol          CAS 64-17-5  (1913)
Ethanol; CH3.CH2.OH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       sp  non-aq 25°C 100%  U    M                   1978MBa (22027) 261
                                         K(FeA+L)=0.8
Medium: benzene. A=Tetraphenylporphyrin-thiocarbide
********************************************************************************
C2H6OS                 HL                     CAS 60-24-2  (841)
2-Mercaptoethanol; HS.CH2.CH2.OH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       gl  oth/un   ?   0.0  U        B2=6.6         1961AMa (22064) 262
********************************************************************************
C2H7NO                  L    Ethanolamine     CAS 141-43-5  (1057)
2-Aminoethanol; H2N.CH2.CH2.OH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       oth oth/un 25°C 0.43M U        K1=1.90   B2=3.05   1966SKe (22402) 263
********************************************************************************
C2H8N2                  L    Ethylenediamine  CAS 107-15-7  (23)
1,2-Diaminoethane; H2N.CH2.CH2.NH2
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       gl  none   25°C  0.0  C   H                   1998DFd (23153) 264
                                         K(Fe(CN)6+HL)=2.80
                                         K(Fe(CN)6+H2L)=4.80
                                         K(Fe(CN)6+2H2L)=7.09
                                         K(Fe(CN)6H2L+H2L)=2.29
Constants are for ion pair formation. DH(Fe(CN)6+HL)=-3.7 kJ mol-1;
```

DH(Fe(CN)6+H2L)=3.4; DH(Fe(CN)6+2H2L)=12.2; DH(Fe(CN)6H2L+H2L)=8.8.

Fe++ gl alc/w 30°C 5% M K1=4.28 1994RRb (23154) 265

Medium: 5% v/v EtOH/H2O, 0.10 M KNO3.

Fe++ gl KCl 25°C 1.0M C K1=4.26 B2= 7.73 1987MIa (23155) 266
B3=10.17

Fe++ gl KNO3 25°C 1.0M C TIH R K1=4.34 B2=7.65 1984PAa (23156) 267
B3=9.70

IUPAC evaluation. DH(K1)=-21.1, DH(K2)=-22.4, DH(K3)=-22.8 kJ mol-1

Fe++ oth oth/un ? ? U K1=4.37 B2=7.65 1969MMb (23157) 268
K3=1.99

Data from survey of literature data

Fe++ cal KCl 25°C 1.0M U H 1960CPa (23158) 269

DG(K1)=-24.66 kJ mol-1, DH=-21.1, DS=12; DG(B2)=-43.68, DH=-43.5, DS=0.8;
DG(B3)=-55.39, DH=-66.3, DS=-36

Fe++ gl oth/un 25°C 1.40M U K1=4.34 B2=7.34 1957PBa (23159) 270
K3=2.05

Fe++ EMF KCl 30°C 1.0M U K1=4.28 B2=7.53 1941BJa (23160) 271
K3=1.99

Method: H electrode

****

C2H8O7P2 H4L HEDPA CAS 2809-21-4 (436)

1-Hydroxyethane-1,1-diphosphonic acid; CH3.C(OH)(PO3H2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	KNO3	25°C	0.10M	C		K1=12.9		1997DBb (23366)	272
							K(FeL+H)=4.87			
							K(FeHL+H)=3.3			
Fe++	gl	KCl	25°C	0.10M	U		K1=9.05		1967KLa (23367)	273
							K(Fe+HL)=5.31			
							K(2Fe+H-1L))=19.59			
							K(2Fe+L)=13.89			
							K(2Fe+HL)=7.99			

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C2H9NO6P2 H4L IDPA CAS 32545-63-4 (1335)

Imino-N,N-bis(methylenephosphonic acid); HN(CH2PO3H2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	KNO3	25°C	0.1M	C		K1=7.70		1985MMa (23453)	274
							B(FeHL)=14.35			
							B(FeH2L)=19.34			

****
C3H4N2 L Pyrazole CAS 288-13-1 (367)
1,2-Diazole, pyrazole; cyclo(-NH.N:CH.CH:CH-)

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ vlt NaNO3 25°C 0.10M U K1=0.84 B2=1.08 1968CWa (23572) 275
B3=1.28
B4=1.52
****
C3H4N2 L Imidazole CAS 288-32-4 (90)
1,3-Diazole, imidazole; C3H4N2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ sp non-aq 20°C 100% U 1990ABa (23879) 276
K(FeP(DMSO)+L)=5.81
K(FePL+L)=3.87
In DMSO. FeP = phthalocyaninatoiron(II)

Fe++ sp non-aq 20°C 100% U M 1978KBb (23880) 277
K(FeA+2L)=7.46
Medium: DMSO, 0.1 M Et4NClO4. A=Phthalocyanine

Fe++ kin oth/un 25°C 0.10M U H 1978TMa (23881) 278
K(Fe(CN)5+L)=5.26
Medium: LiClO4. DH1=-38.0 kJ mol-1, DS1=-29 J K-1 mol-1

Fe++ sp oth/un 25°C 0.05M U I M 1976HFa (23882) 279
K(FeA(OH)+HL+L)=5.08
K(FeA+2L)=6.00
Medium: 0.05 M hexadecyltrimethylammonium bromide. FeA=hemin. Data also for
0.5 M Na dodecylsulfate

Fe++ oth KNO3 30°C 0.16M U K1=1.81 B2=3.04 1966SKc (23883) 280

Fe++ gl KCl 0°C .058M U T K1=3.31 B2=6.41 1961SMa (23884) 281
25 C: K1=3.20, K2=3.17; 45 C: K1=3.25, K2=2.96
****
C3H4N2S HL Imidazolethiol CAS 872-35-5 (1823)
2-Mercaptoimidazole; C3H3N2.SH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl NaClO4 25°C 0.10M U K1=5.67 B2=10.04 1977STc (23970) 282
****
C3H4O3 HL Pyruvic acid CAS 127-17-3 (1152)
2-Oxopropanoic acid; CH3.CO.COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo

```
-------------------------------------------------------------------------------
Fe++       gl  NaClO4 25°C 3.00M C        K1=0.69        1978FGa (24050) 283
*******************************************************************************
C3H4O4                H2L    Malonic acid     CAS 141-82-2  (79)
Propanedioic acid; CH2(COOH)2
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe++       gl  KCl    25°C  1.0M C        K1=2.24        1987MIa (24441) 284
-------------------------------------------------------------------------------
Fe++       gl  NaClO4 25°C 1.00M C        K1=2.17   B2=3.21   1977DEa (24442) 285
-------------------------------------------------------------------------------
Fe++       vlt NaClO4 25°C 0.50M U        B2=2.22        1954SLb (24443) 286
-------------------------------------------------------------------------------
Fe++       vlt oth/un   ?   1.0M U        K1=2.8         1951SCa (24444) 287
*******************************************************************************
C3H6O2S               H2L    Thiolactic acid  CAS 79-42-5  (366)
2-Mercaptopropanoic acid;  CH3.CH(SH).COOH
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe++       gl  NaClO4 30°C 0.10M U        K1=6.22   B2=11.17  1988NDa (25142) 288
*******************************************************************************
C3H7NO2                HL    Alanine          CAS 56-41-7  (86)
2-Aminopropanoic acid; H2N.CH(CH3).COOH
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe++       gl  alc/w  30°C   5%  M        K1=6.97        1994RRb (26170) 289
Medium: 5% v/v EtOH/H2O, 0.10 M KNO3.
-------------------------------------------------------------------------------
Fe++       gl  KCl    25°C  1.0M C        K1=2.53        1987MIa (26171) 290
-------------------------------------------------------------------------------
Fe++       gl  KCl    20°C  1.0M U      T K1=3.54        1959PEc (26172) 291
-------------------------------------------------------------------------------
Fe++       gl  oth/un 25°C 0.01M U        B2=7.3         1950ALa (26173) 292
*******************************************************************************
C3H7NO2                HL    B-Alanine        CAS 107-95-9  (575)
3-Aminopropanoic acid; H2N.CH2.CH2.COOH
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe++       gl  oth/un 20°C 0.01M U        B2=4           1950ALa (26454) 293
*******************************************************************************
C3H7NO2                HL    Sarcosine        CAS 107-97-1  (87)
N-Methyl-2-aminoethanoic acid; CH3.NH.CH2.COOH
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe++       gl  KCl    20°C  1.0M U        K1=3.52        1959PEc (26601) 294
```

****

C3H7NO2S H2L Cysteine CAS 52-90-4 (96)
2-Amino-3-mercaptopropanoic acid; H2N.CH(CH2.SH)COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	sol	oth/un	25°C	->0	U		B2=11.77 B(FeL(OH))=12.77	1955TKa (26773)	295
Fe++	gl	oth/un	20°C	0.01M	U		K1=6.2	1952ALa (26774)	296

****

C3H7NO3 HL Serine CAS 56-45-1 (49)
2-Amino-3-hydroxypropanoic acid; H2N.CH(CH2.OH)COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	NaClO4	25°C	3.00M	U		K1=4.30 B2=7.38 B3=10.30	1973WIa (27127)	297
Fe++	gl	KNO3	40°C	0.20M	U	T H	K1=3.62 B2=6.36	1968RMb (27128)	298
15 C: K1=3.67, K2=2.78. DH(B2)=-6.3 kJ mol-1, DS=100 J K-1 mol-1									
Fe++	oth	oth/un	25°C	0.0	U		B2=7.7	1964SYa (27129)	299
Fe++	gl	KCl	20°C	1.0M	U		K1=3.43	1959PEc (27130)	300
Fe++	gl	oth/un	20°C	0.01M	U		B2=7.0	1950ALa (27131)	301

****

C3H8NO5P H3L Glyphosate CAS 1071-83-6 (1617)
N-(Phosphonomethyl)glycine; H2O3P.CH2.NH.CH2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	KNO3	25°C	0.1M	C		K1=6.87 B2=11.18 B(FeHL)=12.79	1985MMa (27403)	302

****

C3H8N2O L Dimethylurea CAS 96-31-1 (2021)
1,3-Dimethylurea; CH3.NH.CO.NH.CH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	vlt	NaClO4	25°C	0.20M	U		K1=-0.15 B2=0.08 K3=1.20 K4=-0.15	1985MCc (27475)	303

****

C3H8N2O L Ethylurea CAS 625-52-5 (2020)
N-Ethylurea; H2N.CO.NH.C2H5

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo

Fe++ vlt NaClO4 25°C 0.20M U K1=0.041 B2=0.24 1985MCc (27483) 304
K3=-0.097
K4=0.11
K5=0.84
K6=0.079

****

C3H8N2O2 HL CAS 71292-18-7 (356)
2,3-Diaminopropanoic acid; H2N.CH2.CH(NH2).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	oth/un	20°C	0.01M	U		B2=5.0	1952ALa (27550)	305

****

C3H8OS2 H2L BAL CAS 59-52-9 (379)
2,3-Dimercaptopropan-1-ol; HS.CH2.CH(SH).CH2(OH)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	KCl	30°C	0.10M	U		B2=15.78 B(Fe2L3)=28	1962LJa (27657)	306

****

C3H8O2S HL 1-Thioglycerol CAS 96-27-5 (1848)
3-Mercapto-1,2-propanediol HS.CH2.CH(OH).CH2.OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	NaClO4	20°C	0.10M	U	TI	K1=13.37	1986NDb (27710)	307

****

C3H8O3S3 H3L Unithiol CAS 74-61-3 (1271)
2,3-Dimercaptopropanesulfonic acid; HS.CH2.CH(SH).CH2.SO3H

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	sp	NaCl	25°C	0.1M	U		K1=6.02 B2=11.42	1999PAa (27785)	308

Also published in Zh. Neorg.Khim. (1999) 44, 590

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	sp	oth/un	?	0.20M	U		B2=7.64	1972OFa (27786)	309

****

C3H9N L n-Propylamine CAS 107-10-8 (2356)
1-Aminopropane; H2N.CH2.CH2.CH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	sp	non-aq	23°C	100%	U	M	K(FeA+L)=2.58 K(FeAL+L)=1.33	1982HDa (27831)	310

Medium: toluene. A='capped' porphyrin

****

C3H9N L iso-Propylamine CAS 75-31-0 (157)
2-Propylamine; CH3.CH(CH3).NH2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	sp	non-aq	25°C	100%	U	M	K(FeA2B2+L=FeA2L+B)=4.00 K(FeA2BL+L=FeA2L2+B)=3.08 K(FeB2C2+L=FeBC2L+B)=4.30 K(FeBC2L+L=FeC2L2+B)=3.26	1994STa (27844)	311

K(FeA2D2+L=FeA2DL+D)=1.18; K(FeC2D2+L=FeC2DL+D)=0.52. Medium: CH2Cl2
A=dmgdiphenylborate, B=CH3CN, C=dmgdifluoroborate, D=Pyridine

****

C3H9N3O2 HL CAS 471915-95-4 (8549)
2,3-Diamino-N-hydroxypropanamide;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	KCl	25°C	0.20M	C		K1=4.34 B(FeHL)=12.28 B(FeH-1L)=-5.54	2002ECa (27983)	312

****

C3H10NO3P H2L (1986)
1,1-Dimethyl-1-aminomethylphosphonic acid; H2N.C(CH3)2.PO3H2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	KCl	25°C	0.10M	U		K1=4.68 B2=8.61 K(Fe+HL)=3.07	1969DMd (28075)	313

****

C3H11NO6P2 H4L (6735)
N-Methylimino-N,N-bis(methylenephosphonic acid); CH3.N(CH2PO3H2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	KNO3	25°C	0.10M	C		K1=9.12 K(FeL+H)=6.97 K(FeHL+H)=4.28	1993SKc (28448)	314

****

C3H12NO9P3 H6L NTPA CAS 6419-19-8 (2920)
Nitrilotris(methylenephosphonic acid); N(CH2PO3H2)3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	KNO3	25°C	0.10M	C		K1=12.7 K(FeL+H)=6.4 K(FeHL+H)=6.30	1997DBb (28561)	315
Fe++	gl	KNO3	25°C	0.10M	C		K1=13.5 K(FeL+H)=6.49 K(FeHL+H)=5.41 K(FeH2L+H)=4.2	1989SAa (28562)	316

Fe++ EMF NaClO4 25°C 1.0M U K1=15.3 1987PLa (28563) 317
K(Fe+HL)=9.9
K(Fe+H2L)=6.0

Fe++ gl alc/w 25°C 10% U K1=12.60 1987SHa (28564) 318
K(FeL+H)=7.00
K(FeHL+H)=5.67
K(FeH2L+H)=4.36

In 10% ethanol/H2O; I=0.1 M NaClO4.

****

C4H3N3O3S H3L Thiovioluric CAS 23036-77-3 (2000)
2-Thio-4,5,6(H)-pyrimidinetetrone 5-oxime

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo

---

Fe++ gl NaNO3 25°C 0.50M C 1984HNb (28719) 319
B3=8.60

Fe++ sp NaNO3 25°C 0.50M U 1981DDa (28720) 320
B3=9.16

Using pH titrations, B3=9.04

Fe++ gl NaNO3 25°C 0.10M C 1979DDb (28721) 321
K(Fe+3H2L)=9.04

Fe++ sp oth/un 20°C 0.10M U 1971TTa (28722) 322
K(Fe+4H2L)=19.6

Medium: 50% dioxan, 0.1 M NaClO4

****

C4H3N3O4 H3L Violuric acid CAS 26351-19-9 (1208)
2,4,5,6-(1H,3H)Pyrimidinetetrone-5-oxime, 5-isonitrosobarbituric acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo

---

Fe++ gl NaCl 25°C 0.10M C 2002KSa (28746) 323
K(Fe+H2L)=2.96

Fe++ gl NaNO3 25°C 0.50M C 1984HNb (28747) 324
B3=8.65

Fe++ sp NaNO3 25°C 0.50M U 1981DDa (28748) 325
B3=8.92

Using pH titrations, B3=8.60

Fe++ gl NaNO3 25°C 0.50M U 1978DDa (28749) 326
B3=8.60

By spectrophotometry: B3=8.4

****

C4H4N2 L Pyrazine CAS 290-37-9 (620)

1,4-Diazine, Pyrazine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	sp	oth/un	23°C	?	U	M	K(Fe(CN)5L+H)=0.065	1983JSa (28792)	327

****

C4H4N2O2S H2L Thiobarbituric CAS 504-17-6 (4279)
4,6-Dihydroxy-2-mercaptopyrimidine, 2-thiobarbituric acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	NaClO4	31°C	0.10M	U	T H	K1=5.82 B2=10.21	1984SJa (28888)	328

Also data for 18 and 42 C. DH(K1)=-59.5 kJ mol-1, DS(K1)=-84.6 J K-1 mol-1
DH(K2)=-42.0, DS(K2)=-54.4.

****

C4H4O4 H2L Fumaric acid CAS 110-17-8 (289)
trans-Butenedioic acid; HOOC.CH:CH.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	NaClO4	37°C	0.15M	C		K1=2.78 B2=4.99 B3=7.19	1974CCa (29198)	329

****

C4H6N2 L 2-Me-Imidazole CAS 693-98-1 (122)
2-Methyl-1,3-diazole; C3H3N2.CH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	sp	non-aq	25°C	100%	U	M	K(FeA2B2+L=FeA2BL+B)=2.41 K(FeA2BL+L=FeA2L2+B)=-1.00 K(FeB2C2+L=FeBC2L+B)=3.20 K(FeBC2L+L=FeC2L2+B)=1.00	1994STa (29481)	330

Medium: CH2Cl2. A=Dimethylglyoximediphenylborate, B=CH3CN, C=dmgdifluoro-
borate, D=Pyridine

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	sp	non-aq	20°C	100%	U	M	K(FeALC+L=FeAL2+C)=-3.80 K(FeBLC+L=FeBL2+C)=-4.62 K(FeAC2+L=FeACL+C)=1.58 K(FeBC2+L=FeBCL+C)=-0.28	1993PMa (29482)	331

In toluene. A=Tetramesitylporphine, B=Tetraphenylporphine, C=Tosylmethyliso-
cyanide. K(FeAL+L)=4.95, K(FeBL+L)=4.89

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	nmr	non-aq	25°C	100%	U	M	K(FeA+L=FeAL)=0.87	1979HSa (29483)	332

Medium: MeCN solution, A=tetraMe-1,4,8,11-tetraazocyclotetradecatetraene

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	vlt	non-aq	20°C	100%	U	M		1978KBb (29484)	333

K(FeA+L)=2.84
K(FeA+2L)=4.84
Medium: DMSO. A=Phthalocyanine. Cyclic voltammetry also used

****

C4H6N2 L 4-Me-Imidazole CAS 822-36-6 (353)
4-Methyl-1,3-diazole; C3H3N2.CH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	kin	none	38°C	0.0	U	T H		2000YWa (29527)	334
							K(FeC+L)=1.27		

FeC: cytochrome c. Method: 1H nmr in D2O. Also data at 42C. K(FeC+L)=1.58. DH=135 kJ mol-1, DS=459 J K-1 mol-1.

****

C4H6N2 L N-Me-Imidazole CAS 616-47-7 (354)
N-Methyl-1,3-diazole; C3H3N2.CH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	EMF	KCl	25°C	1.00M	U		K1=2.43	1995NTa (29585)	335
Fe++	sp	non-aq	25°C	100%	U	M		1994BGb (29586)	336
							K(FeA+L)=5.41		

Medium:Toluene. A:(OC2O)-linked capped porphyrin

Fe++	sp	non-aq	23°C	100%	U	M		1982HDa (29587)	337
							K(FeA+L)=3.68		

Medium: toluene. A='capped' porphyrin

Fe++	sp	non-aq	23°C	100%	U	HM		1980ELa (29588)	338
							K(FeA+L)=2.90		

Medium: toluene. A= "Capped" porphyrin. DH=-26 kJ mol-1.

Fe++	sp	non-aq	25°C	100%	U	M		1980ELa (29589)	339
							K(FeA+L)=3.31		

Medium: toluene. A="Homologous capped" porphyrin

Fe++	sp	non-aq	23°C	100%	U	M		1979BEa (29590)	340
							K(FeA+L)=3.31		
							K(FeAL+L)=0.77		

Medium: toluene. A="Capped Homologous" Porphyrin. At 0 C, K(FeAL+O2)=0.92

Fe++	sp	non-aq	23°C	100%	U			1979BEa (29591)	341
							K(FeA+L)=2.90		

Medium: toluene. FeA=a substituted porphyrinato-Fe(II)
K(FeAL+O2)=0.65

Fe++	vlt	non-aq	20°C	100%	U	M		1978KBb (29592)	342
							K(FeA+2L)>7.5		

Medium: DMSO. A=Phthalocyanine

****

C4H6N2S HL Methimazole CAS 60-56-0 (1824)
N-Methyl-2-mercaptoimidazole; C3H2N2(CH3).SH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	NaClO4	25°C	0.10M	U		K1=5.83	B2=10.81	1977STc (29662)	343

****

C4H6O4 H2L Succinic acid CAS 110-15-6 (112)
1,4-Butanedioic acid; HOOC.CH2.CH2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	NaClO4	37°C	0.15M	C		K1=1.42	B2=2.92	1974CCa (29972)	344

****

C4H6O4S H2L Thiodiacetic CAS 123-93-3 (140)
2,2'-Thiodiglycolic acid, Thiodiethanoic acid; HOOC.CH2.S.CH2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	NaClO4	25°C	0.50M	U		K1=2.45	B2=3.82	1972NAa (30215)	345
Fe++	gl	NaClO4	25°C	0.10M	U		K1=2.88	B2=5.24	1970PPa (30216)	346
							K(Fe+HL)=1.61			

****

C4H6O4S H3L Thiomalic acid CAS 70-49-5 (109)
2-Mercaptosuccinic acid, 2-Sulfanyl-1,4-butanedioic acid; HOOC.CH(SH).CH2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	NaClO4	30°C	0.10M	U		K1=5.85	B2=10.76	1988NDa (30330)	347

****

C4H6O5 H2L Malic acid CAS 617-48-1 (393)
2-Hydroxybutane-1,4-dioic acid, Hydroxy-succinic acid; HOOC.CH2.CH(OH).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	NaClO4	20°C	0.10M	U		K1=2.5		1964TIb (30627)	348

By ion exchange: K1=2.68

****

C4H6O5 H2L Diglycolic acid CAS 110-99-6 (243)
Di(carboxy)methyl ether, 2,2'-Oxydiethanoic acid; HOOC.CH2.O.CH2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	KCl	25°C	0.10M	C		K1=2.48		1984MMg (30872)	349
							K(FeL+H)=2.09			
Fe++	gl	KNO3	25°C	0.10M	U		K1=2.63		1975MTc (30873)	350

Fe++ gl NaClO4 25°C 0.50M U K1=2.18 1972NAd (30874) 351

****

C4H6O6 H2L D-Tartaric acid CAS 147-71-7 (93)

D-Tartaric acid, D-2,3-Dihydroxybutanedioic acid; HOOC.CH(OH).CH(OH).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	nmr	none	25°C		U	M	K(Fe+H2L=FeHL+H)=1.11	1990GKc	(30974) 352

****

C4H6O6 H2L L-Tartaric acid CAS 87-69-4 (92)

L-Tartaric acid, L-2,3-Dihydroxybutanedioic acid; HOOC.CH(OH).CH(OH).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	ix	oth/un	30°C	dil	C	T	K1=2.17	1992LHb	(31237) 353

Medium: 0.2-5.0 mM tartaric acid eluent. At 40 C, K1=2.21

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	nmr	none	25°C		U	M	K(Fe+H2L=FeHL+H)=1.16	1990GKc	(31238) 354

Data for d,l-Tartaric acid

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	dis	NaClO4	20°C	0.10M	U		K1=2.69 B2=4.68	1969MBe	(31239) 355
Fe++	gl	NaClO4	25°C	1.00M	U		K1=1.43 B2=2.50	1968BRb	(31240) 356
Fe++	ix	NaClO4	20°C	0.10M	U		K1=2.24	1964TIa	(31241) 357
Fe++	vlt	oth/un	?	?	U		K2=4.85	1945TOa	(31242) 358

****

C4H7NO2 HL (8137)

(S)-Azetidine-2-carboxylic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	KNO3	25°C	0.10M	C		K1=4.3 B2= 8.10	1989ARa	(31441) 359

****

C4H7NO2 HL CAS 57-71-6 (6204)

But-2,3-dione monoxime; CH3.CO.C(:NOH).CH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	alc/w	25°C	75%	U		K1=8.2 B2=13.60 K3=4.2	1986BTa	(31455) 360

Medium: 75% MeOH/H2O, 0.1 M NaClO4

****

C4H7NO4 H2L Aspartic acid CAS 56-84-8 (21)

Aminobutanedioic acid; H2N.CH(CH2.COOH).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo

```
--------------------------------------------------------------------------------
Fe++       gl  KNO3   25°C 0.10M M        K1=5.34   B2= 8.57  1981GVa (31853) 361
--------------------------------------------------------------------------------
Fe++       gl  KCl    20°C  1.0M U        K1=4.34        1959PEc (31854) 362
--------------------------------------------------------------------------------
Fe++       gl  oth/un 20°C 0.01M U        B2=8.5         1952ALa (31855) 363
********************************************************************************
C4H7NO4               H2L    IDA              CAS 142-73-4  (118)
Iminodiethanoic acid; HN(CH2.COOH)2
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       EMF NaClO4 20°C 1.00M C        K1=6.10   B2=10.55  2000BMa (32249) 364
Method: Pt/Fe+++/Fe++ and glass electrodes.
--------------------------------------------------------------------------------
Fe++       gl  KCl    25°C  1.0M C        K1=5.45   B2= 9.82  1987MIa (32250) 365
--------------------------------------------------------------------------------
Fe++       gl  NaClO4 25°C 0.50M U        K1=5.54   B2=9.81   1972NAc (32251) 366
--------------------------------------------------------------------------------
Fe++       gl  KNO3   20°C 0.10M U        K1=5.8    B2=10.1   1964ANa (32252) 367
********************************************************************************
C4H8N2O2              H2L    Dimethylglyoxim  CAS 95-45-4  (2032)
2,3-Butanedione dioxime, Dimethylglyoxime; CH3.(C:NOH).(C:NOH).CH3
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       oth oth/un 27°C    ?  U        B2=7.25        1957SRb (32539) 368
********************************************************************************
C4H8N2O3               HL    Asparagine       CAS 70-47-3  (17)
2-Aminobutanedioic acid 4-amide; H2N.CH(CH2.CO.NH2).COOH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       gl  NaCl   25°C 1.00M C        K1=3.43   B2=5.90   1996BFb (32695) 369
--------------------------------------------------------------------------------
Fe++       gl  NaClO4 25°C 3.00M C        K1=4.366  B2=7.57   1974BWa (32696) 370
                                         B3=10.259
--------------------------------------------------------------------------------
Fe++       gl  oth/un 20°C 0.01M U        B2=6.5         1950ALa (32697) 371
********************************************************************************
C4H8N2O3               HL    Gly-Gly          CAS 556-50-3  (54)
Glycyl-glycine; H2N.CH2.CO.NH.CH2.COOH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       gl  KCl    20°C  1.0M U        K1=2.62        1959PEc (33023) 372
********************************************************************************
C4H9NO2                HL    Aminoisobutyric  CAS 144-90-1  (188)
2-Amino-2-methylpropanoic acid; H2N.C(CH3)2.COOH
--------------------------------------------------------------------------------
```

```
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe++       gl  KCl    20°C  1.0M U        K1=3.48        1959PEc (33837) 373
*************************************************************************
C4H9NO2                HL    2-Aminobutyric   CAS 2835-81-6  (571)
2-Aminobutanoic acid; CH3.CH2.CH(NH2).COOH
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe++       gl  KCl    20°C  1.0M U        K1=3.37        1959PEc (33913) 374
*************************************************************************
C4H9NO3                HL    Threonine        CAS 72-19-5  (48)
2-Amino-3-hydroxybutanoic acid; H2N.CH(CH(OH).CH3)COOH
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe++       gl  NaCl   37°C 0.15M U    M                   1986XHa (34298) 375
                                        B(FeHL)=12.44
                                        B(FeH2L)=15.10
                                        B(FeH-1L(His))=3.446
-------------------------------------------------------------------------
Fe++       gl  KNO3   40°C 0.20M U T H    K1=3.69   B2=6.50   1968RMb (34299) 376
At 15 C: K1=3.76, K2=2.86. DH(B2)=-8.4 kJ mol-1, DS=96.1 J K-1 mol-1
-------------------------------------------------------------------------
Fe++       gl  KCl    20°C  1.0M U        K1=3.30        1959PEc (34300) 377
*************************************************************************
C4H10N2O2              HL                    CAS 1883-09-6  (45)
2,4-Diaminobutanoic acid; H2N.CH2.CH2.CH(NH2)COOH
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe++       gl  oth/un 20°C 0.01M U        K1=5.7         1952ALa (34568) 378
*************************************************************************
C4H11N                  L    iso-Butylamine   CAS 78-81-9  (2355)
1-Amino-2-methylpropane; H2N.CH2.CH(CH3).CH3
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe++       sp  non-aq 23°C 100%  U    M                   1982HDa (34730) 379
                                        K(FeA+L)=2.07
Medium: toluene. A='capped' porphyrin
*************************************************************************
C4H11N                  L    Butylamine       CAS 109-73-9  (159)
1-Aminobutane; CH3.CH2.CH2.CH2.NH2
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe++       sp  non-aq 25°C 100%  U    M                   1994STa (34765) 380
                                        K(FeA2B2+L=FeA2BL+B)=5.60
                                        K(FeA2BL+L=FeA2L2+B)=4.70
```

K(FeB2C2+L=FeBC2L+B)=5.90
K(FeBC2L+L=FeC2L2+B)=4.67
K(FeA2D2+L=FeA2DL+D)=3.54; K(FeA2DL+L=FeA2L2+D)=2; K(FeC2D2+L=FeC2DL+D)=2.23
Medium: CH2Cl2. A=dmgdiphenylborate, B=CH3CN, C=dmgdifluoroborate, D=py

****

C4H11N L t-Butylamine CAS 75-64-9 (158)
2-Amino-2-methylpropane; H2N.C(CH3)3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	sp	non-aq	25°C	100%	U	M		1994STa (34784)	381
							K(FeA2B2+L=FeA2BL+B)=1.40		
							K(FeA2BL+L=FeA2L2+B)=0.04		
							K(FeB2C2+L=FeBC2L+B)=1.78		
							K(FeBC2L+L=FeC2L2+B)=0.85		

Medium: CH2Cl2. A=Dimethylglyoximediphenylborate, B=CH3CN, C=dmgdifluoro-borate, D=Pyridine

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	sp	non-aq	23°C	100%	U	M		1982HDa (34785)	382
							K(FeA+L)=0.90		

Medium: toluene. A='capped' porphyrin

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	sp	non-aq	23°C	100%	U	M		1980ELa (34786)	383
							K(FeA+L)=2.50		

Medium: toluene. A= "Capped" porphyrin.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	sp	non-aq	23°C	100%	U	M		1979BEa (34787)	384
							K(FeA+L)=2.23		

Medium: toluene. A="Capped Homologous" Porphyrin

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	sp	non-aq	23°C	100%	U			1979BEa (34788)	385
							K(FeA+L)=2.50		

Medium: toluene. FeA=a substituted porphyrinato-Fe(II)

****

C4H11NO2 L Diethanolamine CAS 111-42-2 (89)
2,2'-Iminodiethanol; HN(CH2.CH2.OH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	oth	oth/un	25°C	0.43M	U		K1=2.37 B2=3.67	1966SKe (34957)	386

Medium: CH2OHCH2NH3NO3

****

C4H11NO8P2 H5L CAS 2439-99-8 (2129)
N-Carboxymethyl-N,N-bis(methylenephosphonic acid); HOOC.CH2.N(CH2.PO3H2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	KNO3	25°C	0.10M	C		K1=11.9	2000SDa (35105)	387
							K(FeL+H)=6.14		
							K(FeHL+H)=4.56		

K(FeL+OH)=4.1

****

C4H11N3O2 HL CAS 471915-94-3 (8550)
2,4-Diamino-N-hydroxybutanamide;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	KCl	25°C	0.20M	C				2002ECa (35176)	388
							B(FeHL)=14.02			

****

C4H13N3 L Dien CAS 111-40-0 (584)
1,4,7-Triazaheptane, 2,2'Iminobis(ethylamine), diethylenetriamine;
NH2.(CH2)2.NH.(CH2)2.NH2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	KCl	25°C	1.0M	C		K1=5.66	B2= 9.61	1987MIa (35778)	389
Fe++	cal	KCl	25°C	0.10M	U	H			1961CPa (35779)	390
							DH(B2)=-54.2 kJ mol-1			
Fe++	gl	KCl	30°C	1.0M	U T H		K1=6.23	B2=10.36	1952JHa (35780)	391

40 C: K1=6.03, K2=3.95. DH(K1)=-37.6 kJ mol-1, DH(K2)=-33.4

****

C5H4NCl L CAS 626-60-8 (322)
3-Chloropyridine; C5H4N.Cl

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	sp	non-aq	23°C	100%	U	M			1980ELa (36024)	392
							K(FeA+L)=1.53			

Medium: toluene. A= "Capped" porphyrin.

****

C5H4N2O2 HL CAS 98-97-5 (1879)
Pyrazine-2-carboxylic acid; cyclo(-CH:CH.N:C(COOH).CH:N-)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	sp	NaClO4	25°C	0.10M	U	M	K1=3.4	B2=6.1	1981TBa (36051)	393
							B3=7.7			
Fe++	sp	NaClO4	25°C	1.0M	C		K1=4.10	B2= 7.71	1979MMi (36052)	394
							B3=10.51			
							K(Fe+HL=FeL+H)=1.40			
							K(FeL+HL=FeL2+H)=0.81			
							K(FeL2+HL=FeL3+H)=0.10			
Fe++	sp	NaClO4	25°C	1.00M	U		K1=4.1	B2=7.71	1977MAa (36053)	395
							B3=10.51			

****

C5H4N2O3S H2L Thioorotic acid (4335)
1,2,3,6-Tetrahydro-2-thio-6-oxo-4-pyrimidinecarboxylic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	NaCl	20°C	0.15M	U		K1=3.92	1979DZe (36076)	396
							K(Fe+HL)=2.40		

****
C5H4N2O4 H2L Orotic acid CAS 65-86-1 (624)
1,2,3,6-Tetrahydro-2,6-dioxo-4-pyrimidinecarboxylic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	NaCl	20°C	0.15M	U		K1=4.67	1979DZe (36112)	397
							K(Fe+HL)=2.57		

****
C5H4N4O HL Hypoxanthine CAS 68-94-0 (1174)
6-Hydroxypurine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	oth/un	20°C	0.01M	U		K1=3.9	1953ALa (36190)	398

****
C5H5N L Pyridine CAS 110-86-1 (31)
Pyridine, Azine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	nmr	none	RT	0	U			1997LCb (36624)	399
							K(FeC+L)=0.33		

Medium: D2O. FeC is cytochrome C.

Fe++	nmr	non-aq	24°C	100%	U	M		1991LSd (36625)	400
							K(FeA+L)=2.65		
							K(FeAL+L)=1.60		

Medium: MeCN. A=N,N'-ethylene-bis(trifluoroacetylacetoneiminate)

Fe++	sp	non-aq	20°C	100%	U			1985PEa (36626)	401
							K(FeAS2+L=FeASL+S)=5.59		
							KFeASL+L=FeAL2+S)=2.48		

Medium (S): DMSO. A=phthalocyanin

Fe++	sp	non-aq	20°C	100%	U			1985PEb (36627)	402
							K(FeABS+L=CoABL+S)=6.43		
							K(FeABL+L=CoAL2+B)=-1.34		

Medium (S): DMSO. A=phthalocyanin. B=CO

Fe++	sp	non-aq	23°C	100%	U	HM		1980ELa (36628)	403
							K(FeA+L)=1.88		

Medium: toluene. A= "Capped" porphyrin. DH=-22.0 kJ mol-1

```
--------------------------------------------------------------------------------
Fe++       sp  non-aq 25°C 100%  U    M                  1980ELa (36629) 404
                                        K(FeA+L)=2.17
Medium: toluene. A="Homologous capped" porphyrin
--------------------------------------------------------------------------------
Fe++       vlt non-aq 20°C 100%  U    M                  1978KBb (36630) 405
                                        K(FeA+L)=3.10
                                        K(FeA+2L)=4.98
Medium: DMSO. A=Phthalocyanine. K(FeA+2L)=4.47 by spectroscopy
--------------------------------------------------------------------------------
Fe++       gl  KNO3   25°C 0.50M U        K1=0.6    B2=0.90   1973BJa (36631) 406
--------------------------------------------------------------------------------
Fe++       gl  oth/un 25°C 0.50M U        K1=0.71        1950BJa (36632) 407
                                        B4=6.7 ?
Medium: 0.5 M C5H5N.HNO3
********************************************************************************
C5H5NO                  L    3-Pyridinol      CAS 109-00-2  (1475)
3-Hydroxypyridine; C5H4N.OH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       kin NaClO4 25°C 0.10M U                        1998CWa (36707) 408
                                        K(Fe(CN)5(H2O)+L)=4.88
Medium: 0.1 M LiClO4, pH=5
********************************************************************************
C5H5NO                 HL    4-Pyridinol      CAS 626-64-2  (1876)
4-Hydroxypyridine, Pyridin-4-one;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       kin NaClO4 25°C 0.10M U                        1998CWa (36712) 409
                                        K(Fe(CN)5(H2O)+L)=2.40
Medium: 0.1 M LiClO4, pH=5.
********************************************************************************
C5H5NOS                 L                     CAS 1121-31-9  (3052)
3-Mercaptopyridine 1-oxide; C5H4N(-O)(SH)
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       gl  oth/un 20°C 0.01M U        K1=4.7         1956ARb (36731) 410
********************************************************************************
C5H5NO2                HL                     CAS 35940-93-3  (3618)
3-Furancarboxaldehyde oxime  (3-Furfuraldoxime); C4H3O.CH(:N.OH)
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       gl  diox/w 20°C  60%  U  I     K1=5.20        1979GBd (36815) 411
                                        B(FeHL2)=21.98
********************************************************************************
C5H5N3O4              H2L                     CAS 59048-06-5  (6096)
```

N-Methylvioluric acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	NaNO3	25°C	0.50M	C			1984HNb (36877)	412
							B3=9.38			
Fe++	gl	NaNO3	25°C	0.50M	C			1978VNa (36878)	413
							B3=9.38			

****

C5H5N5O L CAS 700-02-7 (3033)
Adenine N-Oxide;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	oth/un	25°C	?	U		K1=2.80		1960PEb (37003)	414

****

C5H5O2F3 HL CAS 367-57-7 (163)
1,1,1-Trifluoropentane-2,4-dione; CF3.CO.CH2.CO.CH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	alc/w	25°C	75%	C		K1=4.72	B2= 9.01	1998ERa (37052)	415
							B3=12.2			

Medium: 75% v/v EtOH/H2O, 0.10 M KCl

****

C5H6 HL Cyclopentadiene CAS 542-92-7 (4288)
Cyclopentadiene; cyclo(-CH:CH.CH2.CH:CH-)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	sp	NaClO4	25°C	0.10M	U		B2=18.9		1972BSf (37076)	416

****

C5H6N2 L 2-Methylpyrazin CAS 109-08-0 (1785)
2-Methylpyrazine, 2-Methyl-1,4-diazine; C4H3N2.CH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	sp	NaCl	25°C	0.10M	U	M			1976SHa (37134)	417
							K(Fe(CN)X+L=Fe(CN)L+X)=3.6			

X= Dimethylpyrazine

****

C5H6N2O2S HL CAS 15112-09-1 (8298)
N-Methyl-2-thiobarbituric acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	NaClO4	31°C	0.10M	U	T H	K1=5.92	B2=10.41	1984SJa (37325)	418

Also data for 18 and 42 C. DH(K1)=-65.8 kJ mol-1, DS(K1)=-104 J K-1 mol-1
DH(K2)=-43.1, DS(K2)=-56.3.

****
C5H6O4S3 H2L (7055)
Trithiocarboglycolic acid; HOOC.CH2.S.CS.S.CH2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	alc/w	25°C	20%	U	T H	K1=8.13	B2=14.13	1994BSc (37466)	419

****
C5H6O7 H3L (8107)
Carboxymethyltartronic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	KCl	25°C	0.10M	C		K1=3.67	1984MMg (37489)	420
							K(FeL+H)=2.70		

****
C5H7NO3 HL CAS 29917-12-2 (5671)
2,3,4-Pentanetrione-3-oxime;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	EMF	oth/un	25°C	0.50M	U		B2=6.02	1984RCb (37512)	421
							B3=9.44		

****
C5H7NO6P2 H4L CAS 186599-36-0 (7613)
2,6-Pyridinediphosphonic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	KNO3	25°C	0.10M	C		K1=10.12 B2=15.45	1998CMb (37562)	422
							K(Fe(OH)2L+H)=11.38		
							K(Fe(OH)L+H)=9.81		
							K(FeL+H)=4.50		
							K(FeHL+H)=3.36		

K(FeL2+H)=6.51, K(FeHL2+H)=4.78, K(FeH2L2+H)=4.18,
K(FeH3L2+H)=3.57.

****
C5H7N3 L (1482)
2-Amino-4-methyl-1,3-diazine; C4H2N2(NH2)(CH3)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	kin	NaCl	25°C	0.10M	U			1993FMa (37577)	423
							Kout(Fe(CN)5H2O+L)=1.30		

At pH 6-7, phosphate buffer. Data also for bis-bipyridyl-xylenes and hexane

****
C5H7N3O2 L (6254)
1-Carbamido-3-methyl-pyrazol-5-one; CH3.C3H2N2(:O).CO.NH2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo

```
--------------------------------------------------------------------------------
Fe++       gl  diox/w 25°C  50%  U        K1=7.37   B2=13.19  1979PDa (37597) 424
********************************************************************************
C5H8N2                  L                       CAS 1759-84-0  (173)
1,2-Dimethylimidazole; C3H2N2(CH3)2
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       sp  non-aq 20°C 100%  U    M                  1993PMa (37625) 425
                                        K(FeALC+L=FeAL2+C)=-4.54
                                        K(FeBLC+L=FeBL2+C)=-7.04
                                        K(FeAC2+L=FeACL+C)=0.08
                                        K(FeBC2+L=FeBCL+L)=-2.07
In toluene. A=Tetramesitylporphine, B=Tetraphenylporphine, C=Tosylmethyliso-
cyanide. K(FeAL+L)=2.92, K(FeALCO+L=FeAL2+CO)=-4.22
--------------------------------------------------------------------------------
Fe++       sp  non-aq 23°C 100%  U TI M                  1982HDa (37626) 426
                                        K(FeA+L)=4.40
                                        K(FeAL+L)=0.31
Medium: toluene. A=Tetra(4-methoxy)phenylporphyrin. At 45 C, K(FeAL+L)=2.19.
In DMF: K=2.09
--------------------------------------------------------------------------------
Fe++       sp  non-aq 23°C 100%  U    M                  1982HDa (37627) 427
                                        K(FeA+L)=3.89
Medium: toluene. A='capped' porphyrin
--------------------------------------------------------------------------------
Fe++       sp  non-aq 23°C 100%  U    M                  1980ELa (37628) 428
                                        K(FeA+L)=3.06
Medium: toluene. A= "Capped" porphyrin.
--------------------------------------------------------------------------------
Fe++       sp  non-aq 25°C 100%  U    M                  1980ELa (37629) 429
                                        K(FeA+L)=3.61
Medium: toluene. A="Homologous capped" porphyrin
--------------------------------------------------------------------------------
Fe++       sp  non-aq 23°C 100%  U    M                  1979BEa (37630) 430
                                        K(FeA+L)=3.61
Medium: toluene. A="Capped Homologous" Porphyrin
--------------------------------------------------------------------------------
Fe++       sp  non-aq 23°C 100%  U T                    1979BEa (37631) 431
                                        K(FeA+L)=3.61
Medium: toluene. FeA=a substituted porphyrinato-Fe(II)
--------------------------------------------------------------------------------
Fe++       vlt non-aq 20°C 100%  U    M                  1978KBb (37632) 432
                                        K(FeA+2L)=2.38
                                        K(FeA+2L)=3.43
Medium: DMSO. A=Phthalocyanine. Cyclic voltammetry also used
********************************************************************************
C5H8O2                 HL    Acetylacetone    CAS 123-54-6  (164)
Pentane-2,4-dione; CH3.CO.CH2.CO.CH3
--------------------------------------------------------------------------------
```

```
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe++       gl  alc/w  25°C  75%  C  I     K1=6.38   B2=11.60  1998ERa (37958) 433
                                         B3=13.73
Medium: 75% v/v EtOH/H2O, 0.10 M KCl
In H2O, 0.10 M KCl: K1=4.97, B2=9.04, B3=10.8
-------------------------------------------------------------------------
Fe++       dis NaClO4 25°C 0.10M C        K1=5.2         1986SNa (37959) 434
Method: rate of distribution of volatile ligand between aqueous phase and
inert gas phase. K(H+L)=9.17 assumed.
-------------------------------------------------------------------------
Fe++       sp  non-aq 25°C 100%  U    M                  1967BGb (37960) 435
                                         K(FeL2+py) > 4
                                         K(FeL2py+py)=2.25
                                         K(FeL2py2+py)=1.40
Medium:benzene
-------------------------------------------------------------------------
Fe++       gl  oth/un 30°C  0.0  U        K1=5.07   B2=8.67   1954IHa (37961) 436
MEDIUM: 0 corr
-------------------------------------------------------------------------
Fe++       gl  diox/w 30°C  75%  U        K1=9.71   B2=18.19  1953UFb (37962) 437
*************************************************************************
C5H9NO2                HL                      CAS 14401-90-2  (6205)
Pent-2,4-dione monoxime; CH3.CO.CH2.C(:NOH).CH3
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe++       gl  alc/w  25°C  75%  U        K1=7.7    B2=12.90  1986BTa (38472) 438
                                         K3=4.0
Medium: 75% MeOH/H2O, 0.1 M NaClO4
*************************************************************************
C5H9NO2                HL    Proline          CAS 147-85-3  (44)
Pyrrolidine-2-carboxylic acid; C4H8N.COOH
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe++       gl  KCl    20°C  1.0M U        K1=4.07        1959PEc (38612) 439
-------------------------------------------------------------------------
Fe++       gl  oth/un 20°C 0.02M U        B2=8.3         1950ALa (38613) 440
*************************************************************************
C5H9NO3                HL    Hydroxyproline   CAS 51-35-4  (416)
4-Hydroxy-2-pyrrolidinecarboxylic acid; C4H7N(OH)(COOH)
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe++       gl  KCl    20°C  1.0M U        K1=3.94        1959PEc (38730) 441
*************************************************************************
C5H9NO4               H2L    Glutamic acid    CAS 56-86-0  (22)
2-Aminopentanedioic acid; H2N.CH(CH2.CH2.COOH)COOH
-------------------------------------------------------------------------
```

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	KNO3	25°C	0.10M	M		K1=5.08		1981GVa (39078)	442
Fe++	gl	KCl	20°C	1.0M	U		K1=3.52		1959PEc (39079)	443
Fe++	gl	oth/un	20°C	0.01M	U		K1=4.6		1952ALa (39080)	444

C5H9NO4 H2L MIDA CAS 4408-64-4 (190)
N-Methyliminodiethanoic acid; CH3.N(CH2.COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	NaClO4	25°C	0.50M	C	M	K1=6.18	B2=11.53	2001SFa (39250)	445
							K(Fe(NO)+L)=6.86			
							K(Fe(NO)L+L)=4.63			
Fe++	gl	KCl	25°C	0.10M	C		K1=6.71	B2=11.76	1986MDa (39251)	446
							K(Fe+HL)=2.29			
Fe++	gl	KNO3	25°C	0.10M	U		K1=6.65		1977TIa (39252)	447
Fe++	gl	KCl	20°C	0.10M	U		K1=6.65	B2=12.02	1955SAa (39253)	448

C5H9NS2 HL CAS 25769-03-3 (3623)
Pyrrolidine-N-carboxydithioic acid; C4H8N-CSSH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	sp	alc/w	25°C	75%	U				1970PNa (39332)	449
							B3=12.69			

Medium: 75% MeOH, 0.3 M NaClO4

C5H9N3 L Histamine CAS 51-45-6 (103)
4(5)-(2'-Aminoethyl)imidazole; C3H3N2.CH2.CH2.NH2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	KCl	25°C	.058M	U	T	K1=5.80	B2=10.06	1961SMa (39535)	450

0 C: K1=6.05, K2=4.30; 45 C: K1=5.38, K2=3.98

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	KNO3	30°C	1.0M	U		K1=9.60	B2=16.09	1956HFb (39536)	451

C5H9N3O5 H2L CAS 85594-21-4 (9125)
2-(Acetylamino)-N,N'-dihydroxypropanediamide;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	vlt	KNO3	25°C	0.10M	C				2004YYa (39581)	452
							K1eff=8.03			

Method: square wave voltammetry. Medium pH 7.0.

****

C5H9N3S HL (1822)
2-Mercaptohistamine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	NaClO4	25°C	0.10M	U		K1=5.40	B2=11.37	1977STc (39607)	453

****

C5H10NO7P H4L PMIDA CAS 5994-61-6 (2433)
N-(Phosphonomethyl)iminodiethanoic acid; H2O3P.CH2.N(CH2.COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	KNO3	25°C	0.10M	C		K1=11.6		2000SDa (39673)	454
							K(FeL+H)=5.45			
							K(FeHL+H)=3.6			
Fe++	gl	NaCl	25°C	0.10M	U		K1=9.86	B2=13.20	1993DLa (39674)	455
							B(FeHL)=15.27			
							B(FeH2L2)=28.51			
							B(FeH-1L)=-0.97			

****

C5H10N2O3 HL Glutamine CAS 56-85-9 (18)
2-Aminopentanedioic acid 5-amide; H2N.CH(CH2.CH2.CO.NH2)COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	NaClO4	25°C	3.00M	U		K1=4.43	B2=7.26	1973WIa (39816)	456

****

C5H11N L Piperidine CAS 110-89-4 (105)
Perhydropyridine; cyclo(-CH2.CH2.CH2.NH.CH2.CH2-) C5H11N

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	sp	non-aq	25°C	100%	U	M			1994STa (40446)	457
							K(FeA2B2+L=FeA2BL+B)=3.85			
							K(FeA2BL+L=FeA2L2+B)=2.18			
							K(FeB2C2+L=FeBC2L+B)=4.11			
							K(FeBC2L+L=FeC2L2+B)=2.38			

Medium: CH2Cl2. A=Dimethylglyoximediphenylborate, B=CH3CN, C=dmgdifluoro-
borate, D=Pyridine

****

C5H11NO2 HL Valine CAS 72-18-4 (43)
2-Amino-3-methylbutanoic acid; H2N.CH(CH(CH3)2)COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	alc/w	30°C	5%	M		K1=6.91		1994RRb (40704)	458

Medium: 5% v/v EtOH/H2O, 0.10 M KNO3.

```
--------------------------------------------------------------------------------
Fe++       gl  KCl    20°C  1.0M U      T K1=3.39        1959PEc (40705) 459
--------------------------------------------------------------------------------
Fe++       gl  oth/un 20°C 0.01M U        B2=6.8         1950ALa (40706) 460
********************************************************************************
C5H11NO2S              HL    Methionine       CAS 63-68-3  (42)
2-Amino-4-(methylthio)butanoic acid; H2N.CH(CH2.CH2.S.CH3)COOH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       gl  KCl    20°C  1.0M U        K1=3.24        1959PEc (41090) 461
--------------------------------------------------------------------------------
Fe++       gl  oth/un 20°C 0.01M U        B2=6.7         1950ALa (41091) 462
********************************************************************************
C5H11NO2S             H2L    Penicillamine    CAS 52-66-4  (350)
DL-2-Amino-3-mercapto-3-methylbutanoic acid; (CH3)2C(SH)CH(NH2)COOH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       oth NaClO4 35°C 0.10M U        K1=8.80   B2=15.10  1998GAc (41258) 463
Method: electrophoresis.  Medium: 0.10 M HClO4, 0.01 M H2L
********************************************************************************
C5H11NS2               HL                    CAS 147-84-2  (2126)
Diethyldithiocarbamic acid; (CH3.CH2)2N.CSSH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       ISE non-aq 25°C 100%  U        K1=7.5    B2=15.2   1984LSb (41350) 464
                                          B3=19.7
Medium: DMSO, 0.1 M NaClO4; Ag-electrode
--------------------------------------------------------------------------------
Fe++       sp  alc/w  25°C  75%  U                    1970PNa (41351) 465
                                          B3=11.34
Medium: 75% MeOH, 0.3 M NaClO4
********************************************************************************
C5H12N2O                L    Diethylurea      CAS 623-76-7  (2022)
1,3-Diethylurea; (CH3.CH2.NH)2.CO
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       vlt NaClO4 25°C 0.20M U        K1=-0.40  B2=-0.10  1985MCc (41458) 466
                                          K3=0.54
                                          K4=0.63
                                          K5=-0.15
********************************************************************************
C5H12N2O2              HL    Ornithine        CAS 1069-31-4  (46)
2,5-Diaminopentanoic acid; H2N.CH2.CH2.CH2.CH(NH2)COOH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
```

```
Fe++       gl  KCl    20°C  1.0M U        K1=3.09        1959PEc (41573) 467
--------------------------------------------------------------------------------
Fe++       gl  oth/un 20°C 0.01M U        K1=5.0         1952ALa (41574) 468
********************************************************************************
C6H3N3O7               HL    Picric acid      CAS 88-89-1  (593)
2,4,6-Trinitrophenol; HO.C6H2(NO2)3
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       con mixed  25°C  20%  C                        1994SSb (42109) 469
                                          K(FeC+L)=1.93
Medium:20% w/w propylene carbonate/ethylene carbonate.
FeC=ferrocene.
********************************************************************************
C6H4N4O                HL                    CAS 900-47-0  (3083)
4-Hydroxypteridine;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       gl  oth/un 20°C 0.01M U        K1=3.4    B2=5.9    1954AHb (42278) 470
********************************************************************************
C6H4N4O2              H2L    Lumazine         CAS 487-21-8  (3084)
2,4-Dihydroxypteridine (2,4-Pteridinediol)
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       gl  oth/un 20°C 0.01M U        K1=2.9    B2=5.6    1953ALa (42286) 471
********************************************************************************
C6H4O4                 H2L                   CAS 615-94-1  (1280)
2,5-Dihydroxy-1,4-benzoquinone;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       gl  KCl    30°C  25%  M TIH    K1=7.26   B2=13.30  1991GDe (42304) 472
Medium: 35% Dioxan/H2O, 0.1 M NaClO4. Other solvents and backgrounf concs.
********************************************************************************
C6H4O5                 H2L    Comenic acid     CAS 499-78-5  (2544)
3-Hydroxypyran-4-one-6-carboxylic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       sp  oth/un 25°C 0.10M U        B2=7.30        1974SNb (42318) 473
********************************************************************************
C6H5NO2                HL    Picolinic acid   CAS 98-98-6  (391)
2-Pyridine-carboxylic acid; C5H4N.COOH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       gl  NaClO4 35°C 1.00M U T      K1=4.35   B2=8.95   1984PHa (42531) 474
                                          B3=12.23
```

Fe++ gl NaClO4 30°C 0.10M U I K1=4.81 B2=8.39 1981RMa (42532) 475
K3=2.91

Fe++ gl NaNO3 20°C 0.10M U K1=4.90 B2=9.00 1960ANb (42533) 476
K3=3.30

Fe++ sp KNO3 25?°C 0.20M U 1958BRa (42534) 477
B3=11.30

****

C6H5NO3 HHL CAS 824-40-8 (878)
Pyridine-2-carboxylic acid N-oxide (Picolinic acid N-oxide); C5H4N(O)COO

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo

---

Fe++ gl NaClO4 30°C 0.10M U I K1=3.40 B2=6.24 1981RMa (42833) 478

****

C6H5NO4 H2L 4-Nitrocatechol CAS 3316-09-4 (890)
1,2-Dihydroxy-4-nitrobenzene; O2N.C6H3(OH)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo

---

Fe++ gl NaClO4 30°C 0.05M U TIH K1=14.72 B2=25.62 1986NDa (42924) 479
I=0.1, 40 C: K1=13.07, B2=22.76; 50 C: K1=12.91, B2=22.45
I=0.1, 30 C:K1=13.53, B2=23.52; I=0.2, 30 C:K1=13.08, B2=23.02

****

C6H5NO4 HL CAS 78901-24-3 (885)
4-Hydroxypyridine-2-carboxylic acid N-oxide; C5H3N(O)(OH).COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo

---

Fe++ gl NaClO4 30°C 0.10M U I K1=3.67 B2=6.74 1981RMa (42969) 480

****

C6H6NO5P H3L CAS 145432-83-3 (7384)
6-Phosphonopyridine-2-carboxylic acid; HOOC.C5H3N.PO3H2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo

---

Fe++ gl KNO3 25°C 0.10M C K1=8.70 B2=13.80 1998CMb (43221) 481
K(Fe(OH)2L+H)=10.77
K(Fe(OH)L+H)=9.09
K(FeL+H)=3.46
K(FeL2+H)=5.13
K(FeHL2+H)=3.83

****

C6H6N2O HL CAS 873-69-8 (1258)
Pyridine-2-aldoxime; C5H4N.CH:NOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo

---

```
Fe++       gl  KNO3   24°C 0.10M U        K1=9.4    B2=17.40  1962BEa (43293) 482
                                          K3=5.1
-------------------------------------------------------------------------------
Fe++       sp  oth/un 25°C .045M U T H                  1962HIa (43294) 483
                                          B3=24.85
                                          K(FeL3+H)=7.13
B3=25.13(18 C),24.70(28.5 C),24.43(32.5 C). DH(B3)=-84 kJ mol-1,DS=200
K=7.14(18 C),7.11(35 C); DH(K)=-3,DS=126.6. K'=3.33(33 C); DH(K')=4, DS=80
-------------------------------------------------------------------------------
Fe++       sp  oth/un   ?     ?  U        K1=3           1959IHa (43295) 484
                                          K3=7.0
*******************************************************************************
C6H6N2O                 L    Nicotinamide     CAS 98-92-0  (1473)
Pyridine-3-carboxylic acid amide, Vitamin PP, C5H4N.CO.NH2
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe++       oth none    0°C    ?  U        K1=1.00   B2=1.80   1971KAc (43341) 485
Method: freezing point depression
*******************************************************************************
C6H6N2O2               HL                        (8281)
3-Hydroxy-2-amidocarboxypyridine, Hydroxypicolinamide;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe++       gl  KNO3   25°C 0.10M C        K1=5.24   B2= 9.48  1990ARa (43374) 486
                                          K(FeL2+L)=4.08
*******************************************************************************
C6H6N2O2               HL                     CAS 5657-61-4  (1430)
Nicotinylhydroxamic acid; C5H4N.CO.NH.OH
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe++       sp  KCl    25°C 0.50M C        B2=17.20       1991LEc (43436) 487
                                          B3=23.47
                                          B(FeHL2)=20.03
                                          B(FeH2L2)=22.51
*******************************************************************************
C6H6N2O4               HL    Methylorotic     CAS 706-36-2  (2611)
3N-Methyl-2,4-dihydroxypyrimidine-6-caboxylic acid, methylorotic acid;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe++       gl  NaCl   20°C 0.15M U        K1=5.50        1979DZc (43473) 488
                                          K(Fe+HL)=2.30
*******************************************************************************
C6H6O2                H2L    Catechol         CAS 120-80-9  (534)
1,2-Dihydroxybenzene, pyrocatechol; HO.C6H4.OH
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
```

Fe++ gl alc/w 30°C 5% M K1=7.98 1994RRb (43753) 489
Medium: 5% v/v EtOH/H2O, 0.10 M KNO3.

Fe++ gl NaClO4 30°C 0.10M M TIH K1=13.89 B2=25.80 1986DNa (43754) 490
Data for 0.05-0.20 M NaClO4. Extrap. to I=0.0, K1=14.50, B2=26.83.
Data for 30-50 C. DH(K1)=-34.7 kJ mol-1.

Fe++ gl KNO3 25°C 1.0M U 1968TMa (43755) 491
K(Fe+H2L=FeHL+H)=-5.71
K(Fe+H2L=FeL+2H)=-14.332
K(FeL+H2L=FeL2+2H)=-16.740

****

C6H6O3 H3L Pyrogallol CAS 87-66-1 (696)
1,2,3-Trihydroxybenzene; C6H3(OH)3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	NaClO4	30°C	0.10M	M	TIH	K(Fe+HL)=12.88 K(Fe+2HL)=23.66	1986DNa (43958)	492

Data for 0.05-0.20 M NaClO4. Extrap. to I=0.0, K(Fe+HL)=13.01,
K(Fe+2HL)=24.25. Data for 30-50 C. DH(Fe+HL)=-29.4 kJ mol-1.

****

C6H6O8S2 H4L Tiron CAS 149-45-1 (104)
4,5-Dihydroxybenzene-1,3-disulfonic acid; (HO)2.C6H2(SO3H)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	NaClO4	30°C	0.05M	U	TIH	K1=13.83 B2=24.30	1986NDa (44425)	493

I=0.1, 40 C: K1=13.95, B2=25.00; 50 C: K1=13.70, B2=24.61
I=0.1, 30 C:K1=14.30, B2=25.66; I=0.2, 30 C:K1=14.80, B2=26.43

****

C6H6O9 H4L Ditartronic ac (8108)
Di(2-Propane-1,3-dioic acid)ether;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	KCl	25°C	0.10M	C		K1=4.41 K(FeL+H)=3.22	1984MMg (44536)	494
Fe++	gl	KCl	25°C	0.10M	C		K1=4.41 K(FeL+H)=3.22	1984MMg (44537)	495

****

C6H7N L Picoline CAS 109-06-8 (320)
2-Methylpyridine; C5H4N.CH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	vlt	non-aq	25°C	100%	U	M		1978KBb (44609)	496

K(FeA+L)=1.35
K(FeA+2L)=2.30
Medium: DMSO. A=Phthalocyanine
****
C6H7N L beta-Picoline CAS 108-99-6 (324)
3-Methylpyridine; C5H4N.CH3

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ vlt non-aq 20°C 100% U M 1978KBb (44699) 497
K(FeA+L)=3.08
K(FeA+2L)=4.64
Medium: DMSO. A=Phthalocyanine
****
C6H7N L gamma-Picoline CAS 108-89-4 (325)
4-Methylpyridine; C5H4N.CH3

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ vlt non-aq 20°C 100% U M 1978KBb (44821) 498
K(FeA+L)=4.04
K(FeA+2L)=5.87
Medium: DMSO. A=Phthalocyanine

Fe++ vlt non-aq 20°C 100% U 1978KBb (44822) 499
K(Fe(phthalocyanine)+L)=1.42
Medium: DMSO
****
C6H7NO HL 2-Aminophenol CAS 95-55-6 (2868)
2-Amino-1-hydroxybenzene; HO.C6H4.NH2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl none 20°C 0.0 U K1=3.66 B2=6.34 1961PEb (44927) 500

Fe++ gl none 20°C 0.0 U K1=8.0 1959SIb (44928) 501
****
C6H7NO L CAS 7295-76-3 (3095)
3-Methoxypyridine; C5H4N.OCH3

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ kin NaClO4 25°C 0.10M U 1998CWa (44992) 502
K(Fe(CN)5(H2O)+L)=5.25
Medium: 0.1 M LiClO4, pH=5
****
C6H7NO L CAS 620-08-6 (3096)
4-Methoxypyridine; C5H4N.OCH3

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo

---
Fe++ kin NaClO4 25°C 0.10M U 1998CWa (45016) 503
K(Fe(CN)5(H2O)+L)=5.29
Medium: 0.1 M LiClO4, pH=7.
****
C6H7NO4S HL (3122)
3-Amino-4-hydroxybenzenesulfonic acid; (HO)(H2N)C6H3.SO3H

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl none 20°C 0.0 U K1=3.32 B2=6.13 1961PEb (45083) 504
****
C6H7N3O L CAS 1452-63-7 (3097)
Pyridine-2-carboxylic acid hydrazide; C5H4N.CO.NH.NH2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl oth/un 20°C 0.01M U K1=8.4 1956ARd (45100) 505
****
C6H7N3O4 H2L CAS 54784-33-7 (6082)
1,3-Dimethyl-5-nitroso-barbituric acid; 1,3-Dimethylvioluric acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl NaNO3 25°C 0.50M C 1984HNb (45151) 506
B3=10.25

Fe++ gl NaNO3 25°C 0.50M C 1977VNa (45152) 507
B3=10.25
****
C6H8N2 L 2-Picolylamine CAS 29722-36-9 (502)
2-(Aminomethyl)pyridine; C5H4N.CH2NH2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ cal NaCl 25°C 0.15M C H K1=4.105 B2=7.441 1987ENa (45353) 508
B3=10.116
DH(K1)=-24.6 kJ mol-1, DS=-4 J K-1 mol-1; DH(B2)=-44, DS=-6; DH(B3)=-86,
DS=-96

Fe++ gl oth/un 30°C ->0 U K1=3.82 B2=7.16 1959GFa (45354) 509
****
C6H8N4B- L (7237)
Bis(pyrazol-1-yl)borate; (C3H3N2)2BH2-

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ dis non-aq 25°C 100% U 1996KSa (45438) 510
K(Fe+2HL=FeL2(org)+2H)=-3.96
By solvent extraction into CHCl3

****

C6H8O2 HL CAS 765-70-8 (8322)
3-Methylcyclopentane-1,2-dione;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	alc/w	30°C	5%	M	M	K1=6.74 B2=11.92 K(Fe(bpy)+L)=7.31 K(FeA+L)=5.89 K(FeB+L)=4.82 B(Fe(ala)L)=14.21	1994RRb (45453)	511

Medium: 5% v/v EtOH/H2O, 0.10 M KNO3. B(Fe(val)L)=14.08, B(Fe(en)L)=11.54
H2A is oxalic acid; H2B is catechol.

****

C6H8O6 H2L Ascorbic acid CAS 50-81-7 (285)
Ascorbic acid (Vitamin C);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	KNO3	30°C	0.10M	C	M	K(Fe(phen)+L)=7.98 K(Fe(bpy)+L)=8.12 K(Fe(en)+L)=6.35 K(Fe(baea)+L)=5.98	1984BPc (45636)	512

K(Fe(dipropylenetriamine)+L) = 5.34; baea=bis(aminoethyl)amine

Fe++	EMF	NaClO4	20°C	1.00M	U		K1=-0.27 B2=1.54	1981MOc (45637)	513

Ascorbic acid treated as HL. Antimony electrode used

Fe++	gl	NaClO4	37°C	0.15M	C		K1=7.09	1974CCa (45638)	514
Fe++	gl	NaClO4	25°C	3.00M	C		B(FeHL)=0.21 K(Fe+HL=FeL+H)-6.58	1974UWa (45639)	515

****

C6H8O6S H3L CAS 99-68-3 (3692)
(Carboxymethylthio)butanedioic acid; HOOC.CH(S.CH2.COOH).CH2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	KNO3	25°C	0.05M	M		K1=6.75	1975DPb (45694)	516

****

C6H8O7 H3L Citric acid CAS 77-92-9 (95)
2-Hydroxypropane-1,2,3-tricarboxylic acid; HOOCCH2.CH(OH)(COOH).CH2COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	NaCl	25°C	1.0M	C		K1=3.33 B2= 6.27 B(FeHL)=7.478 B(FeHL2)=10.60	2000KKc (46087)	517

```
                                        B(FeH-1L2)=-0.86
--------------------------------------------------------------------------------
Fe++       nmr none   25°C       U    M                  1990GKc (46088) 518
                                        K(Fe+H3L=FeH2L+H)=1.61
--------------------------------------------------------------------------------
Fe++       gl  KNO3   37°C 0.15M C        K1=4.56        1979ADb (46089) 519
                                        B(FeHL)=8.72
                                        B(FeH2L)=11.2
                                        B(FeHL2)=12.2
                                        B(Fe2H-2L2)=-5.4
--------------------------------------------------------------------------------
Fe++       EMF KNO3   25°C 0.10M U        K1=4.80        1974FMa (46090) 520
                                        B(FeHL)=8.62
--------------------------------------------------------------------------------
Fe++       gl  NaClO4 20°C 0.10M U        K1=4.4         1964TIb (46091) 521
                                        K(Fe+HL)=2.65
--------------------------------------------------------------------------------
Fe++       gl  NaClO4 25°C  1.0M U        K1=3.08        1954HSa (46092) 522
                                        K(Fe+HL)=2.12
                                        K(FeH-1L= FeH-2L+H)=3.0
********************************************************************************
C6H9NO6               H3L                     CAS 41035-84-1  (4367)
N-Carboxymethyl-L-aspartic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       gl  KCl    25°C  0.1M U        K1=7.80   B2=14.20  2002KNa (46376) 523
                                        B(FeHL)=12.24
                                        B(Fe(OH)L)=5.87
--------------------------------------------------------------------------------
Fe++       gl  KCl    25°C  1.0M C        K1=7.66        1979MBg (46377) 524
                                        K(Fe+HL)=2.72
                                        K(Fe+H2L)=2.70
                                        K(Fe+OH+L)=14.39
                                        K(Fe+2OH+L)=11.38
********************************************************************************
C6H9NO6               H3L    NTA              CAS 139-13-9  (191)
Nitrilotriethanoic acid; N(CH2.COOH)3
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       oth NaClO4 35°C 0.10M U    M   K1=9.97        1998GAc (46799) 525
                                        K(FeL+A)=5.06
Method: electrophoresis.  Medium: 0.10 M HClO4, 0.01 M H2L
H2A: penicillamine
--------------------------------------------------------------------------------
Fe++       gl  KCl    25°C 0.10M U        K1=8.90   B2=11.98  1994MMd (46800) 526
                                        *K(FeL(H2O))=-10.82
--------------------------------------------------------------------------------
Fe++       gl  KCl    25°C  1.0M C        K1=8.05   B2=11.53  1987MIa (46801) 527
```

Fe++ vlt oth/un 20°C 0.20M U T K2=4.0 1971BFa (46802) 528
K(Fe+HL)=1.0
B2(10 C)=4.30; 40 C=3.95. K(Fe+HL)(10 C)=1.0; 40 C, =2.2

Fe++ gl KCl 20°C 0.10M U T K1=8.83 1955SAa (46803) 529

Fe++ EMF KCl 20°C 0.10M U T K1=8.84 1951SFa (46804) 530
Method: H electrode

Fe++ EMF KCl 20°C 0.10M U K1=8.82 1951SHa (46805) 531
K(FeLOH+H)=10.6
Method: H electrode

****

C6H9N3O2 HL Histidine CAS 71-00-1 (1)
2-Amino-3-(4'-imidazolyl)propanoic acid; H2N.CH(CH2.C3H3N2)COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	kin	oth/un	25°C	0.10M	U	H	K(Fe(CN)5+L)=5.77		1978TMa (47551)	532

Medium: LiClO4. For N1 isomer. DH=-40.9 kJ mol-1, DS=-25 J K-1 mol-1.
For N3 isomer, K=3.46, DH=-26.7, DS=-21

Fe++	gl	none	21°C	0.0	M		K1=5.25	B2=9.69	1974YAa (47552)	533

Fe++	gl	NaClO4	25°C	3.00M	U	T	K1=5.88	B2=10.43	1970WIa (47553)	534

Fe++	gl	KNO3	15°C	0.20M	U	T	K1=5.39	B2=8.74	1969RMb (47554)	535

K1(40 C)=5.28, K2(40 C)=3.22

Fe++	gl	KCl	25°C	.058M	U	T	K1=5.85	B2=10.15	1961SMa (47555)	536

0 C, K1=6.65, K2=4.70; 45 C, K1=5.42, K2=4.74

Fe++	gl	oth/un	20°C	0.01M	U		B2=9.3		1952ALa (47556)	537

****

C6H9N3O2S H2L Thiolhistidine CAS 13552-61-9 (5659)
1-Amino-2-(2-Mercaptoimidazole)-propionic acid;

Fe++	gl	NaClO4	25°C	0.10M	U		K1=5.80	B2=11.11	1982TSb (47639)	538

****

C6H10N2O2 HL Nioxime CAS 492-99-9 (1098)
Cyclohexane-1,2-dione-dioxime; C6H8(:NOH)2

Fe++	vlt	alc/w	25°C	10%	U		K1=9.03	B2=17.29	1974ANb (47705)	539

****

C6H10O4S H2L CAS 111-17-1 (139)
3,3'-Thiodipropanoic acid; HOOC.CH2.CH2.S.CH2.CH2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	KNO3	25°C	0.05M	M		K1=4.15		1975DPb (48181)	540

C6H10O4S2 H2L CAS 7244-02-2 (438)
1,2-Bis(carboxymethylthio)ethane; HOOC.CH2.S.CH2.CH2.S.CH2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	NaClO4	25°C	0.10M	U		K1=2.73		1971PPb (48241)	541
							K(Fe+HL)=2.03			

C6H10O6 H2L CAS 23243-68-7 (242)
1,2-Bis(carboxymethoxy)ethane; HOOC.CH2.O.CH2.CH2.O.CH2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	KNO3	25°C	0.10M	U		K1=2.35		1975MTc (48339)	542

C6H10O7 HL Galacturonic CAS 685-73-4 (290)
D-Galacturonic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	vlt	NaClO4	25°C	0.10M	U		K1=3.09	B2=5.58	1990DGa (48388)	543
Fe++	gl	NaClO4	25°C	1.0M	U		K1=3.09	B2= 5.58	1989DGa (48389)	544
Fe++	gl	NaClO4	37°C	0.15M	C		K1=9.7	B2=18.3	1974CCa (48390)	545

C6H11NO4 H2L CAS 5336-17-4 (345)
N-Ethyliminodiethanoic acid; C2H5.N(CH2.COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	KCl	25°C	0.10M	C		K1=6.72	B2=11.68	1986MDa (48601)	546

C6H11NO4S H3L CAS 58033-48-5 (3124)
N-2-Mercaptoethyliminodiethanoic acid; HS.CH2.CH2.N(CH2.COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	KCl	20°C	0.10M	U		K1=11.72		1955SAa (48611)	547
							K(Fe+HL)=5.87			

C6H11NO5 H2L HIMDA CAS 93-62-9 (192)
N-(2-Hydroxyethyl)iminodiethanoic acid; HO.CH2.CH2.N(CH2.COOH)2

```
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Fe++       EMF KCl    20°C 0.10M U        K1=6.78   B2=10.00  1955SAa (48725) 548
******************************************************************************
C6H12N2O4             H2L    EDDA             CAS 5657-17-0  (119)
1,2-Diaminoethane-N,N'-diethanoic acid; HOOC.CH2.NH.CH2.CH2.NH.CH2.COOH
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Fe++       gl  KCl    25°C  1.0M C        K1=8.63   B2=10.67  1987MIa (49238) 549
******************************************************************************
C6H12N2O4             H2L    N,N-EDDA         CAS 5835-29-0  (2333)
1,2-Diaminoethane-N,N-diethanoic acid; H2N.CH2.CH2.N(CH2.COOH)2
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Fe++       gl  KCl    20°C 0.10M U        K1=9.81   B2=13.67  1955SAa (49300) 550
                                          K(Fe+HL)=3.84
******************************************************************************
C6H13NO2               HL    Leucine          CAS 61-90-5  (47)
2-Amino-4-methylpentanoic acid; H2N.CH(CH2.CH(CH3)2)COOH
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Fe++       gl  KCl    20°C  1.0M U      T K1=3.42        1959PEc (50073) 551
******************************************************************************
C6H13NO2               HL    Norleucine       CAS 616-06-8  (602)
2-Aminohexanoic acid (2-Aminocaproic acid) CH3.(CH2)3.CH(NH2).COOH
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Fe++       gl  oth/un 20°C 0.01M U        B2=8.6         1950ALa (50178) 552
******************************************************************************
C6H13NO4               HL    Bicine           CAS 150-25-4  (2124)
N,N-Bis(2-hydroxyethyl)glycine; (HO.CH2.CH2)2N.CH2.COOH
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Fe++       oth KNO3   20°C 0.10M U        K1=5           1965JMa (50359) 553
Method: paper electrophoresis
------------------------------------------------------------------------------
Fe++       gl  KCl    30°C 0.10M U        K1=4.31   B2=7.31   1953CCa (50360) 554
******************************************************************************
C6H14N2O               L                        (2357)
1-Oxa-4,7-diazacyclononane; Cyclo(-((CH2)2.NH)2(CH2)2.O.-)
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Fe++       gl  KNO3   25°C 0.10M U        K1=5.00        1990CCa (50712) 555
```

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C6H14N2O2 HL Lysine CAS 56-87-1 (41)
2,6-Diaminohexanoic acid; H2N.(CH2)4.CH(NH2)COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	oth/un	20°C	0.01M	U		K1=4.5	1952ALa (50822)	556

****

C6H14N2O2 HL CAS 69749-17-3 (1546)
2-Amino-N-hydroxyhexanamide; CH3.(CH2)3.CH(NH2).CO.NH.OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	KCl	25°C	0.50M	U		B2=23.29 B(FeHL)=17.36 B(FeH2L2)=32.95 B(FeHL2)=29.31 B3=27.77	1991LEb (50851)	557

B(FeHL3)=35.66, B(FeH2L3)=41.98, B(Fe(OH)L2)=15.98

****

C6H14N2O3 HL 5-Hydroxylysine CAS 13204-98-3 (1585)
2,6-Diamino-5-hydroxyhexanoic acid; H2N.CH2.CH(OH).CH2.CH2.CH(NH2).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	NaClO4	25°C	0.10M	U		K1=3.1	1965NCa (50871)	558

****

C6H14N2S L (5635)
1-Thia-4,7-diazacyclononane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	NaNO3	25°C	0.10M	U		K1=5.9 B2=12.00	1987HDa (50889)	559

****

C6H14N4O2 HL Arginine CAS 74-79-3 (40)
2-Amino-5-guanidopentanoic acid; H2N.CH((CH2)3.NH.C(:NH)(NH2)COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	oth/un	25°C	?	U	T	K1=2.86	1960PEd (51006)	560
K1=3.29(17 C)									
Fe++	gl	oth/un	20°C	0.01M	U		K1=3.20	1952ALa (51007)	561

****

C6H15NO3 Triethanolamine CAS 102-71-6 (447)
Tris-(2-hydroxyethyl)amine; L

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	oth	oth/un	25°C	0.43M	U		K1=2.27 B2=3.59	1966SKe (51289)	562

Medium: CH2OHCH2.NH3NO3
****
C6H15NS HL CAS 1942-52-5 (2595)
2-(Diethylamino)ethanethiol;(CH3.CH2)2N.CH2.CH2.SH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl NaClO4 20°C 0.10M U TI K1=12.00 B2=19.06 1986NDb (51353) 563
****
C6H15N3 L CAS 4730-54-5 (26)
1,4,7-Triazacyclononane; cyclo(-NH.CH2.CH2.NH.CH2.CH2.NH.CH2.CH2-)

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl KNO3 20°C 0.10M U T H K1=14.51 B2=20.93 1997BAa (51408) 564
At 32 C, K1=13.75. DH(K1)=-106.9 kJ mol-1. DS(K1)=351 J K-1 mol-1.
****
C6H15N3O2 HL CAS 52760-35-7 (6670)
Lysine hydroxamic acid; H2N.(CH2)4.CH(NH2)CO.NHOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl KCl 25°C 0.20M C 2002ECa (51425) 565
B(FeHL)=14.92
****
C6H15N3O3 L (6613)
1,3,5-Triamino-1,3,5-trideoxy-cis-inositol,5-Amino-5-deoxy-streptamine;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl KNO3 25°C 0.10M C K1=6.40 B2=11.18 1998GMa (51450) 566
****
C6H15O3P L CAS 122-52-1 (1723)
Triethylphosphite; (C2H5O)3P

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ sp non-aq 23°C 100% U M 1980ELa (51511) 567
K(FeA+L)=3.24
Medium: toluene. A= "Capped" porphyrin.
****
C6H18N4 L Trien-tetramine CAS 112-24-3 (11)
1,4,7,10-Tetraazadecane; H2N.CH2.CH2.NH.CH2.CH2.NH.CH2.CH2.NH2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl KCl 25°C 1.0M C K1=7.12 1987MIa (52097) 568

Fe++ cal KCl 25°C 0.10M U H 1961SPb (52098) 569
DG(K1)=-43.89 kJ mol-1, DH(K1)=-25.3, DS=62.8 J K-1 mol-1

```
--------------------------------------------------------------------------------
Fe++       gl  KCl    40°C 1.30M U T H                  1952JHa (52099) 570
                                          B(Fe3L2)=3.70
B(Fe3L2)=3.92(30C), DH=-38 kJ mol-1. At 35 C: DH(K1)=-38
--------------------------------------------------------------------------------
Fe++       gl  oth/un 30°C  1.0M U T      K1=8.31        1952JHa (52100) 571
40 C: K1=8.08
--------------------------------------------------------------------------------
Fe++       gl  KCl    20°C 0.10M U        K1=7.8         1950SCa (52101) 572
********************************************************************************
C6H18N4                 L    Tren             CAS 4097-89-6  (817)
2,2',2''-Triaminotriethylamine; (H2N.CH2.CH2)3N
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       cal KCl    25°C 0.10M U   H                  1960PCa (52196) 573
DG(K1)=-49.53 kJ mol-1, DH=-26.4, DS=-77 J K-1 mol-1
--------------------------------------------------------------------------------
Fe++       gl  KCl    20°C 0.10M U        K1=8.8         1950PSa (52197) 574
********************************************************************************
C7H5N                   L    Cyanobenzene     CAS 100-47-0  (4406)
Cyanobenzene, benzonitrile; C6H5.CN
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       sp  non-aq 25°C 100%  U    M                  1994STa (52568) 575
                                       K(FeA2B2+L=FeA2BL+B)=-1.70
                                       K(FeA2BL+L=FeA2L2+B)=-3.48
                                       K(FeC2B2+L=FeC2BL+B)=-2.23
                                       K(FeC2BL+L=FeC2L2+B)=-4.00
Medium: CH2Cl2. A=Dimethylglyoximediphenylborate, B=Pyridine, C=Dimethyl-
difluoroborate
********************************************************************************
C7H5NO4                 H2L    Quinolinic acid  CAS 89-00-9  (567)
2,3-Pyridinedicarboxylic acid; C5H3N.(COOH)2
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       gl  NaClO4 25°C 1.00M U T      K1=1.42        1984PHa (52625) 576
--------------------------------------------------------------------------------
Fe++       sp  oth/un 15°C 0.10M U        K1=3.2    B2=3.8    1963MSa (52626) 577
K1 measured in the presence of 0.02 M KCN
********************************************************************************
C7H5NO4                 H2L                     CAS 499-80-9  (566)
2,4-Pyridinedicarboxylic acid; C5H3N.(COOH)2
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       gl  oth/un 25°C  dil  U        K1=4.84   B2=8.10   1970OMa (52652) 578
********************************************************************************
```

C7H5NO4 H2L CAS 100-26-5 (2528)
2,5-Pyridinedicarboxylic acid, Isocinchomeronic acid; C5H3N.(COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	oth/un	25°C	dil	U		K1=5.91 B3=10.60	B2=9.32	1970OMa (52667)	579
Fe++	sp	oth/un	15°C	0.10M	U		K1=3.4	B2=3.8	1963MSa (52668)	580

K1 measured in the presence of 0.02 M KCN

****

C7H5NO4 H2L Dipicolinic aci CAS 449-83-2 (418)
2,6-Pyridinedicarboxylic acid; C5H3N.(COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	NaClO4	25°C	1.00M	U	T	K1=6.65	B2=10.78	1984PHa (52769)	581
Fe++	sp	oth/un	15°C	0.10M	U		K1=3.3	B2=3.6	1963MSa (52770)	582

K1 measured in the presence of 0.02 M KCN

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	NaNO3	20°C	0.10M	U		K1=5.71	B2=10.36	1960ANb (52771)	583

****

C7H5NO4 H2L Cinchomeronic CAS 490-11-9 (2852)
3,4-Pyridinedicarboxylic acid, Cinchomeronic acid; C5H3N.(COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	sp	oth/un	15°C	0.10M	U		B2=5.0 B3=4.9		1963MSa (52841)	584

B2 measured in the presence of 0.02 M KCN

****

C7H5N3O HL CAS 35252-03-0 (3142)
2-Hydroxypyrido[3',4'-b]pyrazine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	oth/un	20°C	0.01M	U		K1=5.4	B2=9.9	1954AHb (53089)	585

****

C7H6NO2Cl HL CAS 7120-43-6 (3782)
5-Chloro-2-hydroxybenzaldehyde oxime (5-chlorosalicylaldoxime)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	diox/w	20°C	75%	U		K1=8.2	B2=14.60	1965BEb (53387)	586

Medium: 75% dioxan, 0.1 M NaClO4

****

C7H6NO3Br H2L CAS 87353-69-3 (207)
4-Bromosalicylhydroxamic acid; Br.C6H3(OH).CO.NH.OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	EMF	diox/w	30°C	50%	U		K1=6.90		1977DJa (53395)	587

Medium: 50% dioxan, 0.1 M NaClO4

****

C7H6NO3Br H2L CAS 5798-94-7 (206)

5-Bromosalicylhydroxamic acid; Br.C6H3(OH).CO.NH.OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	EMF	diox/w	30°C	50%	U		K1=7.92		1977DJa (53406)	588

Medium: 50% dioxan, 0.1 M NaClO4

****

C7H6NO3Cl H2L (205)

3-Chlorosalicylhydroxamic acid; Cl.C6H3(OH).CO.NH.OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	EMF	diox/w	30°C	50%	U		K1=6.81		1977DJa (53415)	589

Medium: 50% dioxan, 0.1 M NaClO4

****

C7H6N2O4 HL CAS 1595-15-9 (3754)

2-Hydroxy-5-nitrobenzaldehyde oxime (5-nitrosalicylaldoxime)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	diox/w	20°C	75%	U		K1=6.9	B2=12.50	1965BEb (53492)	590

Medium: 75% dioxan, 0.1 M NaClO4

****

C7H6N2O4 H2L CAS 2683-49-0 (3753)

4-Aminopyridine-2,6-dicarboxylic acid (4-aminodipicolinic acid)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	KNO3	20°C	0.10M	U		K1=6.68	B2=12.53	1965ABa (53507)	591

****

C7H6N2O5 H2L CAS 831-51-6 (208)

5-Nitrosalicylhydroxamic acid; O2N.C6H3(OH).CO.NH.OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	EMF	diox/w	30°C	50%	U		K1=5.63		1977DJa (53522)	592

Medium: 50% dioxan, 0.1 M NaClO4

****

C7H6OS HL Thiobenzoic CAS 98-91-9 (6294)

Thiobenzoic acid; C6H5.COSH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	diox/w	30°C	60%	U		K1=4.3	B2=8.1	1972OTc (53555)	593

Medium: 60% v/v dioxan, 1 M (K,Na)NO3

****

C7H6O2 HL Salicylaldehyde CAS 90-02-8 (193)

2-Hydroxybenzaldehyde, Salicylaldehyde; HO.C6H4.CHO

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	diox/w	25°C	50%	U		K1=4.22	B2=7.62	1949MMa (53620)	594

****

C7H6O2S H2L Thiosalicylic CAS 147-93-3 (236)

2-Mercaptobenzoic acid; HS.C6H4.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	alc/w	50°C	45%	U	T H	K1=5.72	B2=10.34	1968RSh (53904)	595

Medium: 45% EtOH, 0.15 M. K1=5.45(30 C),5.57(40 C);K2=4.41(30 C),4.48(40 C).
DH(K1)=21.3 kJ mol-1(25 C),DS=175 J K-1 mol-1; DH(K2)=12.9, DS=130

****

C7H6O2S2 H2L CAS 89677-36-1 (5448)

3-(2-Thiophene)-2-mercaptopropenoic acid; C4H3S.CH:C(SH).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	diox/w	25°C	0.10M	U		K1=8.23	B2=14.73	1977WVa (53930)	596

****

C7H6O3 H2L Salicylic acid CAS 69-72-7 (14)

2-Hydroxybenzoic acid, Salicylic acid; HO.C6H4.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	cal	alc/w	25°C	100%	U	H			1990PJa (54194)	597

Medium: MeOH. DG(K1)=-27.4 kJ mol-1, DH=-4.1; DG(B2)=-47.5; DH=-32.3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	alc/w	25°C	100%	M				1988LTa (54195)	598
							K(Fe+HL)=4.8			
							K(Fe+2HL)=8.3			

Medium: MeOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	KCl	20°C	0.10M	U		K1=6.55	B2=11.25	1958PEe (54196)	599

****

C7H6O6S H3L CAS 5965-83-3 (399)

5-Sulfosalicylic acid, 2-Hydroxy-5-sulfobenzoic; HO3S.C6H3(OH).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	sp	diox/w	25°C	20%	U	I M	K1=5.85	B2=11.35	1988SIc (54974)	600
							B(FeLA)=13.10			

In 0.1 M NaClO4. In 50% EtOH/H2O, K1=5.10, K2=4.70, B(FeLA)=11.75
A=Alizarin maroon

Fe++ gl KCl 20°C 0.10M U K1=5.90 B2=9.9 1958PEe (54975) 601
****
C7H7NO2 H2L Salicylaldoxime CAS 94-67-7 (1486)
2-Hydroxybenzaldehyde oxime; HO.C6H4.CH:N.OH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl diox/w 20°C 75% U 1965BEb (55308) 602
K(Fe+HL)=9.38
K(FeHL+HL)=7.35
Medium: 75% dioxan, 0.1 M NaClO4
****
C7H7NO2 HL CAS 3222-47-7 (3154)
6-Methylpyridine-2-carboxylic acid; CH3.C5H3N.COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl NaNO3 20°C 0.10M U K1=4.10 B2=7.50 1960ANb (55428) 603
K3=2.7
****
C7H7NO2 HL CAS 495-18-1 (184)
Benzohydroxamic acid; C6H5.CO.NH.OH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl diox/w 37°C 30% C M B2=8.74 1983MAd (55496) 604
B(Fe(bpy)L)=9.42
****
C7H7NO3 H2L CAS 89-73-6 (204)
2-Hydroxybenzohydroxamic acid (salicylhydroxamic acid); HO.C6H4.CO.NHOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ EMF diox/w 30°C 50% U K1=7.74 1977DJa (55593) 605
Medium: 50% dioxan, 0.1 M NaClO4
****
C7H7NO3 HL CAS 548-93-6 (3156)
3-Hydroxyanthranilic acid (2-Amino-3-hydroxybenzoic acid)

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl oth/un 20°C 0.0 U K1=3.8 B2=8.3 1961PEb (55626) 606

Fe++ gl oth/un 20°C ? U K1=7.7 1959SIb (55627) 607
****
C7H7NO3 HL CAS 1197-10-0 (3759)
6-(Hydroxymethyl)pyridine-2-carboxylic acid; HO.CH2.C5H3N.COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---

Fe++ gl oth/un 25°C ? U K1=3.91 B2=7.13 1962GOa (55650) 608
****
C7H7NO4 HL CAS 17209-50-6 (886)
4-Methoxypyridine-2-carboxylic acid N-oxide; C5H3N(O)(OCH3).COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl NaClO4 30°C 0.10M U I K1=3.88 B2=7.10 1981RMa (55662) 609
****
C7H7N3O2 H2L CAS 4463-97-2 (1654)
2,6-Pyridinedialdoxime;C5H3N.(CH:NOH)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl KCl 25°C .025M U K1=5.380 1977HMa (55739) 610
K(FeH3L+H)=2.523
K(FeH2L+H)=4.481
K(FeHL+H)=4.899
K(FeL+H)=7.211

Fe++ sp oth/un 25°C 0.0 U H 1965HIa (55740) 611
K(FeL2+H)=7.40
K(FeHL2+H)=5
DH(FeL2+H)=0 kJ mol-1, DS=142 J K-1 mol-1
****
C7H8N2O HL CAS 5451-39-8 (3157)
2-Acetylpyridine oxime; C5H4N.C(:N.OH).CH3

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ sp KCl 28°C 0.50M U B2=12.73 1960BTb (55798) 612
****
C7H8N4 L (2641)
4,4'-(5,5')-Bisimidazolylmethane; C3H3N2.CH2.C3H3N2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl KNO3 30°C 0.16M U K1=4.47 B2=8.37 1965DFa (55965) 613
sulphate present; slightly low?
****
C7H8N4S L CAS 3608-75-1 (1799)
2-Pyridinecarboxaldehyde thiosemicarbazone; C5H4N.CH:N.NH.CS.NH2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ sp oth/un 25°C 0.10M U 1975LMb (56022) 614
B(FeH3L2)=44.9
B(FeH2L3)=41.7
B(FeHL3)=38.4
B3=34.2

****
C7H9N L 2,4-Lutidine CAS 108-37-4 (319)
2,4-Dimethylpyridine; C5H3N.(CH3)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	vlt	non-aq	20°C	100%	U	M	K(FeA+L)=1.43 K(FeA+2L)=1.70	1978KBb (56199)	615

Medium: DMSO. A=Phthalocyanine
****
C7H9N L 2,6-Lutidine CAS 108-44-1 (723)
2,6-Dimethylpyridine; C5H3N.(CH3)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	vlt	non-aq	20°C	100%	U	M	K(FeA+L)=1.66 K(FeA+2L)=1.95	1978KBb (56221)	616

Medium: DMSO. A=Phthalocyanine
****
C7H9N L 3,4-Lutidine CAS 583-58-4 (2056)
3,4-Dimethylpyridine; C5H3N.(CH3)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	sp	non-aq	23°C	100%	U	M	K(FeA+L)=2.26	1980ELa (56258)	617

Medium: toluene. A= "Capped" porphyrin.
****
C7H9N L 3,5-Lutidine (323)
3,5-Dimethylpyridine; C5H3N.(CH3)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	sp	alc/w	25°C	8%	U	I	K(Fe(CN)5py+L=FeX5L+py)=-0.008	1976BBa (56287)	618

Medium: 8% MeOH/H2O (0.047 mol fraction). Data also for 0.10, 0.16, 0.23 mf. MeOH/H2O. Data also for EtOH/H2O, t-BuOH/H2O,and glycerol/H2O mixtures
****
C7H9NO3S2 HL (940)
2-(Thiophene-2-aldimino)ethane sulfonic acid; C4H3S.CH:N.CH2.CH2.SO3H

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	NaClO4	25°C	0.10M	U		K1=4.63 B2=8.41	1982MSa (56457)	619

****
C7H9N3O2S2 L (6945)
1-Ethoxycarbonyl-3-thiazole-2-ylthiourea; C3H2NS.NHCSNHCOOC2H5

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	alc/w	25°C	60%	U		K1=6.21		1994KEa (56501)	620

Medium: 60 % EtOH/H2O, 0.1 M NaNO3

****

C7H10N2 L CAS 42088-91-5 (3134)

2-(Methylaminomethyl)pyridine (2-Picolylmethylamine)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	oth/un	30°C	->0	U		K1=3.53	B2=6.26	1959GFa (56612)	621

****

C7H11NO6P2 H4L CAS 4712-06-5 (4470)

Amino(phenyl)methylenediphosphonic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	KCl	25°C	0.10M	U		K1=10.40		1969DMd (56941)	622
							K(Fe+HL)=7.37			
							B(Fe2L)=15.62			

****

C7H12N2O2 H2L Heptoxime CAS 530-97-2 (1304)

1,2-Cycloheptanedione dioxime; C7H10(:NOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	diox/w	20°C	75%	U		K1=13.22	B2=24.65	1981HFa (57067)	623
Fe++	gl	NaClO4	20°C	0.10M	C				1980MHa (57068)	624
							K(Fe+HL)=10.46			
							K(Fe+2HL)=20.01			

****

C7H13NO4 H2L CAS 16578-07-5 (341)

N-Propyliminodiethanoic acid; CH3.CH2.CH2.N(CH2.COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	KCl	25°C	0.10M	C		K1=6.59	B2=11.88	1986MDa (57529)	625
							B(FeL(OH))=11.28			

****

C7H13NO4S H2L (3184)

N-(2-Methylthioethyl)iminodiethanoic acid; CH3.S.CH2.CH2.N(CH2.COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	EMF	KCl	20°C	0.10M	U		K1=7.12	B2=10.72	1955SAa (57546)	626

Method: H electrode

****

C7H13NO5 H2L CAS 62117-07-1 (3171)

N-(2-Methoxyethyl)iminodiethanoic acid; CH3.O.CH2.CH2.N(CH2.COOH)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ EMF KCl 20°C 0.10M U K1=6.81 B2=10.73 1955SAa (57574) 627
Method: H electrode
****
C7H14N2O2 HL CAS 111652-03-0 (8138)
Azetidine-1-(2-aminobutanoic acid);

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl KNO3 25°C 0.10M C K1=5.8 1989ARa (57700) 628
****
C7H21N2O10P3 H6L (7004)
N-(2-Hydroxyethyl)-1,2-diaminoethane-N,N'N'-trimethylenephosphonic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl KCl 25°C 0.10M U K1=12.84 1974KRd (58372) 629
K(Fe+HL)=9.04
K(Fe+H2L)=4.49
****
C8H5NO2 HL Isatin CAS 91-56-5 (7844)
2,3-Indolinedione;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl alc/w 30°C 5% M M K1=8.94 B2=16.19 1994RRb (58409) 630
K(Fe(bpy)+L)=9.22
K(FeA+L)=7.55
K(FeB+L)=6.65
B(Fe(ala)L)=16.12
Medium: 5% v/v EtOH/H2O, 0.10 M KNO3. B(Fe(val)L)=15.98, B(Fe(en)L)=13.46
H2A is oxalic acid; H2B is catechol.
****
C8H5NO3 L CAS 524-38-9 (8323)
N-Hydroxyphthalimide;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl alc/w 30°C 5% M M K1=4.90 B2= 8.95 1994RRb (58423) 631
K(Fe(bpy)+L)=5.66
K(FeA+L)=4.38
K(FeB+L)=3.85
K(FeL+ala)=7.63
Medium: 5% v/v EtOH/H2O, 0.10 M KNO3. K(FeL+val)=7.52, B(Fe(en)L)=9.89
H2A is oxalic acid; H2B is catechol.
****
C8H5NO6 H3L CAS 536-20-9 (3813)
Pyridine-2,4,6-tricarboxylic acid; C5H2N(COOH)3

```
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       sp  oth/un 15°C 0.10M U        K1=2.2    B2=3.7    1963MSa (58450) 632
K1 measured with 0.02 M KCN
********************************************************************************
C8H6N2O                HL                     CAS 5423-54-1  (3217)
4-Hydroxy-1,5-naphthyridine;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       gl  oth/un 20°C 0.01M U        K1=5.8    B2=10.7   1954AHb (58737) 633
********************************************************************************
C8H6N2O                HL                     CAS 17056-99-4  (3220)
5-Hydroxyquinoxaline;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       gl  oth/un 20°C 0.01M U        K1=6.8         1954AHb (58746) 634
********************************************************************************
C8H6N2O                HL                     CAS 17057-00-0  (3218)
8-Hydroxy-1,6-naphthyridine;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       gl  oth/un 20°C 0.01M U        K1=5.9    B2=10.5   1954AHb (58752) 635
********************************************************************************
C8H6N2O                HL                     CAS 70730-36-8  (3219)
8-Hydroxy-1,7-naphthyridine;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       gl  oth/un 20°C 0.01M U        K1=6.2    B2=11.7   1954AHb (58757) 636
********************************************************************************
C8H6N2O                HL                       (6290)
8-Hydroxycinnoline, (2-Hydroxybenzo)pyrimidine;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       gl  oth/un 20°C 0.10M U        K1=6.7         1954AHb (58767) 637
********************************************************************************
C8H6N2O                HL    8-Quinazolinol   CAS 7757-02-2  (3221)
8-Hydroxyquinazoline;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       gl  oth/un 20°C 0.01M U        K1=6.6    B2=12.2   1954AHb (58777) 638
********************************************************************************
C8H6N2S                 L                       (3814)
2-(2'-Pyridyl)-1,3-thiazole;
```

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ sp oth/un 25°C 0.10M U K1=2.7 B2=6.0 1968EHa (58794) 639
B3=8.8
Medium: NH2OH.HCl, pH=2.9
****
C8H6N2S L CAS 53911-41-4 (3815)
4-(2'-Pyridyl)-1,3-thiazole;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl oth/un 25°C 0.10M U K1=4.06 B2=7.10 1968EHa (58802) 640
B3=12.61
****
C8H6N4 L CAS 10199-00-5 (3791)
2,2'-Bis(1,3-diazine) (2,2'-bipyrimidine); C4H3N2.C4H3N2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ sp NaCl ? 0.20M U 1963BMa (58810) 641
B3=7.53
****
C8H7NO4 HL CAS 24195-03-7 (4498)
4-Methylpyridine-2,4-dicarboxylic acid,4-methyl ester; CH3.C5H2N(COOH)(COOCH3)

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ sp oth/un 25°C dil U K1=3.75 B2=6.51 1970OMa (59145) 642
****
C8H7NO4 HL CAS 17848-79-2 (4499)
5-Methylpyridine-2,5-dicarboxylic acid, 5-methyl ester; CH3.C5H2N(COOH)(COOCH3)

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ sp oth/un 25°C dil U K1=3.82 B2=6.08 1970OMa (59148) 643
****
C8H7N3 L CAS 18653-75-3 (3792)
2-(2'-Pyridyl)imidazole;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ EMF KNO3 25°C 0.10M U K1=4.097 B2=7.90 1967EHc (59183) 644
B3=11.600
****
C8H7N3 L CAS 16576-78-6 (3793)
4-(2'-Pyridyl)imidazole;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---

```
Fe++       gl  KNO3   25°C 0.10M U        K1=4.93   B2=9.02   1967EHb (59190) 645
                                          B3=13.76
**************************************************************************
C8H8N4                  L    Hydralazine      CAS 86-54-4  (3197)
1-Hydrazinophthalazine;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe++       gl  NaCl   37°C 0.15M U        B2=7.824       1984AMb (59402) 646
                                          B3=11.651
--------------------------------------------------------------------------
Fe++       gl  oth/un 22°C 0.10M U        K1=4.9    B2=9.5    1957FEa (59403) 647
                                          B3=13.8
**************************************************************************
C8H8O3                 HL    Mandelic Acid    CAS 611-72-3  (80)
2-Phenyl-2-hydroxyethanoic acid; C6H5.CH(OH).COOH
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe++       sp  NaClO4 30°C 0.10M U        K1=2.18   B2=3.60   1975KAd (59828) 648
**************************************************************************
C8H8O3                 HL                    CAS 673-22-3  (3194)
4-Methoxysalicylaldehyde; CH3O.C6H3(OH).CHO
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe++       gl  diox/w 30°C  75%  U        K1=4.30   B2=7.55   1967KBb (59979) 649
Medium: 75% dioxan, 0.1 M NaClO4
**************************************************************************
C8H8O4                 HL                    CAS 520-45-6  (4478)
3-Acetyl-2-hydroxy-6-methylpyran-4-one, Dehydroethanoic acid;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe++       gl  diox/w 35°C  50%  U        K1=3.11   B2=5.78   1971MAa (60087) 650
Medium: 50% dioxan, 0.1 M NaClO4
**************************************************************************
C8H8O5                H2L                    CAS 5629-08-3  (679)
7-Oxy-bicyclo[2.2.1]-hept-5-ene-2,3-dicarboxylic acid;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe++       gl  NaCl   37°C 0.15M U                         1988HYa (60125) 651
                                          B(FeHL)=10.66
                                          B(FeH2L)=13.25
                                          B(FeHL2)=14.58
**************************************************************************
C8H9NO2                HL                    CAS 1726-86-9  (1487)
2-Hydroxy-5-methylbenzaldehyde oxime; CH3.C6H3(OH).CH:NOH
--------------------------------------------------------------------------
```

```
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe++       gl  NaClO4 20°C 0.10M U        K1=9.7    B2=17.40  1965BEb (60195) 652
*************************************************************************
C8H9NO2                HL                      CAS 2446-50-6  (8185)
N-Methyl-benzohydroxamic acid;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe++       vlt non-aq 25°C 100%  C                        1992SSe (60266) 653
                                        B3=14.4
Medium: acetonitrile, 0.20 M Et4NPF6. Method: cyclic voltammetry.
*************************************************************************
C8H9NO2S               HL                      CAS 104-18-7  (4575)
(4-Aminophenylthio)ethanoic acid; H2N.C6H4.S.CH2.COOH
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe++       gl  KNO3   25°C 0.05M M        K1=3.97        1975DPb (60372) 654
*************************************************************************
C8H9NO3               H2L                      CAS 26071-07-8  (209)
5-Methylsalicylhydroxamic acid; CH3.C6H3(OH).CO.NH.OH
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe++       EMF diox/w 30°C  50%  U        K1=8.65        1977DJa (60437) 655
Medium: 50% dioxan, 0.1 M NaClO4
*************************************************************************
C8H9NO4                HL                      CAS 78257-51-9  (887)
4-Ethoxypyridine-2-carboxylic acid N-oxide; C2H5O.C5H3N-O(COOH)
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe++       gl  NaClO4 30°C 0.10M U  I     K1=3.80   B2=6.97   1981RMa (60478) 656
*************************************************************************
C8H9NO4               H2L                        (4520)
Dehydroethanoic acid oxime;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe++       gl  diox/w 35°C  50%  U                        1971MAa (60493) 657
                                      K(Fe+HL)=2.92
                                      K(Fe+2HL)=5.33
Medium: 50% dioxan, 0.01 M NaClO4
*************************************************************************
C8H9N3O7               H2L    Uramildiacetic   CAS 13055-06-5  (185)
5-Amino-2,4,6-trioxo-1,3-perhydrodiazimino-N,N-diethanoic acid;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
```

Fe++ oth KNO3 25°C 0.10M U K1=10.56 1972FVa (60632) 658
****
C8H11N L CAS 69376-33-6 (542)
2,4,6-Trimethylpyridine; C5H2N.(CH3)3

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ vlt non-aq 20°C 100% U M 1978KBb (60945) 659
K(FeA+L)=0.24
Medium: DMSO. A=Phthalocyanine
****
C8H11NO8 H4L CAS 7408-20-0 (2608)
Amino-di(butanedioic acid);HN(CH(COOH)CH2.COOH)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl KCl 25°C 0.1M U K1=9.00 B2=14.85 2002KNa (61206) 660
B(FeHL)=13.53
B(FeH2L)=17.36
B(Fe(OH)L)=4.40
****
C8H12N4B- L (7238)
(Pyrazol-1-yl)dihydro(3,5-dimethylpyrazol-1-yl)borate; C3H3N2.BH2.C3HN2(CH3)2-
---
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ dis non-aq 25°C 100% U 1996KSa (61544) 661
K(Fe+2HL=FeL2(org)+2H)=-3.82
By solvent extraction into CHCl3
****
C8H12N4O3 HL His-Gly CAS 2578-58-7 (274)
Histidyl-glycine; H2N.CH(CH2.C3H3N2).CO.NH.CH2.COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl none 21°C 0.0 M K1=4.20 1974YAa (61629) 662
****
C8H13NO6S H3L (5675)
2-Mercapto-1-aminoethane-N,N,S-triethanoic acid; HOOC.CH2.S.CH2.CH2.N(CH2COOH)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl NaClO4 25°C 0.10M U K1=8.94 1975POa (61823) 663
K(Fe+HL)=2.11
****
C8H14N2O2 H2L Octoxime CAS 18310-14-0 (1303)
1,2-Cyclooctanedione dioxime; C8H12(:NOH)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---

```
Fe++       gl  diox/w 20°C  75%  U        K1=13.10  B2=24.55  1981HFa (61898) 664
-------------------------------------------------------------------------------
Fe++       gl  NaClO4 20°C 0.10M C                        1980MHa (61899) 665
                                        K(Fe+HL)=10.21
                                        K(Fe+2HL)=19.70
*******************************************************************************
C8H14N2O4             H2L                      CAS 55033-06-2  (8139)
Azetidine-2-carboxy-1-(2-aminobutaneoic acid)
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe++       gl  KNO3   25°C 0.10M C        K1=8.3         1989ARa (61951) 666
Fer another  racemate: K1=7.65
-------------------------------------------------------------------------------
Fe++       gl  KNO3   25°C 0.10M C        K1=8.3         1989ARa (61952) 667
Fer another  racemate: K1=7.65
*******************************************************************************
C8H14O4S3             H2L                         (2526)
3,6,9-Trithiaundecanedioic acid; HOOC.CH2.S.C2H4.S.C2H4.S.CH2.COOH
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe++       gl  NaClO4 25°C 0.10M U        K1=1.88        1971PPc (62122) 668
                                        K(Fe+HL)=0.7
*******************************************************************************
C8H14O7               H2L                         (241)
Di(carboxymethoxy)ethyl ether; (HOOC.CH2.O.CH2.CH2)2O
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe++       gl  KNO3   25°C 0.10M U        K1=2.71        1975MTc (62148) 669
*******************************************************************************
C8H16N2O4             H2L                         (267)
1,2-Diaminoethane-N,N'-di(2-propanoic acid); ((CH3)(COOH).CH.NH.CH2)2
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe++       gl  KNO3   20°C 0.10M U        K1=8.45        1966MKb (62471) 670
*******************************************************************************
C8H16N2O4             H2L                      CAS 13288-40-9  (3237)
1,2-Diaminoethane-N,N'-di(3-propanoic acid); (HOOCCH2CH2NHCH2.)2
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe++       gl  KCl    30°C 0.10M U        K1=6.3         1953CCb (62501) 671
*******************************************************************************
C8H16O2S2             H3L    Dihydrolipoic      (6750)
6,8-Dimercapto-octanoic acid, dihydrolipoic acid; HSCH2.CH2.CH(SH).(CH2)4.COOH
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
```

```
--------------------------------------------------------------------------------
Fe++       gl  none   25°C  0.0  C                        1992BPa (62628) 672
                                      B(FeH6L2)=61.23
                                      B(FeH5L2)=57.21
                                      B(FeH4L2)=51.85
                                      B(FeH4L3)=59.42
B(FeH3L3)=49.73
********************************************************************************
C8H19NO2                L                       CAS 102-79-4  (3841)
N-Butyl-2,2'-iminodiethanol  (butyldiethanolamine);
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       oth oth/un 25°C 0.43M U        K1=2.10   B2=3.35   1966SKe (63033) 673
Medium: CH2OHCH2NH2.HNO3
********************************************************************************
C8H19N3S                L                       CAS 87071-53-2  (719)
1-Thia-4,7,10-triazacyclododecane; cyclo(-S.(C2H4.NH)3.C2H4-)
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       gl  NaClO4 35°C 0.20M C        K1=7.82        1984KKa (63145) 674
********************************************************************************
C8H23N5                 L    Tetren             CAS 112-57-2  (715)
1,4,7,10,13-Pentaazatridecane (Tetraethylenepentamine);
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       gl  none   25°C  0.0  C   H                   1998DFd (63468) 675
                                      K(Fe(CN)6+HL)=3.10
                                      K(Fe(CN)6+H2L)=4.40
                                      K(Fe(CN)6+H3L)=6.50
                                      K(Fe(CN)6+H4L)=8.98
K(Fe(CN)6+H5L)=11.09.  Constants are for ion pair formation.
DH(Fe(CN)6+HL)=-8 kJ mol-1; DH(Fe(CN)6+H2L)=3; DH(Fe(CN)6+H3L)=11.
--------------------------------------------------------------------------------
Fe++       cal KCl    25°C 0.10M U   H                   1964PVa (63469) 676
DH(K1)=-36.4 kJ mol-1, DS=66.9 J K-1 mol-1
--------------------------------------------------------------------------------
Fe++       gl  KCl    25°C 0.10M U        K1=9.85        1963PVa (63470) 677
                                      K(Fe+HL)=4.2
--------------------------------------------------------------------------------
Fe++       gl  none   25°C  0.0  U T H    K1=11.40       1958JSa (63471) 678
K1=11.18(35 C), 10.97(45 C). DH(K1)=-39.1 kJ mol-1, DS=84 J K-1 mol-1
********************************************************************************
C9H5NOBr2               HL                      CAS 521-74-4  (3279)
5,7-Dibromo-8-hydroxyquinoline;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
```

Fe++ gl diox/w 35°C 75% U K1=7.43 B2=14.51 1970GMh (63519) 679
Medium: 75% v/v dioxan, 0.2 M NaClO4

****

C9H5NOClI HL CAS 130-26-7 (1541)
5-Chloro-7-iodo-8-hydroxyquinoline;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	diox/w	25°C	75%	U		K1=7.61	B2=15.41	1958JPa (63527)	680
							K3=4.82			

Medium: 75% dioxan, 0.3 M NaCl

****

C9H5NOCl2 HL CAS 773-76-2 (3278)
5,7-Dichloro-8-hydroxyquinoline;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	diox/w	35°C	75%	U		K1=7.13	B2=14.00	1970GMh (63541)	681

Medium: 75% dioxan, 0.2 M NaClO4

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	diox/w	25°C	75%	U		K1=7.50	B2=14.81	1958JPa (63542)	682
							K3=4.50			

Medium: 75% dioxan, 0.3 M NaCl

****

C9H5NOI2 HL CAS 83-73-8 (3280)
5,7-Di-iodo-8-hydroxyquinoline;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	diox/w	35°C	75%	U		K1=7.40	B2=14.35	1971MAb (63562)	683

Medium: 75% v/v dioxan, 0.1 M NaClO4

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	diox/w	25°C	75%	U		K1=7.40	B2=15.09	1958JPa (63563)	684
							K3=4.25			

Medium: 75% dioxan, 0.3 M NaCl

****

C9H5NO2Br2 HL CAS 16846-41-1 (4666)
5,7-Dibromo-8-hydroxyquinoline N-oxide;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	diox/w	35°C	75%	U		K1=5.93	B2=11.25	1970GMh (63582)	685

Medium: 75% v/v dioxan, 0.2 M NaClO4

****

C9H5NO2Cl2 HL CAS 21168-33-2 (4665)
5,7-Dichloro-8-hydroxyquinoline N-oxide;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	diox/w	35°C	75%	U		K1=5.80	B2=11.43	1970GMh (63592)	686

Medium: 75% v/v dioxan, 0.1 M NaClO4

****

C9H5NO4 HL CAS 22308-86-7 (4607)

3-Nitroso-4-hydroxycoumarin (oximidobenzotetronic acid);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	diox/w	21°C	50%	U		B3=12.70	1970MGd (63606)	687

Medium: 50% dioxan, 0.3 M NaClO4

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	dis	NaClO4	20°C	0.10M	U		B3=13.91	1969MBe (63607)	688

****

C9H5N2O2Cl HL CAS 20254-76-6 (1414)

3-Chloroquinoxaline-2-carboxylic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	alc/w	20°C	5%	U	T	K1=3.40	1982KRa (63620)	689

****

C9H5N3O5 HL CAS 1084-32-8 (4608)

5,7-Dinitro-8-hydroxyquinoline;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	diox/w	35°C	75%	U		K1=4.95 B2=8.87	1970GMh (63627)	690

Medium: 75% dioxan, 0.2 M NaClO4

****

C9H5N3O6 HL CAS 21168-36-3 (4609)

5,7-Dinitro-8-hydroxyquinoline-N-oxide;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	diox/w	35°C	75%	U		K1=3.12 B2=5.15	1970GMh (63635)	691

Medium: 75% v/v dioxan, 0.2 M NaClO4

****

C9H6NOBr HL CAS 1198-14-7 (3281)

5-Bromo-8-hydroxyquinoline;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	diox/w	25°C	75%	U		K1=7.92 B2=16.11 K3=5.30	1958JPa (63643)	692

Medium: 75% dioxan, 0.3 M NaCl

****

C9H6NOCl HL CAS 130-16-5 (1268)

5-Chloro-8-hydroxyquinoline;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo

```
--------------------------------------------------------------------------------
Fe++       gl  diox/w 25°C  60%  U        K1=8.61   B2=16.62  1973SCd (63660) 693
Medium: 60% dioxan, 0.1 M NaClO4
--------------------------------------------------------------------------------
Fe++       gl  diox/w 25°C  75%  U        K1=7.86   B2=15.93  1958JPa (63661) 694
                                         K3=4.50
Medium: 75% dioxan, 0.3 M NaCl
********************************************************************************
C9H6NOF                HL                     CAS 387-97-3  (3283)
5-Fluoro-8-hydroxyquinoline;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       gl  diox/w 25°C  50%  U        B2=15.9        1958TWa (63672) 695
                                         B3=21.3
Medium: 50% dioxan, 0.3 M NaCl
********************************************************************************
C9H6NOI                HL                     CAS 15207-63-1  (3282)
5-Iodo-8-hydroxyquinoline;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       gl  diox/w 25°C  75%  U        K1=7.58   B2=15.71  1958JPa (63682) 696
                                         B3=21.06
Medium: 75% dioxan, 0.3 M NaCl
********************************************************************************
C9H6NO4IS             H2L    Ferron           CAS 547-91-1  (275)
7-Iodo-8-hydroxyquinoline-5-sulfonic acid; (HO)(HO3S)C9H4NI
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       gl  KNO3   25°C 0.10M C        K1=9.53   B2=17.74  1985ZHa (63790) 697
--------------------------------------------------------------------------------
Fe++       gl  oth/un 20°C 0.03M U        K1=6.79        1977KCb (63791) 698
--------------------------------------------------------------------------------
Fe++       gl  diox/w 25°C  50%  U        B2=13.8        1958TWa (63792) 699
                                         B3=18.85
Medium: 50% dioxan, 0.3 M NaCl
********************************************************************************
C9H6N2O2               HL                     CAS 879-65-2  (1413)
Quinoxaline-2-carboxylic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       gl  alc/w  20°C   5%  U T      K1=3.40        1982KRa (63850) 700
********************************************************************************
C9H6N2O3               HL                     CAS 1204-75-7  (1415)
3-Hydroxyquinoxaline-2-carboxylic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
```

```
--------------------------------------------------------------------------------
Fe++       gl  alc/w  20°C   5%  U T      K1=3.31        1982KRa (63852) 701
********************************************************************************
C9H6N2O3               HL                      CAS 5437-99-0  (3865)
5-Nitro-8-hydroxyquinoline;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       gl  diox/w 25°C  60%  U        K1=8.56   B2=16.18  1973SCd (63862) 702
Medium: 60% dioxan, 0.1 M NaClO4
********************************************************************************
C9H6O4                 HL    Ninhydrin        CAS 485-47-2  (2536)
1,2,3-Indantrione monohydrate, Trioxohydrindene monohydrate;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       gl  alc/w  30°C   5%  M    M   K1=6.54   B2=11.70  1994RRb (63950) 703
                                        K(Fe(bpy)+L)=7.23
                                        K(FeA+L)=5.85
                                        K(FeB+L)=5.05
                                        B(Fe(ala)L)=14.13
Medium: 5% v/v EtOH/H2O, 0.10 M KNO3. B(Fe(val)L)=14.04, B(Fe(en)L)=11.48
H2A is oxalic acid; H2B is catechol.
********************************************************************************
C9H7NO                 HL    Oxine            CAS 148-24-3  (504)
8-Hydroxyquinoline (8-quinolinol);
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       gl  diox/w 25°C  60%  U        K1=9.59   B2=18.17  1973SCd (64256) 704
Medium: 60% dioxan, 0.1 M NaClO4
--------------------------------------------------------------------------------
Fe++       sp  mixed    ?   90%  U  I     B2=13.7        1966BAb (64257) 705
Medium: N2H4/H2O.  B2=6.5(5%),6.5(10%),6.9(25%),8.6(50%),10.7(64%),13.0(85%)
--------------------------------------------------------------------------------
Fe++       gl  diox/w 25°C  75%  U        K1=8.58   B2=16.93  1958JPa (64258) 706
                                        B3=22.23
Medium: 75% dioxan, 0.3 M NaClO4
--------------------------------------------------------------------------------
Fe++       gl  diox/w 25°C  50%  U        K1=8.71   B2=16.83  1958TWb (64259) 707
                                        B3=22.13
Medium: 50% dioxan, 0.3 M NaClO4
--------------------------------------------------------------------------------
Fe++       gl  oth/un 20°C 0.01M U        K1=8.0    B2=15.0   1953ALa (64260) 708
--------------------------------------------------------------------------------
Fe++       gl  diox/w 25°C  70%  U        K1=9.83   B2=18.84  1949MMa (64261) 709
********************************************************************************
C9H7NO2                HL                      CAS 1127-45-3  (4614)
8-Hydroxyquinoline-N-oxide;
--------------------------------------------------------------------------------
```

```
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe++       gl  diox/w 25°C  50%  U        K1=10.75  B2=19.60  1970GMb (64403) 710
Medium: 50% dioxan, 0.3 M NaClO4
*************************************************************************
C9H7NO4S             H2L    Sulfoxine        CAS 84-88-8  (448)
8-Hydroxyquinoline-5-sulfonic acid;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe++       sp  mixed    ?   64%  U  I     B2=9.3         1966BAb (64535) 711
Medium: 64% N2H4. B2=6.2(5% N2H4), 5.7(10%), 6.2(25%), 8.0(50%)
-------------------------------------------------------------------------
Fe++       gl  NaCl   25°C 0.30M U        B2=15.7        1958TWa (64536) 712
                                         B3=21.75
-------------------------------------------------------------------------
Fe++       gl  oth/un 20°C 0.01M U        K1=8.4    B2=15.1   1953ALa (64537) 713
*************************************************************************
C9H7N3O2S            H2L    TAR              CAS 2246-46-0  (707)
4-(2'-Thiazolylazo)-resorcinol; C3H2NS.N:N.C6H3(OH)2
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe++       sp  none   25°C  0.0  U                        1985FYa (64703) 714
                                         B3=23.03
-------------------------------------------------------------------------
Fe++       gl  alc/w  25°C  50%  U                        1967NPb (64704) 715
                                         K(Fe+2HL)=21.6
Medium: 50% MeOH, 0.1 M NaClO4
*************************************************************************
C9H8N4O4S2           H2L                        (2879)
Indol-2,3-dione-3-thiosemicarbazone-5-sulfonic acid;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe++       gl  KNO3   37°C 0.15M M        K1=4.3    B2=8.91   1982STa (64862) 716
*************************************************************************
C9H8O3               H2L    o-Coumaric acid  CAS 501-98-4  (6327)
4-Hydroxycinnamic acid; HO.C6H4.CH:CH.COOH
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe++       gl  NaClO4 25°C 0.10M U        K1=11.38  B2=20.29  1975TBb (64884) 717
*************************************************************************
C9H8O4                HL    Acetylsalicylic  CAS 50-78-2  (1240)
2-Acetoxybenzoic acid, Acetylsalicylic acid; CH3.CO.O.C6H4.COOH
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe++       gl  KNO3    RT  0.10M C        K1=2.7    B2= 5.30  1985KLc (64896) 718
```

****
C9H8O4 H3L Caffeic acid CAS 331-39-5 (6037)
3-(3,4-Dihydroxyphenyl)propenoic acid; (HO)2C6H3.CH:CH.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	NaCl	25°C	0.10M	C		K1=3.86 B(FeH-1L)=-3.83 B(FeH-1L2)=-0.36 B(FeH-2L3)=-6.14 B(Fe2L)=6.69	1987LVa (64919)	719

****
C9H9NO2 HL CAS 25355-34-4 (6206)
1-Phenyl-prop-1,2-dione monoxime; C6H5.CO.C(:NOH).CH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	alc/w	25°C	75%	U		K1=13.5 B2=22.90 K3=6.4	1986BTa (65036)	720

Medium: 75% MeOH/H2O, 0.1 M NaClO4
****
C9H10N2O2 HL CAS 52829-64-8 (4627)
2-Acetoacetamidopyridine; C5H4N.NH.CO.CH2.CO.CH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	KNO3	25°C	0.10M	U		K1=5.65	1967HAb (65228)	721

****
C9H10N2O3 HL CAS 62134-49-0 (9110)
N-(2-Pyridyl)-3-carboxypropanamide;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	NaClO4	25°C	0.10M	U		K1=4.19 B2= 6.39	2002GSa (65261)	722

****
C9H10N6B HL CAS 18583-60-3 (7936)
Hydrotris(pyrazolyl)borate;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	dis	non-aq	25°C	100%	C		K(Fe+2HL=FeL2(org)+2H)=4.8	2001KSb (65310)	723

Method: solvent extraction into chloroform.
K: Fe+2HL(org)=FeL2(org)+2H.
****
C9H10O8 H4L CAS 3724-52-5 (1264)
cis-1,2,3,4-Cyclopentanetetracarboxylic acid; C5H6.(COOH)4

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo

Fe++ gl NaClO4 30°C 0.19M U K1=5.55 B2=9.65 1985MSb (65643) 724
****
C9H11NO2 HL Phenylalanine CAS 63-91-2 (2)
2-Amino-3-phenylpropanoic acid; H2N.CH(CH2.C6H5)COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl NaClO4 25°C 3.0M U T K1=3.74 B2=7.19 1972WYa (65934) 725

Fe++ gl KCl 20°C 1.0M U K1=3.26 1959PEc (65935) 726

Fe++ gl oth/un 20°C 0.01M U B2=6.3 1950ALa (65936) 727
****
C9H11NO3 H2L Tyrosine CAS 60-18-4 (4)
2-Amino-3-(4-hydroxyphenyl)propanoic acid; HO.C6H4.CH2.CH(NH2).COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl oth/un 20°C 0.01M U 1952ALa (66219) 728
K(Fe+2HL)=7.1
****
C9H11NO4 H3L DOPA CAS 59-92-7 (5)
2-Amino-3-(3,4-dihydroxyphenyl)propanoic acid;H2NCH(CH2C6H3(OH)2)COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl NaCl 25°C 0.12M U K1=8.80 1978RMc (66396) 729
****
C9H11NO4 HL CAS 18901-23-2 (888)
4-n-Propoxy-pyridine-2-carboxylic acid N-oxide;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl NaClO4 30°C 0.10M U I K1=3.71 B2=6.84 1981RMa (66406) 730
****
C9H11N3O2S HL CAS 51146-75-9 (6170)
N-(2-Hydroxy-3-methoxybenzylidene)thiosemicarbazide; CH3O(OH)C6H3.CH:N.CS.NH.NH2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl diox/w 35°C 50% U I K1=7.84 B2=14.21 1993GJa (66505) 731
Medium: 50% v/v dioxane/H2O, 0.10 M NaClO4.
Also data for 50% dioxane/H2O, 0.0200.2 M NaClO4. At I=0, K1=8.47.
****
C9H14N2O5 L beta-Asp-Pro CAS 66180-29-8 (8142)
Pyrrolidine-2-carboxy-1-(2-amino-4-one-butanoic acid), beta-Aspartly-proline;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl KNO3 25°C 0.10M C K1=4.7 1989ARa (67129) 732

****

C9H15NO6S H3L DCMM CAS 72306-91-3 (8239)
Dicarboxymethyl-N,N-methionine acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	NaCl	25°C	0.50M	C				1980MFc (67469)	733
							K(Fe+HL)=4.66			
							K(FeHL+HL)=3.41			

Addditional methods: conductivity, spectrophotometry

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	KCl	25°C	1.0M	C		K1=6.50	B2=11.38	1979MBg (67470)	734
							K(Fe+HL)=4.66			
							K(FeHL+HL)=3.41			

****

C9H16N2O4 H2L CAS 96287-30-8 (8140)
Azetidine-2-carboxy-1-(2-aminopentanoic acid);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	KNO3	25°C	0.10M	C		K1=5.7		1989ARa (67618)	735

****

C9H17NO5 HL Pantothenic acd CAS 63409-48-3 (2629)
N-(2,4-Dihydroxy-3,3-dimethylbutyryl)-3-aminopropanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	KCl	25°C	0.24M	U		K1=1.38		1980FMd (67814)	736

****

C9H21N3O3 L CAS 221233-44-9 (7658)
cis,cis,cis-2,4,6-Trimethoxycyclohexane-1,3,5-triamine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	KNO3	25°C	0.10M	C		K1=9.03	B2=16.14	1999WKa (68213)	737

****

C9H24N3O9P3 H6L NOTPH CAS 83843-39-3 (224)
1,4,7-Triazacyclononane-N,N',N"-tris(methylenephosphonic acid);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	KNO3	25°C	1.00M	U		K1=18.7		1990BSd (68317)	738
							K(Fe+HL)=12.7			
							K(Fe+H2L)=9.9			
							K(Fe+H3L)=7.2			

****

C10H6N2O HL CAS 6759-78-0 (3316)
5-Cyano-8-hydroxyquinoline;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo

```
--------------------------------------------------------------------------------
Fe++       gl  diox/w 25°C  50%  U        K1=7.10   B2=14.25  1958TWa (68438) 739
                                         K3=6.0
Medium: 50% dioxan, 0.3 M NaCl
********************************************************************************
C10H6N2O4              HL                     CAS 83848-59-3  (1412)
5-Nitroquinoline-8-carboxylic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       gl  alc/w  20°C  50%  U T      K1=4.26        1982KRa (68443) 740
                                         K(FeL+HL=FeHL2)=3.77
********************************************************************************
C10H7NO2               HL                     CAS 132-53-6  (2524)
2-Nitroso-1-naphthol;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       gl  diox/w 21°C  50%  U        K1=8.05   B2=16.19  1970MGd (68645) 741
Medium: 50% dioxan, 0.3 M NaClO4
********************************************************************************
C10H7NO2               HL                     CAS 2598-30-3  (3317)
5-Formyl-8-hydroxyquinoline;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       gl  diox/w 25°C  50%  U        K1=6.90   B2=13.75  1958JPa (68671) 742
                                         K3=5.70
Medium: 50% dioxan, 0.3 M NaCl
********************************************************************************
C10H7NO2               HL    Quinaldic acid   CAS 93-10-7  (2209)
Quinoline-2-carboxylic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       sp  none     ?   0.0  U        B2=5.44        1964PCa (68706) 743
--------------------------------------------------------------------------------
Fe++       sp  KNO3   25°C 0.20M U        B2=5.44        1958BRa (68707) 744
--------------------------------------------------------------------------------
Fe++       gl  oth/un 25°C  0.0  U        K1=3.92   B2=7.67   1955LUa (68708) 745
********************************************************************************
C10H7NO2               HL                     CAS 86-59-9  (873)
Quinoline-8-carboxylic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       gl  alc/w  20°C   5%  U T      K1=6.17   B2=10.28  1982KRa (68759) 746
--------------------------------------------------------------------------------
Fe++       gl  oth/un 25°C  0.0  U        K1=3.68   B2=6.57   1955LUa (68760) 747
********************************************************************************
```

C10H7NO5S H2L CAS 3682-32-4 (1812)
2-Nitroso-1-hydroxynaphthalene-4-sulfonic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	sp	none	?	0.0	U			1958TPa (68883)		748
							B3=18.95			

****
C10H7NO8S2 H3L Nitroso-R acid CAS 525-05-3 (1811)
1-Nitroso-2-hydroxynaphthalene-3,6-disulfonic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	KCl	25°C	0.10M	U		K1=7.85	B2=15.41	1974ANb (69008)	749
							K3=7.50			
Fe++	sp	NaClO4	20°C	1.20M	U		K1=7.60	B2=15.04	1973SBf (69009)	750
							B3=22.13			
							B4=30.63			

****
C10H7N3O4 H2L 1-Ph-violuric (957)
1-Phenyl-alloxan-5-oxime,(1-Phenyl-5-isonitrosobarbituric acid);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	alc/w	18°C	50%	U	T	K1=6.60	B2=11.62	1982SGa (69084)	751

Medium: 50% v/v EtOH/H2O, 0.1 M NaClO4

****
C10H7O2F3 HL CAS 326-06-7 (196)
3-Benzoyl-1,1,1-trifluoroacetone; CF3.CO.CH2.CO.C6H5

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	alc/w	25°C	75%	C		K1=5.80	B2=10.81	1998ERa (69143)	752
							B3=15.73			
							B(FeH-1L)=2.94			
							B(FeH-1L2)=7.36			

Medium: 75% v/v EtOH/H2O, 0.10 M KCl

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	dis	NaNO3	25°C	0.10M	C		K1=4.2	B2=8.0	1994SDc (69144)	753

Method: solvent extraction into CHCl3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	oth/un	?	0.0	U		B2=10.32		1951UFa (69145)	754

****
C10H8N2 L 2,2'-Bipyridyl CAS 366-18-7 (25)
2,2'-Bipyridine; (C5H4N)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	kin	non-aq	25°C	0.10M	U		K1=3.98	B2= 9.09	1998JMa (69552)	755

K3=3.54

Medium: DMF

Fe++ gl alc/w 30°C 5% M K1=4.41 1994RRb (69553) 756

Medium: 5% v/v EtOH/H2O, 0.10 M KNO3.

Fe++ sp none 25°C 0.0 C I 1986DSb (69554) 757

B3=17.77

K(FeL3+3H=Fe+3HL)=-4.63

Data for 0-75.8% w/w 2-PrOH/H2O. In 75.8% 2-PrOH/H2O, B3=14.68, K(FeL3+3H=Fe+3HL)=-6.05

Fe++ sp none 25°C 0.0 C I 1985DHb (69555) 758

B3=17.53

K(Fe+3HL=FeL3+3H)=4.12

Also data for 11-91% w/w DMSO/H2O and formamide/H2O.
In 52% DMSO/H2O, B3=15.05.

Fe++ gl diox/w 37°C 30% C M B2=6.20 1983MAd (69556) 759

B(Fe(bha)L)=9.42

bha: benzohydroxamic acid

Fe++ sp oth/un 25°C 0.01M C H 1982BMg (69557) 760

B3=17.54

By calorimetry in self-medium: DH=-117.15 kJ mol-1. Also data for 10-50% w/w MeOH/H2O, EtOH/H2O, t-BuOH/H2O and glycerol/H2O.

Fe++ sp non-aq 25°C 100% U K1=4.82 1981AWa (69558) 761

Medium: hexamethylphosphoric triamide

Fe++ sp none 25°C 0.0 U T H 1978ABa (69559) 762

B3=17.39

Also at 35-160 C. DH(B3)=-128.7 kJ mol-1. DS=-98.7 J K-1 mol-1

Fe++ cal none 25°C 0.0 C IH 1977BAa (69560) 763

DH(B3)=-100.46 kJ mol-1, DS=-10.5 J K-1 mol-1. DH(Fe+3HL=FeL3+3H)=-74.47, DS=167. Data for 0-64.7% w/w MeOH/H2O. In 64.7%, DH(B3)=-129.1, DS=-136

Fe++ sp none 25°C 0.0 U 1975HLb (69561) 764

K3=17.77

In 8%MeOH 17.87; in 16.4%MeOH 17.89; in 25.2%MeOH 17.78; in 34.4%MeOH 17.72; in 44%MeOH 16.85; in 54%MeOH 16.17; in 64.7%MeOH 15.52

Fe++ dis oth/un 25°C 0.0 U M 1972ARb (69562) 765

K(FeL3+2ClO4=FeL3(ClO4)2)=2.08

K(FeL3+2I=FeL3I2)=1.62

By conductivity: K(FeL3+2ClO4)=2.05, K(FeL3+2I)=1.71, K(FeL3+Cl2)=1.30.

Fe++ sp mixed ? 50% U I 1966BAb (69563) 766

B3=6.8

Medium: 50% N2H4. B3=17.9(0%), 9.0(5%), 8.2(10%), 7.9(25%)

Fe++ dis KNO3 30°C 1.0M U H K1=4.65 1965DDa (69564) 767
B3=17.14

By calorimetry:DH(B3)=-117.0 kJ mol-1, DS=-58 J K-1 mol-1

Fe++ cal NaNO3 20°C 0.10M U H 1963ANb (69565) 768

DH(B3)=-131.0 kJ mol-1, DS=-113 J K-1 mol-1

Fe++ gl NaNO3 20°C 0.10M U 1963ANg (69566) 769
B3=17.45

Fe++ dis KCl 25°C 0.10M U K1=4.20 B2=7.90 1962IMa (69567) 770
K3=9.55

Fe++ sp oth/un 25°C .025M U T H K1=4.2 1950BGa (69568) 771
B3=17.07

35 C: K2 < 5, B3=16.53; DH(K1)=-31.4 kJ mol-1; DH(B3)=-101.7

Fe++ gl oth/un 25°C 0.33M U I K1=4.43 1950KRa (69569) 772
B3=17.58

I=0.01 B3=17.41

Fe++ sp oth/un 25°C 0.0 U K1=4.36 1949KRa (69570) 773

Fe++ EMF oth/un 25°C .008M U 1947DMa (69571) 774
B3=16.4

****

C10H8N2O2 HL CAS 80690-06-8 (874)
5-Aminoquinoline-8-carboxylic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	alc/w	20°C	50%	U	T	K1=7.46 K(FeL+HL=FeHL2)=5.43	1982KRa (69675)	775

****

C10H8N2O2 HL (3318)
8-Hydroxyquinoline-5-carbaldehyde oxime

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	sp	diox/w	25°C	50%	U		B2=14.9 B3=20.2	1958TWa (69684)	776

Medium: 50% dioxan, 0.3 M NaCl

****

C10H8N2O2S HL CAS 15112-10-4 (8299)
N-Phenyl-2-thiobarbituric acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo

Fe++ gl NaClO4 31°C 0.10M U T H K1=6.32 B2=11.21 1984SJa (69691) 777
Also data for 18 and 42 C. DH(K1)=-82.0 kJ mol-1, DS(K1)=-149 J K-1 mol-1
DH(K2)=-46.5, DS(K2)=-60.0. Also data for N-tolyl- derivatives.
****
C10H8O5S H2L CAS 16223-97-7 (2392)
1,2-Dihydroxynaphthalene-4-sulfonic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl NaClO4 25°C 0.10M C K1=8.99 B2=16.49 1977BMd (69807) 778
****
C10H8O8S2 H4L Chromotropic ac CAS 148-25-4 (1875)
1,8-Dihydroxynaphthalene-3,6-disulfonic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl KNO3 27°C 0.10M U K1=6.00 B2= 9.45 1988AIa (69943) 779
****
C10H9NO HL 8-OH-Quinaldine CAS 826-81-3 (998)
2-Methyl-8-hydroxyquinoline;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl diox/w 25°C 50% U K1=8.75 B2=17.10 1958TWa (70046) 780
****
C10H9NO HL CAS 5541-67-3 (999)
5-Methyl-8-hydroxyquinoline;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl diox/w 25°C 50% U B2=16.90 1958TWa (70064) 781
B3=29.68
Medium: 50% dioxan, 0.3 M NaCl
****
C10H9NO7S2 H3L CAS 82-47-3 (6247)
8-Amino-1-hydroxynaphthalene-3,6-disulfonic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl oth/un 20°C 0.0 U K1=2.57 B2=5.5 1961PEb (70220) 782
****
C10H9NO8 H2L CAS 83785-11-9 (685)
2-Nitro-1,4-di(carboxymethoxy)benzene; O2N.C6H3.(OCH2COOH)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl oth/un 30°C ? U K1=4.03 B2=8.29 1985TZa (70234) 783
****
C10H9N3O2 HL CAS 56634-85-6 (1326)
4-Oximino-3-methyl-1-phenyl-2-pyrazolin-5-one;

```
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe++       sp  alc/w  32°C  40%  U                        1968SPb (70390) 784
                                      K(Fe+HL=FeL+H)=3.47
Medium: 40% EtOH, 0.2 M NaClO4
*******************************************************************************
C10H9N5                HL                         (3892)
1-(Pyrimidin-2'-yl)-3-pyridyl-1,2-diazaprop-2-ene;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe++       gl  oth/un 25°C    ?  U        B2=30          1964GHb (70416) 785
                                      K(FeHL2+H)=4.56
                                      K(FeL2+H)=6.09
By spectrophotometry: K(Fe+HL)=6.0, K(Fe+2HL)=14.00
*******************************************************************************
C10H10N4O4S2          H2L                      CAS 78441-02-8  (2880)
N-Methylindol-2,3-dione-3-thiosemicarbazone-5-sulfonic acid;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe++       gl  KNO3   37°C 0.15M M        K1=4.1    B2=8.98   1982STa (70624) 786
*******************************************************************************
C10H10O2               HL    Benzoylacetone   CAS 93-91-4  (197)
1-Phenylbutane-1,3-dione; C6H5.CO.CH2.CO.CH3
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe++       gl  alc/w  25°C  75%  C        K1=6.56   B2=11.97  1998ERa (70725) 787
                                      B3=14.12
Medium: 75% v/v EtOH/H2O, 0.10 M KCl
*******************************************************************************
C10H11NO4             H2L                      CAS 1137-73-1  (2567)
N-Phenyliminodiethanoic acid; C6H5.N(CH2.COOH)2
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe++       gl  KCl    20°C 0.10M U        K1=2.01        1955SAa (71001) 788
*******************************************************************************
C10H11N3                L                      CAS 49612-00-2  (3301)
2-Hydrazino-4-methylquinoline;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe++       gl  oth/un 22°C 0.10M U        K1=4.4    B2=7.8    1957FEa (71079) 789
*******************************************************************************
C10H12N2O4            H2L                      CAS 16598-05-3  (967)
2-Pyridylmethyliminodiethanoic acid; C5H4N.CH2.N(CH2.COOH)2
-------------------------------------------------------------------------------
```

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	NaNO3	20°C	0.10M	C		K1=9.00	1981ANb (71258)	790
Fe++	gl	KNO3	20°C	0.10M	U		K1=8.94	1963IFc (71259)	791

C10H12N4O5 HL Inosine CAS 58-63-9 (2344)
Hypoxanthine-9-beta-D-ribofuranoside;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	oth/un	20°C	0.01M	U		K1=3	1953ALa (71387)	792

C10H12N4O6 H2L Xanthosine CAS 5968-90-1 (1176)
3,9-Dihydro-9-ribofuranosyl-1H-purine-2,6-dione;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	oth/un	20°C	0.01M	U		K1=<2	1953ALa (71487)	793

C10H13N5O5 HL Guanosine CAS 118-00-3 (1402)
2-Aminopurin-6-one-9-riboside;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	oth/un	20°C	0.01M	U		K1=4.3	1953ALa (72009)	794

C10H13N5O5 L CAS 116-92-9 (2174)
Adenosine-N'-oxide;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	none	25°C	0.0	U		K1=6.58	1960PEb (72032)	795

C10H14N4B- L (7239)
Bis(3,5-dimethylpyrazol-1-yl)borate; ((CH3)2C3H)2BH2-

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	dis	non-aq	25°C	100%	U			1996KSa (72128)	796
							K(Fe+2HL=FeL2(org)+2H)=-2.64		

By solvent extraction into CHCl3

C10H14O8S4 H4L CAS 10003-69-7 (3914)
1,1,2,2-Tetrathioethane-S,S',S'',S'''-tetraethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	NaClO4	25°C	0.10M	U		K1=2.68	1973PPc (72626)	797
							B(FeHL)=6.59		

B(FeH2L)=10.22
B(Fe2L)=4.18

Fe++ gl oth/un 25°C 0.10M U K1=1.9 1972PPb (72627) 798
****
C10H15NO L Ephedrine CAS 299-42-3 (1836)
(1-Methylaminoethyl)benzyl alcohol; C6H5.CH(OH)CH(CH3)NHCH3

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl KCl 25°C .058M U T K1=6.25 B2=9.95 1961SMa (72643) 799
K1=6.49(0 C), 5.70(45 C)
****
C10H15N5O4 HL His-Gly-Gly CAS 32999-80-7 (6269)
Histidyl-glycyl-glycine;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl none 21°C 0.0 M K1=3.92 1974YAa (72825) 800
****
C10H16N2O5 H2L gamma-Glu-Pro CAS 53411-63-5 (8143)
Pyrrolidine-2-carboxy-1-(2-amino-5-one-pentanoic acid, Gamma-Glutamyl-proline;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl KNO3 25°C 0.10M C K1=4.2 1989ARa (73058) 801
****
C10H16N2O8 H4L EDDS CAS 52759-67-8 (1100)
1,2-Diaminoethane-N,N'-di-1,4-butanedioic acid; (CH2.NH.CH(COOH)CH2.COOH)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ dis KNO3 20°C 0.10M U K1=10.7 1968MJa (73130) 802
Method: paper electrophoresis
****
C10H16N2O8 H4L EDTA CAS 60-00-4 (120)
1,2-Diaminoethane-N,N,N',N'-tetraethanoic acid, Sequestric acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ sp alc/w 25°C 75% U K1=15.80 1991CMc (73754) 803
K(FeL+H)=3.13
Medium: 75% v/v EtOH/H2O

Fe++ gl KNO3 25°C 0.10M C K1=14.94 1988CMb (73755) 804
K(FeL+H)=2.06

Fe++ gl NaClO4 25°C 1.00M C 1983AHa (73756) 805
K(FeL+H)=2.90

```
Fe++       oth none   25°C  0.0  U        K1=14.3        1977DFa (73757) 806
Calculated from a model.  Constants also for many related Fe++ complexes.
--------------------------------------------------------------------------------
Fe++       vlt oth/un 20°C 0.20M U T                     1972BOa (73758) 807
                                        K(Fe+HL)=6.90
                                        K(Fe+H2L)=3.32
K(Fe+HL)=6.91(10 C), K(30 C)=6.89, K(40 C)=6.88
K(Fe+H2L)=3.36(10 C), K(30 C)=3.32, K(40 C)=3.30
--------------------------------------------------------------------------------
Fe++       vlt oth/un 20°C 0.20M U T                     1971BFa (73759) 808
                                        K(Fe+HL)=6.90
                                        K(Fe+H2L)=3.26
K(Fe+HL)=6.90(10 C), K(30 C)=6.83, K(40 C)=6.87
K(Fe+H2L)=3.38(10 C), K(30 C)=3.40, K(40 C)=3.34
--------------------------------------------------------------------------------
Fe++       cal KNO3   25°C 0.10M U        K1=14.19       1969BNa (73760) 809
                                        K(Fe+HL)=5.47
--------------------------------------------------------------------------------
Fe++       cal KNO3   25°C 0.10M U   H                  1965WHa (73761) 810
DH(K1)=-16.7 kJ mol-1, DS=213 J K-1 mol-1
--------------------------------------------------------------------------------
Fe++       gl  KNO3   20°C 0.10M U        K1=14.2        1964ANa (73762) 811
                                        K(Fe+HL)=6.86
--------------------------------------------------------------------------------
Fe++       gl  KNO3   25°C 0.10M U        K1=14.33       1959SCc (73763) 812
                                        K(FeL+OH)=4.9
                                        K(FeLOH+OH)=4.1
--------------------------------------------------------------------------------
Fe++       EMF KCl    20°C 0.10M U      T K1=14.33       1954SGa (73764) 813
                                        K(Fe+HL)=6.86
                                        K(FeL+H)=1.31
Method: H electrode
--------------------------------------------------------------------------------
Fe++       EMF oth/un 25°C  1.0M U        K1=13.9        1952JLa (73765) 814
Method: H electrode
********************************************************************************
C10H16N5O13P3         H4L    ATP              CAS 56-65-5  (403)
Adenosine-5'-triphosphoric acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       gl  NaCl   25°C 0.12M U        K1=5.11        1978RMc (74729) 815
--------------------------------------------------------------------------------
Fe++       gl  KNO3   25°C 1.00M U    M                  1976RDa (74730) 816
                                        K(FeL+hydroxynorephedrin)=3.94
                                        K(FeL+normetanephrine)=4.07
                                        K(FeL+norpinephrine)=6.30
                                        K(FeL+dopamine)=7.98
--------------------------------------------------------------------------------
Fe++       gl  KNO3   25°C 1.00M U    M                  1976RDa (74731) 817
```

K(FeL+octopamine)=3.78
K(FeL+tyramine)=5.00
K(FeL+norephedrine)=3.34
K(FeL+hydroxyamphetamine)=5.11

****

C10H16O8P2 H4L (6907)
1,2-Diphosphinoethane-P,P,P'P'-tetraethanoic acid;
(HOOC.CH2)2P.CH2.CH2.P(CH2.COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	NaClO4	25°C	0.10M	C		B2=16.44		1992PPb (74946)	818
							B(FeH2L2)=27.51			
							B(FeH4L2)=35.41			
							B(FeH6L2)=41.30			

Additional method: competition with 1,10-phenanthroline

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	NaClO4	25°C	0.10M	C				1982PPc (74947)	819
							B(FeH2L2)=27.51			

****

C10H17NO5 H2L CAS 6243-06-7 (3326)
N-(2-Hydroxycyclohexyl)iminodiethanoic acid; HO.C6H10.N(CH2.COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	KCl	20°C	0.10M	U		K1=7.69	B2=10.69	1964PCa (74987)	820

****

C10H17NO5 H2L (3917)
N-(Tetrahydropyran-2-ylmethyl)iminodiethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	KNO3	20°C	0.10M	U		K1=7.40	1963IFa (75001)	821

****

C10H18N2O4 H2L CAS 96287-33-1 (8141)
Pyrrolidine-2-carboxy-1-(2-aminopentanoic acid);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	KNO3	25°C	0.10M	C		K1=5.6	1989ARa (75207)	822

****

C10H18N2O5 H2L (5608)
1-Oxa-4,7-diazacyclononane-N,N'-diethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	KNO3	25°C	0.10M	U		K1=9.70	1990CCa (75234)	823

****

C10H18N2O7 H3L HEDTA CAS 150-39-0 (392)
N-(Hydroxyethyl)diaminoethane-N,N',N'-triethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	KNO3	25°C	0.10M	C		K1=12.58 K(FeL+H)=2.36	1988CMb (75384)	824
Fe++	vlt	oth/un	20°C	0.20M	U	T	K(Fe+HL)=5.11	1971BFa (75385)	825

K(Fe+HL)(10 C)=5.15, K(30 C)=5.08, K(40 C)=5.08

Fe++	gl	KNO3	25°C	0.10M	U		K1=11.63	1969BNa (75386)	826

2nd method: calorimetry

Fe++	cal	KNO3	25°C	0.10M	U	H		1965WHa (75387)	827

DH(K1)=-25.1 kJ mol-1, DS=128 J K-1 mol-1

Fe++	gl	KNO3	25°C	0.10M	U		K1=12.2 K(FeLOH+H)=8.97 K(FeL(OH)2+H)=10.03	1959SCc (75388)	828
Fe++	gl	KCl	30°C	0.10M	U		K1=11.6	1955CMa (75389)	829

****

C10H18O8 H2L CAS 32775-08-9 (240)

1,12-Dicarboxy-2,5,8,11-tetraoxadodecane; (HOOC.CH2.O.CH2.CH2.O.CH2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	KNO3	25°C	0.10M	U		K1=2.46	1975MTc (75619)	830

****

C10H21N11 L (7006)

1,7-Di(2-(5-tetraazolyl)ethyl)-1,4,7-triazaheptane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	NaNO3	20°C	0.10M	U		K1=15.72	1981ESa (76211)	831

****

C10H23N3O2 L CAS 60350-18-7 (5875)

1,4-Dioxa-7,10,13-triazacyclopentadecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	KNO3	25°C	0.10M	C		K1=7.79 K(FeLOH+H)=9.1	1994CDa (76523)	832

****

C10H24N4 L Cyclam CAS 295-37-4 (8)

1,4,8,11-Tetraazacyclotetradecane; cyclo(-(HN.CH2.CH2.NH.(CH2)3)2-)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	diox/w	25°C	70%	C			2001PAa (76664)	833

K(Fe(Cp)2L+H)=9.21
K(Fe(Cp)2L+2H)=15.27
K(Fe(Cp)2L+3H)=18.46
Medium: 70% v/v dioxan/H2O, 0.10 M KNO3. Fe(Cp)2 is ferrocene.

****

C10H24N4O L (7051)
1-Oxa-4,7,10,13-tetraazacyclopentadecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	KNO3	25°C	0.10M	C		K1=10.34	1994CDa (76709)	834

****

C10H28N6 L PENTEN CAS 4097-90-9 (3315)
N,N,N',N'-Tetra-(2-aminoethyl)diaminoethane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	cal	KCl	25°C	0.10M	U	H	K1=11.05	1964SPb (76872)	835

K calculated. By calorimetry: DH(K1)=-40.3 kJ mol-1, DS=79.4 J K-1 mol-1

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	KCl	20°C	0.10M	U		K1=11.20	1953SMa (76873)	836
							K(Fe+HL)=8.70		
							K(FeL+H)=7.70		

****

C11H8O3S HL CAS 32267-05-3 (3353)
2-Furoyl-2-thenoylmethane; C4H3O.CO.CH2.CO.C4H3S

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	diox/w	30°C	75%	U		K1=10.40 B2=20.05	1953UFe (77158)	837

****

C11H8O4 HL CAS 7555-37-5 (4812)
3-Acetyl-4-hydroxycoumarin

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	diox/w	35°C	50%	U		K1=2.28 B2=4.00	1971MAa (77175)	838

Medium: 50% dioxan, 0.01 M NaClO4

****

C11H8O4 HL CAS 6724-42-1 (6183)
8-Formyl-7-hydroxy-4-methyl-2H-1-benzopyran-2-one; CHO.C9H3O(:O)(CH3)(OH)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	alc/w	35°C	70%	U		K1=6.86 B2=11.85	1984CEa (77199)	839

****

C11H9NO2 HL CAS 92609-55-3 (4827)
5-Acetyl-8-hydroxyquinoline;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo

```
--------------------------------------------------------------------------------
Fe++       gl  diox/w 25°C  60%  U        K1=8.56   B2=16.18  1973SCd (77329) 840
Medium: 60% dioxan, 0.1 M NaClO4
********************************************************************************
C11H9NO3             H2L                      CAS 80690-05-7  (872)
3-Hydroxy-2-methyl-1,4-naphthoquinone monoxime;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       gl  diox/w 30°C 0.10M U        K1=5.83   B2=11.12  1981KSa (77363) 841
                                          K3=5.27
********************************************************************************
C11H9NO3S2            HL                       (939)
2-(Thiophene-2'-aldimino)benzene sulfonic acid; C4H3S.CH:N.C6H4.SO3H
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       gl  NaClO4 25°C 0.10M U        K1=4.23   B2=7.20   1982MSa (77400) 842
********************************************************************************
C11H9NO4             H2L                      CAS 4321-82-7  (4829)
3-Acetyl-4-hydroxycoumarin oxime;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       gl  diox/w 35°C  50%  U                         1971MAa (77418) 843
                                          K(Fe+HL)=2.08
                                          K(Fe+2HL)=3.57
Medium: 50% dioxan, 0.01 M NaClO4
********************************************************************************
C11H9NO4              HL                       CAS 65490-35-9  (6230)
8-Formyl-7-hydroxy-4-methyl-2H-[1]benzopyran-2-one-oxime; (CH3)(OH)C9H3O(:O)CH:NOH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       gl  alc/w  35°C  70%  U        K1=7.87   B2=13.62  1984CEa (77437) 844
********************************************************************************
C11H9N3O              HL                       CAS 10335-29-2  (3937)
2-(2'-Pyridylazo)phenol; C5H4N.N:N.C6H4.OH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       sp  alc/w  20°C  50%  U        B2=26.3         1967ANa (77456) 845
Medium: 50% MeOH, 0.1 M NaClO4
********************************************************************************
C11H9N3O              HL                       CAS 7687-72-1  (3938)
4-(2'-Pyridylazo)phenol; C5H4N.N:N.C6H4.OH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       gl  alc/w  25°C  50%  U        K1=5.6    B2=10.40  1967ANa (77472) 846
```

Medium: 50% MeOH, 0.1 M NaClO4

****

C11H9N3O4 H2L CAS 82628-26-0 (1379)

1-(2-Tolyl)violuric acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	alc/w	18°C	50%	U	T	K1=6.28	B2=10.72	1982SGa (77621)	847

Medium: 50% v/v EtOH/H2O, 0.1 M NaClO4

****

C11H9N3O4 H2L CAS 82628-27-1 (1378)

1-(3-Tolyl)violuric acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	alc/w	18°C	50%	U	T	K1=6.45	B2=11.30	1982SGa (77628)	848

Medium: 50% v/v EtOH/H2O, 0.1 M NaClO4

****

C11H9N3O4 H2L CAS 82628-25-9 (1377)

1-(4-Tolyl)violuric acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	alc/w	18°C	50%	U	T	K1=6.70	B2=11.86	1982SGa (77635)	849

Medium: 50% v/v EtOH/H2O, 0.1 M NaClO4

****

C11H9N3O5S HL (6249)

1,2-Naphthoquinone-4-sulfonic acid 2-semicarbazone; C10H5(:O)(HSO3):N.NH.CO.NH2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	NaClO4	28°C	0.10M	U	T H	K1=5.20	B2=9.85	1980MGd (77641)	850

****

C11H10N4 L PAPHY CAS 2215-33-0 (1305)

Pyridine-2-aldehyde-2'-pyridyl-hydrazone; C5H4N.CH:N.NH.C5H4N

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	EMF	KNO3	20°C	0.10M	U		B2=17.2		1971ANa (77705)	851
Fe++	sp	oth/un	60°C	0.0	U	T H	K(Fe+2HL)=14.39 K(FeHL2+H)=5.60 K(FeL2+H)=6.88		1968GGc (77706)	852

K(Fe+2HL)=17.70(5C),16.57(25C),15.59(40C).DH=-105 kJ mol-1,DS=-38 J K-1 m-1.
K(FeHL2+H)=6.36(5 C),6.08(25 C).DH=--27,DS=38. K(FeL2+H)=7.71(5 C);DH=-26

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	sp	oth/un	25°C	0.0	U		B2=33 K(Fe+2HL)=16.7 K(FeHL2+H)=5.68		1964GHd (77707)	853

K(FeL2+H)=6.57

****

C11H10N4O HL (3939)

3-(2'-Hydroxyphenyl)-1-(pyrimidin-2''-yl)-1,2-diazaprop-2-ene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	alc/w	25°C	50%	U		K1=9.9	B2=18.50	1967ANd (77716)	854

Medium: 50% MeOH, 0.1 M NaClO4

****

C11H12N2O2 HL Tryptophan CAS 73-22-3 (3)

2-Amino-3-(3-indolyl)propanoic acid; H2N.CH(CH2.C8H6N)COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	NaClO4	25°C	3.0M	U		K1=3.92	B2=7.39	1970WIa (78202)	855
							B3=9.5			
Fe++	gl	KCl	20°C	1.0M	U	T	K1=3.43		1959PEc (78203)	856
Fe++	gl	oth/un	20°C	0.01M	U		K2=7.6		1950ALa (78204)	857

****

C11H13O4AsS H2L CAS 36198-36-4 (4870)

Bis(carboxymethyl)-2-(methylthiophenyl)arsine; (HOOC.CH2)2.As.C6H4.S.CH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	oth/un	25°C	0.10M	U		K1=3.80		1971FPa (78744)	858
							K(Fe+HL)=2.32			

****

C11H14N2O4 H2L (1880)

N-(6-Methyl-2-pyridylmethyl)iminodiethanoic acid; CH3C5H3NCH2N(CH2COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	NaNO3	20°C	0.10M	C		K1=8.55		1981ANb (78882)	859

****

C11H14N4OS HL CAS 56566-64-4 (2816)

Biacetylmonoxime-4-phenyl-3-thiosemicarbazone;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	sp	none	25°C	0.0	U		K1=10.146		1975CJb (78938)	860

****

C11H18N2O8 H4L CAS 4408-81-5 (923)

1,3-Diaminopropane-N,N,N',N'-tetraethanoic acid; ((HOOC.CH2)2N.CH2.)2.CH2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	KNO3	20°C	0.10M	U		K1=13.42		1964LAa (79441)	861

K(Fe+HL)=6.30

****

C11H18N4 L CAS 78668-34-5 (6708)
3,6,9,15-Tetraazabicyclo[9.3.1]pentadeca-1(15),11,13-triene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	KNO3	25°C	0.10M	C		K1=12.54	1993CDa (79618)	862

****

C11H20N4O6 H2L ICRF 198 CAS 108430-47-3 (8369)
N,N'-(1-Methyl-1,2-ethanediyl)bis[N-(2-amino-2-oxoethyl)glycine];

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	NaCl	37°C	0.15M	C		K1=9.993	1982HMb (79729)	863
							B(FeHL)=12.208		

****

C11H22N4O4 H2L (6756)
1,4-Diazacycloheptane-N,N'-bis(N-methyl-acetohydroxamic acid);
C5H10N2(CH2.CO.N(OH)CH3)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	sp	KNO3	25°C	0.10M	C			1993SEb (79842)	864
							B(Fe2HL3)=36.2		

****

C11H25N3O2 L (7052)
1,4-Dioxa-7,11,14-triazacyclohexadecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	KNO3	25°C	0.10M	C		K1=6.73	1994CDa (79939)	865
							K(FeLOH+H)=7.81		

****

C11H26N4S L CAS 80846-36-2 (720)
1-Thia-4,7,11,14-tetraazacyclohexadecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	NaClO4	35°C	0.20M	C		K1=10.29	1984KKa (80022)	866

****

C11H27N5 L CAS 29783-72-0 (98)
1,4,7,10,13-Pentaazacyclohexadecane; cyclo(-(NH.CH2.CH2)5.CH2-)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	NaClO4	35°C	0.20M	U		K1=14.57	1982KKb (80032)	867

****

C11H30N6 L (6595)
5-(4'-Amino-2'-azabutane)-5-methyl-3,7-diazanonane-1,9-diamine;

CH3.C(CH2.NH.CH2.CH2.NH2)3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	KCl	25°C	0.50M	M		K1=13.4 K(FeL+H)=7.0		1991HLa (80059)	868

C12H6N2Cl2 L CAS 5394-23-0 (3964)
4,7-Dichloro-1,10-phenanthroline;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	sp	alc/w	?	100%	U		B3=12.1		1961HDa (80090)	869

Medium: EtOH, 0.1 M acetate buffer

C12H7N2Br L CAS 40000-20-2 (2750)
5-Bromo-1,10-phenanthroline;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	sp	KNO3	25°C	0.15M	U		K1=5.65 B3=15.98	B2=10.78	1972BOb (80119)	870
Fe++	sp	oth/un	25°C	0.10M	U		K1=5.45 B3=19.7		1959BBa (80120)	871

C12H7N2Cl L CAS 7089-68-1 (3965)
2-Chloro-1,10-phenanthroline;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	sp	KCl	25°C	0.10M	U		B3=11.6		1971IGa (80130)	872

C12H7N2Cl L CAS 1891-14-1 (3966)
4-Chloro-1,10-phenanthroline;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	sp	oth/un	?	0.10M	U		B3=14.8		1961HDa (80132)	873

Acetate buffer

C12H7N2Cl L CAS 4199-89-7 (2751)
5-Chloro-1,10-phenanthroline;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	sp	KNO3	25°C	0.15M	U		K1=5.70	B2=10.72	1972BOb (80143)	874

B3=15.87

Fe++ kin oth/un 25°C 0.10M U 1959BBa (80144) 875
B3=19.7

Fe++ sp oth/un 25°C 0.0 U 1952BGa (80145) 876
B3=19.7
Kinetics also used

****

C12H7N3O2 L CAS 4199-88-6 (449)
5-Nitro-1,10-phenanthroline;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo

---

Fe++ sp none 25°C 0.0 U T H 1978ABa (80171) 877
B3=17.39
Also at 35-107 C. DH(B3)=-136.9 kJ mol-1. DS=-127.2 J K-1 mol-1

Fe++ sp oth/un 35°C 0.0 U T H K1=4.57 1964LAe (80172) 878
B3=14.99
B3=15.64(25 C),14.47(45 C). At 25 C:DH(B3)=-105 kJ mol-1, DS=54 J K-1 mol-1

Fe++ sp oth/un 25°C 0.10M U K1=5.06 1959BBa (80173) 879

Fe++ sp oth/un 25°C =0 U B2=17.8 1952BGa (80174) 880

****

C12H8N2 L Phenanthroline CAS 66-71-7 (144)
1,10-Phenanthroline;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo

---

Fe++ sp none 25°C 0.0 C I 1986DSb (80427) 881
B3=20.50
K(FeL3+3H=Fe+3HL)=-5.35
Data for 0-75.8% w/w 2-PrOH/H2O. In 75.8% 2-PrOH/H2O, B3=16.12,
K(FeL3+3H=Fe+3HL)=-6.57

Fe++ sp none 25°C 0.0 U T H 1978ABa (80428) 882
B3=20.69
Also at 35-107 C. DH(B3)=-130.7 kJ mol-1. DS=-41.7 J K-1 mol-1

Fe++ sp none 30°C 0.0 C I 1978BLb (80429) 883
B3=20.50
K(Fe+3HL=FeL3+3H)=5.35
Data for 0-87.6% w/w EtOH/H2O. In 87.6% EtOH/H2O, B3=16.13,
K(Fe+3HL=FeL3+3H)=5.03.

Fe++ dis oth/un 25°C 0.0 U M 1972ARb (80430) 884
K(FeL3+2ClO4)=2.13
K(FeL3+2I)=1.77

By conductivity: K(FeL3+2ClO4)=2.08; K(FeL3+2I)=1.82; K(FeL3+2NO3)=1.45;
K(FeL3+2Br)=1.30; K(FeL3+2Cl)=1.34

Fe++ sp oth/un 25°C 0.15M U K1=5.84 B2=11.20 1972BOb (80431) 885
B3=16.45
Medium: K2SO4.

Fe++ sp mixed ? 64% U I 1966BAb (80432) 886
B3=8.8
Medium: 64% N2H4. B3=20.2(0%), 11.3(5%), 10.5(10%), 10.1(25%), 9.15(50%)

Fe++ sp oth/un 45°C 0.0 U T H 1964LAe (80433) 887
B3=18.77
B3=20.22(25 C),19.58(33 C). DH(B3)=-130.8 kJ mol-1, DS=-46 J K-1 mol-1

Fe++ cal NaNO3 20°C 0.10M U H 1963ANb (80434) 888
DH(B3)=-137.9 kJ mol-1, DS=-64.4 J K-1 mol-1

Fe++ sp NaNO3 20°C 0.10M U 1963ANg (80435) 889
B3=21.3

Fe++ dis KCl 25°C 0.10M U K1=5.86 B2=11.11 1962IMa (80436) 890
K3=10.03

Fe++ sp alc/w ? 50% U I 1961HDa (80437) 891
B3=16.2
Medium: 50% EtOH, 0.1 M actate buffer. B3=18.5(0% EtOH)

Fe++ sp KCl 25°C 0.01M U K1=5.85 1959BBa (80438) 892

Fe++ EMF oth/un 25°C 0.00 U K1=5 1956SSa (80439) 893
B3=21.3
K3=9.85
Spectrophotometry also used

Fe++ sp oth/un 25°C 0.10M U 1955IMa (80440) 894
B3=21.15

Fe++ EMF oth/un 20°C 0.01M U 1955MCa (80441) 895
B3=21.3

Fe++ sp oth/un 25°C 0.63M U K1=5.89 1950KLa (80442) 896
Medium: 0.625 M H2SO4

Fe++ sp none 25°C 0.0 U 1948LKa (80443) 897
B3=21.3
By kinetics B3=21.5

Fe++ EMF oth/un 25°C 0.01M U 1946DNa (80444) 898
B3=21.0

****
C12H8N2O HL CAS 1891-19-6 (3967)
5-Hydroxy-1,10-phenanthroline;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl oth/un ? 0.10M U 1961HDa (80546) 899
K(Fe+3HL)=11.7(?)
Acetate buffer.
****
C12H8N2O3S HL CAS 33388-36-2 (3996)
1,10-Phenanthroline-5-sulfonic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ sp mixed ? 64% U I 1966BAb (80547) 900
B3=8.4
Medium: 64% N2H4. B3=11.7(5%), 11.0(10%), 9.9(25%), 9.1(50%)
****
C12H9N3 L CAS 65591-51-7 (2673)
1-(2-Imidazolin-2-yl)isoquinoline;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl NaClO4 25°C 1.00M M K1=6.14 B2=10.98 1978KOb (80619) 901
B3=16.03
****
C12H9N3 L CAS 1137-68-4 (2517)
2-(2'-Pyridyl)benzimidazole;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ sp non-aq 20°C 100% C I K1=5.47 B2= 9.83 1998ENa (80624) 902
K3=3.15
Medium: MeOH. In n50% v/v MeOH/PC, K1=5.65, K2=4.75, K3=4.30
****
C12H10N4 L CAS 6957-24-0 (3373)
Pyridine-2-carbaldehyde azine; C5H4N.CH:N.N:CH.C5H4N

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl oth/un 30°C 0.01M U 1958SBa (80770) 903
K(FeL3+Fe)=2.22
****
C12H10N6O4S H2L CAS 77327-19-6 (8343)
2-[4-Amino-3-(1,2,4-triazolylazo)]napthol-4-sulphonic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl NaClO4 30°C 0.10M U T K1=6.43 B2=10.55 1981GMi (80781) 904

Also data for 40-50 C.

****

C12H11NOS HL Thionalide CAS 93-42-5 (4002)
2-Mercapto-N-(2'-naphthyl)acetamide;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	diox/w	20°C	75%	U		K1=7.0	B2=13.7 B3=19.2	1968BKb (80817)	905

Medium: 75% dioxan, 0.1 M NaClO4

****

C12H11NO3 HL CAS 33273-97-1 (3380)
Ethyl-8-hydroxyquinoline-5-carboxylate;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	diox/w	25°C	50%	U	I	B2=16.2 B3=21.7		1958TWa (80838)	906

Medium: 50% dioxan, 0.3 M NaCl. In 75% dioxan B3=33.7

****

C12H12N2O HL CAS 70301-52-9 (1940)
2-(Hydroxyphenyliminomethyl)pyridine; C5H4N.CH2.NH.C6H4.OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	EMF	KNO3	20°C	0.10M	U		K1=7.39	B2=14.27	1978CSa (81027)	907

****

C12H12N2O3 HL Nalidixic acid CAS 389-08-2 (1401)
1-Ethyl-1,4-dihydro-7-methyl-4-oxo-1,8-naphthyridine-3-carboxylic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	mixed	25°C	75%	U		K1=4.46		1998SJb (81072)	908

Medium: 75% DMSO/H2O, 0.10 M NaClO4.

****

C12H12N4 L (3958)
1-(2'-Pyridyl)-3-(6''-methyl-2''-pyridyl)-1,2-diazaprop-2-ene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	NaNO3	60°C	0.0	M	TI	K1=5.51	B2=11.62	1969GGb (81116)	909

Medium:0 corr. (5 C):K1=6.74,B2=13.06;(15 C):K1=6.55,B2=12.77;(25C):K1=6.37,
B2=12.4;(30C):K1=6.24,B2=12.22;(40C):K1=6.02,B2=11.97;(50C):K1=5.73,B2=11.79

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	NaNO3	60°C	0.0	M	TI	K(FeHL2+H)=5.92 K(FeL2+H)=7.20		1969GGb (81117)	910

Medium:0 corr. (5 C):6.31 and 7.65;(15 C):6.24 and 7.61; (25C):6.16 and 7.53
(30C):6.11 and 7.49; (40C):6.07 and 7.40; (50C):6.02 and 7.35

```
Fe++       gl  oth/un 25°C  0.0  U        B2=26          1964GHa (81118) 911
                                         K(FeHL2+H)=6.28
                                         K(FeL2+H)=7.95
                                         K(Fe+HL)=6.30
                                         K(Fe+2HL)=12.60
**************************************************************************
C12H12N4               HL                       (3935)
1-(3'-Methyl-2-pyridyl)-3-(2''-pyridyl)-1,2-diazaprop-2-ene;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe++       gl  oth/un 25°C  0.0  U        B2=32          1964GHb (81120) 912
                                         K(FeHL2+H)=4.12
                                         K(FeL2+H)=5.61
By spectrophotometry: K(Fe+HL)=7.90, K(Fe+2HL)=15.60
**************************************************************************
C12H12N8B              HL                    CAS 40250-95-1  (7937)
Tetrakis(pyrazolyl)borate;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe++       dis non-aq 25°C 100%  C                         2001KSb (81144) 913
                                         K(Fe+2HL=FeL2(org)+2H)=3.5
Method: solvent extraction into chloroform.
K: Fe+2HL(org)=FeL2(org)+2H.
**************************************************************************
C12H13NO2S              L                       (6236)
Diacetophenylthioamide; (CH3.CO)2CH.CS.NH.C6H5
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe++       sp  alc/w  25°C  60%  U        K1=4.24        1984FNa (81184) 914
Data also for 4-Cl-, 4-Br- and 3-Me- analogues
**************************************************************************
C12H13NO3              HL                      (6219)
Diacetylacetanilide; C6H5.NH.CO.CH(CO.CH3)2
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe++       sp  alc/w  30°C  50%  U        K1=7.01   B2=18.89  1986BNa (81223) 915
**************************************************************************
C12H13N3               L                    CAS 1539-42-0  (932)
bis-((2-Pyridyl)methyl)-amine (Di-2-picolylamine); C5H4N.CH2NHCH2.C5H4N
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe++       gl  KNO3   20°C 0.10M C   H    K1=6.15   B2=12.22  1977AHc (81284) 916
Calorimetry:  DH1=-25.5 kJ mol-1, DS1=30.1; DH(B2)=-71.5, DS(B2)=-6.3
**************************************************************************
C12H14N4               L                       (7104)
```

6,6'-Bis(aminomethyl)-2,2'-bipyridyl;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	KCl	25°C	0.10M	C		K1=8.94 B2=12.48 K(FeL+H)=5.08 *K(FeL)=-9.38	1995WRa (81351)	917

C12H20N2O6 H3L CAS 111652-02-9 (8144)
Azetidine-2-carboxy-1-(4-azaheptane-1,5-dicarboxylic acid);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	KNO3	25°C	0.10M	C		K1=9.2	1989ARa (82010)	918

C12H20N2O8 H4L CAS 61368-60-3 (3389)
1,2-Diaminoethane-N,N'-diethanoic-N,N'-di-2-propanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	KNO3	20°C	0.10M	U		K1=14.18	1966MKb (82132)	919

C12H20N2O8 H4L CAS 2458-58-4 (922)
1,4-Diaminobutane-N,N,N',N'-tetraethanoic acid; (HOOC.CH2)2N.(CH2)4.N(CH2.COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	KNO3	20°C	0.10M	U		K1=13.27	1964LAa (82218)	920

C12H20N2O8 H3L Mugineic acid CAS 69199-37-7 (9036)
2-Carboxy-a-[(3-carboxy-3-hydroxypropyl)amino]-b-hydroxy-1-azetidinebutanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	KNO3	20°C	0.10M	U		K1=8.1	1981STc (82246)	921

C12H20N2O8 H4L BDTA CAS 868-43-9 (1742)
DL-2,3-Diaminobutane-N,N,N',N'-tetraethanoic acid;
(HOOC.CH2)2N.CH(CH3).CH(CH3).N(CH2.COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	EMF	KCl	25°C	0.10M	U		K1=17.08 K(FeL+H)=2.13 K(FeL(OH)+H)=6.0	1971ISa (82299)	922

C12H20N2O8 H4L CAS 22968-57-6 (3992)
meso-2,3-Diaminobutane-N,N,N',N'-tetraethanoic acid;
(HOOC.CH2)2N.CH(CH3).CH(CH3).N(CH2.COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	EMF	KCl	25°C	0.10M	U		K1=15.33 K(FeL+H)=2.3 K(FeL(OH)+H)=6.1	1971ISa (82394)	923

C12H20N2O8S H4L TEDTA CAS 923-74-0 (3394)
2,2'-Thiobis(ethyliminodiethanoic acid); S(CH2.CH2.N(CH2.COOH)2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	KNO3	20°C	0.10M	U		K1=11.57 K(Fe+HL)=6.91	1964ANa (82453)	924
Fe++	gl	KCl	20°C	0.10M	U		K1=11.64 K(Fe+HL)=6.57	1964PCa (82454)	925

C12H20N2O9 H4L EEDTA CAS 923-73-9 (2112)
Oxa-bis(ethyleneimino)diethanoic acid; ((HOOC.CH2)2N.CH2.CH2)2O

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	cal	KNO3	25°C	0.10M	U	H		1965WHa (82530)	926
DH(K1)=-26.8 kJ mol-1, DS=192 J K-1 mol-1									
Fe++	gl	KNO3	20°C	0.10M	U		K1=14.3 K(Fe+HL)=8.2	1964ANa (82531)	927
Fe++	gl	KCl	20°C	0.10M	U		K1=14.9	1964PCa (82532)	928

C12H20N4 L (6709)
3,7,10,16-Tetraazabicyclo[10.3.1]hexadeca-1(16),12,14-triene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	KNO3	25°C	0.10M	C		K1=10.76	1993CDa (82605)	929

C12H21N3O6 H3L CAS 111769-28-9 (8145)
Azetidine-2-carboxy-1-(4-azaheptane-1-amino-1,5-dicarboxylic acid);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	KNO3	25°C	0.10M	C		K1=12.8	1989ARa (82750)	930
For racemic isomer: K1=10.2									
Fe++	gl	oth/un	25°C	0.10M	M		K1=12.1	1983BSd (82751)	931
Medium: 0.10 M KClO4.									

C12H22N2O6 H2L (6394)
1,7-Dioxa-4,10-diazacyclododecan-4,10-diethanoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl R4N.X 25°C 0.10M C K1=11.86 1992ADa (82792) 932
Medium: 0.1 M Me4NNO3
****
C12H22N2O6 H2L (6641)
7,10-Diaza-1,4-Dioxacyclododecane-7,10-diethanoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl R4N.X 25°C 0.10M C K1=11.52 1992ADa (82806) 933
Medium: 0.1 M Me4NNO3
****
C12H22N4O6 H2L ICRF 243 (5772)
DL-NN'-Dicarboxamidomethyl-NN'-dicarboxymethyl-2,3-diaminobutane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl NaCl 37°C 0.15M U K1=10.915 1985HCa (82833) 934
B(FeH-1L)=2.379
B(FeH2L2)=25.214
****
C12H22N4O6 H2L ICRF 226 CAS 83266-80-2 (8370)
N,N'-(1-Ethyl-1,2-ethanediyl)bis[N-(2-amino-2-oxoethyl)glycine];

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl NaCl 37°C 0.15M C K1=9.66 1982HMb (82843) 935
B(FeH-1L)=2.40
B(FeHL)=11.84
****
C12H22N4O6 H2L ICRF 236 (5771)
meso-NN'-Dicarboxamidomethyl-NN'-dicarboxymethyl-2,3-diaminobutane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl NaCl 37°C 0.15M U K1=7.926 1985HCa (82851) 936
B(FeH-1L)=-0.136
B(FeH2L2)=20.229
****
C12H23N3O5 H2L (6393)
1-Oxa-4,7,10-triazacyclododecan-4,10-diethanoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl R4N.X 25°C 0.10M C K1=14.46 1992ADa (82973) 937
B(FeHL)=16.8
Medium: 0.1 M Me4NNO3
****

C12H23N3O6 H3L CAS 117659-73-1 (8147)
1-Amino-8-methyl-1,5,9-tricarboxy-4,8-diazadecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	KNO3	25°C	0.10M	C		K1=11.4	1989ARa (83000)	938

****
C12H26N12 L (7007)
1,10-Di(2-(5-tetraazolyl)ethyl)-1,4,7,10-tetraazadecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	NaNO3	20°C	0.10M	U		K1=11.50	1981ESa (83970)	939

****
C12H26OS L CAS 2180-20-3 (5699)
S,S-Dihexylsulfoxide; C6H13.SO.C6H13

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	ISE	non-aq	25°C	100%	U		K1=5.08 B2=9.45 B3=11.38 B4=12.53 B5=13.40 B6=13.97	1986MMb (83974)	940

Medium: acetone, Bu4NClO4
****
C12H27P L CAS 998-40-3 (170)
Tri-n-butylphosphine; (CH3.(CH2)3)3P

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	sp	non-aq	25°C	100%	U	M	K(FeA+L)=5.49	1980ELa (84134)	941

Medium: toluene. A="Homologous capped" porphyrin
****
C13H7N3 L CAS 1082-19-5 (4008)
4-Cyano-1,10-phenanthroline;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	sp	alc/w	?	100%	U		B3=15.1	1961HDa (84470)	942

Medium: EtOH,0.1 M acetate buffer
****
C13H8O4 H2L (8694)
4,5-Dihydroxyxanthone;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	sp	oth/un	37°C	dil	C			2001KWa (84508)	943

K(2FeA+L)=5.3
Medium: 0.02 M phosphate buffer, pH 5.8. FeA is heme.
****
C13H9NOS HL CAS 3411-95-8 (1683)
2-(2-Hydroxyphenyl)benzothiazole;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl diox/w 25°C 50% U K1=9.20 B2=16.03 1954CFa (84551) 944
****
C13H9NO2BrCl HL CAS 104614-71-3 (9109)
4-Bromo-N-(3-chlorophenyl)-N-hydroxybenzamide;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl diox/w 25°C 50% C M K1=6.68 2001AMc (84576) 945
B(Fe(gly)L)=12.25
Medium: 50% v/v dioxane/H2O
****
C13H9NO2ClF HL CAS 104614-72-4 (9107)
N-(3-Chlorophenyl)-4-fluoro-N-hydroxybenzamide;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl diox/w 25°C 50% C M K1=6.92 2001AMc (84584) 946
B(Fe(gly)L)=12.73
Medium: 50% v/v dioxane/H2O
****
C13H9NO2Cl2 HL CAS 67201-86-9 (9108)
4-Chloro-N-(3-chlorophenyl)-N-hydroxybenzamide;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl diox/w 25°C 50% C M K1=6.72 2001AMc (84592) 947
B(Fe(gly)L)=12.33
Medium: 50% v/v dioxane/H2O
****
C13H9N2Cl L CAS 98068-36-1 (4011)
4-Chloro-2-methyl-1,10-phenanthroline;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ sp alc/w ? 0.10M U B2=4.9 1961HDa (84599) 948
Medium: EtOH, 0.1 M acetate buffer
****
C13H9N3O2S L (693)
2-(2'-Benzothiazolylazo)pyrocatechol;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---

Fe++ sp oth/un 25°C ? U K1=20.086 1988FLa (84627) 949
****
C13H9N3O4S2 H2L CAS 2536-61-0 (4031)
1-(1',3'-Thiazol-2'-ylazo)-2-hydroxynaphthalene-6-sulfonic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl alc/w 25°C 50% U I B2=17.3 1967NPb (84642) 950
Medium: 50% MeOH, 0.1 M NaClO4. B2(0%)=16.7
****
C13H10NO2Cl HL CAS 78154-49-1 (5649)
N-3-Chlorophenylbenzohydroxamic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl diox/w 25°C 50% C M K1=7.07 2001AMc (84736) 951
B(Fe(gly)L)=13.93
Medium: 50% v/v dioxane/H2O

Fe++ gl diox/w 25°C 50% U K1=6.02 B2=11.06 1989PMb (84737) 952
****
C13H10N2 L CAS 3002-77-5 (3400)
2-Methyl-1,10-phenanthroline;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl KCl 25°C 0.10M U K1=4.2 B2=7.9 1953ICa (84780) 953
K3=2.9
****
C13H10N2 L CAS 3003-78-6 (2752)
5-Methyl-1,10-phenanthroline;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ sp KNO3 25°C 0.15M U K1=5.95 B2=11.45 1972BOb (84809) 954
B3=16.55

Fe++ sp oth/un 22°C 0.0 U T H K1=6.11 1967LAe (84810) 955
B3=21.33
B3=21.87(25 C),20.25(35 C),19.45(45 C). DH(B3)=-141 kJ mol-1,DS=-71 J K-1m-1

Fe++ dis KCl 25°C 0.10M U K1=6.46 B2=13.5 1962MBa (84811) 956
B3=21.94

Fe++ sp oth/un 25°C 0.10M U K1=6.05 1959BBa (84812) 957
B3=22.3

Fe++ gl oth/un 20°C =0 U 1952BGa (84813) 958
B3=22.3
****

C13H10N2O L Pyocyanine CAS 83-06-5 (2186)
Pyocyanine;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ sp non-aq 25°C 100% U K1=3.6 1978MSc (84837) 959
Medium: DMSO
****
C13H10N2O3 HL CAS 19357-10-9 (9111)
N-(2-Pyridyl)-2-carboxybenzamide;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl mixed 25°C 40% U K1=5.87 B2=10.32 2002GSa (84861) 960
Medium: 40% v/v DMF/H2O, 0.1 M NaClO4.
****
C13H11NO HL CAS 779-84-0 (3406)
N-Salicylideneaniline; HO.C6H4.CH:N.C6H5

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl diox/w 27°C 50% U K1=8.51 B2=14.36 1972SDb (85035) 961
Medium: 50% dioxan, 0.1 M NaClO4
****
C13H11NO2 H2L CAS 78-75-2 (6258)
3-(Salicylideneamino)phenol; HO.C6H4.CH:N.C6H4.OH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl alc/w 25°C 50% U K1=7.15 B2=12.85 1977DWa (85084) 962
****
C13H11NO2 HL CAS 304-88-1 (181)
N-Phenylbenzohydroxamic acid; C6H5.CO.N(C6H5).OH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ vlt non-aq 25°C 100% C 1992SSe (85146) 963
B3=14.0
Medium: acetonitrile, 0.20 M Et4NPF6. Method: cyclic voltammetry.
****
C13H11N3O2 HL (4985)
2- or 4-Hydroxybenzaldehyde isonicotinylhydrazone;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ kin KCl 25°C 0.20M C 1992DFa (85271) 964
K(Fe+H2L)=5.93
K(FeH2L+H2L)=5.3
Data also for the benzoyl hydrazone. K(Fe+H2L)=6.03, K(FeH2L+H2L)=5.6
****

C13H11N5O2 L CAS 4453-80-9 (8115)
3-Nitro-1,5-diphenylformazan;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl diox/w 30°C 50% C T H K1=6.06 B2=10.98 2001SKb (85313) 965
Medium: 50% v/v dioxane/water, 0.1 M KCl. Data for 20-40 C.
DH(K1)=-26.4 kJ mol-1, DH(K2)=-21.1.
****
C13H12N2O4S H2L CAS 19980-54-2 (1394)
2-Hydroxy-5-methyl-4'-sulfonato-azobenzene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ sp alc/w 25°C 0.10M U K1=10.90 B2=14.52 1981MOb (85375) 966
****
C13H12N4S L Dithizone CAS 60-10-6 (1801)
Diphenylthiocarbazone; C6H5.NH.NH.CS.N:N.C6H5

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ sp NaClO4 25°C 0.10M U K1=4.78 B2=8.99 1973BSe (85457) 967
****
C13H14NO3P H2L CAS 19316-85-7 (1466)
2-Hydroxyphenyl-N-phenylaminomethylphosphinic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl NaClO4 20°C 0.10M U K1=5.20 1985SIb (85562) 968
****
C13H14N2O2S HL CAS 4384-37-1 (4032)
2-(4'-Methylphenylsulfonamido)aniline; CH3.C6H4.SO2.NH.C6H4.NH2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl diox/w ? 50% U K1=9.31 B2=17.45 1968BRa (85593) 969
Medium: 50% dioxan, 0.01 M
****
C13H14N3O5P H2L CAS 80767-75-5 (1467)
2-Hydroxy-4-nitrophenyl-N-(2-pyridylmethyl)aminemethylphosphinic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl NaClO4 20°C 0.10M U K1=5.90 1985SIb (85640) 970
****
C13H14N3O5P H2L CAS 80767-76-6 (1468)
2-Hydroxy-4-nitrophenyl-N-(3-pyridylmethyl)aminemethylphosphinic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---

Fe++ gl NaClO4 20°C 0.10M U K1=5.85 1985SIb (85653) 971
****
C13H15N2O3P H2L CAS 80767-72-2 (1460)
2-Hydroxyphenyl-(N-2-pyridylmethylamino)methylphosphinic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl NaClO4 20°C 0.10M U K1=5.70 1985SIa (85780) 972
****
C13H15N2O3P H2L CAS 80767-73-3 (1461)
2-Hydroxyphenyl-(N-3-pyridylmethylamino)methylphosphinic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl NaClO4 20°C 0.10M U K1=5.75 1985SIa (85793) 973
****
C13H15N2O3P H2L CAS 80767-74-4 (1462)
2-Hydroxyphenyl-(N-4-pyridylmethylamino)methylphosphinic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl NaClO4 20°C 0.10M U K1=5.80 1985SIa (85806) 974
****
C13H15N2O4P H3L CAS 80767-78-8 (1463)
2-Hydroxyphenyl-(N-2-pyridylmethylamino)methylphosphonic acid;
C6H4(OH)CH(PO3H2).NH.CH2.C5H4N

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl NaClO4 20°C 0.10M U K1=7.80 1985SIa (85819) 975
K(Fe+HL)=3.90
****
C13H15N2O4P H3L CAS 85946-85-6 (1464)
2-Hydroxyphenyl-(N-3-pyridylmethylamino)methylphosphonic acid;
C6H4(OH)CH(PO3H2).NH.CH2.C5H4N

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl NaClO4 20°C 0.10M U K1=7.85 1985SIa (85832) 976
K(Fe+HL)=3.90
****
C13H15N2O4P H3L CAS 85946-86-7 (1465)
2-Hydroxyphenyl-(N-4-pyridylmethylamino)methylphosphonic acid;
C6H4(OH)CH(PO3H2).NH.CH2.C5H4N

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl NaClO4 20°C 0.10M U K1=7.90 1985SIa (85845) 977
K(Fe+HL)=3.95
****

C13H15N3O2 HL CAS 16832-24-9 (6)
N3-Benzyl-L-histidine; H2N.CH(CH2.C3H2N2(CH2.C6H5))COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	none	21°C	0.0	M		K1=5.65 B2=10.24	1974YAa (85885)	978

****

C13H19N3O4 H2L (6689)
N,N'-((Pyridine-2,6-diyl)bis-methylene)bis-sarcosine; C5H3N(CH2.N(CH3)CH2.COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	NaNO3	25°C	0.10M	U		K1=10.44	1992BSb (86071)	979

****

C13H19N3O8 H3L b-Asp-b-Asp-Pro CAS 91921-49-2 (8149)
Pyrrolidine-2-carboxy-N-(1,5-dicarboxy-1-amino-4-azaheptane-3,7-dione);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	KNO3	25°C	0.10M	C		K1=4.6	1989ARa (86078)	980

****

C13H20NO4P H3L (1471)
2-Hydroxyphenyl-N-(cyclohexylamino)methylphosphonic acid;
C6H4(OH)CH(PO3H2).NH.C6H11

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	NaClO4	20°C	0.10M	U		K1=6.80	1985SIb (86090)	981
							K(Fe+HL)=3.35		

****

C13H22N2O8 H4L CAS 1798-14-7 (921)
(Pentamethylenedinitrilo)tetraethanoic acid; ((HOOC.CH2)2N.CH2.CH2)2CH2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	KNO3	20°C	0.10M	U		K1=10.8	1964ANa (86194)	982
							K(Fe+HL)=6.4		

****

C13H22N4 L (6710)
3,7,11,17-Tetraazabicyclo[11.3.1]heptadeca-1(17),13,15-triene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	KNO3	25°C	0.10M	C		K1=9.34	1993CDa (86323)	983
							K(Fe(OH)L+H)=10.91		

****

C13H24N2O6 H2L (5610)
1,11-Dioxa-4,8-diazacyclotridecane-N,N'-diethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo

```
--------------------------------------------------------------------------------
Fe++       gl  R4N.X  25°C 0.10M C        K1=8.38        1998CCd (86412) 984
                                         K(FeL+H)=5.14
Medium: 0.10 M Me4NNO3.
********************************************************************************
C14H8N4O4Cl2S         H2L                        (6672)
7-((3,5-Dichloro-2-pyridyl)azo)-8-hydroxyquinoline-5-sulfonic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       vlt KNO3   25°C 0.10M U                        1993HKa (86621) 985
                                         B(Fe+2HL)=27.74
For 3,5-dibromo analogue K=27.73
********************************************************************************
C14H9NO4              H2L    Alizarin Maroon  CAS 3963-78-8  (1052)
3-Amino-1,2-dihydroxyanthraquinone;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       sp  diox/w 25°C  20%  U  I M   K1=6.40   B2=11.80  1988SIc (86812) 986
                                         B(FeLA)=13.10
Medium: 20% dioxan/H2O, 0.1 M NaClO4. In 50% EtOH/H2O, K1=6.20, K2=5.05,
B(FeLA)=11.75, H2A=sulfosalicylic acid
********************************************************************************
C14H12NO2Cl            HL                      CAS 67055-92-9  (6301)
N-(3-Chlorophenyl)-4-methylbenzohydroxamic acid; CH3.C6H4.CO.N(C6H4Cl)OH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       gl  diox/w 25°C  50%  C    M   K1=7.37        2001AMc (87062) 987
                                         B(Fe(gly)L)=13.59
Medium: 50% v/v dioxane/H2O
--------------------------------------------------------------------------------
Fe++       gl  diox/w 25°C  50%  U        K1=6.25   B2=11.55  1989PMb (87063) 988
Data also for 4-fluoro, 4-chloro, 4-bromo, 4-nitro and 4-methoxy analogues
********************************************************************************
C14H12NO3Cl            HL                      CAS 67135-47-1  (9106)
N-(3-Chlorophenyl)-N-hydroxy-4-methoxybenzamide;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       gl  diox/w 25°C  50%  C    M   K1=7.45        2001AMc (87095) 989
                                         B(Fe(gly)L)=13.80
Medium: 50% v/v dioxane/H2O
********************************************************************************
C14H12N2               L                       CAS 484-11-7  (450)
2,9-Dimethyl-1,10-phenanthroline;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
```

Fe++ dis KCl 25°C 0.10M U K1=<4 1962IMa (87130) 990
****
C14H12N2 L CAS 3248-05-3 (3427)
4,7-Dimethyl-1,10-phenanthroline;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ sp oth/un 25°C 0.10M U K1=5.60 1963BMb (87146) 991
****
C14H12N2 L CAS 3002-81-1 (451)
5,6-Dimethyl-1,10-phenanthroline;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ sp KCl 33°C 0.10M U K1=6.15 1968LAa (87158) 992

Fe++ sp oth/un 25°C 0.0 U T 1968LAa (87159) 993
B3=21.97
Medium: acetate and phosphate buffers. B3(33 C)=21.37, B3(40 C)=20.90,
B3(45 C)=20.60

Fe++ sp oth/un 25°C 0.10M U K1=6.37 1963BMb (87160) 994
****
C14H12N2O3 H2L CAS 28547-20-8 (1395)
2-Hydroxy-5-methyl-4'-carboxy-azobenzene; (HO)(CH3)C6H3.N:N.C6H4.COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ sp alc/w 25°C 0.10M U K1=10.90 B2=14.27 1981MOb (87231) 995
****
C14H12O3 HL Benzilic acid CAS 76-93-7 (710)
Diphenylglycolic acid, (benzilic acid); (C6H5)2C(OH).COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ sp oth/un ? ? U K1=6.2 1976SCb (87349) 996
****
C14H13NO HL CAS 3246-73-9 (5056)
N-(Salicylidene)-2-methylaniline; CH3.C6H4.N:CH.C6H4.OH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl diox/w 27°C 50% U K1=8.63 1972SDb (87368) 997
Medium: 50% dioxan, 0.1 M NaClO4
****
C14H13NO HL CAS 952-81-8 (5057)
N-(Salicylidene)-3-methylaniline; CH3.C6H4.N:CH.C6H4.OH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---

Fe++ gl diox/w 27°C 50% U K1=7.88 1972SDb (87375) 998
Medium: 50% dioxan, 0.1 M NaClO4
****
C14H13NO HL CAS 982-76-3 (5058)
N-(Salicylidene)-4-methylaniline; CH3.C6H4.N:CH.C6H4.OH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl diox/w 27°C 50% U K1=7.33 1972SDb (87385) 999
Medium: 50% dioxan, 0.1 M NaClO4
****
C14H13NO2 HL CAS 889-29-2 (6259)
N-Salicylidene-3-methoxyaniline; HO.C6H4.CH:N.C6H4.OCH3

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl alc/w 25°C 50% U K1=5.55 B2=10.20 1977DWa (87527)1000
****
C14H13N5OS HL (5394)
1-(2-Pyridylmethylideneamino)-3-(salicylideneamino)thiourea;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ sp mixed 25°C 40% U 1985RGa (87614)1001
K1eff=4.25
Medium: 40% DMF, pH 4.5
****
C14H13N5O2 HL (5393)
1-(2-Pyridylmethylideneamino)-3-(salicylideneamino)urea;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ sp mixed 25°C 32% U 1985RGa (87623)1002
K1eff=4.3
Medium: 32% DMF, pH 4.5
****
C14H14N4O3 HL CAS 82845-52-1 (6626)
Pyridoxal isonicotinoylhydrazone;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ kin KCl 25°C 0.20M C 1992DFa (87698)1003
K(Fe+H2L)=5.11
K(FeH2L+H2L)=5.00
Data also for the benzoyl hydrazone. K(Fe+H2L)=5.00, K(FeH2L+H2L)=4.9

Fe++ sp KNO3 25°C 0.10M U 1990VHa (87699)1004
K(Fe+2H2L=FeH4L2)=6.98
K(Fe+2HL=FeH2L2)=12.47
Medium: succinic-succinate buffer

****
C14H16NO3P H2L CAS 25881-35-0 (1469)
Phenyl-N-(benzylamino)methylphosphonic acid; C6H5.CH(PO3H2).NH.CH2.C6H5

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	NaClO4	20°C	0.10M	U		K1=6.50	1985SIb	(87809)1005
							K(Fe+HL)=3.10		

****
C14H16NO4P H3L CAS 61146-25-6 (1470)
2-Hydroxyphenyl-N-(benzylamino)methylphosphonic acid; C6H4(OH)CH(PO3H2).NH.CH2.C6H5

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	NaClO4	20°C	0.10M	U		K1=6.90	1985SIb	(87822)1006
							K(Fe+HL)=3.50		

****
C14H16NO3+ HL (5071)
2-(Trimethylammoniummethylcarbonyl)-1,3-indanedione;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	oth/un	25°C	0.02M	U		K1=6.05	1971BMd	(87829)1007

Medium: 0.02 M HL, 0.02 M Mohr's salt
****
C14H16N2O8 H4L CAS 40774-59-2 (1901)
1,2-Diaminobenzene-N,N,N',N'-tetraethanoic acid; C6H4(N(CH2.COOH)2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	NaClO4	25°C	1.00M	C			1985NKa	(87950)1008
							K(FeL+H)=2.41		

****
C14H16N4O3++ L Toxogonine (6013)
1,1'-Oxydimethylene-bis(4-pyridinium aldoxime) dianion; O(CH2.NC5H4.CH:NOH)2++

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	sp	oth/un	23°C	0.05M	U			1986BHb	(88023)1009
							Keff(FeAP+L)=3.87		
							Keff(FeNP+L)=3.45		

At pH 6-7 (FeAP) and >11.8 (FeNP). FeAP=amminopentacyanoferrate(II) and
FeNP=nitrosylpentacyanoferrate(II). Data also for the trimethylene analogue
****
C14H17N2O4P H3L (1472)
2-Hydroxyphenyl-N-(2-(2'-pyridyl)ethylamino)methylphosphonic
acid;C6H4(OH)CH(PO3H2)NHCH2CH2C5H4N

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo

```
Fe++       gl  NaClO4 20°C 0.10M U        K1=7.75        1985SIb (88042)1010
                                         K(Fe+HL)=3.60
********************************************************************************
C14H22N2O8            H4L    CDTA             CAS 482-54-2  (200)
trans-1,2-Diaminocyclohexane-N,N,N',N'-tetraethanoic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       gl  NaClO4 25°C 1.00M C                         1983AHa (88645)1011
                                         K(FeL+H)=2.88
--------------------------------------------------------------------------------
Fe++       vlt oth/un 18°C 0.20M U T                       1972BOa (88646)1012
                                         K(Fe+HL)=9.30
                                         K(Fe+H2L)=6.38
At 28 C: values are: 9.32, 6.30;  35 C: 9.26, 6.32;  40 C: 9.26, 6.28
--------------------------------------------------------------------------------
Fe++       cal KNO3   25°C  1.0M U   H                   1965WHa (88647)1013
DH(K1)=-27.6 kJ mol-1, DS=255 J K-1 mol-1
--------------------------------------------------------------------------------
Fe++       vlt NaClO4 30°C  1.0M U        K1=16.27       1963RSa (88648)1014
********************************************************************************
C14H23N3O10           H5L    DTPA             CAS 67-43-6  (238)
Diethylenetriamine-pentaethanoic acid; HOOC.CH2.N(CH2.CH2.N(CH2.COOH)2)2
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       EMF NaClO4 20°C 1.00M C                         2000BMa (89232)1015
                                         K(Fe+CrL)=4.95
Method: Pt/Fe+++/Fe++ and glass electrodes.
--------------------------------------------------------------------------------
Fe++       EMF NaClO4 25°C 1.00M U        K1=17.0        1985PLb (89233)1016
                                         K(Fe+HL)=12.5
--------------------------------------------------------------------------------
Fe++       cal KNO3   25°C 0.10M U   H                   1965WHa (89234)1017
DH(K1)=-32.2 kJ mol-1, DS=205 J K-1 mol-1
--------------------------------------------------------------------------------
Fe++       EMF oth/un 20°C 0.10M U        K1=15.97       1959ANd (89235)1018
                                         K(FeL+Fe)=2.98
                                         K(Fe+HL)=10.71
--------------------------------------------------------------------------------
Fe++       gl  KNO3   25°C 0.10M U        K1=16.5        1959VCa (89236)1019
                                         K(FeL+H)=5.30
                                         K(FeL+OH)=5.01
                                         K(FeLOH+OH)=4.37
--------------------------------------------------------------------------------
Fe++       gl  oth/un 20°C 0.10M U        K1=16.55       1958DRa (89237)1020
********************************************************************************
C14H24N2O7            H3L                      (3440)
N-(2-Hydroxycyclohexyl)ethylenediamine-N,N',N'-triethanoic acid;
--------------------------------------------------------------------------------
```

```
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe++       gl  oth/un 25°C 0.10M U        K1=13.24       1960SAc (89493)1021
*************************************************************************
C14H24N2O8            H4L    HMDTA            CAS 1633-00-7  (920)
1,6-Diaminohexane-N,N,N',N'-tetraethanoic acid; ((HOOC.CH2)2N.CH2.CH2.CH2)2
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe++       gl  KNO3   20°C 0.10M U        K1=11.0        1964ANa (89574)1022
                                         K(Fe+HL)=6.6
*************************************************************************
C14H24N2O8            H4L    EDTP               (2936)
Diaminoethane-N,N,N',N'-tetrapropanoic acid; (HOOC.CH2CH2)2N.CH2CH2.N(CH2CH2.COOH)2
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe++       gl  KCl    30°C 0.10M U        K1=6.2         1953CCb (89681)1023
*************************************************************************
C14H24N2O10                   EGTA             CAS 67-42-5  (349)
Ethyleneglycol-O,O'-bis(2-aminoethyl ether)-N,N,N',N'-tetraethanoic acid; H4L
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe++       cal KNO3   25°C 0.10M U   H                    1965WHa (89861)1024
DH(K1)=-21.7 kJ mol-1, DS=154.7 J K-1 mol-1
-------------------------------------------------------------------------
Fe++       gl  KNO3   20°C 0.10M U        K1=11.81       1964ANa (89862)1025
                                         K(Fe+HL)=6.4
-------------------------------------------------------------------------
Fe++       gl  KNO3   20°C 0.10M U        K1=11.92       1963FCa (89863)1026
                                         K(Fe+HL)=6.93
*************************************************************************
C14H25N3O6            H3L                      (8146)
Azetidine-2-carboxy-1-(1-amino-5-azadecane-1,6-dicarboxylic acid);
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe++       gl  KNO3   25°C 0.10M C        K1=6.6         1989ARa (90069)1027
*************************************************************************
C14H25N3O7            H3L                      (5397)
1-Oxa-4,7,10-triazacyclododecane-4,7,10-triethanoic acid;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe++       gl  R4N.X  25°C 0.10M U        K1=16.55       1988ADa (90082)1028
                                         K(Fe+HL)=8.94
*************************************************************************
C14H25N5                L                    CAS 80251-43-0  (5459)
3,6,10,13,19-Pentaazabicyclo[13.3.1]nonadecane-1(19),15,17-triene;
```

```
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       gl  NaClO4 35°C 0.20M U    M   K1=10.76       1982KKb (90129)1029
Ternary complex with O2
********************************************************************************
C14H26N2O7            H2L                      (1567)
1,4,10-Trioxa-7,13-diazacyclopentadecane-N,N'-diethanoic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       cal R4N.X  25°C 0.10M U   H                    1989DSa (90188)1030
DH(FeL)=-14.6 kJ mol-1; DS=197; (estimated values).
--------------------------------------------------------------------------------
Fe++       gl  R4N.X  25°C 0.10M C        K1=13.0?       1987DDb (90189)1031
********************************************************************************
C14H30N4O2            H2L                      (316)
4,4,9,9-Tetramethyl-5,8-diazadodecane-2,11-dione dioxime;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       gl  NaCl   25°C 0.10M C                        1978PRa (90672)1032
                                        K(Fe+H2L=FeHL+H)=-3.51
                                        K(Fe+HL)=8.8
********************************************************************************
C14H36N6               L    TAPEN           CAS 4879-98-5  (5715)
N,N,N',N'-Tetrakis(3-aminopropyl)diaminoethane; (-CH2.N(CH2.CH2.CH2.NH2)2)2
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       gl  KNO3   25°C 0.50M M        K1=7.92        1986GMa (90898)1033
                                        B(FeHL)=17.48
                                        B(FeH2L)=26.26
********************************************************************************
C14H37N7               L                        CAS 298-85-5  (5606)
1,4,7,10,13,16,19-Heptaazacycloheneicosane;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       gl  NaClO4 25°C 0.15M C    M                   1992ABa (90912)1034
                                        K(FeA+3H+L)=31.03
                                        K(FeA+4H+L)=39.15
                                        K(FeA+5H+L)=44.39
                                        K(FeA+H3L)=3.4
K(FeA+H4L)=5.1, K(FeA+H5L)=6.6. FeA=Fe(CN)6----
--------------------------------------------------------------------------------
Fe++       gl  NaClO4 25°C 0.15M C        K1=12.09       1991BBa (90913)1035
                                        B(FeHL)=17.73
                                        K(FeL+H)=5.64
                                        K(Fe+HL)=7.97
```

****

C14H37N7 L (6456)
2,5,8,11,14,17,20-Heptaazaheneicosane; CH3.(NH.(CH2)2)6.NH.CH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	NaClO4	25°C	0.15M	C	M	K(FeA+4H+L)=40.40 K(FeA+5H+L)=46.45 K(FeA+6H+L)=50.92 K(FeA+H4L)=3.6	1992ABa	(90926)1036

K(FeA+H5L)=4.9, K(FeA+H6L)=6.0, K(FeA+H7L)=6.9, B(FeA+7H+L)=54.3.
FeA=Fe(CN)6----.

****

C15H9N3O4Cl2S H2L (6673)
1-((3,5-Dichloro-2-pyridyl)azo)-2-hydroxynaphthalene-4-sulfonic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	vlt	KNO3	25°C	0.10M	U		B2=34.14	1993HKa	(90936)1037

For 3,5-dibromo analogue B2=34.08. For 3,5-dichloro...-1-hydroxynaphthalene-
analogue B2=25.85, 3,5-dibromo analogue K=25.81

****

C15H10O7 H5L Quercetin CAS 117-39-5 (5101)
3,5,7-Trihydroxy-2-(3',4'-dihydroxyphenyl)-1-benzopyran-4-one;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	sp	non-aq	25°C	100M	C		K1eff=-0.82	2001ADb	(91021)1038

Medium: MeOH, 0.2 M acetate buffer, pH 5.0. K1eff: Al+HnL=AlL

****

C15H11N3 L CAS 1148-79-4 (488)
2,2':6'2"-Terpyridine; C5H4N.C5H3N.C5H4N

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	sp	oth/un	23°C	0.50M	U	M	B2=21.26	1984SWa	(91154)1039
Fe++	sp	NaCl	25°C	0.10M	U T H		B2=20.4	1981BSa	(91155)1040

DH(B2)=-113 kJ mol-1; DS(B2)=-13 J K-1 mol-1

Fe++	kin	oth/un	25°C	var	U		K1=7.1 B2=20.9	1966HHa	(91156)1041
Fe++	sp	oth/un	23°C	0.10M	U		B(FeH2L2)=20.4	1956MLa	(91157)1042
Fe++	sp	oth/un	?	0.10M	U		B2=18.0 K(Fe+2H2L=FeL2+4H)=3.7	1954BWa	(91158)1043

****

C15H11N3O4S H2L (5130)
7-Phenylazo-8-hydroxyquinoline-5-sulfonic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ vlt KNO3 25°C 0.10M U K1=13.76 1993HKa (91336)1044
For 4-chlorophenyl analogue K=13.49
****
C15H11N3O7S2 H3L CAS 17852-90-3 (5131)
7-(4-Sulfophenylazo)-8-hydroxyquinoline-5-sulfonic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ sp NaClO4 25°C 0.10M U K1=9.70 1993HKb (91349)1045
****
C15H11N3O8S2 H4L (6674)
7-((2-Hydroxy-5-sulfophenyl)azo)-8-hydroxyquinoline-5-sulfonic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ sp NaClO4 25°C 0.10M U 1993HKb (91357)1046
K(Fe+HL)=10.73
****
C15H12N2O3 HL CAS 86443-19-8 (4065)
Ethyl 4-hydroxy-1,10-phenanthroline-3-carboxylate;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ sp alc/w ? 100% U 1961HDa (91439)1047
K(Fe+3HL)=13.0(?)
Medium: EtOH, 0.1 M acetate buffer
****
C15H12N4 L (4056)
2-Picolinealdehyde 2'-quinolylhydrazone; C5H4N.CH:N.NH.C9H6N

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl diox/w 25°C 50% U K1=10.44 B2=20.62 1965HRa (91453)1048
****
C15H12O2 HL Diphenylacac CAS 120-46-7 (362)
1,3-Diphenylpropane-1,3-dione, Dibenzoylmethane; C6H5.CO.CH2.CO.C6H5

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl diox/w 30°C 75% U K1=11.15 B2=21.50 1953UFe (91547)1049
****
C15H14NO3Cl HL CAS 113581-14-9 (9105)
N-(3-Chlorophenyl)-4-ethoxy-N-hydroxybenzamide;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo

```
--------------------------------------------------------------------------------
Fe++       gl  diox/w 25°C  50%  C    M   K1=7.65        2001AMc (91704)1050
                                          B(Fe(gly)L)=14.17
Medium: 50% v/v dioxane/H2O
********************************************************************************
C15H14N2O2             HL                        (1393)
2-Hydroxy-5-methyl-4'-acetyl-azo-benzene; (HO)(CH3).C6H3.N:N.C6H4.CO.CH3
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       sp  alc/w  25°C 0.10M U        K1=10.30  B2=14.04  1981MOb (91713)1051
********************************************************************************
C15H16N2O2             HL                     CAS 7397-15-1  (6853)
Peonolphenylhydrazone;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       gl  diox/w 20°C  75%  U T      K1=13.58  B2=26.76  1991NNa (91925)1052
30 C: K1=13.28, K2=12.92; 40 C: K1=13.15, K2=12.53
********************************************************************************
C15H17N4OBr            HL                     CAS 14357-53-2  (712)
2-(5-Bromo-2-pyridylazo)-5-diethylaminophenol; BrC5H3N.N:N.C6H3(OH)N(CH3)2
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       sp  KCl    25°C    ?  U        B2=10.67       1988WSa (91979)1053
********************************************************************************
C15H23N3O4             HL                        (5972)
2,6-Bis(3-carboxy-1,2-dimethyl-2-azapropyl)pyridine;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       oth oth/un 25°C 0.10M U        K1=11.93       1988BPa (92296)1054
Data also for 3-carboxy-azabutyl and 3-carboxy-4-methyl-2-azapentyl ligands.
********************************************************************************
C15H23N3O4            H2L                        (6690)
N,N'-((Pyridine-2,6-diyl)bis-methylene)bis-N-methylalanine;
C5H3N(CH2.N(CH3)CH(CH3)COOH)2
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       gl  NaNO3  25°C 0.10M U        K1=10.84       1992BSb (92301)1055
********************************************************************************
C15H23N3O8            H3L    g-Glu-g-Glu-Pro  CAS 91921-50-5  (8150)
2-Carboxypyrrolidine-N-(1,6-dicarboxy-1-amino-5azanonane-4,9-dione);
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       gl  KNO3   25°C 0.10M C        K1=4.4         1989ARa (92310)1056
********************************************************************************
```

C15H27N3O6 H3L CAS 96287-34-2 (8148)
Pyrrolidine-2-carboxy-N-(1-amino-1,6-dicarboxy-5-azanonane);

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl KNO3 25°C 0.10M C K1=6.6 1989ARa (92470)1057
****
C16H9N2OBr3 HL CAS 84317-74-8 (5169)
1-(2,4,6-Tribromophenylazo)-2-hydroxynaphthalene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl mixed 25°C 75% U K1=6.34 1972MCb (92652)1058
Medium: 75% acetone, 0.1 M KNO3
****
C16H10N4O8S2 H2L Ferene CAS 79551-14-7 (5410)
3-(2-Pyridyl)-5,6-bis(2-(5-furyl sulfonic acid)-1,2,4-triazine;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ sp none 25°C 0.0 U 1984HRa (92680)1059
B3=14.9
****
C16H11N2OBr HL CAS 7150-24-5 (5172)
1-(4-Bromophenylazo)-2-hydroxynaphthalene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl mixed 25°C 75% U K1=7.13 B2=13.67 1972MCb (92698)1060
Medium: 75% acetone, 0.1 M KNO3
****
C16H11N2OCl HL CAS 24390-65-6 (5170)
1-(2-Chlorophenylazo)-2-hydroxynaphthalene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl mixed 25°C 75% U K1=6.75 B2=12.56 1972MCb (92713)1061
Medium: 75% acetone, 0.1 M KNO3
****
C16H11N2OCl HL CAS 10149-93-6 (5171)
1-(4-Chlorophenylazo)-2-hydroxynaphthalene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl mixed 25°C 75% U K1=7.04 B2=13.50 1972MCb (92728)1062
Medium: 75% acetone, 0.1 M KNO3
****
C16H11N2OI HL CAS 25023-35-2 (5173)
1-(4-Iodophenylazo)-2-hydroxynaphthalene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo

---

Fe++ gl mixed 25°C 75% U K1=7.36 B2=14.07 1972MCb (92743)1063
Medium: 75% acetone, 0.1 M KNO3

****

C16H11N2O2Cl H2L CAS 3566-94-7 (3474)
1-(5-Chloro-2-hydroxyphenylazo)-2-hydroxynaphthalene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo

---

Fe++ gl diox/w 30°C 75% U K1=18.01 1952SNa (92760)1064

****

C16H11N3O3 HL CAS 6410-09-9 (5151)
1-(2-Nitrophenylazo)-2-hydroxynaphthalene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo

---

Fe++ gl mixed 25°C 75% U K1=4.42 1972MCb (92797)1065
Medium: 75% acetone, 0.1 M KNO3

****

C16H11N3O3 HL CAS 6410-46-1 (5152)
1-(4-Nitrophenylazo)-2-hydroxynaphthalene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo

---

Fe++ gl mixed 25°C 75% U K1=5.32 B2=10.01 1972MCb (92812)1066
Medium: 75% acetone, 0.1 M KNO3

****

C16H11N3O3S HL CAS 35778-69-9 (4090)
Diphenylthiovioluric acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo

---

Fe++ sp diox/w ? 33% U B2=5.20 1960SBa (92825)1067
Medium: 33% dioxan, 0.2 M KNO3

****

C16H11N3O4 HL (2910)
1,3-Diphenyl-5-hydroxyimino-hexahydropyrimidine-2,4,6-trione;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo

---

Fe++ gl diox/w 30°C 75% C K1=5.82 B2=11.19 1978MGb (92834)1068

****

C16H12N2O HL CAS 842-07-9 (5156)
1-Phenylazo-2-hydroxynaphthalene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo

---

Fe++ gl mixed 25°C 75% U K1=8.88 B2=16.94 1972MCb (92918)1069
Medium: 75% acetone, 0.1 M KNO3

****
C16H12N2O2 H2L CAS 9486-98-2 (3462)
1-(2-Hydroxyphenylazo)-2-hydroxynaphthalene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl mixed 25°C 75% U 1972MCb (92952)1070
K(Fe+HL)=11.96
K(FeHL+HL)=11.25
Medium: 75% acetone, 0.1 M KNO3
****
C16H12N2O2 H2L CAS 14934-27-1 (5157)
1-(4-Hydroxyphenylazo)-2-hydroxynaphthalene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl mixed 25°C 75% U 1972MCb (92970)1071
K(Fe+HL)=11.24
K(FeHL+HL)=10.90
Medium: 75% acetone, 0.1 M KNO3
****
C16H12N2O4S H2L CAS 13964-82-4 (3475)
1-(4-Sulfophenylazo)-2-hydroxynaphthalene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl mixed 25°C 75% U K1=4.90 B2=8.98 1972MCb (92998)1072
Medium: 75% acetone, 0.1 M KNO3
****
C16H12N2O8S2 H4L (6676)
1-((2-Hydroxy-5-sulfophenyl)azo)-2-hydroxynaphthalene-6-sulfonic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ sp NaClO4 25°C 0.10M U K1=23.87 1993HKb (93039)1073
****
C16H12N2O8S2 H4L (6675)
2-((2-Hydroxy-5-sulfophenyl)azo)-1-hydroxynaphthalene-4-sulfonic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ sp NaClO4 25°C 0.10M U K1=21.71 1993HKb (93044)1074
****
C16H13N5 H3L (2840)
2,2'-Dipyridylketone-2-pyridylhydrazone; C5H4N.NH.N:C(C5H4N)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ sp NaCl 25°C 0.10M U B2=7.47 1983HSb (93357)1075
K(Fe+2HL)=5.25

****
C16H13N5O4 HL CAS 75272-98-9 (8459)
2,4-Dihydro-4-[(2-hydroxyphenyl)azo]-5-methyl-2-(4-nitrophenyl)-3H-pyrazol-3-one;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl alc/w 25°C 70% U K1=13.89 B2=25.40 1994RAb (93391)1076
Medium: 70% v/v EtOH/H2O, 0.1 M NaCl.
****
C16H14N2O HL (1318)
2-(2-Hydroxynaphthyliminomethyl)pyridine;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl diox/w 25°C 50% A K1=7.81 B2=14.66 1981RUa (93412)1077
Medium: 50% dioxan, 0.1 M NaClO4
****
C16H16N2O4 H2L CAS 1762-46-5 (4084)
Diethyl 2,2'-bipyridyl-5,5'-dicarboxylate; (CH3.CH2O.CO.C5H3N.)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ sp diox/w ? 75% U K1=2.5 B2=4.5 1961JPa (93692)1078
B3=6.5
Medium: 75% dioxan, 0.1 M H2SO4
****
C16H18N2O4S HL Penicillin G CAS 69-57-8 (942)
Benzylpenicillin;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl mixed 30°C 50% U K1=5.04 B2=9.40 1980TSa (93806)1079
Medium: 50% v/v acetone/H2O
****
C16H18N2O5S HL Penicillin V CAS 87-08-1 (943)
Phenoxymethylpenicillinic acid, 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic
acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl mixed 30°C 50% U K1=4.40 B2=8.37 1980TSa (93816)1080
Medium: 50% v/v acetone/H2O
****
C16H22N2O8P2 H6L CAS 20708-36-5 (5194)
2,2'-(Ethylenedi-imino)bis(2-hydroxybenzylphosphonic acid);

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ EMF KCl ? 0.10M U K1=25.0 1968MRc (94162)1081
K(Fe+H2L)=17.45

****
C16H22N4O L (3471)
2-(N-(2-Dimethylaminoethyl)-N-(4-methoxybenzyl)amino)pyrimidine;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl KCl 25°C 0.06M U T K1=5.65 B2=9.39 1961SMa (94197)1082
K1=6.30(0 C), 5.25(45 C)
****
C16H28N2O8 H4L (2850)
1,8-Diaminooctane-N,N,N',N'-tetraethanoic acid; ((HOOCCH2)2N(CH2)4)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl KNO3 20°C 0.10M U K1=10.96 1964ANa (94791)1083
K(Fe+HL)=6.71
****
C16H28N4O8 H4L DOTA CAS 60239-18-1 (1017)
1,4,7,10-Tetraazacyclododecane-1,4,7,10-tetraethanoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl R4N.X 25°C 0.10M C K1=20.22 1992CDd (94893)1084
B(FeHL)=24.48
Medium: 0.10 M Me4NNO3.
****
C16H30N2O8 H2L CAS 72912-01-7 (1568)
1,4,10,13-Tetraoxa-7,16-diazacyclooctadecane-N,N'-diethanoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl R4N.X 25°C 0.10M C H K1=7.88 1989DSa (95040)1085
By calorimetry: DH(FeL)=0.5 kJ mol-1; DS=150; (estimated values).
****
C16H34OS L CAS 1986-89-6 (5700)
S,S-Dioctylsulfoxide; C8H17.SO.C8H17

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ ISE non-aq 25°C 100% U K1=5.16 B2=9.54 1986MMb (95482)1086
B3=11.50
B4=12.75
B5=13.64
B6=14.13
Medium: acetone, Bu4NClO4
****
C16H35O2P HL CAS 13525-99-0 (2135)
Di(2-ethylhexyl)phosphinic acid; (2-C2H5C6H12)2P(O)OH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo

---
Fe++ dis NaClO4 25°C 1.00M C I 1987SMb (95500)1087
K(Fe+4HL=FeH2L4+2H)=8.41
K(Fe+6HL=FeH4L6+2H)=14.69
Data also for 0.1 M Na2SO4 medium. Distrib. into Isopar-H (ESSO)
****
C16H36N4 L CAS 3713-77-7 (5391)
1,6,11,16-Tetraazacycloeicosane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ cal NaClO4 25°C 0.15M C HM 1988BMg (95527)1088
Kout(Fe(CN)6+H4L)=3.62
DH(Fe(CN)6+H4L)=-4.6 kJ mol-1, DS(Fe(CN)6+H4L)=54 J K-1 mol-1.
****
C16H38N6O2 L O-BisDien CAS 43090-52-4 (5479)
1,4,7,13,16,19-Hexaaza-10,22-dioxacyclotetracosane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl KCl 25°C 0.10M U M K1=6.35 1993MUa (95625)1089
K(FeL+Fe)=3.85
K(Fe2H-1L+H)=7.41
K(Fe+H3L)=2.15
K(FeH2L+SO4)=3.82
****
C16H40N8 L CAS 297-11-0 (5588)
1,4,7,10,13,16,19,22-Octaazacyclotetracosane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl NaClO4 25°C 0.15M C M 1992ABa (95658)1090
K(FeA+4H+L)=39.73
K(FeA+5H+L)=46.06
K(FeA+6H+L)=51.07
K(FeA+H4L)=4.1
K(FeA+H5L)=5.5, K(FeA+H6L)=7.1. FeA=Fe(CN)6----
****
C16H42N8 L (6457)
2,5,8,11,14,17,20,23-Octaaza-tetracosane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl NaClO4 25°C 0.15M C M 1992ABa (95678)1091
K(FeA+4H+L)=40.71
K(FeA+5H+L)=48.66
K(FeA+6H+L)=54.38
K(FeA+H4L)=2.7
K(FeA+H5L)=3.9, K(FeA+H6L)=5.2, K(FeA+H7L)=6.4, B(FeA+7H+L)=58.84.
FeA=Fe(CN)6----.

****
C17H12N2O3 H2L (2040)
1-(2-Carboxyphenylazo)-2-hydroxynaphthalene; HOOC.C6H4.N:N.C10H6.OH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl NaClO4 25°C 0.01M U K1=6.78 1981GMe (95702)1092
****
C17H13NO3S H2L CAS 119516-70-0 (6185)
7-Hydroxy-8((2-mercaptophenyl)iminomethyl)-4-methyl-2H-1-benzopyran-2-one;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl diox/w 20°C 70% U T H K1=15.37 1988KOb (95748)1093
25 C:K=14.97; 32 C: K=14.45; 45 C:K=13.48. DH=-133.5 kJ mol-1, DS=-161
****
C17H13N5O5 HL CAS 158728-44-0 (8460)
2-[[4,5-Dihydro-3-methyl-1-(4-nitrophenyl)-5-oxo-1H-pyrazol-4-yl]azo]benzoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl alc/w 25°C 70% U K1=20.04 B2=33.04 1994RAb (95782)1094
Medium: 70% v/v EtOH/H2O, 0.1 M NaCl.
****
C17H14N2O HL CAS 2046-17-5 (5214)
1-(2-Methylphenylazo)-2-hydroxynaphthalene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl mixed 25°C 75% U K1=9.45 B2=17.80 1972MCb (95795)1095
Medium: 75% acetone, 0.1 M KNO3
****
C17H14N2O HL CAS 6756-41-8 (5215)
1-(4-Methylphenylazo)-2-hydroxynaphthalene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl mixed 25°C 75% U K1=9.62 B2=18.46 1972MCb (95810)1096
Medium: 75% acetone, 0.1 M KNO3
****
C17H14N2O2 HL CAS 1229-55-6 (5216)
1-(2-Methoxyphenylazo)-2-hydroxynaphthalene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl mixed 25°C 75% U K1=11.84 B2=22.87 1972MCb (95829)1097
Medium: 75% acetone, 0.1 M KNO3
****
C17H14N2O2 HL CAS 13441-91-1 (5217)
1-(4-Methoxyphenylazo)-2-hydroxynaphthalene;

```
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       gl  mixed  25°C  75%  U        K1=11.42  B2=22.14  1972MCb (95844)1098
Medium: 75% acetone, 0.1 M KNO3
********************************************************************************
C17H16N4O2S            HL                     CAS 202867-34-3  (7313)
2-[2-(5-Methylbenzothiazolyl)azo]-5-dimethylaminobenzoic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       sp  alc/w   RT   16%  C                        1998FZa (96109)1099
                                        B2eff=10.79
Medium: 16% EtOH/H2O, 0.5% sodium dodecyl sulfate.
********************************************************************************
C17H19N3                L    Antazoline       CAS 91-75-8  (3486)
2-(N-(Benzyl)-N-phenylaminomethyl)-1,4,5H-1,3-diazole, antistine;
C3H5N2.CH2.N(C6H5)CH2.C6H5
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       gl  KCl    25°C 0.06M U T      K1=6.45        1961SMa (96264)1100
K1=7.40(0 C), 6.12(45 C)
********************************************************************************
C17H20N4O6             HL    Riboflavin       CAS 83-88-5  (1438)
7,8-Dimethyl-10(D-1'-ribityl)isoalloxazine, Vitamin B2, Vitamin H
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       gl  oth/un 20°C 0.01M U        K1=7.1         1953ALa (96336)1101
********************************************************************************
C17H21NO                L    Benadryl         CAS 58-73-1  (3492)
N,N-Dimethyl-2-(diphenylmethoxy)ethylamine;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       gl  KCl    25°C .058M U T      K1=5.85   B2=9.74   1961SMa (96371)1102
K1=6.05(0 C), 5.50(45 C)
********************************************************************************
C17H22NO3+             HL                       (5224)
2-(Triethylammoniummethylcarbonyl)-1,3-indanedione;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       gl  oth/un 25°C 0.02M U        K1=6.22        1971BMd (96397)1103
Medium: 0.02 M HL,0.02 M Mohr's salt
********************************************************************************
C17H23N3O4             H2L                      (6691)
N,N'-((Pyridine-2,6-diyl)bis-methylene)bis-proline;
--------------------------------------------------------------------------------
```

```
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe++       gl  NaNO3  25°C 0.10M U        K1=12.68       1992BSb (96411)1104
*************************************************************************
C17H25N5O2              L    Prizidilol       CAS 73793-66-5  (8367)
3-[2-(-t-Butylamino-2-hydroxypropoxy)phenyl]-6-hydrazinopyridazine;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe++       gl  NaCl   37°C 0.15M U                        1984AMb (96479)1105
                                    B(FeHL)=12.737
*************************************************************************
C17H30N4O8            H4L    TRITA            CAS 60239-20-5  (1018)
1,4,7,10-Tetraazacyclotridecane-1,4,7,10-tetraethanoic acid;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe++       gl  KNO3   25°C 0.10M C        K1=17.56       1992CDd (96647)1106
                                    B(FeHL)=21.94
*************************************************************************
C18H12N2                L                     CAS 6135-89-5  (3498)
5-Phenyl-1,10-phenanthroline;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe++       sp  oth/un 25°C    ?  U                        1952BGa (96863)1107
                                    B3=21.1
*************************************************************************
C18H12N4O4S            HL                       (7221)
8-Hydroxy-7-(8-quinolyl)azo-5-quinolinesulfonic acid; C9H6N.N:N.C9H4(OH)
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe++       sp  NaCl   25°C 0.10M U        K1=11.88  B2=33.78  1990NOa (96872)1108
*************************************************************************
C18H12N6                L                     CAS 3682-35-7  (1891)
2,4,6-Tris(2-pyridyl)-1,3,5-triazine; C3N3(C5H4N)3
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe++       sp  oth/un 23°C 0.50M U    M   B2=11.05       1984SWa (96879)1109
-------------------------------------------------------------------------
Fe++       sp  oth/un 20°C  dil  U        B2=11.45       1972FEc (96880)1110
                                    K(FeL2+H)=2.40
-------------------------------------------------------------------------
Fe++       oth oth/un   ?  0.50M U  I     K1=5.04   B2=11.86  1971LPa (96881)1111
                                    K(FeL2+H)=2.56
I=2.0: K1=5.72, B2=12.53, K(FeL2+H)=2.76; I=5.0: K(FeL2+H)=3.10
-------------------------------------------------------------------------
Fe++       sp  NaCl   25°C 0.10M U        B2=12.4        1968PMb (96882)1112
```

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--------------------------------------------------------------------------------
Fe++       sp  oth/un 25°C 0.06M U        B2=10.24       1966BCb (96883)1113
********************************************************************************
C18H15N3O3S            HL                     CAS 69423-73-0  (4137)
Di-2-tolylthiovioluric acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       sp  mixed    ?   33%  U        B2=5.60        1960SBa (97002)1114
Medium: 33% acetone, 0.2 M KNO3
********************************************************************************
C18H15N3O3S            HL                     CAS 69423-74-1  (4138)
Di-3-tolylthiovioluric acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       sp  mixed    ?   33%  U        B2=6.08        1960SBa (97004)1115
Medium: 33% acetone, 0.2 M
********************************************************************************
C18H15N3O3S            HL                     CAS 61625-17-0  (4139)
Di-4-tolylthiovioluric acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       gl  diox/w 30°C  25%  M T H    K1=4.81   B2= 8.75  1978MGe (97012)1116
Medium: 25% dioxane/H2O, 0.10 M NaClO4. Data for 40, 45 and 50 C. DH(K1)=
-39.6 kJ mol-1, DS(K1)=-38.9 J K-1 mol-1; DH(K2)=-51.8, DS(K2)=-92.5.
--------------------------------------------------------------------------------
Fe++       sp  mixed    ?   33%  U        B2=5.80        1960SBa (97013)1117
Medium: 33% acetone, 0.2 M KNO3
********************************************************************************
C18H18N4               L                      CAS 16858-01-8  (1528)
Tris(2-pyridylmethyl)amine; (C5H4NCH2)3N
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       gl  KNO3   20°C 0.10M C   H    K1=8.65        1977AHc (97259)1118
                                         K(FeL(OH)+H)=8.78
DH1=-32.7 kJ mol-1, DS1=54.0
--------------------------------------------------------------------------------
Fe++       gl  KNO3   20°C 0.10M U   H    K1=8.7         1970WAa (97260)1119
By calorimetry, DH=-32.6 kJ mol-1, DS=53.9 J K-1 mol-1
********************************************************************************
C18H20N2O6             H4L                    CAS 10328-28-6  (3501)
Ethylenedinitrilo-N,N'-bis(2'-hydroxyphenyl)-N,N'-diethanoic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       vlt NaClO4 25°C 0.10M U        K1=14.26       1964SCa (97394)1120
********************************************************************************
```

C18H22N4O4 H2L CAS 2444-14-6 (3502)
N,N'-Bis(2-pyridylmethyl)diaminoethane-N,N'-diethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	oth/un	25°C	0.10M	U		K1=12.4	1965LCa	(97540)1121

****
C18H30N4O12 H6L TTHA CAS 869-52-3 (694)
Triethylenetetraaminehexaethanoic acid;((HOOC.CH2)2N.CH2.CH2.N(CH2.COOH).CH2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	EMF	NaClO4	25°C	0.10M	U		K1=17.1 B2=27.3 K(FeL+H)=8.67 K(FeHL+H)=3.25 K(FeH2L+H) < 2 K(FeL+OH)=4.98	1965SCb	(98029)1122

K(FeLOH+OH)=4.19, K(Fe2L+OH)=5.27, K(Fe2LOH+OH)=5.18
****
C18H32N4O8 H4L TETA CAS 60239-22-7 (1019)
1,4,8,11-Tetraazacyclotetradecane-1,4,8,11-tetraethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	KNO3	25°C	0.10M	C		K1=13.09 B(Fe2L)=15.55 B(FeH-1L)=4.16	1992CDd	(98201)1123

****
C19H12N5Cl L (7176)
4-Chloro-2,6-bis(benzimidazol-2-yl)-pyridine; ClC5H2N(C7H5N2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	EMF	alc/w	20°C	70%	C		K(FeL2+H)=17.4 K(FeHL2+H)=10.08 K(FeH2L2+H)=6.66 K(FeH3L2+H)=4.61	1995ELa	(98994)1124

Medium: 70% v/v EtOH
****
C19H13N3O4S H2L CAS 85413-91-9 (4144)
1-Hydroxy-2-(8'-quinolylazo)naphthalene-4-sulfonic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	alc/w	25°C	50%	U		K2=9.4	1967ANd	(99029)1125

Medium: 50% MeOH, 0.1 M NaClO4
****
C19H13N5 L (6734)
2,6-Bis(benzimidazol-2-yl)pyridine;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ sp mixed 20°C 50% C T H K1=6.00 B2=11.26 2002ELa (99059)1126
Medium: 50% v/v propylenecarbonate/MeOH. Data for 4-32 C. At 4 C, K1=5.90, K2=5.05 K3=4.0. DH(B2)=50.52 kJ mol-1, DS(B2)=43.28 J K-1 mol-1.

Fe++ sp non-aq 20°C 100% C I K1=5.90 B2=10.70 1996ELa (99060)1127
Medium: MeOH. Also data for the 4-hydroxy- and 4-chloro-2,6-bis(imidazol-2'-yl)pyridine ligands.

Fe++ sp non-aq 25°C 100% U H K1=5.46 B2=10.11 1993SGa (99061)1128
B3=13.60
Medium: MeOH. Data also from magnetic measurements

Fe++ sp alc/w 20°C 100% U K1=5.54 B2=9.66 1992SLa (99062)1129
B3=13.51
Medium: MeOH; also effect of added CHCl3 studied
****
C19H19N7O6 H3L Folic acid CAS 75708-92-8 (194)
Pteroylglutamic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl oth/un 20°C 0.01M U B2=7.9 1953ALa (99286)1130
****
C19H31N3O4 H2L (6692)
N,N'-(Pyridine-2,6-diyl)bis-methylene)bis-N-methylvaline;
C5H3N(CH2.N(CH3)CH(CH(CH3)2)COOH)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl NaNO3 25°C 0.10M U K1=10.05 1992BSb (99450)1131
****
C20H14N2O HL (5291)
1-(1-Naphthylazo)-2-hydroxynaphthalene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl mixed 25°C 75% U K1=7.54 1972MCb (99599)1132
Medium: 75% acetone, 0.1 M KNO3
****
C20H14N2O HL CAS 2653-64-7 (5292)
1-(2-Naphthylazo)-2-hydroxynaphthalene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl mixed 25°C 75% U K1=7.80 1972MCb (99614)1133
Medium: 75% acetone, 0.1 M KNO3
****

C20H14N4 L CAS 63283-05-6 (4146)
2,2':6',2'':6'',2'''-Quaterpyridine;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ sp oth/un 25°C 0.01M U H K1=8.28 B2=14.93 1964BOa (99740)1134
Medium:H2SO4. DH(K1)=-31.4 kJ mol-1, DS=50 K J-1 mol-1; DH(K2)=-56.4, DS=-63
****
C20H14N4O6S2 H2L FerroZine CAS 28048-33-1 (2785)
3-(2-Pyridyl)-5,6-diphenyl-1,2,4-triazine-4,4'-disulfonic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ sp none 25°C 0.0 U 1976GIa (99742)1135
B3=15.56
****
C20H24N2O12S2 H6L CAS 3625-85-3 (5755)
N,N'-Bis(2-hydroxy-5-sulfobenzyl)-diaminoethane-N,N'-diethanoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl KNO3 25°C 0.10M C K1=19.75 1988CMb (100026)1136
K(FeL+H)=6.25
K(FeHL+H)=4.73
****
C21H13N3O HL (6256)
1-(2'-Quinolylazo)-acenaphthylen-2-ol; C9H6N.N:N.C12H6.OH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl diox/w 30°C 75% U IH K1=8.20 B2=14.92 1979SGd (101013)1137
****
C21H24N4 L (931)
Tris((6-methyl-2-pyridyl)methyl)-amine; (CH3.C5H3N.CH2)3N

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl KNO3 20°C 0.10M C K1=4.46 1977AHc (101245)1138
****
C21H30O2 HL Delta-THC CAS 5957-75-5 (1206)
D'-6a,10a-Tetrahydrocannabinol;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl non-aq 30°C 100% U B2=21.781 1976WPa (101383)1139
B(FeHL)=7.785
B(FeHL2)=10.436
Medium: t-BuOH, 0.15 M Bu4NNO3
****
C22H15N3O HL (6255)

1-(4'-Methyl-2'-quinolylazo)-acenaphthylen-2-ol; CH3.C9H5N.N:N.C12H6.OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	diox/w	30°C	75%	U	IH	K1=8.85		1979SGd (101521)	1140

****

C22H23N2O8Cl H2L Aureomycin CAS 56235-18-8 (3515)
Chlorotetracycline;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	oth/un	20°C	0.01M	U		K1=5.7	B2=10.40	1956ARd (101759)	1141

****

C22H24N2O8 H2L Tetracycline CAS 60-54-8 (2201)
Tetracycline;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	NaClO4	25°C	0.10M	C		B(FeHL)=5.80 B(FeH2L)=11.49		1996SJa (101813)	1142
Fe++	gl	oth/un	20°C	0.01M	U		K1=5.3	B2=9.30	1956ARd (101814)	1143

****

C22H24N2O9 H2L Oxotetracycline CAS 79-57-2 (2202)
Oxytetracycline, 5-Hydroxy-tetracycline;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	oth/un	20°C	.005M	U		K1=5.6	B2=10.40	1956ARd (101882)	1144

****

C22H28N4O8 H2L CAS 388603-36-9 (8004)
4,10-Bis(2-hydroxy-5-nitrobenzyl)-4,10-diaza-1,7-dioxadodecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	R4N.X	25°C	0.10M	C		K1=13.7 B(FeH2L)=25.6 B(FeHL)=19.4		2001CCb (102022)	1145

Medium: 0.10 M Me4NCl.

****

C22H34N6O2 L BISBAMP (5868)
3,9,17,23,29,30-Hexaaza-6,20-dioxatricyclo[23.3.1.1]triaconta-1(20),11,13,15(30),25
,27-hexaene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe++	gl	KCl	25°C	0.10M	U	M	K1=6.64 K(FeL+H)=7.64 B(FeH-1L)=1.55		1993MUa (102241)	1146

K(FeHL+SO4)=2.8

****

C24H16N2 L Bathophenan CAS 1662-01-7 (2749)
4,7-Diphenyl-1,10-phenanthroline;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	sp	alc/w	25°C	100%	U		K1=6.1 B3=22.7	1972LBa	(102857)1147
Fe++	oth	mixed	25°C	30%	U		B3=21.7	1970LPa	(102858)1148

Method: platinum electrode. Medium: <0.05,30% CH3CN.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	sp	alc/w	18°C	10%	U		K2=21.8	1960NSa	(102859)1149

Medium: EtOH

****

C24H34N4O12 H6L (5480)
1,4-Bis(2,5,5-tris(carboxymethyl)-2,5-diazapentyl)benzene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	KNO3	25°C	0.10M	C		K1=13.54 K(FeL+H)=9.81 K(FeHL+H)=5.28 K(FeH2L+H)=2.99 K(FeH3L+H)=2.23	1983NMa	(103225)1150

****

C24H34N6O6 H2L CAS 247158-53-8 (7573)
1,7-Bis(2-hydroxy-5-nitrobenzyl)-4,10-dimethyl-1,4,7,10-tetraazadodecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	R4N.X	25°C	0.10M	C		K1=13.4 B(FeH2L)=26.9 B(FeHL)=20.3	2001CCb	(103229)1151

Medium: 0.10 M Me4NCl.

****

C24H54N8O3 L O-BisTren CAS 64819-97-2 (5473)
7,19,30-Trioxa-1,4,10,13,16,22,27,33-octaazabicyclo[11.11.11]pentatriacontane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	KCl	25°C	0.10M	U	M	B(Fe2H-1L)=3.62 B(FeH2L)=23.22 K(FeH2L+SO4)=1.6 K(Fe2H-1L+SO4)=2.64	1993MUa	(103573)1152

****

C24H60N12 L CAS 24904-24-3 (5837)

1,4,7,10,13,16,19,22,25,28,31,34-Dodecaazacyclohexatriacontane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	NaClO4	25°C	0.15M	C	M	K(Fe(CN)6+H5L)=4.57 K(Fe(CN)6+H6L)=5.16 K(Fe(CN)6+H7L)=5.96 K(Fe(CN)6+H8L)=6.96 K(Fe(CN)6+H9L)=7.53	1992BBa (103587)	1153

****

C25H22N6O2 L CAS 160488-19-7 (7710)
N,N'-1,3-Propanediylbis-(2,2-bipyridyl-5-carboxamide);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	sp	non-aq	25°C	100%	C		B2=12.1 B(Fe2L2)=18.6 B(Fe2L3)=25.50	2000FBa (103616)	1154

Medium: methanol, 0.10 M Bu4N[CF3SO3].

****

C25H28N4O10 L CAS 752-13-6 (2940)
Tetraacetylriboflavine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	nmr	non-aq	38°C	100%	U		K1=2.0 B3=5.83	1975LHa (103676)	1155

In acetone. B3 measured by ESR at 38 C, K1 by spectrophotometry at 25 C

****

C25H48N6O8 H3L Desferrioxamine CAS 70-51-9 (2488)
Desferrioxamine B; NH2.((CH2)5.NOH.CO.C2H4.CO.NH)2.(CH2)5.NOH.CO.CH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	NaNO3	20°C	0.1M	U		K(Fe+H2L)=7.2 K(Fe+H3L)=3.8	1963AEa (103803)	1156

****

C26H24P2 L CAS 28240-60-0 (2280)
Ethylenebis(diphenylphosphine); (C6H5)2P.CH2.CH2.P(C6H5)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	sp	non-aq	25°C	100%	U	I	K1=4.07 B2=7.10	1995MFa (103929)	1157

In MeCN(60%(v/v))-toluene mixtures. I=0.05 M Et4NBF4
In 30%: B1=4.01; 40%: 4.08; 50%: 4.25

****

C26H28N6 L CAS 16858-02-9 (933)
N,N,N',N'-Tetrakis-(2-pyridylmethyl)-diaminoethane;

```
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       sp  KNO3   20°C 0.10M C   H    K1=14.61       1977AHc (104002)1158
Calorimetry:  DH1=-75.5 kJ mol-1, DS1=22.2
--------------------------------------------------------------------------------
Fe++       cal KNO3   20°C 0.10M U   H    K1=14.6        1970WAa (104003)1159
DH=-69.8 kJ mol-1, DS=41.4 J K-1 mol-1
********************************************************************************
C27H30N4O9            H6L    Trencam            (5754)
2,2',2"-Tri(2,3-dihydroxybenzamidoethyl)amine; N(C2H4.NH.CO.C6H3(OH)2)3
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       sp  KNO3   25°C 0.10M C        K1=12.6        1987RLa (104473)1160
                                         K(FeL+H)=11.2
********************************************************************************
C27H30O16             H4L    Rutin              CAS 153-18-4  (4169)
3,3',4',5,7-Pentahydroxyflavone-3-beta-rutinoside;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       sp  non-aq 25°C  100M C                         2001ADb (104506)1161
                                         K1eff=-1.99
Medium: MeOH, 0.2 M acetate buffer, pH 5.95.  K1eff: Al+HnL=AlL
********************************************************************************
C28H22N2O8S2          H2L                     CAS 4403-90-1  (2911)
1,4-Di(4-methylanilino)anthraquinone;       (Alizarin cyanin green)
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       sp  oth/un 25°C    ?  U        K1=5.34   B2=9.3    1978ISb (104663)1162
********************************************************************************
C30H27N3O15           H6L    Enterobactin     CAS 28384-96-5  (2259)
Enterobactin; cyclo-((OH)C6H3(OH).CO.NH.CH.CO.CH2)3
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe++       vlt R4N.X  22°C 0.40M U                         1985LEb (105190)1163
                                         K(Fe+H6L=FeL+6H)=-39.5
                                         K(FeL+H)=10.4
                                         K(FeHL+H)=7.7
                                         K(FeH2L+H)=7
********************************************************************************
C30H48N8O6            H2L                     CAS 210773-11-8  (7576)
1,13-Bis(2-hydroxy-5-nitrobenzyl)-4,7,10,16-tetramethyl-1,4,7,10,13,16-hexaazaoctad
ecane;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
```

Fe++ gl R4N.X 25°C 0.10M C K1=10.0 2001CCb (105335)1164
B(FeH3L)=31.4
B(FeH2L)=25.1
B(FeHL)=17.7
B(FeH-1L)=0.5
Medium: 0.10 M Me4NCl.
****
C30H50N6O2 L CAS 380446-61-7 (8002)
3,7,11,19,23,27-Hexaaza-33,34-dihydroxy-15,31-dimethyltricyclotetratriaconta-1,13,15,17,29,30-hex
---
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl KCl 25°C 0.10M U K1=12.51 2001WMa (105369)1165
K(FeL+H)=10.16
K(FeHL+H)=7.93
K(FeH2L+H)=5.34
K(FeL+Fe)=8.39
K(Fe2L+H)=4.31, *K(Fe2L)=-10.23, *K(Fe2(OH)L)=-11.34, *K(Fe2(OH)2L)=-12.93
****
C32H38N6O2 H2L CAS 185675-92-7 (7485)
15,31-Dimethyl-3,11,19,27,33,35-hexaazapentacyclohexatriacontadodeca-34,36-diol;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ gl KCl 25°C 0.10M C K1=15.32 1999WMa (105694)1166
B(FeHL)=26.0
B(FeH2L)=35.24
B(FeH3L)=40.10
B(Fe2L)=25.20
B(Fe2HL)=31.22; B(Fe2H-1L)=15.29.
****
C33H36N4O6 L Bilirubin CAS 635-65-4 (2623)
Bilirubin

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ vlt oth/un 23°C 0.05M U 1974NHa (105897)1167
Keff=7.54
Medium: 0.05 M phosphate buffer, pH 8
****
C34H54O8 H2L Lasalocid CAS 25999-20-6 (2335)
Lasalocid acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe++ cal alc/w 25°C 100% U T H 1990PJa (106132)1168
Medium: MeOH. DG(K1)=-28.6 kJ mol-1, DH=-6.6; DG(B2)=-51.5, DH=-27

Fe++ gl alc/w 25°C 100% M K1=5.0 B2=9.0 1988LTa (106133)1169

Medium: MeOH
****
C36H46N4 H2L Octaethylporph. CAS 2683-82-1 (1794)
2,3,7,8,12,13,17,18-Octaethyl-21H,23H-porphine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	sp	oth/un	25°C	0.10M	U			1991MAc (106367)	1170
							*K(FeP(H2O))=-4.8		

In micellar dodecyl sulfate solution (5%), 0.1 M Me4NBr.
****
C36H60N8O8 L CAS 121925-84-6 (7152)
Cyclo(Gly-eLL-Gly)2 (eLL=N,N'-ethylene-bridged (S)-leucyl-(S)-leucine
---
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	sp	non-aq	25°C	100%	U		K1=3.62 B2=5.98	1994MKa (106453)	1171

Medium: MeCN
****
C36H60O30 L a-Cyclodextrin CAS 10016-20-3 (6946)
alpha-Cyclodextrin, Cyclohexaamylose;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	sol	none	25°C		C			1998WTa (106462)	1172
							K(Fe(Cp)2+L)=2.14		
							K(Fe(Cp)2L+L)=3.37		

Fe(Cp)2 is ferrocene.

Fe++	nmr	NaCl	25°C	0.10M	U	M		1994MWa (106463)	1173
							K(FeA5B+L=FeA5BL)=1.18		

A=CN, B=1,8-Bis(pyrazinium)octane. For B=1,9-Bis(pyrazinium)nonane, K=1.98;
B=1,10-Bis(pyrazinium)decane, K=2.89; B=1,11-Bis(pyrazinium)undecane, K=3.18
****
C36H66N6O24 L a-Cyclodextrin CAS 207395-12-8 (7800)
Hexakis(2-amino)-alpha-cyclodextrin;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	vlt	oth/un	25°C	0.10M	C			1996GLa (106543)	1174
							K(Fe(CN)6+L)=5.48		

Medium: 0.1 M aminoacetonitrile buffer, pH 5.3. Method: cyclic voltammetry
Also data for the heptamer and octamer aminocyclodextrin.
****
C37H44N2O13S H6L MeThymol Blue (428)
3,3'-Bis(N,N-di(carboxymethyl)aminomethyl)thymolsulfonephthalein;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	gl	KNO3	30°C	0.0	U	T H	K1=10.75	1978SSj (106594)	1175

Extrapolated from data for I=0.1-1.0 M KNO3. Data for 40 C.
DH(K1)=-23 kJ mol-1, DS(K1)=128 J K-1 mol-1.

****

C42H42NP3 L (7145)
tris(2-Diphenylphosphinoethyl)amine

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	sp	non-aq	25°C	100%	U		K1=5.37	1995MFa	(106941)1176

In MeCN(60%(v/v))-toluene mixtures. I=0.05 M Et4NBF4

****

C42H42P4 L (6540)
Tris(2-(diphenylphosphino)ethyl)phosphane; P(CH2CH2P(C6H5)2)3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	sp	non-aq	25°C	100%	U		K1=6.00	1995MFa	(106943)1177

In MeCN(60%(v/v))-toluene mixtures. I=0.05 M Et4NBF4

****

C42H70O35 L b-Cyclodextrin CAS 7585-39-9 (7611)
Cycloheptaamylose;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	sol	none	25°C		C			1998WTa	(106990)1178
							K(Fe(Cp)2+L)=4.22		

Fe(Cp)2 is ferrocene.

****

C44H30N4 H2L Tetraphenylpor. CAS 917-23-7 (1781)
5,10,15,20-Tetraphenyl-21H,23H-porphine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	vlt	non-aq	25°C	100%	U	M		1996NSa	(107061)1179
							K(FeL+2py=FeL(py)2)=5.7		
							K(FeL+2A=FeLA2)=5.6		
							K(FeL+2C=FeLC2)=5.6		
							K(FeL+2D=FeLD2)=6.7		

Method: cyclic voltammetry. Medium: DMF. A=4-Cyanopyridine,
C=3,4-Dimethylpyridine, D=N-Methylimidazole. Also data for other porphyrins.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	kin	non-aq	25°C	100%	U		K1=8.0	1985FTa	(107062)1180

Medium: pyridine : In 3,5-dichloro-py: K1=6.0, in 3-cyano-py: K1=6.2

****

C48H80O40 L g-Cyclodextrin CAS 17465-86-0 (7612)
Cyclooctaamylose;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	sol	oth/un	25°C		U			1998WTa	(107428)1181

K(Fe(Cp)2+L)=2.96

Fe(Cp)2 is ferrocene.

****

C52H46N4O12S4 H4L (6861)

5,10,15,20-Tetrakis(2,6-dimethyl-3-sulfonatophenyl)porphin;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	vlt	NaNO3	?	0.20M	C			1991KZa (107476)	1182
							*K(FeL)=-9.7		

****

Polymer DNA (4185)

Deoxyribonucleic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	sp	NaCl	25°C	0.02M	C	M		2003MWa (108146)	1183
							Keff(Fe(phen)3+L)=3.155		
							Keff(Fe(phen)2A+L)=4.782		
							Keff(Fe(phen)A2+L)=4.612		

L is calf thymus DNA. Medium: 5mM Tris (pH 7.2), 0.02 M NaCl.
A is 4,7-diphenyl-1,10-phenanthroline. Data for 0.005-0.12 M NaCl.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	vlt	NaCl	25°C	0.01M	C	M		2000AIa (108147)	1184
							K(Fe(bipy)3+L)=3.34		
							K(Fe(phen)3+L)=4.46		

Method: differential pulse voltammetry.
Medium: 0.01 M NaCl, 0.01 M Tris, pH 7.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	vlt	oth/un	RT	0.01M	U			1996PAa (108148)	1185
							K1eff=3.81		

Medium: 0.01 M tris buffer, pH 7. Metal is ferrocenylnucleobase complex.
Host-guest interaction.

****

Polymer (5381)

Methaemoglobin;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	oth	oth/un	26°C	?	U	M		1968GGa (108259)	1186
							K(MeHb+A)=5.2		

Method: Scatchard plot, MeHb=methaemoglobin, A=CN

****

Polymer RNA (4205)

Ribonucleic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe++	vlt	oth/un	RT	0.01M	U			1996PAa (108415)	1187
							K1eff=4.08		

Medium: 0.01 M tris buffer, pH 7. Fe is ferrocenylnucleobase complex.
Host-guest interaction.
****
e- HL Electron (442)
Electron;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ oth none 50°C 0.00 U T 1972LEc (484)1188
K=-9.23(-74mV,50 C)
K: Fe3O4(s)+8H + 8e=3Fe(s)+4H2O. K=-4.67(-49mV,150 C), -4.32(-56 mV,250 C), -6.41(-99mV,350 C). Method: combination of thermodynamic data
---
Fe+++ oth none 50°C 0.00 U T 1972LEc (485)1189
K=-35.6(-1.14V,50 C)
K: Fe2O3(s)+H2O+2e=2HFeO2-. K=-29.1(-1.22V,150 C), -27.0(-1.4V,250 C), -25.9 (-1.6V,350 C). Method: combination of thermodynamic data
---
Fe+++ oth none 50°C 0.00 U T 1972LEc (486)1190
K(Fe3++e-=Fe2+)=12.80(821mV)
K=11.91(1.00V,150 C), 11.08(1.15V,250 C), 10.27(1.27V,350 C)
Method: combination of thermodynamic data

Fe+++ EMF NaClO4 25°C 0.10M U T 1972WLa (487)1191
K=13.013(769.8mV,25 C)
K: Fe(III) + e. K=13.514(745.8mV,5 C), 13.389(752.2mV, 10 C), 13.263(758.3mV ,15 C), 13.138(764.2mV,20 C), 12.888(775.2mV,30 C), 12.762(780.3mV,35 C)

Fe+++ oth none 25°C 0.0 M H 1968LCd (488)1192
DH(Fe + e = Fe++) = -41.8 kJ mol-1

Fe+++ EMF none 25°C 0.0 U 1968MRd (489)1193
K(Fe(CN)6+e)=6.103 (361.0 mV)

Fe+++ EMF none 25°C 0.0 U T H 1967HIa (490)1194
K(Fe(CN)6+e)=6.00, 355 mV
DH=-111.6 kJ mol-1, DS=-259 J K-1 mol-1, 15-30 C

Fe+++ EMF oth/un 25°C var U 1966MOa (491)1195
K(Fe(CN)5H2O+e)=6.96 (412 mV)

Fe+++ EMF none 25°C 0.0 U 1966ROa (492)1196
K(Fe(CN)6+e)=6.160, 364.4 mV

Fe+++ EMF none 25°C 0.0 U 1965LBa (493)1197
K(Fe(CN)6+e)=6.160 (364.4 mV)

Fe+++ EMF oth/un 90°C 4.0M U 1963SSe (494)1198
K=-10.13(-730 mV)
Medium: KOH. K: Fe(OH)4+e=Fe(II)(OH)4

```
--------------------------------------------------------------------------------
Fe+++      EMF NaClO4 25°C  2.0M U                        1962ZSa   (495)1199
                                        K(Fe+e=Fe(II))=12.47(737.5 mV)
--------------------------------------------------------------------------------
Fe+++      cal none   25°C  0.0  U   H                    1958FOa   (496)1200
Medium: HClO4, I=0 corr. DH(Fe+e=Fe(II))=-39.9 kJ mol-1
--------------------------------------------------------------------------------
Fe+++      EMF none   25°C  0.0  M                        1958LAa   (497)1201
                                        K'=15.35 (908 mV)
K': FeOOH(s) + 3H + e = Fe + 2H20. Alternative value: K'=15.87, 939 mV
--------------------------------------------------------------------------------
Fe+++      EMF KNO3   25°C 0.25M U  I                     1958SPa   (498)1202
                                        K(Fe+e=Fe(II))=12.66(749 mV)
Medium:HNO3. In I=1 M: K=12.61(746 mV)), I=4 M: K=12.88(762 mV). In 1 M HCl:
K=12.37(732 mV), 1 M HClO4: K=12.97(767 mV), 0.5 M H2SO4: K=11.39(674 mV)
--------------------------------------------------------------------------------
Fe+++      oth none   25°C  0.0  U                        1957WOa   (499)1203
                                        K=36(710 mV)
K: Fe(VI)O4+3H2O+3e=FeOOH(s)+5OH. From thermodynamic data
--------------------------------------------------------------------------------
Fe+++      EMF NaClO4 25°C 0.10M U  I                     1937SSa   (500)1204
                                        K(Fe+e=Fe(II))=12.67(749 mV)
Medium: HClO4. At I=0.5 to 1 M: K=12.53(741 mV). At I=0: K=13.07(770.1 mV)
--------------------------------------------------------------------------------
Fe+++      EMF none   25°C  0.0  U                        1935KTa   (501)1205
                                        K=6.02(356.0 mV)
K: Fe(CN)6+e=Fe(II)(CN)6
--------------------------------------------------------------------------------
Fe+++      EMF KCl    21°C  1.0M U                        1928DAa   (502)1206
                                        K(Fe(CN)6+e)=8.24(198+283 mV)
                                        K(Fe(CN)5(NH3)+e)=6.43
                                        K(Fe(CN)5(NO2)+e)=8.86
                                        K(Fe(CN)5(H2O)+e)=8.43
--------------------------------------------------------------------------------
Fe+++      EMF oth/un 80°C  40%  U                        1920GGa   (503)1207
                                        K=23.6(0.55 V)
Medium:40 % NaOH. K: Fe(VI)O4+3e=Fe(III)
********************************************************************************
AsO4---               H3L    Arsenate         CAS 7778-39-4  (1557)
Arsenate;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      oth none   25°C  0.0  M                        1997SAb  (1143)1208
Ks(Fe(AsO4)(s)+H=Fe+HAsO4)=-9.45.  Calculated from thermodynamic data.
--------------------------------------------------------------------------------
Fe+++      oth oth/un 25°C  0.0  U                        1990SAa  (1144)1209
                                        *K(FeL(s)+H=Fe+HL)=-10.20
Calculated from thermodynamic data.
--------------------------------------------------------------------------------
```

```
Fe+++      gl  NaNO3  25°C 3.00M C                        1988KRb  (1145)1210
                                        B(1,-2,1)=0.11
                                        B(1,-3,1)=-1.34
B(p,q,r): pM+qH+rH3L=MpHq(H3L)r.
-------------------------------------------------------------------------------
Fe+++      sol oth/un 20°C  var  U                        1956CHc  (1146)1211
                                        Kso(FeL)=-20.24
*******************************************************************************
BO4H4-                  HL    Borate           CAS 10043-35-3  (991)
Borate; B(OH)4-
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe+++      gl  NaNO3  25°C 0.10M C                        2002MDa  (1307)1212
                                        K(Fe+B(OH)4=Fe(H2BO4)+2H)=3.67
K(Fe+B(OH)4=Fe(OH)(H2BO4)+3H)=1.16, K(Fe+B(OH)4=Fe(OH)2(H2BO4)+2H)=-1.72
-------------------------------------------------------------------------------
Fe+++      gl  NaClO4 25°C 0.70M C  I                     1997BTb  (1308)1213
                                        K(Fe+B(OH)3=FeB(OH)4+H)=-2.27
Addtional method: Pt/Fe electrode. At I=0.0, K(Fe+B(OH)4=FeB(OH)4)=7.53,
K(Fe+B(OH)3=FeB(OH)4+H)=-1.71,
-------------------------------------------------------------------------------
Fe+++      sp  oth/un 25°C 0.68M U        K1=1.0    B2=2.0    1980EKa  (1309)1214
Method: UV spectroscopy
-------------------------------------------------------------------------------
Fe+++      oth oth/un   ?   var  U        K1=8.5    B2=15.6   1964BUb  (1310)1215
                                        B3=20.3
-------------------------------------------------------------------------------
Fe+++      sp  oth/un   ?     ?  U        K1=8.58   B2=15.54  1961SHd  (1311)1216
*******************************************************************************
Br-                     HL    Bromide          CAS 10035-10-6  (19)
Bromide;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe+++      sp  NaClO4 20°C 0.40M U        K1=-0.09       1988FWa  (1927)1217
-------------------------------------------------------------------------------
Fe+++      gl  oth/un 25°C 0.53M U T      K1=1.15        1977NIa  (1928)1218
-------------------------------------------------------------------------------
Fe+++      dis NaClO4 25°C  4.0M U        K1=-0.10  B2=0.00   1972STb  (1929)1219
-------------------------------------------------------------------------------
Fe+++      sp  NaClO4 20°C  3.0M U T H    K1=0.33   B2=-0.06  1971TSi  (1930)1220
At I-0 corr: 10 C: K1=0.53,K2=-0.10; 20 C: K1=0.68,K2=-0.01; 30 C: K1=0.88,
K2=0.05; 40 C: K1=1.06,K2=0.14.  DH(K1)=25.5 kJ mol-1, DH(K2)=11.3
-------------------------------------------------------------------------------
Fe+++      sp  none   25°C  0.0  U   H    K1=0.72        1970KVa  (1931)1221
DH(K1)=27.2 kJ mol-1
-------------------------------------------------------------------------------
Fe+++      kin NaClO4  2°C  1.0M U                       1969CEa  (1932)1222
                                        K1in=-1.47
```

K1out=-0.70
Medium: LiClO4. 1.6 C. Spectrophotometry also used

Fe+++ dis NaClO4 25°C 1.0M U K1=-0.12 B2=-0.38 1969MWb (1933)1223

Fe+++ sp NaClO4 20°C 1.20M U K1=-0.15 1967MAh (1934)1224

Fe+++ sp KNO3 20°C 0.47M U I K1=0.36 1957YTa (1935)1225
K1=0.27 (I=2.7), 0.22 (I= 1.2 to 2.3). Also for Mg(NO3)2 and Al(NO3)3 media
---
Fe+++ sp NaClO4 25°C 1.20M U K1=-0.21 B2=-0.70 1955LRa (1936)1226

Fe+++ sp NaClO4 27°C 1.0M U H K1=-0.30 1942RSa (1937)1227
Medium: Na/HClO4. At I=0 corr. K1=0.60, DH(K1)=26 kJ mol-1, DS=96 J K-1 m-1

Fe+++ EMF none 20°C 0.0 U K1=0.49 1939LIa (1938)1228
****
BrO3- HL Bromate (6017)
Bromate;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ dis NaClO4 25°C 1.0M U T H K1=0.36 B2=0.01 1971MHb (2412)1229
Medium: HClO4. DH(K1)=15.9 kJ mol-1, DS=59 J K-1 m-1, DH(K2)=18.8, DS=56
K1=0.26(15 C); K1=0.30, K2=-0.52(20 C); K1=0.44,K2=-0.35(30 C)
****
CN- HL Cyanide CAS 74-90-8 (230)
Cyanide;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp KCl 25°C 0.10M C T H 2002PCb (2675)1230
K(FeA+CN)=6.55
Data for 10-35 C. DH(FeA+CN)=-75 kJ mol-1, DS=-123 J K-1 mol-1.
A is N-acetyl-microperoxidase

Fe+++ vlt none ? 0.0 U M 1991CHd (2676)1231
K(Fe(CN)6+Me4N)=0.76; K(Fe(CN)6+2Me4N)=1.7; K(Fe(CN)6+3(Me4N)=3.3.
Method: Cyclic Voltammetry

Fe+++ sp NaNO3 25°C 0.10M U M 1982WPa (2677)1232
K(2FeA+4L=2FeAL2)=5.66
A=Tetrakis(4-N-methylpyridyl)porphyrin

Fe+++ nmr non-aq 20°C 100% U M 1978WYa (2678)1233
K(FeA+L)=4.28
K(FeAL+L)=3.04
Medium: DMSO-d6. A=Protoporphyrin-IX-chloride

Fe+++ nmr non-aq 20°C 100% U K1=4.28 B2=7.32 1975WYa (2679)1234

Medium: DMSO

Fe+++ sp NaClO4 25°C var U 1973MHa (2680)1235
K(Fe+Mo(CN)8)=2.6

Fe+++ sp NaClO4 25°C 1.0M U 1972EWa (2681)1236
K(Fe(CN)5OH+H)=8.4

Fe+++ sp oth/un 0°C var U 1970EJb (2682)1237
K(Fe2(CN)10+Fe2L10=2Fe2L10)=5

Fe+++ cal oth/un 25°C 0.0 U H 1965WCa (2683)1238
B6=43.6
DH(B6)=-293.2 kJ mol-1. By thermodynamic calculations B6 also 43.9

Fe+++ cal oth/un 25°C var U H 1964GHc (2684)1239
DH(B6)=-284.2 kJ mol-1

Fe+++ cal oth/un 25°C ? U H 1961GUa (2685)1240
DB(B6)=-297.1 kJ mol-1

Fe+++ sp oth/un 20°C var U M 1961MAi (2686)1241
K(Fe+Mo(IV)L8)=4.14

Fe+++ oth none 25°C 0.0 U 1956SMa (2687)1242
B6=31
Method: combination of thermodynamic data

Fe+++ cal oth/un ??? ? U H 1951YAa (2688)1243
DH(B6)=-223.4 kJ mol-1

****

CO3-- H2L Carbonate CAS 465-79-6 (268)
Carbonate;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sol	NaClO4	25°C	0.20M	C	M	B2=7.40 K(Fe+H2O+L=Fe(OH)L+H)=-3.83	1992BSa	(3227)1244

Solubility study of hematite (Fe2O3) suspensions. Constants at I=0

****

C6N6Co--- H3L Cyanocobaltate (5470)
Hexacyanocobaltate; [Co(CN)6]---

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaClO4	25°C	0.30M	U	I	K1=2.21 Kout(Fe(H2O)x+L)=1.74	1982MSf	(3490)1245
Fe+++	sp	oth/un	30°C		U		K(Fe(CN)5(H2O)+L)=1.4	1974EFa	(3491)1246

```
**************************************************************************
C6N6Fe----            H4L                        (2191)
Hexacyanoferrate (II); Fe(II)(CN)6----
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe+++      sol oth/un 25°C  var  U                        1956TGb  (3567)1247
                                        Kso(Fe4L3)=-40.52
**************************************************************************
C6N6Fe---             H3L    Ferricyanide       (2491)
Hexacyanoferrate (III); Fe(III)(CN)6---
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe+++      sp  oth/un 25°C 0.30M U  I     K1=1.91         1982MSf  (3646)1248
                                        Kout(Fe(H2O)x+L)=1.52
--------------------------------------------------------------------------
Fe+++      sp  oth/un 30°C       U                        1974EFa  (3647)1249
                                        K(Fe(CN)5(H2O)+L)=1.2
--------------------------------------------------------------------------
Fe+++      kin NaClO4 25°C 0.50M U T      K1=0.5          1967SSf  (3648)1250
                                        K1out=1.54
Medium: HClO4. Spectrophotometry also used. K1out=0.79(9 C)
--------------------------------------------------------------------------
Fe+++      sp  NaClO4 26°C  1.0M U  I     K1=1.32         1951IDa  (3649)1251
Medium: NaClO4, 0.1 M HClO4. In 1 M NaNO3, 0.1 M HNO3 K1=1.18. 0.5 M HClO4:
K1=1.56
**************************************************************************
C8N8Mo----            H4L                        (5471)
Octacyanomolybdate; [Mo(CN)8]----
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 0.30M U        K2=5.15         1982MSf  (3700)1252
                                        Kout(Fe(H2O)x+L)=2.41
**************************************************************************
Cl-                    HL    Chloride         CAS 7647-01-0  (50)
Chloride;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 0.10M C  I     K1=0.67   B2= 1.37  2005BYa  (4838)1253
Data for I=0.1-8.5 m NaClO4 and for 0.1-8.2 m HClO4. At I=0.7 m NaClO4,
K1=0.43, B2=-0.41. At I=5.0 m, K1=0.70, B2=-0.28
--------------------------------------------------------------------------
Fe+++      kin NaClO4 25°C  2.0M U                        2001BCc  (4839)1254
                                        K(FeA2+Cl)=-1.69
Medium: 2.0 M NaClO4/NaX/HClO4. HA=N-methylacetohydroxamic acid.
--------------------------------------------------------------------------
Fe+++      sp  NaCl   25°C  0.0  C T H    K1=-0.366 B2=-1.74  2001ZPa  (4840)1255
```

Calc. from data (10-100 C) for 0.2-5.8 m NaCl, using Pitzer and Helgeson act. coeffs. DH(K1)=24.7 kJ mol-1, DS=75.0;DH(K2)=9.9, DS=6.1;DH(B4)=71.4

Fe+++ oth oth/un 25°C 1.0M C K1=0.58 1999IFa (4841)1256
Method: EXAFS. Medium: 1.0 M HClO4.

Fe+++ kin KNO3 25°C 0.10M C K1=1.53 1997EHa (4842)1257

Fe+++ oth none 25°C 0.0 C I K1=1.28 B2= 1.16 1995MYa (4843)1258
By extrapolation of literature data using Pitzer equations.
At I=0.72 M, K1=0.57, B2=0.13.

Fe+++ sp NaClO4 20°C 0.40M U K1=0.49 1988FWa (4844)1259

Fe+++ sp none 25°C 0.0 U IH 1986BLb (4845)1260
K3=-0.82
K4=-2.11

Fe+++ sp oth/un 25°C 2.74M U K1=0.73 B2=0.26 1981BKe (4846)1261
Medium: mixed HCl-HClO4 solutions.

Fe+++ sp NaClO4 25°C 2.60M U H K1=0.81 B2=1.06 1979SPa (4847)1262
DH(K1)=13.39 kJ mol-1. DH(B2)=22.18 kJ mol-1

Fe+++ sp oth/un 25°C 1.0M C K1=0.47 1978PTa (4848)1263
Kout(Fe+Cl)=0.15
Medium: 1.0 M Fe(ClO4)3/HClO4, pH 0.30

Fe+++ EMF oth/un 90°C 0.00 U TI K1=1.38 1977NTa (4849)1264

Fe+++ ix alc/w 20°C 60% U K1=1.39 1976BFb (4850)1265
Medium: 60%(vol) MeOH; for 60% EtOH K1=1.47, 60% PrOH K1=1.26

Fe+++ gl NaCl 25°C 0.68M U K1=0.44 B2=0.08 1976BKb (4851)1266

Fe+++ con oth/un 25°C 1.00M U I K1=0.52 1976HBc (4852)1267

Fe+++ kin oth/un 25°C 1.00M U I K1=0.48 B2=0.59 1976SDa (4853)1268
Kout(Fe+Cl)=0.34

Fe+++ oth NaClO4 21°C 0.10M U T K1=0.92 1976YKa (4854)1269

Fe+++ sp mixed 25°C ? U T K1=4.30 B2=7.30 1974WSa (4855)1270
Medium: DMF(wet), 0.2 M NaClO4. K1=4.3(16 C)

Fe+++ sp oth/un ? ? U K1=0.16 1972KKf (4856)1271

Fe+++ dis NaClO4 25°C 4.0M U K1=0.88 B2=0.80 1972STb (4857)1272

Fe+++ dis non-aq 25°C 100% U 1972WIa (4858)1273

K(H+FeCl4)=2.3
K(HFeCl4+Cl)=1.7
Medium: methylisobutylketone

Fe+++ EMF non-aq 25°C 100% U 1971DTb (4859)1274
B3=15.55
K4=4.25
Medium: SeOCl2, 0.5 M (C2H5)4NClO4

Fe+++ sp oth/un rt var U B2=0.06 1971KGa (4860)1275
K(FeL2+3H+4L-=H3FeL6)=-6.67

Fe+++ sp NaClO4 25°C 6.0M U TI K1=2.04 1971KRc (4861)1276
Medium: (H,Na)ClO4. K1=2.08(I=6.5), 2.19(I=7.6), 2.23(I=8.2).
At I=8.2: K1=2.12(12.3 C), 2.35(44.1 C)

Fe+++ sol none 25°C 0.0 U 1971MSj (4862)1277
Kso(Fe(OH)2.86Cl0.14)=-38.4
Kso(Fe(OH)2.5Cl0.5)=-32.3

Fe+++ oth non-aq 99°C 100% U 1971TEb (4863)1278
K(FeL3(s)+SbL3=SbL2+FeL4)=-1.5
Medium: SbCl3. Method: current-voltage

Fe+++ sp non-aq 25°C 100% U K1=4.74 B2=7.19 1970LHa (4864)1279
Medium: DMSO, 0.1 M NaClO4

Fe+++ nmr oth/un 25°C var U K1=0.7 1970LSa (4865)1280
Method: esr

Fe+++ sp NaClO4 25°C 0.50M U I K1=0.75 1970RSc (4866)1281
Medium: HClO4. K1=0.72(I=1), 0.99(I=3), 1.24(I=4), 1.56(I=5), 2.04(I=6)

Fe+++ sp NaClO4 20°C 0.15M U K1=0.6 1969FOb (4867)1282
K(Fe+ClO4)=0.3

Fe+++ oth none 50°C 0.0 U T K1=1.96 B2=2.62 1969HEa (4868)1283
B3=1.76
B4=0.05
Estimated from literature data. At 100 C: K1=2.94, B2=3.63, B3=3.00, B4=1.63
At 150 C: K1=3.98, B2=4.72, B3=4.30, B=3.23

Fe+++ dis oth/un 290°C 100% U 1969JSb (4869)1284
K(2FeCl4=Fe2Cl7+Cl)=-3.40
Medium: KFeCl4. Method: gas chromatography

Fe+++ sp NaClO4 20°C 1.20M U M K1=0.66 B2=0.81 1969MAd (4870)1285
B3=0.83
K(Fe+L+SO4)=2.98

Fe+++ dis oth/un 25°C 1.0M U K1=0.63 B2=0.74 1969MWb (4871)1286
Medium: HClO4

Fe+++ EMF oth/un 25°C 4.0M U I K1=1.02 B2=1.0 1969NPb (4872)1287
At I=1.0 M: K1=0.57

Fe+++ EMF oth/un 25°C ? U K1=1.9 B2=2.35 1969PSe (4873)1288
K3=-1.0

Fe+++ sp non-aq rt 100% U 1968DPb (4874)1289
K(Fe2Cl6=FeCl2++FeCl4-)=-3.52
Medium: butylacetate

Fe+++ kin NaClO4 1°C 2.0M U K1=0.23 1968NMc (4875)1290
Medium: LiClO4

Fe+++ EMF NaClO4 25°C 4.0M U I K1=0.5 B2=-0.3 1968PSc (4876)1291
At I=1.0 M, K1=0.3

Fe+++ sp non-aq 25°C 100% U K1=3.62 1968WAa (4877)1292
K2=2.10
Medium: DMSO, 0.10 M NaClO4?

Fe+++ sp oth/un 0.0 U 1967DPa (4878)1293
K4=-2.54 to -2.24

Fe+++ EMF oth/un 25°C 0.0 U 1967LPb (4879)1294
K(Ferricenylmethyl+L)=1.0

Fe+++ EMF oth/un 25°C 0.0 U 1967NPf (4880)1295
K(Fe(C5H5)2+L)=0.45

Fe+++ cal NaClO4 25°C var U IH 1967VLf (4881)1296
Medium: HClO4. DH(K1)=-3.22(I=8),1.67(I=7),8.94(I=5),12.1(I=4),13.9(I=3),
16.6(I=2) kJ mol-1. Also thermodynamic data at other temp. and I

Fe+++ oth NaClO4 25°C 8.0M U I K1=3.13 1967VLf (4882)1297
From survey of literature data. Medium: HClO4
K1=2.46(I=7),1.50(I=5),1.10(I=4),0.76(I=3),0.53(I=2),1.38(I=0 corr)

Fe+++ cal NaClO4 33°C 4.0M U TIH 1967VLf (4883)1298
Medium: HClO4. DS(K1)=54.3(10 C),73.2(55 C)J K-1 mol-1 plus many other data
---
Fe+++ gl NaCl 25°C 0.50M U 1966BCa (4884)1299
Ks(FeH2.7)=3.04
Ks(FeH2.7Cl0.3)=2.95

Fe+++ con oth/un 25°C var U 1966KWa (4885)1300
K1in/K1out=-0.37
Also used: pressure-jump

Fe+++ sp non-aq 25°C 100% U K1=3.72 B2=5.76 1966WRa (4886)1301
Medium:Me2SO, 0.1 M NaClO4, 0.02 M HClO4

Fe+++ sp non-aq 100% U I 1965DCa (4887)1302
B4/B2 > 10
Medium:MeCONMe2

Fe+++ sp non-aq 25°C 100% U IH 1965SLb (4888)1303
K3/K4=-1.55
Medium: pyridine, K3/K4=1.42 in Me2NCHO; >= 3 in MeCN,MeNO2
DH=49.3 kJ mol-1, DS=133.8 J K-1 mol-1 in pyridine

Fe+++ con oth/un 25°C var U K1=1.32 1964HMa (4889)1304
At 1 bar. K1=-0.4(2100 bar)

Fe+++ cal oth/un ? i U IH 1964PCa (4890)1305
DH(K1)=17.9(I=1.0), 14.4(I=3.7) kJ mol-1

Fe+++ oth oth/un 0.0 U 1964VGa (4891)1306
K3K4=-4.54
Method:electrical migration or transference number

Fe+++ sp NaClO4 23°C 10.0M U I K1=1.68 1963HCa (4892)1307
Medium:5 M NaClO4+5 M HClO4. K1=1.62(+4 M HClO4),1.54(+3 M),1.45(+2 M), 1.39 (+1 M HClO4). In 5 M HClO4:K1=1.68,1.30(4 M),0.89(3 M),0.70(2 M),0.59(1 M)

Fe+++ oth NaClO4 25°C 2.0M U M 1963PDa (4893)1308
K(Fe(C5H5)2+L)=0.48

Fe+++ dis non-aq 22°C 100% U I 1962MSf (4894)1309
K(H(org)+FeCl4(org))=6.15
Medium: benzene. K: H(org)+FeCl4(org)=HFeCl4(org). K=6.3(C6H5Cl), 4(o-C6H4Cl2), 4.2(C6H5NO2)

Fe+++ EMF NaClO4 25°C 1.0M U T H K1=0.46 1962WGa (4895)1310
Medium: HClO4. K1=0.36(14.3,16 C), 0.49(30.1 C), 0.57(35.4 C), 0.68(44.3 C)
DH(K1)=18 kJ mol-1, DS=70.7 J K-1 mol-1(25C). By calorimetry: DH(K1)=19

Fe+++ sp NaClO4 25°C 1.0M U T H K1=0.47 1962WGa (4896)1311
medium: HClO4. K1=0.56(35 C), 0.66(45 C). Also in 3.5 M HClO4.
DH(K1)=17 kJ mol-1, DS=65.7 J K-1 mol-1(25C)

Fe+++ sp NaClO4 25°C 0.50M U IH K1=0.64 1961SRb (4897)1312
Medium: HClO4. DH(K1)=21 kJ mol-1, DS=100 J K-1 mol-1(25 C)
In 0.5 M DClO4 in D2O: K1=0.94, DH(K1)=18

Fe+++ dis NaClO4 25°C 0.20M U I K1=0.78 1961WKb (4898)1313
Medium: HClO4. K1=0.71(I=0.3), 0.66(I=1.0).
In 0.97 M HCl: K(Fe+3Cl+2(C8H17)3NHCl(C6H6)=((C8H17)3NH)2FeCl5(C6H6))=3.51

```
-------------------------------------------------------------------------------
Fe+++      ix  none   25°C  0.0  U        K2=>-0.7       1960MAc  (4899)1314
                                          K3=-1.40
                                          K4=-1.92
                                          K(FeCl4+H=HFeCl4)=2.7
-------------------------------------------------------------------------------
Fe+++      sp  NaClO4 22°C 1.38M U   H                   1959CCa  (4900)1315
Medium: HClO4. DH(K1)=25 kJ mol-1
-------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 2.50M U  IH    K1=0.62        1959CNa  (4901)1316
Medium: HClO4, K1=0.76(C=3),1.10(C=4),1.96(C=6),3.13(C=8),3.47(8.5),3.79(9).
DH(K1)=16(C=3), -9.6(C=8.5) kJ mol-1, DS=67(C=3), 34(C=8.5) J K-1 mol-1.
-------------------------------------------------------------------------------
Fe+++      con non-aq 20°C 100%  U                      1959GBb  (4902)1317
                                          K(FeCl3POCl3=POCl2+FeCl4)=-2
Medium: POCl3
-------------------------------------------------------------------------------
Fe+++      dis oth/un 25°C  0.0  U        K2=-0.57       1959MEb  (4903)1318
                                          K3=-2.96
-------------------------------------------------------------------------------
Fe+++      sp  diox/w 30°C 100%  U  I                   1959MKa  (4904)1319
                                          K(FeCl3+HCl=HFeCl4)=0.85
K=2.6(THF), 2.7(Bu2O), 4.0(i-Pr2O)
-------------------------------------------------------------------------------
Fe+++      sp  non-aq 30°C 100%  U        K1=2.88   B2=3.99   1959RWa  (4905)1320
Medium: CH3CONHCH3
-------------------------------------------------------------------------------
Fe+++      sp  non-aq   ?  100%  U                      1956SCa  (4906)1321
                                          K4=2.34
Medium: pyridine
-------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 1.20M U        K1=0.61   B2=0.79   1955LRa  (4907)1322
-------------------------------------------------------------------------------
Fe+++      sp  none   20°C  0.0  U                      1953GJa  (4908)1323
                                          K3=-0.14
                                          K4=-1.98
-------------------------------------------------------------------------------
Fe+++      EMF none   16°C  0.0  U        K1=1.45        1950BAa  (4909)1324
-------------------------------------------------------------------------------
Fe+++      sp  NaClO4 20°C  2.0M U        K1=0.76   B2=1.06   1943OLa  (4910)1325
                                          K3=-0.06
-------------------------------------------------------------------------------
Fe+++      EMF KNO3   25°C 0.53M U        K1=0.36        1942BRa  (4911)1326
-------------------------------------------------------------------------------
Fe+++      sp  none   25°C  0.0  U  IH    K1=1.48   B2=2.13   1942RSa  (4912)1327
                                          K3=-1.0
I=0 corr. DH(K1)=36 kJ mol-1, DS=150 J K-1 mol-1. In 1 M NaClO4, 26.5 C:
K1=0.62, K2=0.11, K3=-1.40
-------------------------------------------------------------------------------
Fe+++      sp  NaClO4   ?  .665M U        K1=0.11        1941BFa  (4913)1328
```

```
-------------------------------------------------------------------------------
Fe+++      EMF none   20°C  0.0  U        K1=1.41        1939LIa  (4914)1329
-------------------------------------------------------------------------------
Fe+++      EMF none   25°C  0.0  U        K1=0.61        1937MOb  (4915)1330
-------------------------------------------------------------------------------
Fe+++      EMF oth/un 25°C  var  U  I     K1=0.48        1929PKa  (4916)1331
At I=0 corr.: K1=1.30
*******************************************************************************
ClO2-                  HL    Chlorite         CAS 13898-47-0  (6143)
Chlorite;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe+++      kin NaClO4  5°C 1.00M U        K1=1.12        1993FEa  (6009)1332
-------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 1.00M U        K1=1.14        1991FGa  (6010)1333
*******************************************************************************
ClO3-                  HL    Chlorate         CAS 7790-93-4  (971)
Chlorate;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe+++      dis oth/un 25°C  1.0M U T H    K1=-0.40  B2=-0.80  1971MHb  (6035)1334
Medium: HClO4. DH(K1)=22.2 kJ mol-1,DS=67 J K-1 mol-1; DH(K2)=-74.9,DS=-259.
K1=-0.54,K2=0(15 C); K1=-0.47,K2=-0.2(20 C); K1=-0.34,K2=-0.7(30 C)
*******************************************************************************
ClO4-                  HL    Perchlorate      CAS 7001-90-3  (287)
Perchlorate;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe+++      nmr non-aq 25°C 100%  U        K1=2.04   B2=3.92   1989SKb  (6240)1335
                                         K(FeA3+L)=0.48
Medium: acetonitrile. A=3,4,5,6,7,8-hexamethyl-1,10-phenanthroline
-------------------------------------------------------------------------------
Fe+++      sp  NaClO4 20°C 0.40M U        K1=0.0         1988FWa  (6241)1336
-------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C  var  U        K1=0.7         1973MHa  (6242)1337
-------------------------------------------------------------------------------
Fe+++      sp  NaClO4 20°C 0.15M U        K1=0.3         1969FOb  (6243)1338
-------------------------------------------------------------------------------
Fe+++      EMF oth/un 25°C  0.0  U                       1967LPb  (6244)1339
                                         K(ferricenylmethyl+L)=1.77
-------------------------------------------------------------------------------
Fe+++      EMF oth/un 25°C  0.0  U                       1967NPf  (6245)1340
                                         K(Fe(C4H5)2+ +L)=1.2
-------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C .044M U  I     K1=0.57        1959SYa  (6246)1341
K1=0.83(I=0.024 M), 1.15(I=0 corr.)
-------------------------------------------------------------------------------
```

```
Fe+++      sp  NaClO4 19°C 0.15M U  I     K1=0.53        1954SYa  (6247)1342
K1=1.28(I=0 corr.)
-------------------------------------------------------------------------------
Fe+++      sp  none     ?   0.0  U        K1=-0.32       1952SUb  (6248)1343
*******************************************************************************
CrO4--                H2L    Chromate         CAS 7738-94-5  (2382)
Chromate;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe+++      sol none   25°C  0.0  M T H    K1=7.8         1996BPd  (6487)1344
                                          Kso(KFe3(CrO4)2(OH)6)=-18.4
Method: solubility of KFe3(CrO4)2(OH)6 at pH 1.5-3.0 (HClO4)
and 4-35 C. DH(K1)=19.1 kJ mol-1, DS(K1)=214 J K-1 mol-1.
-------------------------------------------------------------------------------
Fe+++      gl  none   25°C    0  U        K1=7.77        1994OEa  (6488)1345
                                          Kso(FeOHL.2Fe(OH)3)=-99.8
-------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 0.20M U T H                   1972BTc  (6489)1346
                                          *K1=0.29
1 C: *K1=0.09. 9.3 C; *K1=0.17. 17.2 C; *K1=0.23. DH(*K1)=12.9 kJ mol-1
-------------------------------------------------------------------------------
Fe+++      kin NaClO4 25°C 1.00M U                       1969EHb  (6490)1347
                                          *K1=-0.37
By spectrophotometry: *K1=-0.35
-------------------------------------------------------------------------------
Fe+++      sp  oth/un  0°C .084M U                       1963EKa  (6491)1348
                                          *K1=0.15
*******************************************************************************
F-                     HL    Fluoride         CAS 7644-39-3  (201)
Fluoride;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe+++      sp  KCl    25°C 0.10M C T H                   2002PCb  (6868)1349
                                          K(FeP+F)=1.58
                                          K(FeA+F)=0.08
Data for 10-35 C. DH(FeP+F)=-8.4 kJ mol-1, DS=2 J K-1 mol-1. DH(FeA+F)=
-7.0, DS=-22. P is sperm whale myoglobin; A is N-acetyl-microperoxidase
-------------------------------------------------------------------------------
Fe+++      dis NaClO4 25°C 0.30M C  I     K1=11.22       1997SSe  (6869)1350
Method: extraction of 59Fe from 0.3 M NaClO4/HClO4 into benzene/
thenoyltrifluoroacetone. Data for 0-0.308 mole fraction MeOH in H2O.
-------------------------------------------------------------------------------
Fe+++      EMF NaCl   25°C 0.68M C        K1=5.155  B2= 9.11  1996SBa  (6870)1351
                                          B3=11.96
                                          B4=13.72
                                          B(FeH-1F)=1.39
Method: Pt/Fe(III),Fe(II) electrode, glass electrode, fluoride i.s.e.
Medium: 0.68 m NaCl.
```

```
-------------------------------------------------------------------------------
Fe+++      oth none   25°C  0.0  C  I     K1=6.03   B2=10.66  1995MYa  (6871)1352
                                           B3=13.66
By extrapolation of literature data using Pitzer equations.
At I=0.72 M, K1=5.24, B2=9.46, B3=11.84.
-------------------------------------------------------------------------------
Fe+++      ISE KNO3   25°C 0.10M C    M   K1=5.30   B2=9.53   1987YHa  (6872)1353
                                           K3=3.0
K(FeA+F)= 3.46(H3A=NTA), 3.31(H3A=HEDTA), 1.7(H4A=EDTA), 1.5(H4A=CDTA)
-------------------------------------------------------------------------------
Fe+++      con oth/un 25°C 0.50M U  I     K1=5.32   B2=9.03   1976HBb  (6873)1354
-------------------------------------------------------------------------------
Fe+++      ISE NaClO4 25°C 0.50M C  I                     1975JOb  (6874)1355
                                           K(Fe+HF=FeF+H)=2.28
Method: F ion selective electrode. At I=1.0 M NaClO4, K(Fe+HF=FeF+H)=2.19.
-------------------------------------------------------------------------------
Fe+++      gl  oth/un 20°C 3.30M U  I     K1=4.36   B2=8.61   1975KFa  (6875)1356
                                           K3=4.03
                                           K4=3.85
-------------------------------------------------------------------------------
Fe+++      nmr oth/un   ?   var  U                     1970LSa  (6876)1357
                                           K6=-0.3
-------------------------------------------------------------------------------
Fe+++      ISE NaClO4 25°C 0.50M U        K1=5.16   B2=9.07   1969ALa  (6877)1358
                                           B3=12
Using redox: K1=5.19, B2=9.12, B3=12.05
-------------------------------------------------------------------------------
Fe+++      sp  NaClO4  2°C  1.0M U                     1969CEb  (6878)1359
                                           K(Fe+HF=FeF+H)=2.22
Medium: LiClO4
-------------------------------------------------------------------------------
Fe+++      vlt NaClO4   ?   1.0M U        K1=5.41   B2=9.85   1969SGh  (6879)1360
                                           K3=2.49
Medium: HClO4. Method: also quinhydrone electrode
-------------------------------------------------------------------------------
Fe+++      nmr oth/un 20°C 0.50M U  I     K1=5.34   B2=9.19   1969VSa  (6880)1361
                                           K3=2.95
Method: nmr
-------------------------------------------------------------------------------
Fe+++      sp  alc/w    ?  100%  U        K1=5.46   B2=10.21  1968SGk  (6881)1362
                                           K3=3.78
                                           K4=3.30
                                           K5=2.83
                                           K6=2.78(2.68?)
Medium:EtOH
-------------------------------------------------------------------------------
Fe+++      ISE NaClO4 25°C  1.0M U        K1=5.06             1968SRc  (6882)1363
Method:F membrane electrode
-------------------------------------------------------------------------------
Fe+++      cal NaClO4 25°C 0.50M U   H                  1967AHa  (6883)1364
```

DH(K1)=9.8 kJ mol-1, DS=131.7 J K-1 mol-1. By redox,I=0: DH(K1)=14.2, DS=163

Fe+++ EMF NaClO4 25°C 1.0M U K1=2.23 B2=3.17 1967WCa (6884)1365
K3=0.08

Fe+++ oth oth/un ? var U K1=5.76 B2=10.20 1964BSc (6885)1366
Method:refractometry.

Fe+++ EMF NaClO4 25°C 0.50M U 1964PCa (6886)1367
K(Fe+HF=FeF+H)=2.21
K(FeF+HF=FeF2+H)=1.05
K(FeF2+HF=FeF3+H)=-0.20

Fe+++ EMF NaClO4 27°C 0.50M U 1961YAa (6887)1368
K(Fe+HF=FeF+H)=2.26
K(FeF+HF=FeF2+H)=1.04

Fe+++ cal NaClO4 25°C 0.50M U H 1959SCe (6888)1369
DH(*K1)=-2.4 kJ mol-1, DS=35 J K-1 mol-1; DH(*K2)=-7.0, DS=-3.8; DH(*K3)=
-8.5, DS=-28

Fe+++ kin NaClO4 0°C 0.05M U K1=5.40 1957SMa (6889)1370

Fe+++ EMF NaClO4 25°C 0.50M U T H K1=5.17 B2=9.09 1956CHb (6890)1371
K3=2.91
At 15 C: K1=5.13, K2=3.91, K3=2.85. 35 C: K1=5.25, K2=4.00, K3=3.00
DS(K1)=126 J K-1 mol-1, DS(K2)=96, DS(K3)=75 ? At 0.11 C K1=5.03

Fe+++ ix oth/un 25°C 0.35M U 1956KAb (6891)1372
K(FeF6+H=HFeF6)=4.51
Medium: KF

Fe+++ EMF NaClO4 25°C 0.50M U H 1955PAa (6892)1373
DH(K1)=9.8 kJ mol-1, DS=130 J K-1 mol-1; DH(K2)=7.41, DS=100; DH(K3)=12.5,
DS=96. At I=0 corr: DS(K1)=163, DS(K2)=121, DS(K3)=105

Fe+++ EMF NaClO4 25°C 0.50M U T H 1955YAa (6893)1374
K(Fe+HF=FeF+H)=2.26
K(FeF+HF=FeF2+H)=0.99
K(FeF2+HF=FeF3+H)=-0.10
At 5 C: *K1=2.30, *K2=1.12, *K3=-0.04. At 50 C: *K1=2.23, *K2=0.94,*K3=-0.52
DH(*K1)=-2.6 kJ mol-1, DS=62 J K-1 mol-1; DH(*K2)=-6.9, DS=10

Fe+++ EMF NaClO4 25°C 0.50M U K1=5.21 B2=9.16 1953HWa (6894)1375
K3=2.70

Fe+++ kin NaClO4 0°C 0.50M U K1=4.99 B2=8.88 1953HWa (6895)1376
K3=3.00

Fe+++ sp NaClO4 25°C 0.52M U K1=5.14 1953SAa (6896)1377

```
--------------------------------------------------------------------------------
Fe+++      sp  none     ?   0.0  U   H    K1=4.90        1951EUa  (6897)1378
DH(K1)=31 kJ mol-1, DS=205 kJ mol-1
--------------------------------------------------------------------------------
Fe+++      EMF NaClO4 25°C 0.50M U                      1949DRa  (6898)1379
                                       K(Fe+HF=FeF+H)=2.28
                                       K(FeF+HF=FeF2+H)=1.02
                                       K(FeF2+HF=FeF3+H)=-0.24
--------------------------------------------------------------------------------
Fe+++      sp  oth/un   ?   var  U        K1=5.30        1947BKb  (6899)1380
--------------------------------------------------------------------------------
Fe+++      EMF KNO3   25°C 0.53M U        K1=5.15   B2=9.15   1942BRa  (6900)1381
--------------------------------------------------------------------------------
Fe+++      EMF none   20°C  0.0  U        K1=5.52        1939LIa  (6901)1382
********************************************************************************
HPO3--                H2L    Phosphite        CAS 13598-36-2  (6305)
Phosphite;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      sp  oth/un 24°C  0.0  U                      1966MAi  (7509)1383
                                       K(Fe+HL)=4.71
                                       K(FeHL+HL)=2.92
Medium: 0 corr. By redox: K(Fe+HL)=5.0, K(FeHL+HL)=2.17
--------------------------------------------------------------------------------
Fe+++      sp  alc/w  21°C 100%  U T      K1=5.77   B2=9.11   1964POb  (7510)1384
                                       K3=3.04
Medium: MeOH
********************************************************************************
H2PO2-                 HL    Hypophosphite    CAS 6303-21-5  (6304)
Hypophosphite;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      kin NaClO4 25°C 1.00M U                      1969EDa  (7645)1385
                                       K(Fe+H3L=FeH2L+H)=2.18
--------------------------------------------------------------------------------
Fe+++      sp  oth/un 20°C 0.20M U        K1=4.01   B2=6.79   1967MAk  (7646)1386
                                       K3=2.17
--------------------------------------------------------------------------------
Fe+++      EMF NaClO4 25°C 0.13M U        K1=3.62   B2=6.40   1964NMd  (7647)1387
Medium: 0.13 M HClO4,0.1 H+. No correction for HL
--------------------------------------------------------------------------------
Fe+++      sp  oth/un   ?   var  U        K1=2.77        1950BAb  (7648)1388
********************************************************************************
I-                     HL    Iodide           CAS 10034-85-2  (20)
Iodide;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
```

```
Fe+++      EMF NaClO4 25°C 0.10M U        K1=2.85   B2=1.57   1965NPc  (8025)1389
Medium: HClO4
--------------------------------------------------------------------------------
Fe+++      kin KNO3   25°C 0.09M U  I     K1=1.30        1936HBa  (8026)1390
At I=0 corr. K1=1.88
********************************************************************************
MoO4--                H2L    Molybdate          (443)
Molybdate;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      sol oth/un   ?   var  U        K1=7.90        1964ZLa  (8730)1391
--------------------------------------------------------------------------------
Fe+++      sp  NaClO4   ?  0.05M U        K1=7.86        1963LZa  (8731)1392
                                          B3=16.35
********************************************************************************
NH3                    L    Ammonia          CAS 7664-41-7  (414)
Ammonia
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      sp  NaNO3  30°C 1.50M U    M                   1993BGc  (9153)1393
                                       K(FeA2B+L=FeABL)=1 to 2.18
                                       K(FeABL+L=FeBL2)=2.48 to 3.78
                                       K(FeABC+L=FeBCL)=-0.22to-0.046
                                       K(FeA2B+2L=FeBL2)=4.64 to 4.92
A:H2O. H6B:5,10,15,20-Tetrakis(2,6-dimethyl-3-sulfonatophenyl)porphyrin.
C:OH.
--------------------------------------------------------------------------------
Fe+++      sp  alc/w  25°C  80%  U    M                   1993MBb  (9154)1394
                                       K(FeP+L)=3.34
Medium: 80%MeOH/H2O, 0.1 M KCl. P: porphyrin microperoxidase-8.
--------------------------------------------------------------------------------
Fe+++      gl  R4N.X  25°C 5.00M U        K1=3.8         1985MMa  (9155)1395
--------------------------------------------------------------------------------
Fe+++      oth none   25°C  0.0  U        K1=4.3         1976HMb  (9156)1396
Calculated from linear free energy relationships
--------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 0.95M U    M                   1961JAa  (9157)1397
                                       K(Fe(CN)5A+L=Fe(CN)5L+A)=1.47
                                       K(Fe(CN)5B+L=Fe(CN)5L+B)=0.59
A=SCN, B=N3
********************************************************************************
NH3O                   L    Hydroxylamine;   CAS 5470-11-1  (1808)
Hydroxylamine; NH2.OH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      sp  alc/w  25°C  80%  U                        1993BHa  (9264)1398
                                       K(FeP+L)=2.7
```

Medium: 80%MeOH/H2O. P: porphyrin microperoxidase-8.

****

NO L Nitric oxide CAS 10102-43-9 (850)

Nitric oxide;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	oth/un	25°C	var	C	TIH	K(FeP+NO)=0.15 K'(FeP'+NO)=0.22	2003NYa	(9304)1399

Medium: HClO4/NaClO4 (I=0.01-3.0 M). Data for 10-30 C. DH(K)=-62.3 kJ m-1 DH(K')=-55.2. P: tetra(4-sulfonatophenyl)porphyrin. P': tris(4-sulfonato-

---

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaClO4	25°C	1.0M	U		K((Coen2SO3(OH2)+Fe(CN)5NO)=4	1973SMa	(9305)1400

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sol	oth/un	25°C	dil	U	M		1958YBa	(9306)1401

Ks(HgFe(CN)5L=Hg+Fe(CN)5L)=-8.82 ?, pH=3.7-5

****

NO2- HL Nitrite CAS 7782-77-6 (635)

Nitrite;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	NaClO4	25°C	1.0M	C		K1=2.59 B2=3.7 B3=5.45	1986AEb	(9369)1402

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaClO4	25°C	0.01M	U		K1=2.87	1976TBa	(9370)1403

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	oth/un	35°C	1.0M	U	T H	K(Fe(CN)5+L)=3.24	1966SRa	(9371)1404

Medium: 1 M NaCl,0.2 OH-. K=4.0(10 C), 3.52(25 C). DH=-51.4 kJ mol-1, DS=-105 J K-1 mol-1

****

NO3- HL Nitrate CAS 7697-37-2 (288)

Nitrate;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaClO4	20°C	0.40M	U		K1=-0.22	1988FWa	(9679)1405

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	dis	oth/un	25°C	0.1M	C		Kout(Fe(phen)3+L)=1.57 Kout(Fe(phen)3+2L)=1.75	1984PKb	(9680)1406

Medium: KH2PO4;also for I=0.25 M K1out=1.29, B2out=1.56; I=0.5 M Kout=0.93 I=0.75 K1out=0.57; extraction H2O/CHCl3; phen=phenantroline

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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	NaNO3	25°C	1.0M	U		*Kso(Fe(OH)2L)=2.20	1973DCa	(9681)1407

```
Fe+++      sp  KNO3   25°C  var  U                        1970KSg  (9682)1408
                                        K(Fe+3L+HL)=-1.6
                                        B(FeH3L6)=-2.1  (?)
Medium: HNO3
--------------------------------------------------------------------------------
Fe+++      dis NaClO4 25°C  1.0M U T H    K1=-0.23       1969MSe  (9683)1409
K1=0.12(10 C), -0.09(20 C), -0.28(30 C), -0.55(40 C), DH(K1)=-38 kJ mol-1
--------------------------------------------------------------------------------
Fe+++      con oth/un 25°C    ?  U        K1=0.76        1964HMa  (9684)1410
Pressure 1 bar. K1=0.66(4800 bar)
--------------------------------------------------------------------------------
Fe+++      con oth/un 25°C  0.0  U        K1=1.00        1959MAd  (9685)1411
--------------------------------------------------------------------------------
Fe+++      kin NaClO4 20°C 0.60M U  I     K1=-0.22       1952SYa  (9686)1412
K1=0.83(I=0.066 M), 1.00(I=0 corr.)
--------------------------------------------------------------------------------
Fe+++      sp  NaNO3  26°C  1.0M U        K1=-0.5        1951IDa  (9687)1413
********************************************************************************
N2H4                    L    Hydrazine        CAS 302-01-2  (2117)
Hydrazine; H2N.NH2
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      sp  alc/w  25°C  80%  U                        1993BHa (10081)1414
                                        K(FeP+L)=3.8
Medium: 80%MeOH/H2O.  P: porphyrin microperoxidase-8.
********************************************************************************
N3-                     HL    Azide            CAS 7782-79-8  (441)
Azide;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      sp  KCl    25°C 0.10M C T H                   2002PCb (10209)1415
                                        K(FeP+N3)=4.10
                                        K(FeA+N3)=1.33
Data for 10-35 C. DH(FeP+N3)=-41.0 kJ mol-1, DS=-59 J K-1 mol-1.DH(FeA+N3)
=-19, DS=-38. P is sperm whale myoglobin; A is N-acetyl-microperoxidase
--------------------------------------------------------------------------------
Fe+++      gl  NaClO4 25°C 3.00M C        K1=5.35   B2=8.19   1986NAa (10210)1416
                                        B3=10.13
                                        B4=11.50
                                        B5=12.49
--------------------------------------------------------------------------------
Fe+++      gl  NaClO4 25°C 1.00M C   H    K1=4.51   B2=7.48   1980AVa (10211)1417
                                        B3=9.58
                                        B4=11.0
                                        B5=11.8
--------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 1.00M U        K1=4.30        1976AAa (10212)1418
--------------------------------------------------------------------------------
```

```
Fe+++      sp  oth/un 20°C 0.05M U    M                  1976BAd (10213)1419
                                       K(FeA+L)=5.71
                                       K(FeB+L)=5.37
                                       K(FeC+L)=5.58
                                       K(FeD+L)=5.43
FeA=heme, FeB=alpha-heme, FeC=beta-heme, FeD=alpha2-beta2-(CO)2-heme + other
-------------------------------------------------------------------------------
Fe+++      sp  NaClO4 1.6°C  1.0M U        K1=-0.44      1969CEb (10214)1420
Medium: HClO4
-------------------------------------------------------------------------------
Fe+++      vlt NaClO4 25°C  2.0M U                       1969SNa (10215)1421
                                       B3=10.4
-------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C  1.0M U                       1967CEa (10216)1422
                                       K(Fe+HL=FeL+H)=-0.29
Medium: LiClO4. By kinetics: K=-0.30
-------------------------------------------------------------------------------
Fe+++      sp  NaClO4 28°C 0.25M U  I     K1=0.80        1965MKa (10217)1423
K1=1.00(I=0.15), 1.73(I=0.05)
-------------------------------------------------------------------------------
Fe+++      sp  NaClO4 20°C  0.0  U TIH    K1=4.83        1961BDd (10218)1424
                                       *K1(Fe+HL=FeL+H)=4.83
*K1=-0.12(I=0.75), -0.09(I=0.55), -0.01(I=0.22), -0.06(I=0.11). I=0.25: *K1=
-0.04(15 C), 0.02(25 C), 0.08(35 C). DH(*K1)=10.5 kJ mol-1, DS=34.7 J K-1m-1
-------------------------------------------------------------------------------
Fe+++      sp  oth/un 20°C  0.0  U T H    K1=5.08        1961BDd (10219)1425
Medium: D2O, I=0 corr. *K1=-0.07(23 C), -0.04(28 C), -0.01(33 C).
DH(*K1)=10.5 kJ mol-1, DS=33 J K-1 mol-1
-------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 0.95M U    M                  1961JAa (10220)1426
K(Fe(CN)5SCN+L=Fe(CN)5L+SCN)=0.88
-------------------------------------------------------------------------------
Fe+++      sp  NaNO3  20°C  var  U  IH                   1961WDa (10221)1427
                                       *K1=0.23
DH(*K1)=8.4 kJ mol-1, DS=33 J K-1 mol-1
-------------------------------------------------------------------------------
Fe+++      oth oth/un 25?°C    ?  U   H    K1=5.0         1959BDc (10222)1428
Medium: D2O. DS(K1)=81 kJ mol-1
-------------------------------------------------------------------------------
Fe+++      sp  oth/un   ?  0.05M U        K1=2.51        1959ESa (10223)1429
HL neglected ?
-------------------------------------------------------------------------------
Fe+++      sp  oth/un   ?   dil  U        K1=2.06        1958ESa (10224)1430
                                       *K1=-0.1
HL neglected ?
-------------------------------------------------------------------------------
Fe+++      con oth/un   ?   0.0  U        K1=5.06        1953BAa (10225)1431
-------------------------------------------------------------------------------
Fe+++      sp  oth/un   ?     ?  U   H    K1=4.11        1951EUa (10226)1432
DH(K1)=-18.0 kJ mol-1, DS=20.9 J K-1 mol-1
```

```
--------------------------------------------------------------------------------
Fe+++      sp  oth/un   ?     ?  U        K1=5.30        1950BAa (10227)1433
********************************************************************************
OCN-                   HL    Cyanate          CAS 661-20-1  (6165)
Cyanate, Fulminate;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      kin NaClO4  2°C  1.0M U                         1969CEb (10295)1434
                                        *K1=1.1
Medium: 1M HClO4
--------------------------------------------------------------------------------
Fe+++      sp  NaClO4   ?  0.70M U        K1=2.15   B2=2.56   1966LOa (10296)1435
--------------------------------------------------------------------------------
Fe+++      sp  oth/un       var  U        B2=3.72        1966LPb (10297)1436
********************************************************************************
OH-                    HL    Hydroxide          (57)
Hydroxide;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      EMF NaClO4 25°C 0.10M C  I                     2005BYa (11354)1437
                                        *B1=-2.54
Pt/Fe(3+),Fe(2+) electrode. Data for 0.01-6.0 m NaClO4 and 0.1-6.2 m
HClO4. *B1=-2.179 (I=0), -2.73 (I=0.70 m), -2.77 (I=6.0 m NaClO4).
--------------------------------------------------------------------------------
Fe+++      EMF NaCl   25°C 0.10M C TIH                   2005BYa (11355)1438
                                        *B1=-2.78
Pt/Fe(3+),Fe(2+) electr. Data for I=0.1-6.0 m NaCl, 4-54 C. *B1 includes
effects of Cl- complexation. At I=0.7 m, *B1=-3.21 and  DH=26.0 kJ mol-1.
--------------------------------------------------------------------------------
Fe+++      EMF NaCl   25°C 0.70M C                       2005BYa (11356)1439
Pt/Fe(3+),Fe(2+) electrode.  *Kso(Fe(OH)3)=4.62 (fresh).
lg [Fe+++]=4.62-2.73(pH), indicating solid phase Fe(OH)n, where n=2.73.
--------------------------------------------------------------------------------
Fe+++      gl  NaClO4 25°C  3.0M C                       2003CIa (11357)1440
                                        K(Fe+H2O=FeOH+H)=-3.05
                                        K(Fe+2H2O=Fe(OH)2+2H)=-6.31
                                        K(2Fe+2H2O)=Fe2(OH)2+2H)=-2.96
                                        K(3Fe+4H2O=Fe3(OH)4+4H)=-5.77
At 20 C: K(Fe+3H2O=Fe(OH)3+3H) <-12.7, K(Fe+4H2O=Fe(OH)4+4H)=-22.7
K(12Fe+34H2O=Fe12(OH)34+34H)=-46.1 Results never published
--------------------------------------------------------------------------------
Fe+++      oth oth/un 20°C  0.7M C                       2003SHb (11358)1441
                                        *B2=-6.40
                                        *B3=-15.1
                                        *B4=-22.70
Medium: Uv-treated seawater. Method: adsoprtion of 59Fe-labelled Fe(OH)n
species from EDTA solution onto C18/silica.
--------------------------------------------------------------------------------
```

```
Fe+++      gl  oth/un 25°C 0.74M C TI                    2002LMa (11359)1442
                                        *K1=-2.5
                                        *B2=-6.5
                                        *B3=-13.6
                                        *Kso(Fe(OH)3)=4.13
Salinity = 36%o. Data for 5 and 50 C and seawater salinity, S, 0 to 36%o.
At 5 C and S=36, *K1=-2.8, *B2=-7.6, *B3=-14.7, *Kso(Fe(OH)3)=5.34.
-------------------------------------------------------------------------------
Fe+++      gl  NaNO3  25°C 0.10M C                       2002MDa (11360)1443
                                        *K1=-1.62
                                        *B2=-4.28
                                        *B3=-7.91
-------------------------------------------------------------------------------
Fe+++      sp  KCl    25°C 0.10M C T H                   2002PCb (11361)1444
                                        *K(FeA(H2O))=-9.59
Data for 10-35 C. DH(*K)=33.9 kJ mol-1, DS=-70 J K-1 mol-1.
A is N-acetyl-microperoxidase
-------------------------------------------------------------------------------
Fe+++      gl  NaClO4 25°C 0.70M C  IH                   2000BLa (11362)1445
                                        *K1=-2.74
                                        *B2=-6.1
                                        *Kso=3.84
Data for 0.01-6.0 M. *K1=-2.54 (I=0.10), *K1=-2.18 (I=0). From data at 5-
56 C (I=0.725 m), DH(*K1)=42.7 kJ mol-1. Method: pH and Pt/Fe(III)/Fe(II).
-------------------------------------------------------------------------------
Fe+++      gl  NaCl   25°C 2.84M C                       2000BLa (11363)1446
                                        *B2=-6.86
                                        B(Fe+Cl=Fe(OH)Cl+H)=-3.16
Additional method: Pt/Fe(III),Fe(II) electrode.
-------------------------------------------------------------------------------
Fe+++      EMF NaClO4 20°C 0.70M C                       2000BLb (11364)1447
                                        *Kso(Fe(OH)3)=4.28
Method: Pt/Fe(+++),Fe(++) electrode.
lg [Fe+++]=4.28-2.86(pH), indicating solid phase Fe(OH)n, where n=2.86.
-------------------------------------------------------------------------------
Fe+++      gl  KNO3   20°C  0.1M C  I                   2000DSa (11365)1448
                                        *B2=-6.14
                                        *B(2,2)=-2.79
In 0.05 M KNO3: *B2=-6.40, *B(2,2)=-2.79.
-------------------------------------------------------------------------------
Fe+++      sol oth/un 60°C  0.0  C T                     1999DSc (11366)1449
Method: solubility of hematite in NaCl (0.01-0.02 m)/ NaOH (pH 9.3-13.1).
Ks(0.5Fe2O3+2.5H2O=Fe(OH)4+H)=19.64. Data for 60-300 C.
-------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C  1.0M C                       1999LFa (11367)1450
                                        *K1=-2.72
                                        *B(2,2)=-2.86
-------------------------------------------------------------------------------
Fe+++      sol NaCl   25°C  0.7M C TI                    1999LMb (11368)1451
                                        *K1=-2.52
```

```
                                        *B2=-6.5
                                        *B3=-15
                                        *B4=-22.8
Method: radioanalytical (53Fe). K(Fe(OH)3(s)+3H)=4.16. Data for 5-50 C
and 0.1-5.0 M NaCl. At I=0.0 M, *K1=-2.1, *B2=-6.3, *B3=-14.3, *B4=-22.3.
--------------------------------------------------------------------------
Fe+++      gl  NaClO4 10°C 1.00M U                      1998LFa (11369)1452
                                        *K1=-3.03
                                        *B(2,2)=-2.98
--------------------------------------------------------------------------
Fe+++      gl  NaClO4 25°C 0.70M C                      1997BTb (11370)1453
                                        *K1=-2.75
Addtional method: Pt/Fe electrode.
--------------------------------------------------------------------------
Fe+++      gl  mixed  25°C  80%  C                     1997HMc (11371)1454
                                        *K1=-4.74
Medium: 80% w/w DMSO/H2O, 0.5 M NaClO4.
--------------------------------------------------------------------------
Fe+++      sol oth/un 20°C  0.7M C  I                   1996KNb (11372)1455
                                        *Kso(Fe(OH)3)=4.8-5.0
Medium: coastal seawater. For oceanic seawater, *Kso=4.4-4.6.
Method: dissolved Fe determined via 59Fe.
--------------------------------------------------------------------------
Fe+++      EMF NaCl   25°C 0.68M C                      1996SBa (11373)1456
                                        *K1=-2.754
                                        *B2</=-7
                                        B(FeH-1F)=1.39
Method: Pt/Fe(III),Fe(II) electrode, glass electrode, fluoride i.s.e.
Competition with fluoride. Medium: 0.68 m NaCl.
--------------------------------------------------------------------------
Fe+++      oth none   25°C  0.0  C  I                  1995MYa (11374)1457
                                        *K1=-2.20
                                        *B2=-5.54
                                        *B3=-11.80
                                        *B4=-21.6
By extrapolation of literature data using Pitzer equations.
At I=0.72 M, *K1=-2.62, *B2=-6.0, *B3=-12.5, *B4=-21.8.
--------------------------------------------------------------------------
Fe+++      sol oth/un 25°C 0.72M C                      1995MYa (11375)1458
                                        *B2=-6.0
                                        *B3=-12.5
                                        *Kso(Fe(OH)3)=4.5
By dissolution of Fe(OH)3 in seawater.
--------------------------------------------------------------------------
Fe+++      gl  KNO3   25°C 0.00  C  I                  1994DRa (11376)1459
                                        *K1=-2.18
                                        *B2=-5.6
                                        *B(2,2)=-2.92
                                        *B(12,34)=-48.9
Also data at I=0.1, 0.5, 1 and 3 M. At I=0.1 M, *K1=-2.57, *B2=-5.9,
```

*B(2,2)=-2.88, *B(12,34)=-55.2.

Fe+++ sp NaNO3 30°C 0.20M U M 1993BGc (11377)1460
*K(FeB(H2O)2)=-6.75
H6B:5,10,15,20-Tetrakis(2,6-dimethyl-3-sulfonatophenyl)porphirin.

Fe+++ kin NaCl 25°C 0.10M U 1992ALa (11378)1461
*K(FeA(PO4)(H2O))=-4.02
FeA=purple acid phosphatase.

Fe+++ gl NaClO4 25°C 0.50M U I 1992DEa (11379)1462
*K(Fe(EDTA)(H2O))=-7.2
At I=0.001 M NaClO4, *K=-7.8

Fe+++ gl NaNO3 25°C 0.50M C 1990DJa (11380)1463
*K1=-2.58
*B(2,2)=-3.15
*B2=-6.36
Additional method: spectrophotometry.

Fe+++ gl NaNO3 25°C 0.50M C 1990DJa (11381)1464
*K1=-2.58
*B2=-6.36
*B(2,2)=-3.15

Fe+++ gl NaClO4 25°C 0.0 C I 1990SVb (11382)1465
*K1=-1.98
*B2=-4.4
*B(2,2)=-2.86
*B2=-4.4(min) to -4.65(max). Data for I=0.51-3.50 m NaClO4, extrapolated to I=0 using SIT. At I=1.05 m, *K1=-2.80, *B2=-5.8, *B(2,2)=-2.83.

Fe+++ gl NaCl 25°C 3.0M C 1989MDa (11383)1466
*K1=-4.20
*B(2,2)=-4.64

Fe+++ sp oth/un 25°C 0.00 U I M 1989MMa (11384)1467
*K(FeApy=FeApy(OH)+H)=-9.8
*K(FeBpy=FeBpy(OH)+H)=-9.2
*K(FeCpy=FeCpy(OH)+H)=-10.2
*K(FeDpy+FeDpy(OH)+H)=-9.7
In sodium dodecyl sulphate micelles.py=pyridine. A=protoporphyrin IX; B=deuteroporph.IX dimethyl ester; C=mesoporph.IX di-ester; D=protoporp.IX di-ester

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Fe+++ gl NaNO3 25°C 1.00M C 1988KRb (11385)1468
*K1=-3.01
*B(2,2)=-3.09
*B(3,4)=-6.92

Fe+++ sp NaCl 25°C 0.15M U 1986EMa (11386)1469

```
                                        *K1=-3.05
                                        *B2=-6.31
-------------------------------------------------------------------------------
Fe+++      gl  NaClO4 25°C  1.0M C                      1986KBa (11387)1470
                                        *B(2,2)=-3.20
                                        *K1=-2.73
                                        *B2=-6.29
-------------------------------------------------------------------------------
Fe+++      gl  KNO3   25°C  1.0M C                      1986KBa (11388)1471
                                        *B(2,2)=-3.22
                                        *B(3,4)=-6.98
                                        *K1=-2.77
                                        *B2=-6.61
-------------------------------------------------------------------------------
Fe+++      gl  KCl    25°C  1.0M C                      1986KBa (11389)1472
                                        *B(2,2)=-4.09
                                        *B(3,4)=-7.58
                                        *K1=-3.21
                                        *B2=-6.73
-------------------------------------------------------------------------------
Fe+++      dis none   20°C  0.0  C                      1985IYc (11390)1473
                                        Kso=-39.13 (aged 12 mo)
                                        Kso=-39.74 (aged 36 mo)
Method: extraction using 8-hydroxyquinoline.
-------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 0.10M C  I                  1985MEb (11391)1474
                                        *K1=-2.52
Data for 0-2.0 M NaClO4. At I=0.20 M: *K1-2.64. At I=0.50 M: *K1=-2.69
Also data to 120 MPa.
-------------------------------------------------------------------------------
Fe+++      sp  NaNO3  20°C 0.20M C                      1982DVa (11392)1475
                                        *K1=-2.95
-------------------------------------------------------------------------------
Fe+++      nmr NaClO4 25°C 0.10M U  I                  1982YTa (11393)1476
                                        *K1=-2.72
                                        *B(2,2)=-3.92 (I=2.0)
-------------------------------------------------------------------------------
Fe+++      sp  NaCl   25°C 0.68M C                      1981BKe (11394)1477
                                        *K1=-2.71
                                        *B2=-7.43
-------------------------------------------------------------------------------
Fe+++      sol none   100°C  0.0  C T                  1980TLa (11395)1478
Magnetite solubility under H2. Ks(1/3Fe3O4(s)+H2O=Fe(OH)4+1/6H2+H)=-20.00
K(1/3Fe3O4(s)+1/6H2+5/3H2O=Fe(OH)3)=-11.05.  Data for 100-300 C.
-------------------------------------------------------------------------------
Fe+++      sol NaClO4 80°C    ?  U TI                  1980ZKb (11396)1479
                                        *K1=-1.00
80-200 C
-------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 0.68M U T                   1978BKb (11397)1480
```

```
                                        *K1=-2.72
                                        *B2=-8.60
------------------------------------------------------------------------------
Fe+++      gl  oth/un 25°C 2.00M U                      1978YKa (11398)1481
                                        *K1=-3.85
                                        *B(2,2)=-3.71
------------------------------------------------------------------------------
Fe+++      gl  KNO3   25°C 1.00M M                      1977CBa (11399)1482
                                        *K(FeAL+H2O=FeAL2+H)=-9.41
                                        K(2FeAL=(FeAL)2)=-2.6
H4A=EDTA
------------------------------------------------------------------------------
Fe+++      gl  NaClO4 25°C 2.67M U TI                   1977SPb (11400)1483
                                        *K1=-2.92
                                        *B2=-5.70
                                        *B(2,2)=-3.22
Data for a range of concentrations and T=33 - 80 C
------------------------------------------------------------------------------
Fe+++      gl  oth/un 25°C 0.20M U TI                   1977YKa (11401)1484
                                        K(Fe2(OH)2+2H)=3.46
                                        K=3.15  (50 C)
                                        K=3.41  (80 C)
------------------------------------------------------------------------------
Fe+++      gl  NaClO4 25°C 0.68M U  I     K1=7.28   B2=9.95   1976BKb (11402)1485
In 0.68 M NaNO3: K1=7.04, K2=2.64; in 0.68 M NaCl: K1=7.0, K2=2.76
In seawater: K1=6.80, K2=2.65
------------------------------------------------------------------------------
Fe+++      sol oth/un 25°C 0.72M C                      1976BKc (11403)1486
                                        *Kso(Fe(OH)3)=5.67
                                        *B3=-13.62
Solubility of Fe(OH)3 in seawater, S=36.2. Fe(OH)3 is freshly precipitated
------------------------------------------------------------------------------
Fe+++      gl  NaClO4 25°C 3.00M U                      1975CGb (11404)1487
                                        *K1=-3.1
                                        *B(2,2)=-2.8
                                        *B(12,34)=-46.1
------------------------------------------------------------------------------
Fe+++      ix  NaClO4 18°C  0.1M U       K1=11.66  B2=22.07  1975KIe (11405)1488
                                        K(Fe+3OH)=30.70
                                        K(2Fe+3OH)=24.56
                                        K(2Fe+OH)=22.07
------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C  0.1M U  I                   1975KSc (11406)1489
                                        *K1=-2.78
                                        K(2Fe+2H2O=Fe2(OH)2+2H)=-2.10
In D2O: *K1=-1.41, K=-2.15
------------------------------------------------------------------------------
Fe+++      sp  NaClO4  RT   1.0M C  I                   1975MIb (11407)1490
                                        *K1=-3.07
                                        *B(2,2)=-2.67
```

*K1=-2.43 (I=0.01 M), -2.67 (0.05 M), -2.84 (0.10 M), -2.94 (0.60 M).
*B(2,2)=-2.55 at I=3.0 M NaClO4.

Fe+++ oth mixed 25°C U 1974NKb (11408)1491
*B(2,1)=-1.5
*B(2,2)=-3.0
Medium: 0.4 M glycerol/H2O. Method: Mossbauer spectroscopy

Fe+++ sol NaClO4 25°C U 1973HMa (11409)1492
*K1=-2.51
*Kso=2.51
Medium: HClO4 at various concentrations;*Kso: gamma-FeOOH(s)+3H=Fe + 2H2O

Fe+++ sol NaClO4 26°C 1.00M U 1973KUa (11410)1493
B(FeA(OH))=3.5
B(Fe(A)2(OH)4)=44.6
A=triethanolamine

Fe+++ oth NaClO4 20°C 3.00M U 1973VRa (11411)1494
*B(2,2)=-1.9
Method: Mossbauer spectroscopy

Fe+++ kin NaClO4 18°C 1.00M U I 1972KHa (11412)1495
*K1=-2.9
In 1 M LiNO3, *K1=-2.6. In 1 M KNO3, *K1=-2.7

Fe+++ kin oth/un ? 0.40M U 1972KHa (11413)1496
K(FeCl2 + OH)=-1.9

Fe+++ oth none 50°C 0.00 U T 1972LEc (11414)1497
*K1=-1.63
*B2=-5.44
*B(2,2)=-2.2
*K1=-0.12,*B2=-0.95,*B(2,2)=-0.7(150 C).*K1=0.7,*B2=1.45,*B(2,2)=-0.5(250 C)
*K1=1.2, *B2=2.83, *B(2,2)=-0.8(350 C). Combination of thermodynamic data

---

Fe+++ sp alc/w 25°C 4% U I 1972WEa (11415)1498
*K1=-2.62
in 4% MeOH/H2O, 0.5 M NaClO4. In H2O, *K1=-2.66; 8% MeOH, -2.52;
12%, -2.48; 20%, -2.21; 25%, -2.06; 31%, -2.03

Fe+++ sp alc/w 20°C 20% U T H 1972WEa (11416)1499
*K1=-2.33
Medium: 20% MeOH/H2O, 0.5 M NaClO4. DH(*K1)=48.5 kJ mol-1.
*K1=-2.52(15.5 C), -2.08(30.5 C)

Fe+++ kin oth/un 25°C U 1971HRb (11417)1500
*K2=-5.1

Fe+++ sol none 25°C 0.00 U 1971MSj (11418)1501

```
                                        Kso(Fe(OH)3)=-42.70
--------------------------------------------------------------------------------
Fe+++      EMF NaClO4 25°C 1.00M U                      1971NPa (11419)1502
                                        *K1=-2.78
--------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 0.25M U                      1969BSa (11420)1503
                                        *K1=-2.66
                                        K(2FeOH=Fe2(OH)2)=2.57
--------------------------------------------------------------------------------
Fe+++      sp  NaClO4 20°C 0.15M U  I                   1969FOb (11421)1504
                                        *K1(Fe+H2O=FeOH+H)=-2.8
K(Fe + ClO4-)=0.3. In 0.15 M NaCl, *K1=-3.1. In 0.1 M CaCl2, K1=-3.0
--------------------------------------------------------------------------------
Fe+++      sp  NaClO4 23°C       U                      1969MWa (11422)1505
                                        K(Fe(CN)5NO+OH)=3.4
                                        K'=4.1
K': Fe(CN)5NO-- + 2OH=Fe(CN)5NO2---- + H2O. K(Fe(CN)5NO2 + H)=6.4
Polarography also used
--------------------------------------------------------------------------------
Fe+++      nmr oth/un 20°C 0.10M U        K1=11.3       1969VSa (11423)1506
Method: nmr
--------------------------------------------------------------------------------
Fe+++      cal NaClO4 25°C 3.00M U   H                  1968ASb (11424)1507
DH(*K1)=45.0 kJ mol-1,DS=96; DH(*B(2,2))=41.8,DS=84; DH(*B(3,4))=59.8,DS=92
--------------------------------------------------------------------------------
Fe+++      sol KNO3   25°C  var  U                      1968GSi (11425)1508
                                        Kso=-38.2(fresh)
                                        Kso=-39.2( 48 h)
--------------------------------------------------------------------------------
Fe+++      sp  oth/un 25°C 0.50M U                      1968MDd (11426)1509
                                        K(Fe(CN)5NO+L)=0.5 ?
                                        K(Fe(CN)5NO+2L)=4.50
--------------------------------------------------------------------------------
Fe+++      EMF NaClO4 23°C 3.00M U                      1968RRa (11427)1510
                                        *K1=-2.97
                                        *K2=-6.98
                                        *B(2,1)=-0.98
                                        *B(2,2)=-3.0
--------------------------------------------------------------------------------
Fe+++      EMF NaClO4 25°C 3.00M U T H                  1968ZLa (11428)1511
                                        *K1=-3.00
                                        *B(2,2)=-2.36
*K1=-2.73(35 C), -2.52(45 C), DH=42.6 kJ mol-1,DS=84.4 J K-1 mol-1
*B(2,2)=-2.17(35 C), -2.03(45 C), DH=46.6, DS=114
--------------------------------------------------------------------------------
Fe+++      sol NaClO4 25°C       U                      1967SBa (11429)1512
                                        *K1=-3.1 to 0
                                        *K2=-5 to -0.1
                                        *K3=-7.7 to -1.5
                                        *K4=-16.9 to -7.3
```

*K5=-15.6 to -11.4. Medium: HClO4 (variable). Polynuclear complexes ignored

---

Fe+++ sp KCl 15°C 1.00M U T H 1966SRa (11430)1513
K=6.62
K: Fe(CN)5NO-- + 2OH=Fe(CN)5NO2---- + H2O. K=6.18(25 C), 5.84(35 C).
DH=-67.7 kJ mol-1, DS=-109 J K-1 mol-1

Fe+++ gl oth/un 25°C var U 1965BBd (11431)1514
*K1=-2.90
*K2=-3.38

Fe+++ cal NaClO4 25°C 3.0M U H 1964PCa (11432)1515
DH(*K1)=61.5 kJ mol-1, DH(*B(2,2))=35.1, DH(*B(4,3))=73.6.

Fe+++ oth none 25°C 0.0 U 1963FSa (11433)1516
Kso=-42.7 (alpha-Fe2O3)
Kso(1/2Fe2O3(s)+1.5H2O=Fe+3OH); method:combination of thermodynamic data

---

Fe+++ sp KNO3 20°C 0.10M U 1963PLb (11434)1517
*K1=-2.63

Fe+++ sp alc/w 20°C 66% U 1963PLb (11435)1518
*K1=-1.77
Medium: 66% w/w MeOH/H2O, 0.1 M KNO3

Fe+++ gl NaClO4 25°C 3.0M U 1963SCg (11436)1519
*Kso=3.55 (amorphous inactive)
*Kso=ca.1.4 (alpha-FeOOH)
*Kso(Fe(OH)3(s)+3H=Fe+3H2O) for amorphous inactive Fe(OH)3, *Kso(FeOOH+
3H=Fe+2H2O) for alpha-FeOOH. Redox also used

Fe+++ cal NaClO4 25°C 3.0M U H 1962SCe (11437)1520
DH(*K1)=66.9 kJ mol-1,DS=167; DH(*B2)=71, DS=126; DH(*B(2,2)=36.4, DS=66.1

Fe+++ sp alc/w -59°C 80% U T H 1961BWa (11438)1521
*K1=-2.49
Medium: 80% MeOH. *K1=-2.45(-50 C), -2.04(-25 C), 1.49(0 C), -1.44(20 C)
DH=16.3 kJ mol-1

Fe+++ sp NaClO4 25°C 0.95M U M 1961JAa (11439)1522
K(Fe(CN)5A+OH=Fe(CN)5OH+A=3.18
A=SCN. When A=N3 K=2.30

Fe+++ sol NaClO4 20°C 3.0M U 1961LBa (11440)1523
Ks3=ca.-7 (apparent)
Ks4=-4.50 (2 hr ageing)
Ks4=-5.00 (96 hr ageing)
Ks3(Fe(OH)3(s)=Fe(OH)3); Ks4(Fe(OH)3(s)+OH=Fe(OH)4

Fe+++ oth oth/un 20°C var U 1961LBa (11441)1524

```
                                        K(Fe(OH)3(s)=Fe(OH)3) < -8.7
-------------------------------------------------------------------------------
Fe+++      sp  NaClO4 20°C  3.0M U                      1961MNd (11442)1525
                                        *B(2,2)=-1.17? to 1.06?
-------------------------------------------------------------------------------
Fe+++      sp  none   20°C  0.0  U   H                  1960RSa (11443)1526
                                        *K1=-2.30
DH(*K1)=41.4(18-35 C)
-------------------------------------------------------------------------------
Fe+++      sol oth/un 20°C  dil  U                      1959ASa (11444)1527
                                        K(Fe(OH)3(s)=Fe(OH)3)=-5.85
                                        B3=32.15
                                        Kso=-38
-------------------------------------------------------------------------------
Fe+++      con NaClO4 25°C  3.0M U                      1959BIa (11445)1528
                                        *K1=-3.05
                                        *B2=-6.31
                                        *B(2,2)=-2.96
                                        *B(3,4)=-5.77
-------------------------------------------------------------------------------
Fe+++      sol oth/un   ?   var  U                      1959FEb (11446)1529
                                        K(FeOOH(s)+H2O=Fe(OH)3)=-7
Kso=-37(amorphous), -42.5(alpha-Fe2O3), -44(alpha-FeOOH)
-------------------------------------------------------------------------------
Fe+++      gl  NaClO4 20°C  1.0M U                      1959PEb (11447)1530
                                        *K1=-2.74
                                        *B2=-6.05
                                        *B(2,2)=-2.85
*B(2,2): K(2Fe+2H2O=Fe2(OH)2+2H); method:also redox
-------------------------------------------------------------------------------
Fe+++      EMF none   25°C  0.0  U                      1958LAa (11448)1531
                                        Kso(Fe(OH)3)=-39.43
-------------------------------------------------------------------------------
Fe+++      oth NaClO4 20°C  3.0M U                      1957BRb (11449)1532
                                        *B(2,2)=-2.0
*K1=-3.0 and *K2=-3.3 assumed. Method: magnetic susceptibility.
-------------------------------------------------------------------------------
Fe+++      gl  NaClO4 25°C  3.0M U                      1957BSa (11450)1533
                                        Kso(Fe(OH)3)=-38.7
                                        *Kso=3.96
*Kso: K(Fe(OH)3(s)+3H=Fe+3H2O); method:also redox
-------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C  1.0M U  IH                  1957MIa (11451)1534
                                        *K1=-2.78
                                        *B(2,2)=-2.72
                                        K(2FeOH=Fe2(OH)2)=2.85
*B(2,2): K(2Fe+2H2O=Fe2(OH)2+2H); DH(*K1)=42.7 kJ mol-1, DH(*B(2,2))=51.0,
DH(Fe2(OH)2)=-34.3, DS(*K1)=88, DS(*B(2,2))=117, DS(Fe2(OH)2)=-59. Also I=0
-------------------------------------------------------------------------------
Fe+++      gl  none   ?25   0.0  U                      1957MOa (11452)1535
```

```
                                        Kso(Fe(OH)3)=-36.85
--------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 0.01M U T                    1957TMa (11453)1536
                                        *K1=-2.47
*K1=-2.81(15 C), -2.28(35 C)
--------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 0.02M U  I                   1957TMa (11454)1537
                                        *K1=-2.49
*K1=-2.41(I=0.004), -2.47(I=0.01)
--------------------------------------------------------------------------------
Fe+++      sp  NaClO4 15°C 0.50M U T                    1956CHb (11455)1538
                                        *K1=-2.93
*K1=-2.49(35 C)
--------------------------------------------------------------------------------
Fe+++      sol none   25°C  0.0  U                     1956GWb (11456)1539
                                        K(Fe(OH)3(s)+H)=-2.92
                                        K(Fe(OH)3(s)=Fe(OH)3)=-6.54
--------------------------------------------------------------------------------
Fe+++      oth NaClO4 25°C 3.12M U T H                  1955MSa (11457)1540
                                        *B(2,2)=-2.14
*B(2,2): K(2Fe+2H2O=Fe2(OH)2+2H); DH(*B(2,2))=41.0; *B(2,2)=-2.31(15 C)
-1.99(35 C), -1.79(45 C), -1.60(51 C); method:magnetic susceptibility
--------------------------------------------------------------------------------
Fe+++      sp  NaClO4 15°C 3.12M U T                    1955MSa (11458)1541
                                        *B(2,2)=-2.17
*B(2,2): K(2Fe+2H2O=Fe2(OH)2+2H)=-1.48(51 C)
--------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C  3.0M U  I                   1955MVa (11459)1542
                                        *K1=-2.89
                                        *B(2,2)=-2.58
                                        K(2FeOH=Fe2(OH)2)=3.20
*B(2,2): K(2Fe+H2O=Fe2(OH)2+2H). At I=0 *K1=-2.17, *B(2,2)=-2.88,
+K(Fe2(OH)2)=1.46
--------------------------------------------------------------------------------
Fe+++      EMF NaClO4 15°C 0.50M U                      1954CTa (11460)1543
                                        *K1=-2.93
--------------------------------------------------------------------------------
Fe+++      gl  NaClO4 25°C  3.0M U                      1953HEb (11461)1544
                                        *K1=-3.05
                                        *K2=-3.26
                                        *B(2,2)=-2.91
                                        K(2FeOH=Fe2(OH)2)=3.19
*B(2,2): K(2Fe+2H2O=Fe2(OH)2+2H)
--------------------------------------------------------------------------------
Fe+++      con oth/un 25°C  dil  U                      1953IYa (11462)1545
                                        *K1=-2.83
                                        *K2=-4.59
--------------------------------------------------------------------------------
Fe+++      sp  KCl    25°C 0.50M U    M                 1953KTa (11463)1546
                                        K(Fe(CN)5NO+2OH)=6.05
```

```
-------------------------------------------------------------------------------
Fe+++      sp  none   25°C  0.0  U                        1952SUb (11464)1547
                                        *K1=-1.3
-------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 0.50M U                        1952WTa (11465)1548
                                        *K1=-2.80
-------------------------------------------------------------------------------
Fe+++      kin KNO3   25°C 0.43M U                        1951BBb (11466)1549
                                        *K1=-2.58
-------------------------------------------------------------------------------
Fe+++      EMF oth/un 20°C  var  U                        1951QUa (11467)1550
                                        Kso(Fe(OH)3)=-37.4
-------------------------------------------------------------------------------
Fe+++      sp  none   25°C  0.0  U T                      1951SVa (11468)1551
                                        *K1=-2.19
*K1=-1.93(35 C)
-------------------------------------------------------------------------------
Fe+++      EMF none   18°C  0.0  U                        1950AFa (11469)1552
                                        Kso(Fe(OH)3)=-37.50
-------------------------------------------------------------------------------
Fe+++      gl  oth/un 20°C  var  U                        1949EPa (11470)1553
                                        Kso=-35.5 (fresh)
-------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C .046M U                        1949OSa (11471)1554
                                        *K1=-2.55
-------------------------------------------------------------------------------
Fe+++      gl  oth/un 16°C  var  U                        1945BEa (11472)1555
                                        Kso(Fe(OH)3)=ca.-37
-------------------------------------------------------------------------------
Fe+++      gl  none   25°C  0.0  U T H                    1944LIa (11473)1556
                                        *K1=-1.96
DH(*K1)=76.1; *K1=-2.18(20 C). Also by kinetics
-------------------------------------------------------------------------------
Fe+++      sp  none   20°C  0.0  U T H                    1942RSa (11474)1557
DH(*K1)=51.5 kJ mol-1, DS=130 J K-1 mol-1; DH(K1)=-5.0, DS=209; 20-50 C
-------------------------------------------------------------------------------
Fe+++      gl  none   25°C  0.0  U                        1938LJa (11475)1558
                                        *K1=-2.46
                                        *K2=-4.70
-------------------------------------------------------------------------------
Fe+++      gl  oth/un 25°C  dil  U                        1938OKa (11476)1559
                                        Kso(Fe(OH)3)=-36.35
-------------------------------------------------------------------------------
Fe+++      EMF oth/un 25°C 0.40M U TI                     1934BHa (11477)1560
                                        *K1=-2.74
At I=0 corr *K1=-2.22, at 35 C: *K1=-1.92
-------------------------------------------------------------------------------
Fe+++      gl  oth/un 18°C  var  U                        1933KAa (11478)1561
                                        Kso(Fe(OH)3)=-36.5
Redox also used. At I=0 corr Kso=-37.7 to -39.2
```

```
--------------------------------------------------------------------------------
Fe+++      kin none   15°C  0.0  U                        1928BVa (11479)1562
                                      *K1=-2.20
--------------------------------------------------------------------------------
Fe+++      sp  oth/un 15°C  var  U    M                   1928CSa (11480)1563
                                      K(Fe(CN)5NO+2OH)=3.87
--------------------------------------------------------------------------------
Fe+++      gl  oth/un 18°C  var  U                        1925BRa (11481)1564
                                      Kso(Fe(OH)3)=-37.7
--------------------------------------------------------------------------------
Fe+++      oth oth/un 18°C  dil  U                        1908MUa (11482)1565
                                      Kso(Fe(OH)3)=-35.96
method:combination of thermodynamic data
--------------------------------------------------------------------------------
Fe+++      con oth/un 25°C  var  U                        1906BJa (11483)1566
                                      *K1=-2.60
********************************************************************************
O2                       L    Oxygen           CAS 7782-44-7  (83)
Dioxygen, also oxide; O--, and superoxide, O2-
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      kin NaClO4 25°C  1.0M C                        1983BMd (12628)1567
                                      K(Fe(edta)+O2-)=6.90
Additional method: spectrophotometry. Ligand: superoxide.
Medium pH 10.4, carbonate buffer.
********************************************************************************
O2--                  H2L    Peroxide         CAS 7772-84-1  (2813)
Peroxide; -O.O-
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      kin alc/w  70°C  93%  U                        1967HSd (12662)1568
                                      K(Fe+2H2L)=4.86
Medium: 93% EtOH
--------------------------------------------------------------------------------
Fe+++      sp  NaClO4 22°C  var  U                        1963LRc (12663)1569
                                      K(Fe(OH)(H2O)5+H)=4.55
                                      K(Fe(OH)(H2O)4H2L+H)=2.96
--------------------------------------------------------------------------------
Fe+++      sp  NaClO4 20°C 0.10M U   H                    1951EUa (12664)1570
                                      K(Fe+HL)=9.30
DH(K)=7.5 kJ mol-1; DS=205 J K-1 mol-1
********************************************************************************
PO4---                H3L    Phosphate        CAS 7664-38-2  (176)
Phosphate;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      sp  NaCl   25°C 0.15M C                        2002AMa (13173)1571
```

B(FeHPO4)=19.89
B(FeH2PO4)=20.71
B(Fe(PO4)2)=35.66
B(FeH-2(PO4)2)=32.16
Medium: 0.15 M NaCl/HCl, pH 1.0-2.2. B(FeH-2(PO4)3)=49.35,
B(Fe2H-2(PO4)3)=53.12.

Fe+++ gl NaClO4 10°C 1.00M C 2000LMa (13174)1572
K(Fe2(OH)2+P)=5.90
K(Fe2(OH)2+Fe2P)=4.85
P: H3PO4+H2PO4-

Fe+++ EMF NaClO4 25°C 0 C I 1995CIa (13175)1573
K(Fe+H3L)=-0.2
K(Fe+H2L)=4.0
K(Fe+HL)=10
K(Fe+H3L+H2L)=4.69
K(Fe+2H2L)=7.43, K(Fe+H2L+HL)=11.84, K(Fe+H3L+2H2L)=8.36, K(Fe+3H2L)=9.82
At I=3.0 M: K(Fe+H3L=FeH2L+H)=1.52, K(Fe+H3L=FeHL+2H)=2.65 + others

---

Fe+++ EMF NaClO4 25°C 3.0M C 1992CIa (13176)1574
K(Fe+H3L)=1.41
K(Fe+H3L=FeH2L+H)=1.54
K(Fe+2H3L=FeH4L2+2H)=2.91
K(Fe+2H3L=FeH2L2+4H)=-0.16
K(3Fe+2H3L)=Fe3HL2+5H)7.25, K(3Fe+3H3L=Fe3H2L3+7H)=7.62, K(Fe3HL2+H3L)=2.50,
K(Fe3H4L3+H2L)=3.69, K(3Fe+3H3L=Fe3H4L3+5H)=9.78

Fe+++ gl NaClO4 25°C 3.0M C I 1992CIa (13177)1575
*Kso(Fe+H3L=FeL(am)+3H)=2.85
At I=0: *Kso=4.0, Kso(FeL(am)=Fe+L)=-25.7 by extrapolation using SIT

Fe+++ gl NaNO3 25°C 1.00M C K1=19.50 1988KRb (13178)1576
K(Fe+HL)=9.30

Fe+++ nmr oth/un 25°C ? U M 1985MGa (13179)1577
K(Fe(trien)+L)=1.79

Fe+++ sp NaClO4 25°C 2.50M C T H 1985WPa (13180)1578
K(Fe+H2L)=3.49
K(FeH2L+H2L)=4.9

Fe+++ gl NaClO4 25°C 3.00M C 1974CIa (13181)1579
K(Fe+H3L=FeH2L+H)=1.33
K(2Fe+2H3L=Fe2H3L2+3H)=5.77
K(3Fe+4H3L=Fe3H6L4+6H)=11.65

Fe+++ ix oth/un ? var U 1974FGf (13182)1580
K(Fe+HL)=7.80
K(Fe+2HL)=13.18

```
--------------------------------------------------------------------------------
Fe+++      sp  NaClO4 20°C 0.05M U                      1974FIa (13183)1581
                                       K(Fe(OH)+L)=17.3
                                       K(Fe(OH)L+HL)=6.7
                                       K(Fe+H2O+H2L=FeOHL+3H)=4.33
                                       K(FeOHL+H2L=Fe(OH)HL2+H)=0.45
--------------------------------------------------------------------------------
Fe+++      gl  NaClO4 25°C 0.10M U       K1=10.24       1974RMc (13184)1582
                                       Beff(Fe+L+NTA+fulv. acid)=23.3
                                       B(Fe+L+Citrate+fulvic)=22.15
--------------------------------------------------------------------------------
Fe+++      gl  NaClO4 25°C 0.10M U                      1974RMd (13185)1583
                                       K(Fe+HL)=8.95
                                       K(Fe+FeHL)=6.17
--------------------------------------------------------------------------------
Fe+++      vlt NaClO4 25°C 3.00M U                      1973SZa (13186)1584
                                       K(Fe+H2L)=3.61
                                       K(Fe+HL)=8.13
--------------------------------------------------------------------------------
Fe+++      sol none   25°C  0.0  U                     1972NRa (13187)1585
Kso=-26.43(strengite,FePO4(H2O)2). Estimated values: -28.7(10 C),-23.3(60 C)
--------------------------------------------------------------------------------
Fe+++      sp  oth/un   ?   var  U                     1966FCa (13188)1586
                                       K(2Fe+HL)=11.14
--------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 0.40M U                      1963GSb (13189)1587
                                       K(Fe+H2L)=3.45
                                       K(Fe+HL)=8.36
By EMF (redox) 3.49 and 8.23
--------------------------------------------------------------------------------
Fe+++      oth none   25°C  0.0  U                     1961EWa (13190)1588
                                       Kso(FeH2L(OH)2)=-30.02 amorp.
Kso=-34.56 (strengite, FePO4(H2O)2)
--------------------------------------------------------------------------------
Fe+++      sol none   25°C  0.0  U                     1957CJa (13191)1589
                                       Kso(Fe(H2L)(OH)2)=-34
--------------------------------------------------------------------------------
Fe+++      sp  none     ?   0.0  U                     1957DAa (13192)1590
                                       K(Fe+HL)=9.75
--------------------------------------------------------------------------------
Fe+++      vlt oth/un   ?   var  U                     1954RBa (13193)1591
                                       K(Fe+4H2L)=9.15
--------------------------------------------------------------------------------
Fe+++      sol oth/un 18°C  var  U                     1951ZHa (13194)1592
                                       Kso(FeL)=-21.89
--------------------------------------------------------------------------------
Fe+++      sp  NaNO3  30°C 0.67M U                      1942LKa (13195)1593
                                       K(Fe+HL)=9.35
********************************************************************************
P2O7----              H4L    Pyrophosphate    CAS 2466-09-3  (198)
```

Diphosphate; from (HO)2PO.O.PO(OH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaCl	25°C	0.10M	U			1994ALa	(13586)1594
							K(FeA(H2L)=FeA(H2L)OH+H)=-3.6		
							K(FeA(H2L)OH=FeA(HL)OH+H)=-5.3		

FeA=uteroferrin (=Fe(II)Fe(III)-purple acid phosphatase). Also data for L= PO4---, phenylphosphate, tripolyphosphate and ATP.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	kin	oth/un	25°C	0.0	U			1967SAb	(13587)1595
							K(Fe+H3L)=6.43		
							K(Fe+H2L)=6.97		
							B(Fe2L)=23.4		
Fe+++	sp	oth/un	20°C	0.0	U			1966ASc	(13588)1596
							K(Fe+H2L)=6.62		
							K(Fe+H3L)=6.05		
							K(Fe+2H3L)=11.25		
Fe+++	sp	KNO3	?	2.0M	U	I		1966VVa	(13589)1597
							K(FeSCN+H4L=FeH2L+SCN+2H)=1.17		
							K(Fe+H2L)=5.58		

K=1.26(I=1.5),1.30(I=1.0); K(Fe+H2L)=5.71(I=1.5),5.81(I=1.0),8.08(I=0 corr)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	none	20°C	0.0	U			1965SMj	(13590)1598
							K(Fe+2H2L)=12.38		

By EMF: K=12.07; by distribution: K=12.74

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sol	oth/un	?	var	U			1956YAa	(13591)1599
							K(Fe+2HL)=22.19		
							Kso(Fe4L3)=-22.55 ?		

****

P3O10----- H5L CAS 10380-08-2 (1001)

Tripolyphosphate; from (HO)2PO.O.PO(OH).O.PO(OH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaClO4	20°C	0.10M	U	I		1968ASd	(13858)1600
							K(Fe+H2L)=5.03		
							K(Fe+2HL)=18.85		

At I=0 corr: K(Fe+H2L)=7.03, K(Fe+2HL)=20.63

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaClO4	20°C	0.10M	U	I		1968SAc	(13859)1601
							K(Fe+H3L)=5.04		
							K(Fe+H2L)=5.10		

At I=0 corr: K(Fe+H3L)=6.37, K(Fe+H2L)=7.15

****

ReO4- HL Perrhenate (2581)

Rhenate(VII), Perrhenate;

```
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      dis oth/un 25°C 0.25M C T                    1984PUa (14099)1602
                                        Kout(Fe(phen)3+L)=2.73
Medium: Na2SO4;also for I=075 M K1out=2.56, I=0.5 M Kout=2.62
For I=0.5M,K1out=2.94(20 C), 3.03(15 C), 3.17(10 C); phen=phenantroline
********************************************************************************
S--                   H2L    Sulfide          CAS 7783-06-4  (705)
Sulfide;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      sp  oth/un   ?   dil  U    M                   1956DBb (14375)1603
                                        K(Fe(CN)5NO+L)=5.0
                                        K(Fe(CN05NOL+L)=0.3
--------------------------------------------------------------------------------
Fe+++      EMF oth/un   ?   var  U    M                   1928SPa (14376)1604
                                        K(Fe(CN)5NO+L)=ca.14
********************************************************************************
SCN-                   HL    Thiocyanate      CAS 463-56-9  (106)
Thiocyanate;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      sp  KCl    25°C 0.10M C T H                  2002PCb (14954)1605
                                        K(FeP+SCN)=2.07
                                        K(FeA+SCN)=-0.17
Data for 10-35 C. DH(FeP+L)=-30.1 kJ mol-1, DS=-61 J K-1 mol-1. DH(FeA+L)=
-5.9, DS=-23. P is sperm whale myoglobin; A is N-acetyl-microperoxidase
--------------------------------------------------------------------------------
Fe+++      oth NaClO4  RT  0.20M U        K1=2.74        1995ETa (14955)1606
Method: flow injection analysis with spectrophotometric detection. pH 1.35
--------------------------------------------------------------------------------
Fe+++      sp  KNO3   18°C 0.20M M  I     K1=2.26   B2=3.56   1995ZCa (14956)1607
In 50% propanone/H2O: K1=2.31, K2=1.28
--------------------------------------------------------------------------------
Fe+++      cal non-aq 25°C 100%  U   H  T K1=5.2    B2=9.3    1993OHa (14957)1608
                                        B3=12.5
                                        B4=14.9
                                        B5=16.4
                                        B6=17.1
Medium: N,N-dimethylacetamide, 0.4 M Et4NClO4. DH(K1)=1.8 kJ mol-1;
DH(B2)=-0.1; DH(B3)=-5.6; DH(B4)=-14.1; DH(B5)=-23.6; DH(B6)=-36.5
--------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C  1.0M C  IH    K1=2.11   B2= 3.34  1992OKb (14958)1609
                                        B3=3.82
By calorimetry: DH(K1)=-6 kJ mol-1; DH(B2)=-12, DH(B3)=-26.
Also data for 1.0 M NH4ClO4 medium.
--------------------------------------------------------------------------------
```

```
Fe+++      cal oth/un 25°C 0.10M C   H                  1989HKa (14959)1610
Medium: 0.10 M KSCN. DH(K1)=-4.4 kJ mol-1.
-------------------------------------------------------------------------
Fe+++      dis KCl    24°C 1.00M U   H  T K1=1.55   B2=2.50   1985BJa (14960)1611
                                         K3=0.6
                                         K4=-0.4
-------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 0.50M C  I     K1=2.18        1985MEa (14961)1612
                                         *K(Fe(SCN))=-1.20
At I=1.0 M: K1=2.13, *K(Fe(SCN))=-1.21. At I=1.5 M: K1=2.11,
*K(Fe(SCN))=-1.21. Also data to 120 MPa.
-------------------------------------------------------------------------
Fe+++      sp  non-aq 25°C 100%  U  IH    K1=4.07        1985PWa (14962)1613
Medium: dimethylsulphoxide. K1 extrapolated to I = 0.0
-------------------------------------------------------------------------
Fe+++      nmr NaClO4 25°C  3.0M C        K1=2.53   B2= 3.88  1983KNa (14963)1614
                                         K3=1.31
                                         K4=1.33
                                         K5=-0.32
-------------------------------------------------------------------------
Fe+++      sp  NaNO3  20°C 0.20M C        K1=2.32        1982DVa (14964)1615
-------------------------------------------------------------------------
Fe+++      kin NaClO4 25°C 0.13M U  I     K1=2.4         1978BWa (14965)1616
Medium: 0.1 M HClO4 + 0.005 M Fe(ClO4)3; also data for NaClO4, KClO4, NaNO3,
KNO3, Na2SO4 and K2SO4, I=0.05 - 0.3 M
-------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 0.20M C        K1=2.177       1976JOa (14966)1617
                                         K(FeOH+SCN)=-2.66
-------------------------------------------------------------------------
Fe+++      sp  alc/w  25°C  0.5M U TI     K1=2.53        1976VKd (14967)1618
                                         K1=2.26 (100%H2O)
In  I=0.5 M HNO3 in 50% v/v EtOH/H2H;
For I=0.5 M HNO3 in 50% v/v MeOH/H2H K1=2.67
-------------------------------------------------------------------------
Fe+++      sp  oth/un  rt  0.50M U        K1=2.17        1974CSa (14968)1619
-------------------------------------------------------------------------
Fe+++      sp  KNO3    rt  0.10M U    M                  1972KAg (14969)1620
                                         K(Fe(NTA)+L)=2.40
-------------------------------------------------------------------------
Fe+++      sp  non-aq 25°C 100%  U        K1=2.92   B2=4.91   1971WYa (14970)1621
Medium: DMSO, 0.1 M NaClO4
-------------------------------------------------------------------------
Fe+++      nmr oth/un   ?   var  U        K1=2.0         1970LSa (14971)1622
Method: esr
-------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C  1.0M U T H    K1=2.14        1969CEb (14972)1623
Medium: LiClO4; DH(K1)=-13.0 kJ mol-1. K1=2.33 (1.6 C), 2.21 (15.8 C)
-------------------------------------------------------------------------
Fe+++      sp  NaCl     ?  0.67M U        K1=1.0         1969MMa (14973)1624
-------------------------------------------------------------------------
```

```
Fe+++      sp  non-aq 25°C 100%  U        K1=3.07        1968LCb (14974)1625
Medium: Me2SO, 0.024 M NaNO3
--------------------------------------------------------------------------------
Fe+++      sp  NaClO4 20°C 1.20M U        K1=2.12        1968MAd (14975)1626
--------------------------------------------------------------------------------
Fe+++      EMF NaClO4 25°C  1.0M U        K1=2.10   B2=3.14   1968PCa (14976)1627
--------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C  3.0M U        K1=2.24        1967CSa (14977)1628
Medium: 3 M MgClO4,1.8 H+. By kinetics: K1=2.26
--------------------------------------------------------------------------------
Fe+++      sp  oth/un   ?   var  U    M                  1967LUd (14978)1629
                                       K(FeA+H+L)=-1.10
H4A=EDTA
--------------------------------------------------------------------------------
Fe+++      EMF oth/un 25°C  0.0  U    M                  1967NPf (14979)1630
                                       K(Fe(C5H5)2+L)=1.0
--------------------------------------------------------------------------------
Fe+++      sp  KNO3     ?   2.0M U  I     K1=1.96        1966VVa (14980)1631
K1=1.97(I=1.5), 2.00(I=1), 2.08(I=0.5), 2.11(I=0.4), 3.09(I=0 corr).
--------------------------------------------------------------------------------
Fe+++      dis NaClO4 25°C  3.0M U  I     K1=2.18   B2=3.60   1965MRb (14981)1632
                                       K3=1.40
                                       K4=1.30
                                       K5=-0.7
                                       Kd(FeL4(aq)=FeL4(Et2O))=1.5
Medium:3  MLiClO4),0.2 H+; K6=-0.09, B6=6.14; In 3M LiNO3,0.2 H+: K(M+FeL6)=
-1.1(M=Na+), -0.25(K+), -0.1(Rb+), 0.1(Cs+), -0.1(NH4+)
--------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C  3.0M U TIH    K1=2.19   B2=3.67   1965MRc (14982)1633
                                       K5=0.00
                                       K6=0.035
In LiNO3, I=6.1 M: K1=2.26, B2=3.93; I=1.1: 1.91, 2.99; I=0.1: 2.17, 3.60
I=6.1:DH(K1)=-9.2 kJ mol-1,DS=12 J K-1 mol-1; DH(B2)=24.2,DS=-4
--------------------------------------------------------------------------------
Fe+++      oth NaClO4 25°C 1.40M U        K1=2.35   B2=3.90   1964JMc (14983)1634
                                       K3=1.31
                                       K4=0.66
                                       K5=0.21
Method: paper electrophoresis.
--------------------------------------------------------------------------------
Fe+++      sp  NaClO4 20°C 0.60M U  I     K1=2.15        1964KSe (14984)1635
Medium: HClO4. K1=2.20(I=0.3), 2.27(I=0.15)
--------------------------------------------------------------------------------
Fe+++      sp  NaNO3  23°C  4.0M U        K1=2.1    B2=3.40   1964VMb (14985)1636
                                       K3=0.5
                                       K4=0
                                       K5=K6=0.1
                                       B6=3.7
I=0 corr: K1=3.1, K2=2.2, K3=0.9
--------------------------------------------------------------------------------
```

```
Fe+++      sp  none   22°C  0.0  U  I   T K1=3.11        1962VAa (14986)1637
Also K1 for I=0.3 to 5.0 M LiNO3, NaNO3, NaClO4; forI=0.3 to 2.5 M KNO3 and
I=0.5 to 7.7 M Mg(NO3)2
-------------------------------------------------------------------------------
Fe+++      EMF NaClO4 26°C 0.50M U  I M   K1=2.15   B2=3.27   1961YAa (14987)1638
                                          K(Fe+L+HF=FeLF+H)=3.14
By spectrophotometry K1=2.17(16 C), 2.15(27 C), 2.14(35 C), 2.13(45 C)
DH(K1)=-2.2 kJ mol-1, DS=50 J K-1 mol-1
-------------------------------------------------------------------------------
Fe+++      sp  oth/un   ?   var  U        K1=2.1          1960OHa (14988)1639
-------------------------------------------------------------------------------
Fe+++      vlt NaClO4   ?  0.50M U        K1=1.8          1960TRa (14989)1640
-------------------------------------------------------------------------------
Fe+++      sp  mixed  20°C  20%  U  I     K1=2.68         1959BMc (14990)1641
Medium: 20% w/w acetone/H2O, 0.025 M H. K1=2.82(40%),3.5(80%). With 0.1 M H:
K1=2.43(20%), 2.57(40%), 3.2(80%)
-------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 0.40M U   H    K1=2.16         1958BCb (14991)1642
DH(K1)=-6.7 kJ mol-1.
-------------------------------------------------------------------------------
Fe+++      EMF NaClO4 20°C 0.65M U  I     K1=2.12   B2=3.1    1958PEc (14992)1643
Medium: HClO4. By spectrophotometry, 0.56 M HClO4: K1=2.16, K2=1.15.
At I=0 corr: K1=3.04, K2=1.60
-------------------------------------------------------------------------------
Fe+++      sp  oth/un 20°C 0.08M U  I     K1=2.44         1957YTa (14993)1644
Medium: Mg(NO3)2 at I=0.08. K1=2.13(I=0.5), 2.03(I=1.0), 1.99(1.5 to 3),2.07
(I=4.8), 3.1(0 corr); Also K1 for KNO3, Mg(ClO4)2 and Al(NO3)3 media
-------------------------------------------------------------------------------
Fe+++      EMF NaClO4 25°C 0.50M U  IH  T K1=2.14   B2=3.45   1956LAa (14994)1645
DH(K1)=-6.3 kJ mol-1, DH(K2)=-1.3; data also for 0 corr:K1=3.03, DH(K1)=-6.3
DS=36.4 J K-1 mol-1
-------------------------------------------------------------------------------
Fe+++      sp  oth/un 12°C  var  U        K1=2.30         1955ISa (14995)1646
-------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 1.20M U T    T K1=2.11   B2=3.30   1955LRa (14996)1647
                                          K3=0
                                          *K1(FeL)=-4.2
K1=2.19(5 C), 2.14(15 C), 2.09(35 C), 2.07(45 C). AT I=0 corr: K1=3.03
-------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 1.20M U    M                 1955LRa (14997)1648
                                          B(FeL(SO4))=4.08
                                          B(FeL(SO4)2)=5.69
                                          B(FeLCl)=2.42
                                          B(FeLCl2)=2.08
B(FeLBr)=1.32
-------------------------------------------------------------------------------
Fe+++      sp  oth/un   ?   var  U        K1=2.62         1954JMb (14998)1649
-------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 1.28M U   H  T K1=2.06   B2=3.5    1953BDb (14999)1650
Medium: HClO4. K2 by kinetics. At I=0 corr K1=2.94. DH(K1)=-6.7 kJ mol-1,
```

DS=33 J K-1 mol-1

Fe+++ dis NaClO4 18°C 1.80M U I T K1=2.09 B2=3.84 1951MMa (15000)1651
K3 < -0.74
K4 > 1.80
K5=-0.70
K6=-1.03

In 1.8 M KNO3: K1=1.96, K2=2.02, K3=<-0.41, K4=>-0.14, K5=-1.57, K6=-1.51
In 1.0 M KNO3: K1=1.99. Also other media

Fe+++ sp NaClO4 25°C 0.56M U K1=2.17 1951SSa (15001)1652

Fe+++ sp oth/un rt 0.60M U K1=1.77 1950HMa (15002)1653
Medium: 0.6 M K2SO4

Fe+++ sp alc/w ? 90% U K1=4.70 1947BKa (15003)1654
Medium: 90% w/w EtOH/H2O

Fe+++ sp NaClO4 rt 0.50M U I K1=2.14 1947FOa (15004)1655
Medium: HClO4. In 0.128 M HClO4 K1=2.37. At I=0 corr K1=2.95

Fe+++ sp oth/un ? var U K1=2.3 1946BAa (15005)1656

Fe+++ dis oth/un ? ? U 1944MOa (15006)1657
K4=-2.0

Fe+++ sp NaCl ? 0.66M U K1=1.48 1941BFa (15007)1658

Fe+++ sp NaClO4 ? 1.0M U K1=2.10 1941EBa (15008)1659

Fe+++ sp oth/un ? var U K1=2.29 B2=3.87 1937MOa (15009)1660
K3=-0.22

****

SO3-- H2L Sulfite CAS 7782-99-2 (801)
Sulfite;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo

---

Fe+++ sp NaClO4 10°C 1.00M C 1998LFa (15452)1661
K(Fe2(OH)2+HSO3)=3.37

Fe+++ sp NaClO4 25°C 0.50M U 1992DEa (15453)1662
K(Fe(EDTA)(H2O)+L)=0.79

Fe+++ sp NaCl 25°C 1.0M U T 1972ASa (15454)1663
K(Fe(CN)5NO+Na+L)=-0.35
At 10 C: K=-0.19; 40 C: -0.54

Fe+++ sp NaClO4 25°C 1.0M U 1971CAb (15455)1664
*K1<=-0.4

```
-------------------------------------------------------------------------------
Fe+++      sp  oth/un   ?  0.40M U    M                  1956DBb (15456)1665
                                      K(Fe(CN)5NO+L)1.17
K2?=-0.77 reactants not defined
*******************************************************************************
SO4--                 H2L    Sulfate          CAS 7664-93-9  (15)
Sulfate;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe+++      gl  NaClO4 25°C  3.0M C  I     K1=1.65   B2= 2.68  2002CTa (16187)1666
                                      B(FeHL)=2.36
                                      B(FeH-1L)=-0.49
                                      B(Fe3H-6L3)=-5.8
At I=0, extrapolation using SIT: K1=3.82, B2=5.75, B(FeHL)=3.68
By spectrophotomertry, I=3.0 M: K1=1.55, B2=2.77, B(FeHL)=2.39
-------------------------------------------------------------------------------
Fe+++      sol none   25°C  0.0  M T H                  1996BPc (16188)1667
                                      Kso(KFe3(SO4)2(OH)6)=-11.0
Method: solubility of jarosite, KFe3(SO4)2(OH)6, at pH 1.5-3.0 (HClO4)
and 4-35 C. DH(Kso)=-45 kJ mol-1, DS(Kso)=-350 J K-1 mol-1.
-------------------------------------------------------------------------------
Fe+++      oth none   25°C  0.0  C  I     K1=4.27   B2= 6.11  1995MYa (16189)1668
By extrapolation of literature data using Pitzer equations.
At I=0.72 M, K1=2.58, B2=3.45.
-------------------------------------------------------------------------------
Fe+++      sp  NaClO4 20°C 0.40M U        K1=2.29        1988FWa (16190)1669
-------------------------------------------------------------------------------
Fe+++      gl  NaNO3  25°C 1.00M C        K1=1.53        1988KRb (16191)1670
                                      B(-4,3,1)=-4.34
B(p,q,r): pH+qM+rL=HpMqLr.
-------------------------------------------------------------------------------
Fe+++      oth none    0°C  0.0  U        K1=4.12        1987BSb (16192)1671
Calculated values
-------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 5.00M U   H                  1977AHa (16193)1672
                                      K1out=2.32
DH=16.4 kJ mol-1, DS=99 J K-1 mol-1
-------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 2.67M U T      K1=1.924       1977SPb (16194)1673
K1=2.389(55 C), 3.021(80 C)
-------------------------------------------------------------------------------
Fe+++      gl  oth/un 25°C  0.0  U TI     K1=4.74        1975NTa (16195)1674
I=0(corr); K1=5.18(50 C),6.13(100 C),7.38(150 C).  At 30 C: K1=3.30(I=0.12),
2.75(I=0.50), 1.83(I=2.57). 150 C: 4.63(I=0.25), 4.39(I=0.91), 4.15(I=1.82)
-------------------------------------------------------------------------------
Fe+++      EMF NaClO4 25°C  3.0M U        K1=1.93   B2=2.11   1973NPb (16196)1675
                                      K(Fe+HL)=0.00
-------------------------------------------------------------------------------
Fe+++      vlt NaClO4 25°C 0.06M U  I     K1=2.94        1969SGg (16197)1676
```

Medium: HClO4. At I=0, K1=4.04

Fe+++ EMF NaClO4 25°C 3.0M U T K1=2.23 B2=3.26 1969ZLa (16198)1677
K(Fe2(OH)2+L)=2.51
K(Fe2(OH)2+2L)=3.04
Medium:(Na,H)ClO4. At 35 C: K1=2.40, B2=3.31, K(Fe2(OH)2+L)=2.70,
K(Fe2(OH)2+2L)=3.83. At 45 C: 2.49, 3.34, 2.81, 3.98 respectively

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Fe+++ sp NaClO4 20°C 1.20M U K1=2.06 1967MAh (16199)1678
B(FeLBr)=2.50

Fe+++ sp NaClO4 25°C 1.0M U H K1=2.24 B2=3.18 1963BLa (16200)1679
DH(K1)=-21.5, DH(K2)=60.2 kJ mol-1

Fe+++ sp NaClO4 25°C 0.50M U T H K1=2.30 1963WIa (16201)1680
DH(K1)=26 kJ mol-1, DS=163 J K-1 mol-1. K1=1.93(1 C), 2.11(11 C), 2.30(22 C)
Also by redox and kinetics

Fe+++ sp NaClO4 25°C 0.50M U T K1=2.31 1962DSa (16202)1681
K1=1.98(1.4 C), 2.17(15 C), 2.45(35 C)

Fe+++ sp NaClO4 30°C 1.0M U TIH K1=1.93 1960KUa (16203)1682
Medium: HClO4. DH(K1)=17.6 kJ mol-1, DS=133 J K-1 mol-1. At 20 C: K1=1.83,
K1=1.98(I=0.69), 2.12(I=0.4), 2.39(I=0.2), 2.62(I=0.1), 3.85(I=0)

Fe+++ sp KNO3 20°C 0.10M U I K1=2.66 1959BMc (16204)1683
Medium: HNO3. Also data in Me2CO/H2O mixtures

Fe+++ kin mixed 25°C 39% U K1=5.06 1959JTa (16205)1684
Medium: 38.5 mole % H2O2, x units

Fe+++ EMF oth/un 25°C 1.0M U I K1=2.02 B2=2.32 1959MAd (16206)1685
K3=-0.3
Medium: Na2SO4. Ai I=0 corr. K1=4.04, K2=1.30. Also at I=0.25, 0.75, 1.53

Fe+++ sp NaClO4 25°C 1.20M U M K1=2.23 B2=4.23 1955LRa (16207)1686
K(Fe+HL)=0.78
K(Fe+L+HL)=2.58
B(FeL(SCN))=4.08
B(FeL2(SCN))=5.69

Fe+++ sp NaClO4 19°C 0.15M U I K1=2.36 1954SYa (16208)1687
At I=0 corr. K1=3.85

Fe+++ ix NaClO4 28°C 1.0M U K1=1.98 B2=2.95 1953WDa (16209)1688
Medium: HClO4. By spec. K1=2.03, K2=0.97

Fe+++ kin NaClO4 18°C .066M U I K1=3.02 1952SYa (16210)1689
At I=0 corr. K1=4.18

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S2O3-- H2L Thiosulfate CAS 73686-28-7 (177)
Thiosulfate;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	sp	KNO3	20°C	0.10M	C		K1=2.09	B2=3.07	1997KRa	(16844)1690
							K3=0.62			
Medium: 0.1 M HNO3										
Fe+++	sp	KNO3	20°C	0.10M	U		K1=2.09	B2=3.07	1997KRa	(16845)1691
							K3=0.62			
Data also for I=0.01 and 1.0										
Fe+++	sp	NaClO4	?	0.05M	U		K1=11.98?		1964TVa	(16846)1692
Medium: HClO4										
Fe+++	sp	oth/un	?	var	U		K1=2.55		1959BGg	(16847)1693
Fe+++	sp	oth/un	25°C	0.12M	U		K1=1.98		1957MNa	(16848)1694
Fe+++	sp	KNO3	25°C	0.47M	U	H	K1=2.10		1954PAb	(16849)1695
DH(K1)=41.0 kJ mol-1, DS=178 J K-1 mol-1. K1=1.59(6.1 C). At I=0 corr. 6.1 C K1=3.25, DH(K1)=37.2, DS=197										
Fe+++	sp	oth/un	25°C	var	U		K1=2.65		1948HBa	(16850)1696
Fe+++	EMF	NaNO3	18°C	1.05M	U		K1=1.18		1930SCa	(16851)1697

SeO3-- H2L Selenite CAS 7783-00-8 (2391)
Selenite;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	sol	none	23°C	0	M		K1=11.15		1995RFa	(17058)1698
Ks(Fe2(SeO3)3.6H2O(s)=2Fe+3SeO3)=-41.58										
Fe+++	sp	NaClO4	40°C	1.0M	U	T H			1965HIb	(17059)1699
							K(Fe+H2L=FeHL+H)=0.61			
Medium: Na,HClO4. K=0.51(20 C), 0.54(25 C), 0.56(30 C). DH=16.7 kJ mol-1										
Fe+++	sol	oth/un	20°C	var	U				1957CTa	(17060)1700
							Kso(Fe2L3)=-30.7			

SiO3-- H2L Silicate CAS 7699-41-4 (747)
Silicate; SiO2(OH)2--

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	sol	none	22°C	0.0	C				1979REa	(17210)1701
							K(Fe+H3SiO4)=9.8			

Analysis by atomic absorption spectrometry.

Fe+++	sp	NaClO4	25°C	0.10M	U	H		1973OOb	(17211)1702
							*K1=-0.6		

*DH1=15.8 kJ mol-1, *DS1=41.0. By polarography: *K1=-0.5

Fe+++	sp	NaClO4	25°C	0.10M	U			1965WSa	(17212)1703
							K(Fe+H2L=H+FeHL)=-0.24		
							K(Fe+HL)=9.26		

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WO4-- H2L Tungstate CAS 13783-36-3 (445)

Tungstate;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaCl	?	1.00M	U	M		1973TSa	(17439)1704
							K(Fe+A)=17.8		
							K(Fe+Fe(II)A=Fe(II)+FeA)=4.2		
							K(FeAOH+H)=5.2		
							K'=1.6		

K': 2FeAO(7-) + 2H = (FeA)2O(12-) + H2O. A=SiW11O39(8-)

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CH2O2 HL Formic acid CAS 64-18-6 (37)

Methanoic acid; H.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	oth	oth/un	RT	1.0M	C			1982MDc	(17606)1705
							B6=2.83		

Method: paper electrophoresis. Medium: 0.5 M NaNO3/0.5 M formate buffer, pH 3.75.

Fe+++	ix	NaClO4	?	1.00M	U		K1=1.70	B2=3.70	1973PZa	(17607)1706

Fe+++	EMF	NaClO4	?	1.00M	U	M	K1=1.49	B2=3.4	1972PZa	(17608)1707
							K(3Fe+6L=Fe3(OH)2L6+2H)=13.54			

Fe+++	ix	oth/un	25°C	1.0M	U		K1=1.85	B2=3.61	1962TSa	(17609)1708
							B3=3.95			
							B4=5.4			

Fe+++	EMF	NaClO4	20°C	1.0M	U		K1=3.1		1959PEb	(17610)1709

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CH4N2O L Urea CAS 57-13-6 (2018)

Carbamide, Urea; (H2N)2CO

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	vlt	NaClO4	25°C	0.20M	U		K1=0.78	B2=1.04	1985MCc	(17716)1710
							K3=-0.046			

```
                                        K4=0.52
                                        K5=-0.52
                                        K6=-1.0
-------------------------------------------------------------------------
Fe+++      vlt NaClO4 20°C 0.20M U       K1=0.78   B2=1.04   1980MCa (17717)1711
                                        B3=1.00
                                        B4=1.52
                                        B5=0.95
                                        B6=-0.3
-------------------------------------------------------------------------
Fe+++      sp  NaClO4 20°C 1.20M U    M  K1=0.74   B2=0.98   1970MAe (17718)1712
                                        B3=0.92
                                        B4=0.76
                                        B5=0.44
                                        B6=0.02
B(FeL4(SO4)2)=3.21, B(FeL5(SO4))=1.31
*************************************************************************
CH4N2S                  L    Thiourea         CAS 62-56-6  (51)
Thiocarbamide, Thiourea; (H2N)2CS
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      sp  oth/un 20°C 1.20M U       B2=8.44        1968MAb (17824)1713
-------------------------------------------------------------------------
Fe+++      sp  oth/un 20°C 1.20M U    M                 1968MAb (17825)1714
                                        B(FeL(SO4))=6.63
-------------------------------------------------------------------------
Fe+++      sp  NaClO4 20°C 1.20M U    M  B2=8.4         1968MAd (17826)1715
                                        B(FeLSO4)=6.6
                                        B(Fe(SCN)L)=5.55
*************************************************************************
CH4O                    L    Methyl alcohol   CAS 67-56-1  (597)
Methanol; CH3.OH
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      oth non-aq 21°C 100%  U    M                 1980MKa (17879)1716
                                        K(TPPFeCl+4L)=-3.2
Medium: CH2Cl2. TTPFeCl=Tetraphenylporphyrin ferric chloride.
For octaethylporphyrin ferric chloride, K=-2.3
*************************************************************************
CH5O3P                H2L                    CAS 13590-71-1  (1752)
Methylphosphonic acid; CH3.PO3H2
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      gl  KCl    25°C 0.10M U       K1=9.05        1986NIa (18128)1717
                                        K(Fe+L=FeL(OH)+H)=5.86
                                        K(Fe+L=FeL(OH)2+2H)=-1.08
*************************************************************************
```

CH6O6P2 H4L Medronic acid CAS 1984-15-2 (2384)
Methanediphosphonic acid; CH2(PO3H2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	gl	KCl	25°C	0.10M	U		K1=19.9	B2=26.6	1967KLa (18282)	1718

****

C2HO2Cl3 HL Trichloroacetic CAS 76-03-9 (1205)
Trichloroethanoic acid; Cl3C.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	sp	alc/w	25°C	100%	U		K1=4.09		1971SSg (18332)	1719
Fe+++	EMF	NaClO4	25°C	3.00M	U		K1=0.85	B2=1.08	1970PTb (18333)	1720

****

C2H2O2Cl2 HL CAS 79-43-6 (1282)
Dichloroethanoic acid; Cl2CH.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	sp	oth/un	25°C	1.0M	C		K1=0.73		1978PTa (18394)	1721

Medium: 1.0 M Fe(ClO4)3/HClO4, pH 1.0

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	sp	alc/w	25°C	100%	U		K1=4.06		1973LRa (18395)	1722
Fe+++	gl	NaClO4	20°C	1.00M	U		K1=1.9	B2=3.7	1969PJc (18396)	1723

****

C2H2O3 HL Glyoxylic acid CAS 298-12-4 (1142)
Glyoxylic acid; OHC.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	gl	KCl	25°C	0.10M	U		K1=13.9	B2=26.10	1975SDa (18421)	1724

****

C2H2O4 H2L Oxalic acid CAS 144-62-7 (24)
Ethanedioic acid; (COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	cal	NaNO3	25°C	0.5M	U		K1=7.53	B2=13.64	2000KPb (18886)	1725
							K3=4.85			

DH1=+3.43; DH2=-0.1; DH3=-3.07 kJ/mol

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	gl	non-aq	25°C	100%	C		K1=13.16	B2=23.66	1991MCa (18887)	1726
							B3=30.74			

Medium: DMSO, 0.10 M n-Bu4NClO4.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	vlt	NaClO4	30°C	1.0M	C		K1=7.75		1988GMb (18888)	1727

Method: polarography. Medium pH 5.0.

```
--------------------------------------------------------------------------------
Fe+++      EMF NaClO4 25°C 2.00M C        K1=7.58   B2=13.81  1977DEa (18889)1728
                                          B3=18.60
--------------------------------------------------------------------------------
Fe+++      vlt NaClO4 25°C 1.00M U        K1=7.56        1970GMi (18890)1729
Method : amperometry
--------------------------------------------------------------------------------
Fe+++      EMF NaClO4 25°C 0.50M U        K1=7.53   B2=13.64  1968DMc (18891)1730
                                          B3=18.49
Method: platinum electrode. Medium: LiClO4
--------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C  1.0M U  I     K1=7.59        1966MSb (18892)1731
                                          K(FeOH+HL)=6.83
I=3: K1=7.74
--------------------------------------------------------------------------------
Fe+++      sp  oth/un 25°C 0.50M U T      K1=7.39        1965BSa (18893)1732
                                          K(Fe+HL)=4.35
K1=7.75(5 C), 7.70(15 C), K=4.10(5 C), 4.34(15 C)
--------------------------------------------------------------------------------
Fe+++      ISE oth/un 25°C  0.0  U                       1965PVa (18894)1733
                                          K3=4.27
--------------------------------------------------------------------------------
Fe+++      ix  oth/un   ?  0.50M U        K1=7.54   B2=14.59  1963PBb (18895)1734
                                          B3=20.0
--------------------------------------------------------------------------------
Fe+++      dis NaClO4 20°C 0.10M U                       1963STc (18896)1735
                                          B3=20.46
--------------------------------------------------------------------------------
Fe+++      gl  KNO3   32°C  1.0M U                      1957DSa (18897)1736
                                          K3=4.77
--------------------------------------------------------------------------------
Fe+++      sp  oth/un   ?     ?  U        K1=9.84   B2=16.04  1956BDb (18898)1737
                                          K3=3.70
--------------------------------------------------------------------------------
Fe+++      oth oth/un   ?     ?  U        K1=4.64        1956VPa (18899)1738
                                          B3=19.6
--------------------------------------------------------------------------------
Fe+++      vlt NaClO4 25°C 0.50M U                       1954SLb (18900)1739
                                          B3=17.96
--------------------------------------------------------------------------------
Fe+++      gl  oth/un   ?   0.0  U        K1=9.4    B2=16.2   1949LAa (18901)1740
                                          K3=4
--------------------------------------------------------------------------------
Fe+++      vlt oth/un   ?     ?  U                       1941LIa (18902)1741
                                          B3=21.6
--------------------------------------------------------------------------------
Fe+++      vlt oth/un   ?     ?  U                       1941TOa (18903)1742
                                          B3=23.9
********************************************************************************
C2H3N3                 HL    1,2,4-Triazole   CAS 288-88-0  (381)
```

1,2,4-Triazole; cyclo(-NH.N:CH.N:CH-) C2H3N3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	alc/w	25°C	80%	U			1994HPa (19234)	1743
							K(PeP(H2O)+HL=FePHL+H2O)=2.9		
							K(FeP(H2O)+L=FePH-1L)=5.3		

Medium: 80% v/v MeOH/H2O. FeP: Fe porphyrin microperoxidase-8.

****

C2H3O2Br HL Bromoacetic acd CAS 79-08-3 (1309)
Bromoethanoic acid; Br.CH2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	alc/w	25°C	100%	U		K1=3.89	1971SSg (19278)	1744

Medium: EtOH

****

C2H3O2Cl HL Chloroacetic CAS 79-11-8 (34)
Chloroethanoic acid; ClCH2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	EMF	NaClO4	25°C	1.00M	U		K1=1.93	1971NPa (19362)	1745
							B(2Fe+4L=Fe2L4)=8.95		
							K(Fe+FeOH+4L=Fe2(OH)L4)=6.70		
Fe+++	sp	alc/w	25°C	100%	U		K1=3.89	1971SSg (19363)	1746
Fe+++	EMF	NaClO4	20°C	1.0M	U		K1=2.1	1959PEb (19364)	1747

****

C2H3O2F HL Fluoroacetic ac CAS 144-49-0 (4222)
Fluoroethanoic acid; F.CH2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	NaClO4	20°C	1.00M	U		K1=2.2 B2=3.4	1970KPc (19402)	1748
							B(3Fe+2OH+6L)=9.2		

****

C2H4NF3 L CAS 753-90-2 (6297)
Trifluoroethylamine; CF3.CH2.NH2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	alc/w	25°C	80%	U	M		1993BHa (19434)	1749
							K(FeP+L)=1.3		

Medium: 80%MeOH/H2O. P: porphyrin microperoxidase-8. Also data for L=NH2CH2CN (1.7), NH2CH2CH2CN (2.9), NH2CH2CH2Br (3.2), benzylamine (4.65).

****

C2H4NO2Cl HL CAS 10335-72-5 (2588)
N-(Chloroacetyl)hydroxylamine; ClCH2.CO.NHOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	EMF	NaClO4	25°C	1.00M	U		K1=8.93	1979SRb (19437)	1750
Fe+++	EMF	NaClO4	25°C	1.00M	U		K1=8.93 B2=17.37 K3=7.08	1978SSe (19438)	1751

****

C2H4N2O4 H2L CAS 1687-60-1 (2969)
Oxaldihydroxamic acid; (CO.NH.OH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	oth/un	25°C	0.10M	U		K1=3.44	1957MJa (19447)	1752

****

C2H4O2 HL Acetic acid CAS 64-19-7 (36)
Ethanoic acid; CH3.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	NaClO4	25°C	3.0M	C	I	B*(111)=-1.85; B*(2,2,0)=-2.88 B*(1,2,2)=-3.43; B*(340)=-6.14 B*(363)=-5.66; B*350)=-8.44 B*(3,8,6)=-8.016	2001CTb (19960)	1753

At I=0 (by SIT): B*(1,1,1)=-0.87, B*(1,2,2)=-1.45,B*(3,6,3)=-2.85
B*(pqr):pFe+(q-r)H2O+rHL=Fep(OH)(q-r)Lr

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	NaCl	25°C	3.0M	C		B(FeH-1L)=0.26	1989MDa (19961)	1754
Fe+++	nmr	oth/un	37°C	1.00M	U		K1=2.6 B(Fe2L2)=9.3 B(Fe3L6)=22.8	1982KYb (19962)	1755
Fe+++	sp	alc/w	25°C	100%	U		K1=4.29	1971SSg (19963)	1756
Fe+++	vlt	KNO3	25°C	1.00M	U		K1=3.2 B2=6.3 B3=8.2	1970SRa (19964)	1757
Fe+++	EMF	NaClO4	25°C	3.00M	U		K1=3.23 B2=6.22 B(2Fe+6L=Fe3(OH)2L6+2H)=22.05 B(3Fe+2L=Fe3(OH)3L2+3H)=5.87 B(7Fe+6L=Fe7(OH)9L6+9H)=17.26	1969CNa (19965)	1758
Fe+++	sp	NaClO4	25°C	0.40M	U		K1=2.63	1968DMc (19966)	1759

Medium: LiClO4.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	non-aq	25°C	100%	U		K3=6.17	1964KLa (19967)	1760

Medium: ethanoic acid

Fe+++ EMF KCl 25°C 0.50M U B2=10.32 1961NPa (19968)1761

Medium: HCl

Fe+++ gl oth/un 20°C 0.10M U K1=3.38 B2=6.1 1961SPa (19969)1762
B3=8.7

18-22 C. By spectrophotometry:K1=3.2,B2=6.5,B3=8.3. At I=0.01: K2=2.8

Fe+++ EMF NaClO4 20°C 1.0M U K1=3.2 1959PEd (19970)1763

****

C2H4O2S H2L Thioglycolic CAS 68-11-1 (596)

Mercaptoethanoic acid; HS.CH2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	kin	NaClO4	25°C	0.50M	C		K1=13.49 K(Fe+H2L=FeL+2H)=0.09	1983BMc (20320)1764	

Method: spectrophotometry.

****

C2H4O3 HL Glycolic acid CAS 79-14-1 (33)

2-Hydroxyethanoic acid; HO.CH2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	none	30°C	0.0	U		K1eff=3.90	1976GCa (20539)1765	

Measured at pH 3.0

Fe+++	EMF	NaClO4	20°C	1.00M	U	T	K1=2.5 B(Fe3(OH)2L6)=17.4	1974KRb (20540)1766	
Fe+++	sp	oth/un	25°C	0.10M	U		B2=7.91	1972NBb (20541)1767	

pH 2.5-4

Fe+++	sp	oth/un	?	0.10M	U		K1=4.7	1952BEb (20542)1768	

****

C2H5NO2 HL Glycine CAS 56-40-6 (85)

2-Aminoethanoic acid; H2N.CH2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	alc/w	25°C	61%	U		K1=9.66	1995SDa (21551)1769	

Medium: 61.1 wt % EtOH/H2O, I=0.50 M LiCl.

Fe+++	gl	NaNO3	25°C	0.50M	C		K1=8.57 B(FeHL)=11.33 B(Fe2H-2L2)=12.32	1990DJa (21552)1770	

Additional method: spectrophotometry.

```
Fe+++      gl  NaNO3  25°C 0.50M C        K1=8.57        1990DJa (21553)1771
                                         B(FeHL)=11.33
                                         B(Fe2H-2L2)=12.32
--------------------------------------------------------------------------------
Fe+++      gl  NaClO4 25°C 1.00M U        K1=8           1986ANb (21554)1772
                                         B(FeHL)=11.41
                                         B(Fe2H-2L)=6.80
--------------------------------------------------------------------------------
Fe+++      gl  NaClO4 25°C 6.00M U        K1=9.25        1982BPa (21555)1773
                                         B(FeHL)=12.30
                                         B(FeH2L2)=24.20
                                         B(Fe2L2)=22.29
                                         B(Fe2H2L4)=46.13
Medium: 3.0 M NaClO4 with 3.0 M glycine
--------------------------------------------------------------------------------
Fe+++      sp  NaClO4 20°C  1.0M U        K1=10.0        1958PEd (21556)1774
********************************************************************************
C2H5NO2                HL    Acetohydroxamic  CAS 546-88-3  (2766)
Acetohydroxamic acid, N-Hydroxyacetamide; CH3.CO.NHOH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      gl  KCl    25°C 0.20M C        K1=11.09  B2=20.69  1998FKa (21807)1775
                                         B3=28.80
                                         K(Fe+HL=FeL+H)=1.82
--------------------------------------------------------------------------------
Fe+++      sp  oth/un 25°C  1.0M C                            1985BKb (21808)1776
                                         K(Fe+HL=FeL+H)=1.9
Medium not stated.
--------------------------------------------------------------------------------
Fe+++      sp  NaCl   25°C  1.0M C        K1=10.38  B2=19.16  1984BKb (21809)1777
                                         B3=25.56
--------------------------------------------------------------------------------
Fe+++      EMF NaClO4 25°C 1.00M U        K1=11.42       1979SRb (21810)1778
--------------------------------------------------------------------------------
Fe+++      gl  NaCl   25°C 0.15M M        K1=8.405  B2=17.433 1978BRa (21811)1779
                                         B3=24.618
                                         B(Fe2H-1L6)=16.653
                                         B(FeH-1L3)=43.358
********************************************************************************
C2H6N2O                 L    Methylurea       CAS 598-50-5  (2019)
N-Methylurea; CH3.NH.CO.NH2
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      vlt NaClO4 25°C 0.20M U        K1=0.32   B2=0.70   1985MCc (21968)1780
                                         K3=0.20
                                         K4=0.11
                                         K5=0.11
                                         K6=0.079
```

```
------------------------------------------------------------------------------
Fe+++      vlt NaClO4 20°C 0.20M U        K1=0.32   B2=0.71   1980MCa (21969)1781
                                          B3=0.90
                                          B4=1.0
                                          B5=1.1
                                          B6=1.2
******************************************************************************
C2H6N2O2               HL                     CAS 5549-80-4  (833)
2-Amino-N-hydroxyacetamide, Glycine hydroxamic acid; H2N.CH2.CO.NH.OH
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Fe+++      sp  NaClO4 20°C 0.10M U                      1987KPa (21990)1782
                                          K(Fe+HL)=8.35
------------------------------------------------------------------------------
Fe+++      sp  NaCl   25°C 0.15M U        K1=14.14  B2=22.72  1985EHb (21991)1783
                                          B(FeHL)=17.36
                                          B(FeHL2)=28.94
Alternative model: K1=13.14; B2=22.62; B(FeHL)=17.36; B(FeH3L3)=48.28
------------------------------------------------------------------------------
Fe+++      sp  NaCl   25°C  1.0M C        K1=7.77   B2=13.71  1984BKb (21992)1784
                                          B3=17.63
******************************************************************************
C2H6N2O2                L                     CAS 1000-82-4  (5676)
N-Hydroxymethylcarbamide; NH2.CO.NH.CH2.OH
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Fe+++      gl  NaClO4 20°C 0.10M U                      1984BNa (21997)1785
                                          K(Fe+3HL)=9.4
                                          B3=32.1
******************************************************************************
C2H6O                   L    Ethanol          CAS 64-17-5  (1913)
Ethanol; CH3.CH2.OH
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Fe+++      oth non-aq 21°C 100%  U    M                 1980MKa (22028)1786
                                          K(TPPFeCl+4L)=-3.8
Medium: CH2Cl2. TTPFeCl=Tetraphenylporphyrin ferric chloride.
******************************************************************************
C2H6S                  HL    Ethanethiol      CAS 75-08-1  (6723)
Ethanethiol, ethyl mercaptan; CH3CH2SH
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Fe+++      kin non-aq 25°C 100%  U                      1993HOa (22200)1787
                                          K(L+Fe4S4A4--)=0.079
                                          K(L+Fe4S4A4---)=0.061
                                          K((MoFe3S4A3)2A3+L)=-0.58
```

K((WFe3S4A3)2A3+L) > 0.60
Medium: MeCN. HA=thiophenol
****
C2H7N L Ethylamine CAS 75-04-7 (156)
Ethylamine; CH3.CH2.NH2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	alc/w	25°C	80%	U	M		1993BHa	(22271)1788
							K(FeP+L)=3.65		

Medium: 80%MeOH/H2O. P: porphyrin microperoxidase-8. Also data for L=PrNH2 (1.5), BuNH2 (4.4), tert-BuNH2 (<0.5), MeNH2 (4.0), DiMeNH2 (2.7), Me3N (0).
****
C2H7O2PS2 HL CAS 5930-72-3 (4229)
O,O-Dimethyldithiophosphoric acid; (CH3O)2.PS.SH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	EMF	mixed	25°C	90%	U			1984GGa	(22543)1789
							B3=17.20		

Medium: 90% 2-propanol/H2O. Data for other substituted dithiophosphoric acids
****
C2H8O6P2 H4L CAS 6145-33-1 (3543)
Ethane-1,1-diphosphonic acid; CH3.CH(PO3H2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	NaClO4	25°C	0.5M	C		K1=14.10	1990VKc	(23268)1790
							K(Fe+OH+L)=21.9		
							K(Fe+2OH+L)=25.1		

****
C2H8O7P2 H4L HEDPA CAS 2809-21-4 (436)
1-Hydroxyethane-1,1-diphosphonic acid; CH3.C(OH)(PO3H2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KNO3	25°C	0.10M	C			2002GKc	(23368)1791
							B(Fe2L2)=48.85		
							B(Fe2H-1L2)=44.06		
							B(Fe2H-2L2)=34.55		
							B(FeH3L2)=47.52		
Fe+++	gl	KNO3	25°C	0.10M	C		K1=24.2	1998LDa	(23369)1792
							B(FeHL)=27.4		
							B(FeH-1L)=19.1		
Fe+++	gl	NaClO4	25°C	0.50M	U		K1=14.10	1990VSa	(23370)1793
							B(Fe(OH)L)=21.9		
							B(Fe(OH)2L)=25.1		

```
--------------------------------------------------------------------------------
Fe+++      kin KNO3   30°C 0.10M U T                    1988RRa (23371)1794
                                      K(FeL(OH)+H)=9.67
--------------------------------------------------------------------------------
Fe+++      gl  KCl    25°C 0.10M U       K1=16.21  B2=25.25  1967KLa (23372)1795
                                      K(Fe+H-1L))=21.60
                                      K(2Fe+H-1L))=29.1
********************************************************************************
C2H9NO6P2             H4L    IDPA            CAS 32545-63-4  (1335)
Imino-N,N-bis(methylenephosphonic acid); HN(CH2PO3H2)2
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      gl  KNO3   25°C  0.1M C       B2=30.96       1985MMa (23454)1796
                                      K(FeL+H)=3.90
                                      K(FeL(OH)+H)=10.35
********************************************************************************
C2H16N5O4Co            HL                      (231)
Pentaammineoxalatocobalt(III); Co(NH3)5(HC2O4)
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      sp  NaClO4 28°C 0.30M U       K1=3.25        1974NDa (23473)1797
********************************************************************************
C3H3O4Br              H2L    Bromomalonic     CAS 600-31-7  (6296)
2-Bromo-propanedioic acid, Bromomalonic acid; HOOC.CHBr.COOH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      gl  NaClO4 30°C 0.10M U       K1=6.35   B2=11.83  1976DGd (23537)1798
                                      K3=4.50
********************************************************************************
C3H4N2                  L    Imidazole        CAS 288-32-4  (90)
1,3-Diazole, imidazole; C3H4N2
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      sp  non-aq 25°C 100%  C                    2003TPa (23885)1799
                                      K(FeP+L)=7.5
Medium: CH2Cl2.  P is 2,3,12,13-tetrakis(trifluoromethyl)-5,10,15,20-
tetraphenylporphyrin.
--------------------------------------------------------------------------------
Fe+++      sp  KCl    25°C 0.10M C T H                  2002PCb (23886)1800
                                      K(FeP+L)=2.23
                                      K(FeA+L)=4.16
Data for 10-35 C. DH(FeP+L)=-16.6 kJ mol-1, DS=-13 J K-1 mol-1. DH(FeA+L)=
-29.4, DS=-19. P is sperm whale myoglobin; A is N-acetyl-microperoxidase
--------------------------------------------------------------------------------
Fe+++      sp  alc/w  25°C  80%  U                    1994HPa (23887)1801
                                      K(FeP(H2O)+L=FePL+H2O)=4.38
```

```
                                        K(FeP(H2O)+H-1L=FePH-1L)=6.75
Medium: 80% v/v MeOH/H2O. FeP: Fe porphyrin microperoxidase-8.  Also data
for L=N-methylimidazole (K=4.55), N-acetylimidazole (3.8), N-Cl-N-MeIm (3.9)
--------------------------------------------------------------------------
Fe+++      sp  NaNO3  30°C 0.20M U    M                  1993BGc (23888)1802
                                        K(FeA2B+L=FeABL)=3 to 3.70
                                        K(FeABL+L=FeBL2)=4.48 to 5.51
                                        K(FeABC+L=FeBCL)=-0.046 to 2.9
                                        K(FeA2B+2L=FeBL2)=8.70 to 8.90
A:H2O. H6B:5,10,15,20-Tetrakis(2,6-dimethyl-3-sulfonatophenyl)porphirin.
C:OH.
--------------------------------------------------------------------------
Fe+++      sp  non-aq 25°C 100%  U    M                  1991UHa (23889)1803
                                        K(FeAOCH3+2L=FeA(OCH3)L2)=3.25
                                        K(FeACl+2L=FeAClL2)=6.02
Medium: CH2Cl2. A=Octaethylporphine
--------------------------------------------------------------------------
Fe+++      sp  non-aq 23°C 100%  U    M                  1991YTa (23890)1804
                                        K(FeACl+2L=FeAClL2)=6.24
Medium: CH3CN. A=2,7,12,17-Tetraethyl-3,8,13,18-tetramethylporphine
Data also for other porphines
--------------------------------------------------------------------------
Fe+++      sp  NaNO3  25°C 0.10M U    M                  1982WPa (23891)1805
                                        K(FeA+2L)=5.48
                                        K(2FeA+4L=2FeAL2)=-7.85
A=Tetrakis(4-N-methylpyridyl)porphyrin
--------------------------------------------------------------------------
Fe+++      sp  non-aq 25°C 100%  U T HM                 1978PGa (23892)1806
                                        K(FeAS+2L=FeAL2+S)=4.80
Medium(S): DMSO, 0.04 M NaNO3. A=Tetraphenylporphyrin (TPP) chloride
DH=-44.8 kJ mol-1. 30 C:K=4.70; 35 C:K=4.52; 40 C:K=4.44
--------------------------------------------------------------------------
Fe+++      sp  non-aq 25°C 100%  U   HM                 1978PGa (23893)1807
                                        K(FeAS+2L=FeAL2+S)=4.84
Medium(S): DMSO, 0.04 M NaNO3. A=Protoporphyrin IX (hemin)-chloride
DH=-33.0 kJ mol-1. 30 C:K=4.77; 35 C:K=4.69; 40 C:K=4.56
--------------------------------------------------------------------------
Fe+++      nmr non-aq 20°C 100%  U    M                 1978WYa (23894)1808
                                        K(FeA+2L)=4.8
Medium: DMSO-d6. A=Protoporphyrin-IX-chloride
--------------------------------------------------------------------------
Fe+++      sp  non-aq 30°C 100%  U   H    B2=5.89       1974ARb (23895)1809
Medium: CH2Cl2. DH(B2)=-92.0 kJ mol-1 and DS(B2)=-192.0 J mol-1 K-1.
--------------------------------------------------------------------------
Fe+++      sp  oth/un 25°C  0.0  U   HM                 1964GHf (23896)1810
                                        K(FeA+L)=2.20
                                        K'(FeA(H-1L)+H)=10.34
Medium:0 corr.  DH(K)1=-17.1 kJ mol-1, DS=-17 J K-1 mol-1. DH(K')=-46,
DS=38.  FeA+=ferrimyoglobin
**************************************************************************
```

C3H4O3 HL Pyruvic acid CAS 127-17-3 (1152)
2-Oxopropanoic acid; CH3.CO.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	vlt	NaClO4	30°C	1.0M	C		K1=4.83	B2= 5.52	1988GMb (24051)	1811
							B(Fe(ox)L2)=8.86			
							B(Fe(ox)2L)=9.17			
							B(Fe(cit)L2)=7.01			
Fe+++	sp	NaClO4	20°C	0.10M	U		K(Fe(OH)+L)=9.44		1999PKb (24445)	1812
Fe+++	sp	NaClO4	20°C	0.10M	U	M	K(FeOH+L)=9.44		1999PKb (24446)	1813
Fe+++	gl	NaNO3	25°C	0.50M	C		K1=7.52	B2=13.29	1989SRb (24447)	1814
							B3=16.93			
Fe+++	kin	NaClO4	25°C	0.50M	C		K1=7.57		1977CCb (24448)	1815
Fe+++	EMF	NaClO4	25°C	2.00M	C		K1=7.50	B2=13.04	1977DEa (24449)	1816
							B3=16.6			
Fe+++	gl	NaClO4	30°C	0.10M	U		K1=6.39	B2=12.36	1976DGd (24450)	1817
							K3=5.70			
Fe+++	gl	NaClO4	25°C	0.10M	U		K1=8.04	B2=13.54	1973RMb (24451)	1818
Fe+++	kin	NaClO4	25°C	0.50M	U		K1=7.57		1971CDa (24452)	1819
Fe+++	vlt	NaClO4	25°C	1.00M	U		K1=6.54		1971GMc (24453)	1820
							K(Fe+HL)=2.80			

Method: amperometric titration

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	sp	oth/un	?	?	U		K1=8.25	B2=13.83	1969GSd (24454)	1821
Fe+++	EMF	NaClO4	25°C	0.50M	U		K1=7.46		1968DMc (24455)	1822

Medium: LiClO4

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	vlt	NaClO4	25°C	0.50M	U		B3=15.65		1954SLb (24456)	1823
Fe+++	vlt	oth/un	?	0.02M	U				1951SCa (24457)	1824

****

C3H4O4 H2L Malonic acid CAS 141-82-2 (79)
Propanedioic acid; CH2(COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	sp	NaClO4	20°C	0.10M	U		K(Fe(OH)+L)=9.44		1999PKb (24445)	1812
Fe+++	sp	NaClO4	20°C	0.10M	U	M	K(FeOH+L)=9.44		1999PKb (24446)	1813
Fe+++	gl	NaNO3	25°C	0.50M	C		K1=7.52	B2=13.29	1989SRb (24447)	1814
							B3=16.93			
Fe+++	kin	NaClO4	25°C	0.50M	C		K1=7.57		1977CCb (24448)	1815
Fe+++	EMF	NaClO4	25°C	2.00M	C		K1=7.50	B2=13.04	1977DEa (24449)	1816
							B3=16.6			
Fe+++	gl	NaClO4	30°C	0.10M	U		K1=6.39	B2=12.36	1976DGd (24450)	1817
							K3=5.70			
Fe+++	gl	NaClO4	25°C	0.10M	U		K1=8.04	B2=13.54	1973RMb (24451)	1818
Fe+++	kin	NaClO4	25°C	0.50M	U		K1=7.57		1971CDa (24452)	1819
Fe+++	vlt	NaClO4	25°C	1.00M	U		K1=6.54		1971GMc (24453)	1820
							K(Fe+HL)=2.80			

Method: amperometric titration

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	sp	oth/un	?	?	U		K1=8.25	B2=13.83	1969GSd (24454)	1821
Fe+++	EMF	NaClO4	25°C	0.50M	U		K1=7.46		1968DMc (24455)	1822

Medium: LiClO4

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	vlt	NaClO4	25°C	0.50M	U		B3=15.65		1954SLb (24456)	1823
Fe+++	vlt	oth/un	?	0.02M	U				1951SCa (24457)	1824

B3=15.7

****

C3H6N2O4 H2L CAS 1882-99-1 (8457)
Molonodihydroxamic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KNO3	25°C	1.0M	C	T		1994BBd	(24826)1825
							K(Fe+H2L=FeL+2H)=-0.02		

At 35 C, from kinetic data, K=-0.15. Also data for 40 and 45 C.

****

C3H6O2 HL Propionic acid CAS 79-09-4 (35)
Propanoic acid; CH3.CH2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	alc/w	25°C	100%	U		K1=4.22	1971SSg	(25004)1826
Fe+++	EMF	NaClO4	20°C	1.0M	U		K1=3.45	1959PEa	(25005)1827

****

C3H6O2S H2L Thiolactic acid CAS 79-42-5 (366)
2-Mercaptopropanoic acid; CH3.CH(SH).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	kin	NaClO4	25°C	0.50M	C		K1=13.43	1983BMc	(25143)1828
							K(Fe+H2L=FeL+2H)=-0.16		

Method: spectrophotometry.

****

C3H6O3 HL L-Lactic acid CAS 79-33-4 (82)
L-2-Hydroxypropanoic acid; CH3.CH(OH).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	none	30°C	0.0	U			1976GCa	(25442)1829
							K1eff=3.89		

Measured at pH 3.0

Fe+++	sp	oth/un	?	?	U	M	K1=3.6	1970PKc	(25443)1830
							K(Fe+2L+2OH=FeH-2L2)=26.92		
							K(Fe+A+H-1L)=25.4		

H3A=5-Sulfosalicylic acid

Fe+++	sp	oth/un	?	->0	U		K1=6.4	1952BEb	(25444)1831

****

C3H7NO L DMF CAS 68-12-2 (598)
N,N-Dimethylformamide; HCO.N(CH3)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo

```
Fe+++      nmr non-aq 25°C 100%  U                      1989SKb (25657)1832
                                       K(FeL5+L)=3.22
                                       K(FeL4+2L)=6.30
                                       K(FeL3+3L)=9.7
Medium: acetonitrile
**************************************************************************
C3H7NO2                HL    Alanine          CAS 56-41-7  (86)
2-Aminopropanoic acid; H2N.CH(CH3).COOH
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe+++      sp  alc/w  25°C  80%  U    M                   1993BHa (26174)1833
                                       K(FeP+L)=2.89
Medium: 80%MeOH/H2O. P: porphyrin microperoxidase-8. Also data for L=Gly
(3.46), Val (3.73), Leu (3.99), Phe (4.76), Trp (5.64).
--------------------------------------------------------------------------
Fe+++      gl  NaNO3  25°C 0.50M C        K1=8.80        1993DJa (26175)1834
                                       B(FeHL)=11.03
                                       B(FeH-1L)=6.63
--------------------------------------------------------------------------
Fe+++      vlt KCl    30°C  1.0M U        K1=10.98       1967KMc (26176)1835
--------------------------------------------------------------------------
Fe+++      EMF NaClO4 20°C  1.0M U        K1=10.4        1958PEd (26177)1836
**************************************************************************
C3H7NO2                HL    Sarcosine        CAS 107-97-1  (87)
N-Methyl-2-aminoethanoic acid; CH3.NH.CH2.COOH
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe+++      EMF NaClO4 20°C  1.0M U        K1=9.7         1959PEc (26602)1837
**************************************************************************
C3H7NO2                HL                        (6927)
N-Methylacetohydroxamic acid; CH3.CO.N(OH)CH3
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe+++      gl  KCl    25°C 0.20M C        K1=11.85  B2=21.58  1998FKa (26622)1838
                                       B3=29.36
                                       K(Fe+HL=FeL+H)=3.15
--------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 2.00M C        K1=11.70  B2=21.50  1994CCb (26623)1839
                                       B3=29.44
                                       K(Fe+HL=FeL+H)=2.75
                                       K(FeL+HL=FeL2+H)=0.9
                                       K(FeL2+HL=FeL3+H)=-1.06
**************************************************************************
C3H7NO2                HL                        (7502)
Propanohydroxamic acid; C2H5CONHOH
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
```

```
------------------------------------------------------------------------------
Fe+++      gl  KCl    25°C 0.20M C        K1=11.16  B2=20.74  1998FKa (26631)1840
                                          B3=28.44
                                          K(Fe+HL=FeL+H)=1.83
******************************************************************************
C3H7NO2S              H2L    Cysteine         CAS 52-90-4  (96)
2-Amino-3-mercaptopropanoic acid; H2N.CH(CH2.SH)COOH
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 1.00M U                         1995SJa (26775)1841
                                          K(Fe+H3L=FeHL+2H)=-1.60
                                          K(Fe2+H3L=Fe2HL+2H)=-1.15
Medium: LiClO4
------------------------------------------------------------------------------
Fe+++      dis NaClO4 35°C 0.10M U        K1=13.00       1994TNa (26776)1842
Method: paper electrophoresis. Medium: 0.1 M HClO4
------------------------------------------------------------------------------
Fe+++      kin KCl      ?  0.10M U        K1=13.70       1991JLb (26777)1843
                                          K(FeOH+L)=10.75
                                          K(FeOHL+L)=4.76
------------------------------------------------------------------------------
Fe+++      kin KCl    25°C 0.10M C                      1988JLa (26778)1844
                                          K(Fe(OH)L+L=Fe(OH)L2)=4.76
Method: kinetic study of Fe(III)-cysteine reaction.
------------------------------------------------------------------------------
Fe+++      gl  KNO3   37°C 0.15M M T      K1=10.63  B2=14.01  1979ZJa (26779)1845
At 20 C, 0.15 M KNO3, K1=10.85, B2=14.49.
------------------------------------------------------------------------------
Fe+++      oth oth/un 25°C  ->0  U                         1955TKa (26780)1846
                                          B3=32.10
                                          B(FeL2(OH))=33.30
******************************************************************************
C3H7NO3                HL    Serine           CAS 56-45-1  (49)
2-Amino-3-hydroxypropanoic acid; H2N.CH(CH2.OH)COOH
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Fe+++      gl  NaNO3  25°C 0.50M C                         1997DJb (27132)1847
                                          B(FeHL)=10.80
                                          B(FeH-1L)=5.20
                                          B(FeH-1L2)=12.87
                                          B(FeH-2L)=2.76
B(Fe2H-2L2)=14.50. By spectrophotometry: K1=7.54,  B(FeHL)=10.82,
B(FeH-1L)=5.22.
------------------------------------------------------------------------------
Fe+++      EMF NaClO4 20°C  1.0M U        K1=9.2         1958PEd (27133)1848
******************************************************************************
C3H8NO5P              H3L    Glyphosate       CAS 1071-83-6  (1617)
N-(Phosphonomethyl)glycine; H2O3P.CH2.NH.CH2.COOH
```

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KNO3	25°C	0.1M	C		K1=16.09 B2=23 B(FeHL)=17.63 K(FeL(OH)2+2H)=1.40	1985MMa (27404)	1849

C3H8NO6P H3L Phosphoserine CAS 17885-08-4 (1865)
Serine dihydrogenphosphate, O-Phosphoserine; NH2.CH(CH2.OPO3H2).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KCl	25°C	0.10M	U		K1=10.90	1997ZTa (27466)	1850
Fe+++	gl	KCl	25°C	0.16M	U		K1=14.0 B2=21.40 K(Fe+HL)=6.7	1959OSa (27467)	1851
Fe+++	gl	oth/un	25°C	0.15M	U		K1=>13	1957OSa (27468)	1852

C3H8N2O L Dimethylurea CAS 96-31-1 (2021)
1,3-Dimethylurea; CH3.NH.CO.NH.CH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	vlt	NaClO4	25°C	0.20M	U		K1=-0.046 B2=0.18 K3=1.30 K4=-0.22	1985MCc (27476)	1853
Fe+++	vlt	NaClO4	20°C	0.20M	U		K1=-0.05 B2=0.2 B3=1.49 B4=1.30	1980MCa (27477)	1854

C3H8N2O L Ethylurea CAS 625-52-5 (2020)
N-Ethylurea; H2N.CO.NH.C2H5

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	vlt	NaClO4	25°C	0.20M	U		K1=0.079 B2=0.36 K3=-0.046 K4=0.0 K5=0.95 K6=0.15	1985MCc (27484)	1855
Fe+++	vlt	NaClO4	20°C	0.20M	U		K1=0.1 B2=0.4 B3=0.3 B4=0.3 B5=1.3 B6=1.4	1980MCa (27485)	1856

C3H8N2O2 HL Ala-hydroxamic CAS 16707-85-0 (1582)

2-Amino-N-hydroxypropanamide, Alanine hydroxamic acid; CH3.CH(NH2).CO.NH.OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaClO4	25°C	0.10M	U		K(Fe+H2L=FeHL+H)=1.44	1994OIa (27577)	1857
Fe+++	gl	KCl	25°C	0.20M	C		K1=13.92 B2=21.99 B(FeHL)=17.15 B(FeHL2)=28.36 B(FeH-1L2)=14.54 B(FeHL3)=33.90	1989FSa (27578)	1858

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C3H8N2O2 HL (6666)

beta-Alaninehydroxamic acid; NH2.CH2.CH2.CO.NHOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KCl	25°C	0.20M	C		K1=16.99 B(FeHL)=19.95 B(FeH2L2)=38.30 B(FeH-1L2)=22.11 B(FeH-2L2)=12.12 B(FeH3L3)=55.47, B(FeH2L3)=50.24, B(FeHL3)=42.75.	1995FKa (27607)	1859

****

C3H8N2O3 H2L CAS 55779-32-3 (5500)

Serinehydroxamic acid, 2-Amino-N,3-dihydroxypropionamide; HO.CH2.CH(NH2).CO.NH.OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KCl	25°C	0.50M	C		B2=22.15 B(FeHL)=17.07 B3=28.06 B(FeH2L2)=32.88 B(FeHL2)28.80 B(FeH2L3)=41.17; B(FeH3L3)46.26; B(FeHL3)=34.83; B(FeH-2L2)=22.15	1994LEa (27618)	1860
Fe+++	gl	NaCl	25°C	0.20M	U	I	K1=11.72 B2=20.73 Also data for 43% v/v MeOH/H2O, 52% v/v EtOH/H2O, 59% v/v i-PrOH/H2O, 61% v/v dioxane/H2O.	1994SKb (27619)	1861
Fe+++	sp	NaCl	25°C	0.15M	C		B2=20.75 B(FeHL)=16.26 B(FeH2L2)=31.43 B(FeH3L3)=44.62 B(FeH-1L)=8.06	1988HMa (27620)	1862

****

C3H8N4O2 L CAS 13547-17-6 (5677)

Methylenedicarbamide; NH2.CO.NHCH2NH.CO.NH2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	NaClO4	20°C	0.10M	U		K1=7.7	1984BNa (27641)	1863

****

C3H8OS2 H2L BAL CAS 59-52-9 (379)
2,3-Dimercaptopropan-1-ol; HS.CH2.CH(SH).CH2(OH)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	oth/un	25°C	0.10M	U			1960LMb (27658)	1864
							B(FeL(OH))=30.6		
							B(FeL(OH)(NH3)3)=31.8		

****

C3H9N3O2 HL CAS 471915-95-4 (8549)
2,3-Diamino-N-hydroxypropanamide;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KCl	25°C	0.20M	C		K1=16.41	2002ECa (27984)	1865

****

C3H11NO6P2 H4L (6772)
(Dimethylamino)-N-methylenediphosphonic acid; (CH3)2N.CH(PO3H2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	NaNO3	24°C	0.20M	C		K1=28.8 B2=34.3	1993BRa (28410)	1866
							K(FeL+H)=6.5		
							K(FeHL+H)=1.4		
							K(FeL2+H)=10.3		
							K(FeHL2+H)=9.6		
							K(FeH2L2+H)=5.5, K(FeH3L2+H)=3.9, K(FeH4L2+H)=1.6, K(FeH5L2+H)=1.5		

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C3H12NO9P3 H6L NTPA CAS 6419-19-8 (2920)
Nitrilotris(methylenephosphonic acid); N(CH2PO3H2)3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KNO3	25°C	0.10M	C		K1=21.1	1998LDa (28565)	1867
							B(FeHL)=28.1		
							B(FeH2L)=33.1		
Fe+++	EMF	NaClO4	25°C	1.0M	U		K1=27.6	1987PLa (28566)	1868
Fe+++	gl	R4N.X	20°C	0.1M	C		K1=14.6	1967HEa (28567)	1869
							K(Fe+HL)=9.9		
							K(Fe+H2L)=6.0		

****

C4H2N2S2 H2L CAS 104409-71-4 (569)
1,2-Dicyano-1,2-dimercaptoethylene, Dimercaptomaleonitrile; (NC.C(SH):)2

```
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      sp  non-aq 25°C 100%  U    M                    1972YSb (28618)1870
                                        K(FeL2+A)=5.58
                                        K(FeL2+py)=3.72
                                        K(FeL2+B)=2.75
                                        K(FeL2+C)=2.98
A=triphenylarsine oxide; B=triphenylphosphine oxide; C=triphenylphosphine
*************************************************************************
C4H2O4                H2L    Squaric acid     CAS 2892-51-5  (439)
3,4-Dihydroxy-3-cyclobutene-1,2-dione;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      sp  NaClO4 23°C 1.00M U    M                    1991SJa (28648)1871
                                        K(Fe+HL=FeL+H)=1.33
                                        K(Fe2(OH)2+HL=Fe2(OH)2L+H)=2.4
Medium: LiClO4
-------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 0.50M U T      K1=4.61        1969TWa (28649)1872
K1(40 C)=4.49
*************************************************************************
C4H3N3O                L                        (5683)
Methylisinotrosomalonodinitrile; CH3ON:C(CN)2
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      EMF oth/un 25°C 0.25M U                         1985ROa (28703)1873
                                        K(Fe(OH)2+L)=3.07
                                        K(Fe(OH)2+2L)=5.92
Medium: Na-acetate
*************************************************************************
C4H4N2                 L    Pyridazine       CAS 289-80-5  (1484)
1,2-Diazine, Pyridazine; cyclo(-N:N.CH:CH.CH:CH-)
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      sp  alc/w  25°C  80%  U                         1993HPa (28773)1874
                                        K(FeP+L)=2.25
Medium: 80%MeOH/H2O, pH=7.0.  P: porphyrin microperoxidase-8.
*************************************************************************
C4H4N2                 L    Pyrimidine       CAS 289-95-2  (4247)
1,3-Diazine, pyrimidine;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      sp  alc/w  25°C  80%  U                         1993HPa (28777)1875
                                        K(FeP+L)=1.3
Medium: 80%MeOH/H2O, pH=7.0.  P: porphyrin microperoxidase-8.
*************************************************************************
```

C4H4N2 L Pyrazine CAS 290-37-9 (620)
1,4-Diazine, Pyrazine;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp alc/w 25°C 80% U 1993HPa (28793)1876
K(FeP+L)=1.1
Medium: 80%MeOH/H2O, pH=7.0. P: porphyrin microperoxidase-8.
****
C4H4N2O3 H2L Barbituric acid CAS 67-52-7 (2818)
2,4,6-Trihydroxypyrimidine; C4HN2(OH)3

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl NaCl 25°C 0.1M U K1=3.89 2000KSb (28912)1877
****
C4H5N3O2 HL 6-Aminouricil CAS 873-83-6 (6213)
4-Amino-2,6-dihydroxypyrimidine;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl NaClO4 30°C 0.10M U K1=18.81 B2=34.72 1986JDa (29423)1878
****
C4H5N5O3 H2L (4262)
4-Hydroxy-6-(hydroxyimino)dihydro-2-triazine carboxaldoxime

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp NaClO4 20°C 0.02M U K1=19 1972GNa (29430)1879
K(Fe+HL)=10.05
****
C4H6N2 L 2-Me-Imidazole CAS 693-98-1 (122)
2-Methyl-1,3-diazole; C3H3N2.CH3

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ kin non-aq 25°C 100% U M 1993WSa (29485)1880
K(FeACl+L)=1.26
K(FeBCl+L)=1.40
K(FeCCl+L)=0.30
K(FeDCl+L)=0.32
H2A=8,13-Divinyl-3,7,12,17-tetramethyl-21H,23H-porphine-2,18-dipropanoic ac.
B=dimethyl ester of A, H2C=dibutanoic acid deriv of A, D=dimethyl ester of C

Fe+++ sp oth/un 24°C ? U M 1991HSa (29486)1881
K(FeAClO4+L=FeAL+ClO4)=2.79
K(FeAL+L=FeAL2)=4.32
A=Tetrakis(2,6-dichlorophenyl)porphyrin

Fe+++ sp non-aq 25°C 100% U M 1991UHa (29487)1882

K(FeA(OCH3)+L=FeA(OCH3)L)=0.96
Medium: CH2Cl2. A=Octaethylporphine. With 2-benzylimidazole K=1.66, 2-phenylimidazole K=1.97, 2-ethylimidazole K=0.94
****
C4H6N2 L 4-Me-Imidazole CAS 822-36-6 (353)
4-Methyl-1,3-diazole; C3H3N2.CH3

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp non-aq 25°C 100% U M 1991UHa (29528)1883
K(FeAOCH3+2L=FeA(OCH3)L2)=3.10
K(FeACl+2L=FeAClL2)=5.85
Medium: CH2Cl2. A=Octaethylporphine

Fe+++ sp non-aq 25°C 100% U M 1982QNa (29529)1884
K(FeAL+L)=1.69
Medium: THF. A=Tetraphenyl porphyrin. In toluene: K(FeALSbF6+L) > 7
****
C4H6N2 L N-Me-Imidazole CAS 616-47-7 (354)
N-Methyl-1,3-diazole; C3H3N2.CH3

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp non-aq 25°C 100% C M 1998KWb (29593)1885
K(Fe(P)Cl+2L=Fe(P)L2)=3.52
P=(o-F)(p-OCH3)3-tetraphenylporphyrin; medium: chloroform. In DMF (by voltammetry) K=6.3. Data for other o-X, o-CF3 and 2,6-X-substituted TPP.

Fe+++ EMF KCl 25°C 1.00M U K2=2.92 1995NTa (29594)1886

Fe+++ sp oth/un 24°C ? U M 1991HSa (29595)1887
K(FeAClO4+L=FeAL+ClO4)=1
K(FeAL+L=FeAL2)=4.146
A=Tetrakis(2,6-dichlorophenyl)porphyrin. With N-vinylimidazole, K=3.88, 3.54 respectively
---
Fe+++ sp non-aq 25°C 100% U M 1991UHa (29596)1888
K(FeAOCH3+2L=FeA(OCH3)L2)=0.83
Medium: CH2Cl2. A=Octaethylporphine

Fe+++ sp non-aq 23°C 100% U M 1991YTa (29597)1889
K(FeACl+2L=FeAClL2)=3.25
Medium: CH3CN. A=2,3,7,8,12,17,18-Heptaethyl-13-trifluoromethylporphine
Data also for other porphines

Fe+++ sp non-aq 25°C 100% U T HM 1978PGa (29598)1890
K(FeAS+2L=FeAL2+S)=4.11
Medium(S): DMSO, 0.04 M NaNO3. A=Tetraphenylporphyrin (TPP) chloride
DH=-42.8 kJ mol-1. 30 C:K=3.88; 35 C:K=3.88; 40 C:K=3.74

```
Fe+++      sp  non-aq 25°C 100%  U   HM                  1978PGa (29599)1891
                                          K(FeAS+2L=FeAL2+S)=4.39
Medium(S): DMSO, 0.04 M NaNO3. A=Protoporphyrin IX (hemin)-chloride
DH=-38.0 kJ mol-1. 30 C:K=4.30; 35 C:K=4.18; 40 C:K=4.06
**************************************************************************
C4H6O4                H2L    Succinic acid    CAS 110-15-6  (112)
1,4-Butanedioic acid; HOOC.CH2.CH2.COOH
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe+++      gl  NaClO4 25°C 0.10M U        K1=7.89   B2=13.34  1973RMb (29973)1892
--------------------------------------------------------------------------
Fe+++      sp  R4N.X  25°C 0.50M U        K1=6.88        1968DMc (29974)1893
Medium: LiClO4
--------------------------------------------------------------------------
Fe+++      sp  oth/un   ?     ?  U        K1=7.49        1956PGa (29975)1894
**************************************************************************
C4H6O4                H2L    Me-Malonic Acid  CAS 516-15-2  (816)
Methylpropanedioic acid; HOOC.CH(CH3).COOH
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe+++      kin NaClO4 25°C 0.50M C        K1=7.56        1977CCb (30123)1895
--------------------------------------------------------------------------
Fe+++      gl  NaClO4 30°C 0.10M U        K1=7.15   B2=14.13  1976DGd (30124)1896
                                          K3=5.96
--------------------------------------------------------------------------
Fe+++      kin NaClO4 25°C 0.50M U        K1=7.56        1971CDa (30125)1897
**************************************************************************
C4H6O4S               H2L    Thiodiacetic     CAS 123-93-3  (140)
2,2'-Thiodiglycolic acid, Thiodiethanoic acid; HOOC.CH2.S.CH2.COOH
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe+++      gl  NaClO4 25°C 0.10M U                        1970PPa (30217)1898
                                          K(Fe+HL)=3.63
**************************************************************************
C4H6O4S               H3L    Thiomalic acid   CAS 70-49-5  (109)
2-Mercaptosuccinic acid, 2-Sulfanyl-1,4-butanedioic acid; HOOC.CH(SH).CH2.COOH
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe+++      kin NaClO4 25°C 0.50M C        K1=12.62       1983BMc (30331)1899
                                          K(Fe+H2L=FeL+2H)=0.36
Method: spectrophotometry.
--------------------------------------------------------------------------
Fe+++      gl  KNO3   37°C 0.15M M T      K1=9.01   B2=12.52  1979ZJa (30332)1900
At 20 C, 0.15 M KNO3, K1=9.18, B2=11.98.
**************************************************************************
C4H6O5                H2L    Malic acid       CAS 617-48-1  (393)
```

2-Hydroxybutane-1,4-dioic acid, Hydroxy-succinic acid; HOOC.CH2.CH(OH).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	NaNO3	25°C	0.50M	M	M		1989MAa	(30628)1901
							B(-3,1,1)=-1.5		
							K(2FeH-2L=Fe2H-4L2)=-13.0		
B(p,q,r): pH+qM+rH2L. K(UO2+Fe+H2L=UO2FeH-2L2+6H)=-7.37									
Fe+++	sp	oth/un	?	?	U		K1=10.45	1972GTc	(30629)1902
Fe+++	gl	NaClO4	20°C	0.10M	U		K1=7.1	1964TIb	(30630)1903
							B(Fe2H-2L2)=12.85		
							B(Fe2H-2L3)=17.85		
							B(Fe3H-4L5)=25.97		
By spectrophotometry: K1=7.09									

****

C4H6O5 H2L Diglycolic acid CAS 110-99-6 (243)
Di(carboxy)methyl ether, 2,2'-Oxydiethanoic acid; HOOC.CH2.O.CH2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	NaClO4	25°C	0.50M	U		K1=5.04	1972NAd	(30875)1904

****

C4H6O6 H2L D-Tartaric acid CAS 147-71-7 (93)
D-Tartaric acid, D-2,3-Dihydroxybutanedioic acid; HOOC.CH(OH).CH(OH).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	nmr	none	25°C		U	M		1990GKc	(30975)1905
							K(Fe+H2L=FeHL+H)=1.04		

****

C4H6O6 H2L DL-Tartaric acd CAS 133-37-9 (94)
DL-Tartaric acid,DL-2,3-Dihydroxybutanedioic acid; HOOC.CH(OH).CH(OH).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	NaNO3	25°C	0.50M	M	M		1989MAa	(31019)1906
							K(2FeL=Fe2L2)=-10.9		
Fe+++	gl	NaNO3	25°C	0.50M	U		K1=6.23	1987SRa	(31020)1907
							B(Fe3H-6L3)=9.25		
							B(Fe2H-3L2)=8.75		
Fe+++	sp	NaCl	25°C	1.00M	U			1982KIa	(31021)1908
							K(Fe+3H-1L)=36.7		
Fe+++	sp	NaClO4	25°C	1.00M	U		K1=5.45	1974KPb	(31022)1909
							K(Fe+HL)=2.10		

```
Fe+++      gl  NaClO4 25°C 0.10M U        K1=5.68   B2=10.53  1974RMc (31023)1910
                                         Beff(Fe+L+fulvic acid)=12.74
                                         K(Fe(fulvic acid)+L)=7.36
                                         K(FeL+fulvic acid)=7.06
**************************************************************************
C4H6O6               H2L    L-Tartaric acid  CAS 87-69-4  (92)
L-Tartaric acid, L-2,3-Dihydroxybutanedioic acid; HOOC.CH(OH).CH(OH).COOH
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe+++      nmr none   25°C       U    M                    1990GKc (31243)1911
                                         K(Fe+H2L=FeHL+H)=1.06
Data for d,l-Tartaric acid
--------------------------------------------------------------------------
Fe+++      sp  NaCl   25°C 1.00M U                         1983KIa (31244)1912
                                         K(Fe+2H-1L)=39.6
--------------------------------------------------------------------------
Fe+++      sp  NaClO4 20°C  1.0M C TI                      1980MBb (31245)1913
                                         K(Fe+H2L=FeL+2H)=-0.68
At 8C, K(Fe+H2L=FeL+2H)=-0.74. Also data for MeOH/H2O and n-PrOH/H2O
mixtures.
--------------------------------------------------------------------------
Fe+++      gl  NaClO4 25°C 1.00M C        K1=5.73           1974BVb (31246)1914
                                         B(Fe2H-2L2)=10.9
                                         B(Fe2H-4L2)=6.0
--------------------------------------------------------------------------
Fe+++      gl  NaClO4 25°C 0.10M U        K1=5.68   B2=10.53  1973RMb (31247)1915
--------------------------------------------------------------------------
Fe+++      gl  NaClO4 25°C 0.10M U        K1=6.66   B2=12.30  1973RMb (31248)1916
meso-tartaric acid
--------------------------------------------------------------------------
Fe+++      sp  oth/un   ?     ?  U        K1=9.02           1972GTc (31249)1917
                                         K(Fe+H-2L)=28.69
--------------------------------------------------------------------------
Fe+++      gl  NaClO4 25°C 0.10M U        K1=5.68   B2=10.53  1972RMa (31250)1918
Values quoted for meso form. K1(dl)=6.66, K2(dl)=5.64, B2(meso-dl)=13.46
--------------------------------------------------------------------------
Fe+++      sp  oth/un 25°C  1.0M U                         1967NAb (31251)1919
                                         K(Fe+H2L=FeL+2H)=-0.66 ?
--------------------------------------------------------------------------
Fe+++      gl  NaClO4 20°C 0.10M U        K1=6.49           1964TIa (31252)1920
                                         K(2Fe+2L=Fe2(H-1L)2+2H)=11.87
                                         K(3Fe+3L=Fe3(H-2L)3+6H)=9.48
K(2Fe+2L=Fe2(H-1L)(H-2L)+3H)=9.05
--------------------------------------------------------------------------
Fe+++      dis NaClO4 20°C 0.10M U        B2=11.86          1963STc (31253)1921
--------------------------------------------------------------------------
Fe+++      sp  oth/un   ?     ?  U        K1=7.49           1956PGa (31254)1922
--------------------------------------------------------------------------
Fe+++      vlt oth/un   ?     ?  U        K1=18.06?         1945TOa (31255)1923
```

K3=15.29?

****

C4H6O6 H2L meso-Tartaric CAS 147-73-9 (91)
meso-2,3-Dihydroxybutanedioic acid; HOOC.CH(OH).CH(OH).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	gl	NaClO4	25°C	0.10M	U		K1=6.66	B2=12.30	1974RMc (31428)	1924
							Beff(Fe+L+fulvic acid)=13.83			
							K(Fe(fulvic acid)+L)=8.45			
							K(FeL+fulvic acid)=7.17			

****

C4H7NO2 HL Acetoacetamide CAS 2044-64-6 (1407)
3-Oxobutanamide;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaClO4	25°C	0.5M	C		K1=12.03	1998HCb (31447)	1925

****

C4H7NO2 HL CAS 5687-86-5 (8042)
Cyclopropanecarbohydroxamic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaNO3	25°C	0.10M	C			1996NWa (31459)	1926
							B3=34.80		

****

C4H7NO3 L CAS 7340-09-2 (7021)
O-Acetyacetohydroxamic acid; CH3.CO.NHOCOCH3;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	EMF	NaClO4	25°C	1.00M	U		K1=6.86	1979SRb (31512)	1927

****

C4H7NO3 HL CAS 80393-54-0 (2589)
O-Acetylacethydroxylamine; CH3.CO.CH2.CO.NHOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	EMF	NaClO4	25°C	1.00M	U		K1=6.86	B2=13.34	1978SSe (31514)	1928
							K3=6.33			

****

C4H7NO4 H2L Aspartic acid CAS 56-84-8 (21)
Aminobutanedioic acid; H2N.CH(CH2.COOH).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	EMF	NaClO4	20°C	1.0M	U		K1=11.4	1958PEd (31856)	1929

****

C4H7NO4 H2L IDA CAS 142-73-4 (118)

Iminodiethanoic acid; HN(CH2.COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	EMF	NaClO4	20°C	1.00M	C		K1=10.95	2000BMa (32253)	1930
Method: Pt/Fe+++/Fe++ and glass electrodes.									
Fe+++	gl	KNO3	25°C	0.5M	C		K1=10.90 B2=19.33 B(FeH-1L)=7.73 B(FeH-2L)=4.38 B(Fe2L2)=22.4 B(Fe2H-2L2)=16.90 B(FeHL2)=22.33	1999SEb (32254)	1931
Fe+++	sp	oth/un	25°C	0.10M	U		K1=10.72	1997YSa (32255)	1932
Fe+++	vlt	KCl	25°C	0.20M	C		B2=19.77	1989MAb (32256)	1933
Method: cyclic voltammetry at Pt electrode.									
Fe+++	gl	NaClO4	25°C	1.00M	U		K1=11.13 B(FeHL)=12.02 B(FeH-1L)=8.01	1986ANb (32257)	1934
Fe+++	sp	NaClO4	25°C	0.50M	U		K1=10.72	1972NAd (32258)	1935

****

C4H8N2O3 HL Asparagine CAS 70-47-3 (17)
2-Aminobutanedioic acid 4-amide; H2N.CH(CH2.CO.NH2).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	EMF	NaClO4	20°C	1.0M	U		K1=8.6	1958PEd (32698)	1936

****

C4H8N2O3 HL Gly-Gly CAS 556-50-3 (54)
Glycyl-glycine; H2N.CH2.CO.NH.CH2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	EMF	NaClO4	20°C	1.0M	U		K1=9.1	1958PEd (33024)	1937

****

C4H8N2O4 H2L (6369)
N(1)-Hydroxyasparagine, aspartyl-beta-hydroxamic acid; H2N.CH(CH2.CO.NHOH).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaCl	25°C	0.15M	C		K1=21.06 B2=37.93 B(FeHL)=22.42 B(FeH2L2)=42.03 B(FeH-1L2)=34.88 B(FeH-2L3)=45.36	2002SMb (33133)	1938

```
Fe+++      gl  KCl    25°C 0.20M C                      1993FBa (33134)1939
                                        B(FeHL)=18.82
                                        B(Fe2HL)=31.63
                                        B(Fe2L)=24.25
                                        B(Fe2H-1L)=15.32
B(Fe2H2L)=36.35.
--------------------------------------------------------------------------
Fe+++      gl  KCl    25°C 0.20M C       B2=24.25       1990FBa (33135)1940
                                        B(FeHL)=18.82
                                        B(FeH2L2)=36.35
                                        B(FeHL2)=31.63
                                        B(FeH-1L2)=15.32
**************************************************************************
C4H8N2O4              H2L                    CAS 36244-81-2  (4267)
N-Carboxymethyliminoacethydroxamic acid; HOOC.CH2.NH.CH2.CO.NH.OH
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe+++      sp  NaClO4 20°C 0.10M U       K1=16.05       1981KPa (33142)1941
                                        K(Fe+HL)=8.80
--------------------------------------------------------------------------
Fe+++      sp  NaClO4 20°C 0.10M U       K1=15.26       1972KMb (33143)1942
                                        K(Fe+HL)=10.62
                                        K(FeL+H2O=FeLOH+H)=-4.22
                                        K(FeL(OH)3+2H=FeLOH+2H2O)=11.1
**************************************************************************
C4H8N2O4              H2L                    CAS 5615-93-0  (8458)
Succinodihydroxamic acid;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe+++      gl  KNO3   25°C  1.0M C T                      1994BBd (33149)1943
                                        K(Fe+H2L=FeL+2H)=-0.03
At 35 C, from kinetic data, K=-0.10. Also data for 40 and 45 C.
**************************************************************************
C4H8O2                 HL    Isobutyric acid  CAS 79-31-2  (573)
2-Methylpropanoic acid; CH3.CH(CH3).COOH
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe+++      EMF NaClO4 20°C  1.0M U       K1=4.63        1959PEb (33229)1944
Also quoted: K1=3.6
**************************************************************************
C4H8O2                 HL                     CAS 107-92-6  (1118)
n-Butanoic acid; CH3.CH2.CH2.COOH
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe+++      sp  alc/w  25°C 100%  U       K1=4.11        1971SSg (33337)1945
**************************************************************************
```

C4H8O3 HL CAS 965-70-8 (423)
2-Hydroxybutanoic acid; CH3.CH2.CH(OH).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	none	30°C	0.0	U		K1eff=3.86	1976GCa	(33578)1946

Measured at pH 3.0

****

C4H9NO2 HL Aminoisobutyric CAS 144-90-1 (188)
2-Amino-2-methylpropanoic acid; H2N.C(CH3)2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	EMF	NaClO4	20°C	1.0M	U		K1=10.3	1958PEd	(33838)1947

****

C4H9NO2 HL 2-Aminobutyric CAS 2835-81-6 (571)
2-Aminobutanoic acid; CH3.CH2.CH(NH2).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	EMF	NaClO4	20°C	1.0M	U		K1=9.7	1958PEd	(33914)1948

****

C4H9NO2 HL (2590)
N-Acetylhydroxylamine ethyl ether; CH3.CO.NH.O.C2H5

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	EMF	NaClO4	25°C	1.00M	U		K1=13.33 B2=24.98 K3=11.87	1978SSe	(34035)1949

****

C4H9NO3 HL Threonine CAS 72-19-5 (48)
2-Amino-3-hydroxybutanoic acid; H2N.CH(CH(OH).CH3)COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	EMF	NaClO4	20°C	1.0M	U		K1=8.6	1958PEd	(34301)1950

****

C4H9N3O3 HL (6027)
Glycylglycine hydroxamic acid; H2N.CH2.CO.NH.CH2.CO.NHOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KCl	25°C	0.20M	C		B2=18.90 B3=22.22, B(Fe2L)=16.58 B(FeH2L2)=30.16 B(FeH-2L2)=-3.99 B(FeH2L3)=36.23	1989BMc	(34427)1951

****

C4H9N3O4 H2L CAS 39158-78-0 (4271)

Iminodiacethydroxamic acid; HN(CH2.CO.NH.OH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaClO4	20°C	0.10M	U		K1=14.80 B(Fe2L3)=44.0	1972KMb (34430)1952	

****

C4H10N2O3 HL CAS 4475-93-8 (5892)
Threoninehydroxamic acid;
2-Amino-N,3-dihydroxybutanamide;CH3.CH(OH).CH(NH2).CO.NHOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KCl	25°C	0.50M	C		B2=21.37 B3=27.76 B(FeHL)=16.90 B(FeH2L2)=32.37 B(FeHL2)=28.55	1994LEa (34602)1953	

B(FeHL3)=34.89; B(FeH2L3)=41.16; B(FeH3L3)=46.03; B(FeH-2L2)=22.34
B(FeH-1L3)=19.23

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	NaCl	25°C	0.2M	U	I	K1=11.79 B2=19.03	1994SKb (34603)1954	

Also data for 43% v/v MeOH/H2O, 52% v/v EtOH/H2O, 59% v/v i-PrOH/H2O,
61% v/v dioxane/H2O.

****

C4H11NO8P2 H5L CAS 2439-99-8 (2129)
N-Carboxymethyl-N,N-bis(methylenephosphonic acid); HOOC.CH2.N(CH2.PO3H2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KNO3	25°C	0.10M	U		K1=14.87 K(Fe+HL)=8.82 B(Fe(OH)L)=21.84 B(Fe(OH)2L)=26.95	1973KSg (35106)1955	
Fe+++	gl	KNO3	25°C	0.10M	U		K1=14.65 K(Fe+HL)=8.65 K(FeLOH+H)=7.20	1965WRa (35107)1956	

****

C4H11N3O2 HL CAS 471915-94-3 (8550)
2,4-Diamino-N-hydroxybutanamide;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KCl	25°C	0.20M	C		B(FeHL)=22.06 B(FeH3L2)=45.14 B(FeH2L2)=38.36	2002ECa (35177)1957	

****

C4H11O2PS2 H3L CAS 298-06-6 (210)

O,O'-Diethyldithiophosphoric acid; (C2H5O)2P(S)SH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	EMF	mixed	25°C	90%	U			1984GGa	(35230)1958
							B3=17.82		

Medium: 90% 2-propanol/H20, 0.1 M NaClO4

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sol	none	25°C	0.0	U			1984HAa	(35231)1959
							B3=4.29		

****

C4H13N3 L Dien CAS 111-40-0 (584)
1,4,7-Triazaheptane, 2,2'Iminobis(ethylamine), diethylenetriamine;
NH2.(CH2)2.NH.(CH2)2.NH2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	NaNO3	25°C	0.10M	C		K1=18.76	2002MDa	(35781)1960
							B(FeH-1L)=15.18		
							B(FeH-2L)=10.91		

K(Fe+L+B(OH)4=FeL(H2BO4)+2H)=24.52, K(2Fe+2L+B(OH)4=Fe2L2(BO4)+4H)=43.97

****

C4H14N2O4P2 H2L CAS 37107-07-6 (4287)
Ethylenebis(iminomethylenephosphonous acid)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KNO3	25°C	0.10M	U		K1=10.29	1971MMh	(35830)1961

****

C4H14N2O6P2 H2L EDDPO CAS 1733-49-9 (2435)
1,2-Diaminoethane-N,N'-bis(methylenephosphonic) acid; (H2O3P.CH2.NH.CH2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	EMF	KCl	25°C	0.10M	C		K1=24.65	2002MNa	(35878)1962
							B(FeHL)=31.75		
							B(Fe2L)=28.40		
							B(FeH2L)=37.40		
							B(Fe2HL)=43.70		

Also other constants

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KCl	25°C	0.10M	U		K1=>10	1965DKb	(35879)1963

****

C5H2O2F6 HL HFA CAS 1522-22-1 (195)
1,1,1,5,5,5-Hexafluoropentane-2,4-dione; F3C.CO.CH2.CO.CF3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	dis	NaClO4	25°C	4.0M	C		K1=2.7 B2= 6.80	1986SIc	(35924)1964
							B3=9.6		

K(Fe+3L=FeL3(org))=13.2
Method: distribution from 4.0 M NaClO4 into CCl4.

Fe+++ dis NaClO4 25°C 4.0M C K1=2.7 B2= 6.80 1985IIa (35925)1965
B3=9.8
Method: extraction into CCl4; analysis by spectrophotometry.
K(Fe+3HL(org)=FeL3(org)+3H)=2.7.
****
C5H2O5 H2L Croconic acid CAS 488-86-8 (1643)
4,5-Dihydroxycyclopent-4-ene-1,2,3-trione;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp NaClO4 25°C 0.10M U I K1=4.78 1971AKd (35941)1966
K1(I=0.01)=5.06, K1(I=0.05)=4.88, K1(I=0.5)=4.60
****
C5H5N L Pyridine CAS 110-86-1 (31)
Pyridine, Azine;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp non-aq 25°C 100% C 2003TPa (36633)1967
K(FeP+L)=4.2
Medium: CH2Cl2. P is 2,3,12,13-tetrakis(trifluoromethyl)-5,10,15,20-
tetraphenylporphyrin.

Fe+++ sp non-aq 25°C 100% U M 1996VSa (36634)1968
K(L[Fe((DMG)BPh2)2]2O+L)=-0.7
Medium: CH2Cl2. Also data for L=CH3CN (K=1.6), 4-Nitrophthalonitrile (K=2.3)
Tetracyanoethylene (K=3.7), 1-Methylimidazole (K=3.8), and others.

Fe+++ sp alc/w 25°C 80% U M 1993HPa (36635)1969
K(FeP+L)=2.65
Medium: 80%MeOH/H2O. P: porphyrin microperoxidase-8. Data also for L=4-CN-py
(1.4), 4-Me-py (2.8), 4-NH2-py (4.17), 2-Me-py (<1), 4-Me2N-py (4.58). pH=7.

Fe+++ sp alc/w 25°C 80% U M 1993MBb (36636)1970
K(FeP+L)=2.73
Medium: 80%MeOH/H2O. P: porphyrin microperoxidase-8. Also data for aniline
K=2.67

Fe+++ sp non-aq 25°C 100% U M 1991KTa (36637)1971
K(FeAB+L=FeABL)=1.9
K(FeAC+L=FeACL)=2.0
Medium: benzonitrile, 0.2 M TBA(PF6).A=Octaethylporphyrin, B=C6HF4, C=C6F5
****
C5H5NO HL 2-Pyridinol CAS 142-08-5 (1890)
2-Hydroxypyridine, Pyridin-2-one;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo

```
--------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 1.00M U                      1984TMa (36694)1972
                                        K(Fe+HL=FeL+H)=0.75
--------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C  1.0M C                      1976MPe (36695)1973
                                        K(Fe+HL=FeL+H)=1.3
********************************************************************************
C5H5NO                  L    3-Pyridinol      CAS 109-00-2  (1475)
3-Hydroxypyridine; C5H4N.OH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      gl  NaClO4 25°C 0.10M U                      1998CWa (36708)1974
                                        K(Fe(CN)5(H2O)+L)=3.86
Medium: 0.1 M LiClO4, pH=5
--------------------------------------------------------------------------------
Fe+++      gl  NaClO4 25°C 1.00M C        K1=3.7        1980TMc (36709)1975
                                        K(Fe+HL=FeL+H)=-1.40
--------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C  1.0M C                      1976MPe (36710)1976
                                        K(Fe+HL=FeL+H)=-0.68
********************************************************************************
C5H5NO                 HL    4-Pyridinol      CAS 626-64-2  (1876)
4-Hydroxypyridine, Pyridin-4-one;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      kin NaClO4 25°C 0.10M U                      1998CWa (36713)1977
                                        K(Fe(CN)5(H2O)+L)=2.23
Medium: 0.1 M LiClO4, pH=5
--------------------------------------------------------------------------------
Fe+++      gl  NaClO4 25°C 1.00M C        K1=2.1        1980TMc (36714)1978
                                        K(Fe+HL=FeL+H)=-1.37
********************************************************************************
C5H5NOS                 L                    CAS 23003-22-7  (2904)
3-Hydroxy-2-mercaptopyridine; C5H3N(OH)(SH)
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      sp  alc/w  20°C  40%  C                      2000HAa (36726)1979
                                        K(Fe+H2L=FeHL+H)=2.10
                                        K(Fe+HL)=8.20
Medium: 40% v/v EtOH/H2O, 0.10 M NaClO4.
********************************************************************************
C5H5NO2                HL                    CAS 13161-30-3  (5582)
1-Hydroxypyridin-2(1H)-one, 2-Hydroxypyridine 1-oxide;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      gl  KCl    25°C 0.10M U        K1=10.61  B2=20.11  1993LMc (36753)1980
```

```
                                        K3=7.1
--------------------------------------------------------------------------------
Fe+++      sp  oth/un 25°C 0.10M C        K1=10.3   B2=19.30  1985SRb (36754)1981
                                        K3=7.6
********************************************************************************
C5H5NO2                HL                     CAS 16867-04-2  (2316)
2,3-Dihydroxypyridine, 3-Hydroxypyridin-2(1H)-one; C5H3N(OH)2
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      sp  alc/w  20°C  40%  C                        2000HAa (36785)1982
                                        K(Fe+H2L=FeHL+H)=-0.15
                                        K(Fe+HL)=7.35
Medium: 40% v/v EtOH/H2O, 0.10 M NaClO4.
--------------------------------------------------------------------------------
Fe+++      sp  oth/un 25°C 0.10M C        K1=11.7   B2=21.50  1985SRb (36786)1983
                                        K3=8.1
--------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C  1.0M C                     1976MPe (36787)1984
                                        K(Fe+HL=FeL+H)=2.51
--------------------------------------------------------------------------------
Fe+++      sp  KCl    25°C 1.00M U    M                1972CAb (36788)1985
                                        K(Fe+Cl+HL)=12.13
Medium: 1.0 M HCl
********************************************************************************
C5H5NO2                HL                     CAS 35940-93-3  (3618)
3-Furancarboxaldehyde oxime  (3-Furfuraldoxime); C4H3O.CH(:N.OH)
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      sp  diox/w 21°C  40%  U  I     K1=11.92         1978GMd (36816)1986
--------------------------------------------------------------------------------
Fe+++      gl  diox/w 15°C  75%  U  I     K1=10.91  B2=19.80  1963ASa (36817)1987
                                        K3=6.88
Medium:75% dioxan, 0-0.104 M NaClO4. At 25 C:K1=12.64,K2=10.80,K3=11.50;
Also 35 C. DH(K1)-95.7 kJ mol-1,DS=-78 J K-1 mol-1; DH(K2)-216; DH(K3)=-478
********************************************************************************
C5H5NO2                HL                     CAS 1121-23-9  (2315)
3-Hydroxypyridin-4(1H)-one;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      sp  oth/un 25°C 0.10M C        K1=14.2   B2=25.80  1985SRb (36826)1988
                                        K3=9.3
********************************************************************************
C5H5NO3               H2L                     CAS 99110-85-7  (2195)
1,4-Dihydroxy-2-pyridinone;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
```

```
Fe+++      gl  KCl    25°C 0.10M C        B2=21.31       1992CMc (36842)1989
                                          B(FeHL)=18.5
                                          B(FeL2H)=25.62
                                          B(FeH2L2)=34.26
                                          B3=28.18
B(FeHL3)=35.02, B(FeH2L3)=41.35
-------------------------------------------------------------------------------
Fe+++      sp  NaClO4 26°C 0.10M C                        1987KOb (36843)1990
                                          B3=29.9
*******************************************************************************
C5H5O2F3               HL                     CAS 367-57-7  (163)
1,1,1-Trifluoropentane-2,4-dione; CF3.CO.CH2.CO.CH3
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C  0.5M C        K1=6.60        1998BLa (37053)1991
-------------------------------------------------------------------------------
Fe+++      gl  alc/w  25°C  75%  C        K1=5.56   B2=11.02  1998ERa (37054)1992
                                          B3=13.39
Medium: 75% v/v EtOH/H2O, 0.10 M KCl
-------------------------------------------------------------------------------
Fe+++      dis NaClO4 25°C  4.0M C  I     K1=7.7    B2=14.40  1986SIc (37055)1993
                                          B3=19.8
                                          K(Fe+3L=FeL3(org))=24.0
Method: distribution from 4.0 M NaClO4 into CCl4.
Using MIBK, K(Fe+3L=FeL3(org))=24.4
-------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 0.50M C                        1983HOb (37056)1994
                                          K(Fe+HL=FeL+H)=0.53
-------------------------------------------------------------------------------
Fe+++      dis NaClO4 25°C 4.00M U        K1=7.67   B2=14.40  1982SIa (37057)1995
                                          B3=19.84
*******************************************************************************
C5H6N2OS                L                      CAS 2361-27-5  (2642)
2-Thiophenecarboxylic acid hydrazide; C4H3S.CO.NH.NH2
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 0.10M U                        1981BPc (37211)1996
                                          B3=14.25
                                          K(Fe+3(H-1L))=39.25
*******************************************************************************
C5H6N2O2               HL                     CAS 3326-71-4  (2607)
2-Furanecarboxylic acid hydrazide; C4H3O.CONH.NH2
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 0.10M U                        1981BPc (37304)1997
                                          B3=14.35
                                          K(Fe+3(H-1L))=39.30
```

```
-------------------------------------------------------------------------------
Fe+++      sp  NaClO4 20°C 0.10M U        B2=10.48       1979BBc (37305)1998
                                         B3=14.35
*******************************************************************************
C5H6O4                H2L                      CAS 598-10-7  (70)
Cyclopropane-1,1-dicarboxylic acid; C3H4(COOH)2
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe+++      kin NaClO4 25°C 0.50M C        K1=8.74        1977CCb (37386)1999
*******************************************************************************
C5H6O5                H2L    Ketoglutaric     CAS 328-50-7  (1146)
2-Ketoglutaric acid; HOOC.CH2.CH2.CO.COOH
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe+++      gl  KCl    25°C 0.10M U        K1=5.2    B2=8.20   1975SDa (37473)2000
*******************************************************************************
C5H7NO3                HL                       CAS 29917-12-2  (5671)
2,3,4-Pentanetrione-3-oxime;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe+++      EMF oth/un 25°C 0.50M U        K1=5.90   B2=11.37  1984RCb (37513)2001
                                         B3=16.75
*******************************************************************************
C5H7NO3                HL                         (7204)
N-Hydroxyglutarimide;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe+++      sp  NaClO4 20°C 0.10M U        K1=8.19   B2=14.67  1981KJb (37538)2002
                                         B3=19.34
*******************************************************************************
C5H7NO6P2              H4L                      CAS 186599-36-0  (7613)
2,6-Pyridinediphosphonic acid;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe+++      gl  KNO3   25°C 0.10M C        K1=20.87  B2=28.68  1998CMb (37563)2003
                                         K(Fe(OH)2L+H)=8.36
                                         K(Fe(OH)L+H)=6.40
                                         K(FeL+H)=4.06
                                         K(FeL2+H)=3.86
*******************************************************************************
C5H8N2                  L                       CAS 1759-84-0  (173)
1,2-Dimethylimidazole; C3H2N2(CH3)2
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
```

```
Fe+++      sp  non-aq 25°C 100%  U    M                  1991UHa (37633)2004
                                        K(FeAOCH3+2L=FeA(OCH3)L2)=0.87
Medium: CH2Cl2. A=Octaethylporphine
********************************************************************************
C5H8O2                 HL    Acetylacetone    CAS 123-54-6  (164)
Pentane-2,4-dione; CH3.CO.CH2.CO.CH3
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C  0.5M C        K1=10.5        1998BLa (37963)2005
--------------------------------------------------------------------------------
Fe+++      gl  alc/w  25°C  75%  C  I     K1=10.85  B2=20.00  1998ERa (37964)2006
                                        B3=22.4
Medium: 75% v/v EtOH/H2O, 0.10 M KCl
In H2O, 0.10 M KCl: K1=10.76, B2=19.6, B3=26.8
--------------------------------------------------------------------------------
Fe+++      dis NaClO4 25°C  4.0M C        K1=11.4   B2=20.80  1986SIc (37965)2007
                                        B3=26.7
                                        K(Fe+3L=FeL3(org))=31.4
Method: distribution from 4.0 M NaClO4 into CCl4.
--------------------------------------------------------------------------------
Fe+++      dis NaClO4 25°C 0.10M C        K1=10.5        1986SNa (37966)2008
Method: rate of distribution of volatile ligand between aqueous phase and
inert gas phase. K(H+L)=9.17 assumed.
--------------------------------------------------------------------------------
Fe+++      dis NaClO4 25°C  4.0M C        K1=11.4   B2=20.70  1985IIa (37967)2009
Method: extraction into CCl4; analysis by spectrophotometry.
K(Fe+3HL(org)=FeL3(org)+3H)=0.5.
--------------------------------------------------------------------------------
Fe+++      gl  mixed  25°C  80%  C        K1=10.61  B2=20.30  1985MLa (37968)2010
                                        B3=27.98
Medium: 80% DMSO/H2O
--------------------------------------------------------------------------------
Fe+++      oth NaClO4 25°C  0.0  C  I   T K1=9.25   B2=18.0   1982SLc (37969)2011
                                        B3=24.5
IUPAC evaluation
--------------------------------------------------------------------------------
Fe+++      sp  oth/un 25°C 1.00M U                    1971FNa (37970)2012
                                        K(Fe+HL=FeL+H)=1.55
--------------------------------------------------------------------------------
Fe+++      dis oth/un 20°C 0.10M U        K1=9.17   B2=18.34  1971KOa (37971)2013
--------------------------------------------------------------------------------
Fe+++      vlt diox/w 25°C  50%  U        K2=9.7         1969SMj (37972)2014
                                        K3=7.6
Medium: 50% dioxan, 0.5 M NaClO4
--------------------------------------------------------------------------------
Fe+++      vlt NaClO4 25°C 0.10M U        K2=8.4         1963PBa (37973)2015
                                        K3=6.5
--------------------------------------------------------------------------------
Fe+++      gl  oth/un 30°C  ->0  U        K1=9.8    B2=18.8   1955IFa (37974)2016
```

K3=7.4

Fe+++ sp oth/un 25°C ->0 U K1=11.4 B2=22.10 1953BAa (37975)2017
K3=4.6

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C5H8O4 H2L CAS 595-46-0 (1144)
Dimethylmalonic acid; HOOC.C(CH3)2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	kin	NaClO4	25°C	0.50M	C		K1=7.16	1977CCb	(38211)2018

****

C5H8O4 H2L Glutaric acid CAS 110-94-1 (420)
Pentanedioic acid; HOOC.CH2.CH2.CH2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	NaClO4	20°C	1.00M	M		K1=4.12 B2=6.93	1989MKa	(38319)2019
							K(Fe+HL)=2.50		
							K(Fe+2HL)=5.13		
							K(Fe+3HL)=6.18		
Fe+++	gl	NaClO4	25°C	0.10M	U		K1=7.72 B2=13.12	1973RMb	(38320)2020
Fe+++	sp	NaClO4	25°C	0.50M	U		K1=6.78	1968DMc	(38321)2021

Medium: LiClO4

****

C5H8O7 H2L CAS 40120-71-6 (3022)
2,3,4-Trihydroxypentanedioic acid, Trihydroxyglutaric acid; HOOC.(CH(OH))3.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	oth/un	?	?	U		K1=22.68	1972GTc	(38421)2022
Fe+++	oth	none	?	0.0	U		K1=0.92	1956FGa	(38422)2023

****

C5H9NO2 HL Proline CAS 147-85-3 (44)
Pyrrolidine-2-carboxylic acid; C4H8N.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	EMF	NaClO4	20°C	1.0M	U		K1=10.0	1958PEd	(38614)2024

****

C5H9NO3 HL Hydroxyproline CAS 51-35-4 (416)
4-Hydroxy-2-pyrrolidinecarboxylic acid; C4H7N(OH)(COOH)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	EMF	NaClO4	20°C	1.0M	U		K1=9.0	1958PEd	(38731)2025

****

C5H9NO4 H2L Glutamic acid CAS 56-86-0 (22)
2-Aminopentanedioic acid; H2N.CH(CH2.CH2.COOH)COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	NaNO3	25°C	0.50M	C		K1=11.82 B2=19.80 B(FeHL)=15.38 B(FeH-1L)=8.58 B(Fe2H-2L)=10.51	1997DJb (39081)	2026
By spectrophotometry: K1=11.80, B2=19.76, B(FeHL)=15.36, B(FeH-1L)=8.56, B(FeH-1L2)=16.44.									
Fe+++	gl	NaClO4	25°C	1.0M	M		K1=4.41 B2= 4.09 K(Fe+2HL)=1.48 K(Fe+3HL)=2.36	1991MKa (39082)	2027
Fe+++	EMF	NaClO4	20°C	1.0M	U		K1=12.1	1958PEd (39083)	2028

****

C5H9NO4 H2L MIDA CAS 4408-64-4 (190)
N-Methyliminodiethanoic acid; CH3.N(CH2.COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KNO3	25°C	0.5M	C		K1=10.99 B2=20.72 B(FeH-1L)=7.87 B(FeH-2L)=4.70 B(Fe2L2)=23.75 B(Fe2H-2L2)=18.28	1999SEb (39254)	2029

****

C5H9NO5 H3L (5231)
N-Hydroxyglutamic acid; HOOCCH2CH2CH(NHOH)COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaClO4	20°C	0.10M	U		B2=22.16 K(Fe+HL)=6.54 K(Fe+HL+L)=17.80	1981KJb (39319)	2030

****

C5H9N3 L Histamine CAS 51-45-6 (103)
4(5)-(2'-Aminoethyl)imidazole; C3H3N2.CH2.CH2.NH2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	NaNO3	25°C	0.10M	U		B2=7.05	1993GAa (39537)	2031
Fe+++	gl	KCl	25°C	.058M	U	T	K1=3.72	1961SMa (39538)	2032
0 C: K1=3.76; 45 C: K1=3.15									

****

C5H10N2O4 HL CAS 1955-67-5 (6736)
2-Aminopentanoic-5-hydroxamic acid; HOOC.CH(NH2).CH2.CH2.CO.NOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp NaCl 25°C 0.15M C K1=21.91 2002SMb (40078)2033
B(FeHL)=23.06
B(FeHL2)=41.02
B(FeH-2L)=17.78
B(FeH-2L2)=31.39
B(FeH-2L3)=45.07.

Fe+++ gl KCl 25°C 0.20M C 1993FBa (40079)2034
B(FeHL)=18.92
B(Fe2HL)=31.70
B(Fe2L)=24.10
B(Fe2H-1L)=14.70
B(Fe2H2L)=36.65.
****
C5H10N2O4 H2L (7205)
Glutarodihydroxamic acid; HONH.CO.CH2.CH2.CH2.CO.NHOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl NaNO3 25°C 0.15M C K1=17.09 1986BGc (40083)2035
B(FeHL)=18.97
B(Fe3L4)=69.95
B(Fe2L3)=4.86
B(FeH-1L3)=39.84
B(FeH-2L)=-12.79, B(Fe2H-2L3)=30.15

Fe+++ sp NaClO4 20°C 0.10M U 1981KJb (40084)2036
K(Fe+HL)=11.61
B(Fe2(OH)L2)=56.74
K(2Fe+2HL+2L)=66.34
****
C5H10OS2 HL CAS 110-50-9 (591)
(Butoxy)dithiomethanoic acid; CH3.CH2.CH2.CH2O.CSSH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ dis oth/un 25°C 0.25M U 1982SAa (40157)2037
B3=17.2
****
C5H10O3 HL CAS 53103-75-6 (4295)
2-Ethoxypropanoic acid; CH3.CH(OC2H5).COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp oth/un ? ? U K1=2.92 B2=5.64 1970PKd (40245)2038
****
C5H11NO2 HL Valine CAS 72-18-4 (43)

2-Amino-3-methylbutanoic acid; H2N.CH(CH(CH3)2)COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	EMF	NaClO4	20°C	1.0M	U		K1=9.6	1958PEa	(40707)2039

****

C5H11NO2 HL (7503)
N-(2-Propyl)acetohydroxamic acid; CH3CON(C3H7)OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KCl	25°C	0.20M	C		K1=12.04 B2=21.94 B3=29.64	1998FKa	(40901)2040
							K(Fe+HL=FeL+H)=2.78		

****

C5H11NO2S HL Methionine CAS 63-68-3 (42)
2-Amino-4-(methylthio)butanoic acid; H2N.CH(CH2.CH2.S.CH3)COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	oth	NaClO4	35°C	0.10M	C		K1=7.95 B2=12.65	1996TEa	(41092)2041
Method: paper electrophoresis.									
Fe+++	dis	NaClO4	35°C	0.10M	U		K1=7.95	1994TEa	(41093)2042
Methd: Paper electrophoresis; Medium: 0.1 HClO4.									
Fe+++	EMF	NaClO4	20°C	1.0M	U		K1=9.1	1958PEd	(41094)2043

****

C5H11NO2S H2L D-Penicillamine CAS 52-67-5 (1323)
D-2-Amino-3-mercapto-3-methylbutanoic acid; (CH3)2C(SH)CH(NH2)COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KNO3	37°C	0.15M	M	T	K1=11.02 B2=15.79	1979ZJa	(41185)2044
At 20 C, 0.15 M KNO3, K1=11.27, B2=16.25.									

****

C5H11NO2S H2L Penicillamine CAS 52-66-4 (350)
DL-2-Amino-3-mercapto-3-methylbutanoic acid; (CH3)2C(SH)CH(NH2)COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaClO4	25°C	1.00M	U		K(Fe+H3L=FeHL+2H)=-1.20	1995SJa	(41259)2045
							K(Fe2+H3L=Fe2HL+2H)=-0.42		
Medium: LiClO4									
Fe+++	kin	NaClO4	25°C	0.50M	C		K1=11.15 K(Fe+H2L=FeL+2H)=-1.17	1983BMc	(41260)2046
Method: spectrophotometry.									

****

C5H11NO2S2 HL CAS 1528-32-9 (2127)
Di(2-hydroxyethyl)dithiocarbamic acid; (HO.CH2.CH2)2N.CSSH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	gl	NaClO4	25°C	1.00M	U		K1=5.70	B2=10.51	1996BCg (41297)	2047
							B3=16.32			

****
C5H12NO4P HL CAS 51276-47-2 (5704)
2-Amino-4-(methylhydroxyphosphoryl)butanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	NaClO4	23°C	0.10M	U		K1=10.04	1990YTa (41444)	2048

****
C5H12N2O L Diethylurea CAS 623-76-7 (2022)
1,3-Diethylurea; (CH3.CH2.NH)2.CO

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	vlt	NaClO4	25°C	0.20M	U		K1=-0.22	B2=0.08	1985MCc (41459)	2049
							K3=0.46			
							K4=0.66			
							K5=-0.097			
Fe+++	vlt	NaClO4	20°C	0.20M	U		K1=-0.2	B2=0.1	1980MCa (41460)	2050
							B3=0.5			
							B4=1.2			
							B5=1.1			

****
C5H12N2O2 HL Ornithine CAS 1069-31-4 (46)
2,5-Diaminopentanoic acid; H2N.CH2.CH2.CH2.CH(NH2)COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	NaClO4	20°C	1.0M	U		K1=8.7	1958PEd (41575)	2051

****
C5H12N2O2 HL CAS 36207-49-5 (834)
2-Amino-N-hydroxypentanamide; CH3.CH2.CH2.CH(NH2).CO.NH.OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	gl	KCl	25°C	0.50M	C		B2=22.90		1991LEa (41591)	2052
							B3=27.58			
							B(FeHL)=16.91			
							B(FeHL2)=28.50			
							B(FeH2L2)=32.84			

B(Fe2H-2L2)=21.87; B(FeHL3)=35.03; B(FeH2L3)=41.54; B(FeH-1L3)=18.48;
B(Fe2H-1L3)=35.17; B(FeH-1L2)=15.65

****

C5H12N2O2S HL Met-hydroxamic CAS 19253-87-3 (5992)
2-Amino-4-(methylthio)butanehydroxamic acid, Methionine hydrox.a.;
CH3.S.CH2.CH2.CH(NH2).CO.NHOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	gl	NaCl	30°C	0.20M	U	I	K1=11.42	B2=18.88	1997SKb	(41605)2053

In 42% v/v MeOH/H2O, 0.20 M NaCl, K1=11.6, K2=8.54. In 59% v/v i-PrOH/H2O, 0.20 M NaCl, K1=12.40, K2=8.74.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaCl	25°C	0.15M	U		K1=12.73	1986EMa	(41606)2054
							B(FeHL)=16.26		
							B(FeHL2)=26.12		
							B(FeH2L2)=30.94		
							B(Fe2L3)=38.24		

****

C5H13NO8P2 H4L (3714)
N-(2'-Carboxyethyl)iminobis(methylenephosphonic acid)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KNO3	25°C	0.10M	U		K1=16.3	1965WRa	(41769)2055

****

C5H13N2O2+ HL CAS 14122-13-5 (8321)
Betaine hydroxamic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	sp	NaCl	25°C	1.0M	C		K1=7.28	B2=13.41	1984BKb	(41788)2056
							B3=16.46			

****

C5H14NO5P H2L CAS 5994-60-5 (1302)
N,N'-Bis(2-hydroxyethyl)aminomethylphosphonic acid; (HO.CH2.CH2)2N.CH2.PO3H2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	NaClO4	20°C	0.10M	U			1970KMa	(41844)2057
							K(Fe+OH+HL)=19.19		
							K(Fe(OH)HL=Fe(OH)L+H)=-4.28		
							K(FeOHL=Fe(OH)H-2L+2H)=-13.67		
							K(Fe(OH)L+2OH)=14.21		

****

C6H2O4Cl2 H2L Chloranilic acd CAS 87-88-7 (1281)
3,6-Dichloro-2,5-dihydroxy-1,4-benzoquinone;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	sp	oth/un	35°C	0.15M	U	T H	K1=5.75	B2=9.83	1967CAa	(42049)2058

K1=5.91(15 C),5.81(25 C); B2=9.95(15 C),9.84(25 C). DH(K1)=-14.0 kJ mol-1, DS=-64.4(?) J K-1 mol-1; DH(B2)=-10.9, DS=-15.1(?)

Fe+++ sp oth/un 35°C 0.15M U T H K1=5.16 B2=9.24 1967CAa (42050)2059
K1=5.82(15 C),5.51(25 C); B2=9.74(15 C),9.47(25 C)
DH(K1)=-61.4 kJ mol-1,DS=102(?) J K-1 mol-1; DH(B2)=-10.9,DS=-30.9(?)
****
C6H3N3O7 HL Picric acid CAS 88-89-1 (593)
2,4,6-Trinitrophenol; HO.C6H2(NO2)3

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp oth/un 21°C 0.40M U K1=1.80 1955BKa (42110)2060
B3=3.10
Medium:0.2-0.9(some EtOH)
****
C6H4N2O5 HL CAS 50-28-5 (505)
2,4-Dinitrophenol; HO.C6H3(NO2)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl non-aq 25°C 100% C K1=3.26 B2= 5.64 1984FMa (42228)2061
Medium: DMSO, 0.10 M KClO4.

Fe+++ sp oth/un 21°C 0.40M U K1=1.05 1955BKa (42229)2062
B3=3.27
Medium:0.2-0.7(some EtOH)
****
C6H4O8Br2S2 H4L (4396)
4,5-Dibromo-1,2-dihydroxybenzene-3,6-disulfonic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp KNO3 20°C 0.10M U K1=21.1 B2=35.70 1971AHa (42331)2063
K3=10.5
****
C6H5NO2 HL Picolinic acid CAS 98-98-6 (391)
2-Pyridine-carboxylic acid; C5H4N.COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl NaClO4 25°C 0.10M C 1986LLb (42535)2064
K3=4.37

Fe+++ gl NaClO4 35°C 1.00M U T K1=5.66 1984PHa (42536)2065
B(Fe(OH)L2)=25.19
B(Fe2(OH)2L4)=52.79

Fe+++ sp NaClO4 25°C 2.67M U T H 1982BPb (42537)2066
K(Fe+HL=FeL+H)=0.45
Data also available when T=35, 50, 65 and 75. DH=8.4 kJ mol-1

```
Fe+++      gl  KCl    25°C 0.50M U    M   K1=6.02        1980EEa (42538)2067
                                           K(Fe(OH)+HL=FeL+H2O)=3.32
ternary complex with pyridoxine (pyridoxol, vitamin B6)
--------------------------------------------------------------------------------
Fe+++      gl  NaClO4 20°C 0.10M U         B2=12.88       1964TIa (42539)2068
                                           B(FeL2(OH))=23.92
                                           B(Fe2L4(OH)2)=50.72
--------------------------------------------------------------------------------
Fe+++      EMF NaNO3  25°C 0.10M U         K2=12.80       1960ANa (42540)2069
                                           B(FeL2(OH))=23.84
                                           B(Fe2L4(OH)2)=50.76
                                           K(FeL2OH+H)=2.96
                                           K(2(FeL2OH=Fe2L4(OH)2)=3.06
********************************************************************************
C6H5NO2                HL    Nicotinic acid   CAS 59-67-6  (419)
3-Pyridine-carboxylic acid; C5H4N.COOH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      gl  NaClO4 35°C 1.00M U         K1=4.52        1984PHa (42671)2070
                                           B(Fe2L3)=16.11
********************************************************************************
C6H5NO3                HL    2-Nitrophenol    CAS 88-75-5  (510)
2-Nitrohydroxybenzene; HO.C6H4.NO2
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      gl  NaClO4 25°C 0.10M U         K1=5.99        1966JMb (42735)2071
********************************************************************************
C6H5NO3               H2L                     CAS 874-24-8  (4356)
3-Hydroxypyridine-2-carboxylic acid; C5H3N.(OH)(COOH)
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      sp  alc/w  25°C  40%  C         K1=11.85  B2=23.70  1993ABe (42749)2072
                                           K(Fe+HL)=12.03
                                           K(FeL+HL=FeL2+H)=2.70
                                           K(FeL+H)=2.53
                                           K(Fe+LH2=FeHL+H)=2.72
Medium: 40% v/v MeOH/H2O, 0.10 M NaClO4.
********************************************************************************
C6H5NO3                HL    3-Nitrophenol    CAS 554-84-7  (739)
3-Nitrophenol; HO.C6H4.NO2
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 0.10M U         K1=5.93        1969DMb (42770)2073
--------------------------------------------------------------------------------
Fe+++      sp  KNO3   23°C 0.50M U  I      K1=6.69        1968MCb (42771)2074
In 0.027 M NaClO4: K1=7.05
```

```
--------------------------------------------------------------------------------
Fe+++      gl  NaClO4 25°C 0.10M U        K1=6.95        1966JMb (42772)2075
--------------------------------------------------------------------------------
Fe+++      sp  oth/un 25°C  0.0  U        K1=7.78        1955MIa (42773)2076
********************************************************************************
C6H5NO3                HL    4-Nitrophenol    CAS 100-02-7  (454)
4-Nitrohydroxybenzene; HO.C6H4.NO2
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      gl  non-aq 25°C 100%  C        K1=7.04   B2=12.40  1984FMa (42801)2077
                                         B3=16.59
Medium: DMSO, 0.10 M KClO4.
--------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 0.10M U        K1=5.05        1969DMb (42802)2078
--------------------------------------------------------------------------------
Fe+++      sp  KNO3   23°C 0.50M U  I     K1=5.60        1968MCb (42803)2079
In 0.027 M NaClO4: K1=5.86
--------------------------------------------------------------------------------
Fe+++      gl  NaClO4 25°C 0.10M U        K1=5.74        1966JMb (42804)2080
--------------------------------------------------------------------------------
Fe+++      sp  oth/un 25°C  0.0  U        K1=5.74        1955MIa (42805)2081
********************************************************************************
C6H5NO4                H2L    3-Nitrocatechol  CAS 6665-98-1  (2685)
1,2-Dihydroxy-3-nitrobenzene; O2N.C6H3(OH)2
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      gl  KCl    25°C 0.10M M        K1=15.71  B2=28.92  1986HAc (42860)2082
********************************************************************************
C6H5NO4                H2L    4-Nitrocatechol  CAS 3316-09-4  (890)
1,2-Dihydroxy-4-nitrobenzene; O2N.C6H3(OH)2
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      gl  KCl    25°C 0.10M M        K1=15.53  B2=28.63  1984HAc (42925)2083
                                         B3=38.22
--------------------------------------------------------------------------------
Fe+++      gl  oth/un 27°C 0.10M M        K1=17.08  B2=30.51  1978ASa (42926)2084
                                         K3=9.51
********************************************************************************
C6H5NO9S2              H4L                      (3710)
4-Nitroso-5,6-dihydroxybenzene-1,3-disulfonic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      sp  NaCl     ?  0.10M U        K1=16.42  B2=28.45  1967BHa (42973)2085
                                         K3=6.49
********************************************************************************
C6H5OBr                HL    2-Bromophenol    CAS 95-56-7  (3673)
```

2-Bromophenol; HO.C6H4.Br

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	NaClO4	25°C	0.10M	U		K1=6.98	1966JMb	(43004)2086
Fe+++	sp	oth/un	25°C	0.0	U		K1=7.19	1965EHb	(43005)2087

C6H5OBr HL 3-Bromophenol CAS 591-20-8 (3674)
3-Bromophenol; HO.C6H5.Br

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	NaClO4	25°C	0.10M	U		K1=7.65	1966JMb	(43009)2088

C6H5OBr HL 4-Bromophenol CAS 106-41-2 (456)
4-Bromophenol; HO.C6H4.Br

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	KNO3	23°C	0.50M	U	I	K1=7.72	1968MCb	(43019)2089
In 0.02 M NaClO4: K1=7.89									
Fe+++	gl	NaClO4	25°C	0.10M	U		K1=8.00	1966JMb	(43020)2090
Fe+++	sp	none	25°C	0.0	U		K1=8.10	1955MIa	(43021)2091

C6H5OCl HL 2-Chlorophenol CAS 95-57-8 (3671)
2-Chlorophenol; HO.C6H4.Cl

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaClO4	25°C	0.10M	U		K1=6.07	1969DMb	(43029)2092
Fe+++	gl	NaClO4	25°C	0.10M	U		K1=7.26	1966JMb	(43030)2093
Fe+++	sp	oth/un	25°C	0.0	U		K1=7.32	1965EHb	(43031)2094

C6H5OCl HL 3-Chlorophenol CAS 108-43-0 (3672)
3-Chlorophenol; HO.C6H4.Cl

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaClO4	25°C	0.10M	U		K1=6.88	1969DMb	(43039)2095
Fe+++	gl	NaClO4	25°C	0.10M	U		K1=7.52	1966JMb	(43040)2096
Fe+++	sp	oth/un	25°C	0.0	U		K1=7.89	1965EHb	(43041)2097

C6H5OCl HL 4-Chlorophenol CAS 106-48-9 (1631)

4-Chlorophenol; HO.C6H4.Cl

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaClO4	25°C	0.10M	U		K1=6.95	1969DMb (43051)	2098
Fe+++	gl	NaClO4	25°C	0.10M	U		K1=7.95	1966JMb (43052)	2099
Fe+++	sp	oth/un	25°C	0.0	U		K1=7.92	1965EHb (43053)	2100

****

C6H5OF HL 2-Fluorophenol CAS 367-12-4 (3678)

2-Fluorophenol; HO.C6H4.F

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	NaClO4	25°C	0.10M	U		K1=7.19	1966JMb (43057)	2101
Fe+++	sp	oth/un	25°C	0.0	U		K1=7.33	1965EHb (43058)	2102

****

C6H5OF HL 3-Fluorophenol CAS 372-20-3 (3679)

3-Fluorophenol; HO.C6H4.F

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	NaClO4	25°C	0.10M	U		K1=7.77	1966JMb (43061)	2103
Fe+++	sp	oth/un	25°C	0.0	U		K1=7.77	1965EHb (43062)	2104

****

C6H5OF HL 4-Fluorophenol CAS 371-41-5 (3680)

4-Fluorophenol; HO.C6H4.F

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	NaClO4	25°C	0.10M	U		K1=8.29	1966JMb (43065)	2105
Fe+++	sp	oth/un	25°C	0.0	U		K1=9.38	1965EHb (43066)	2106

****

C6H5OI HL 2-Iodophenol CAS 533-58-4 (3675)

2-Iodophenol; HO.C6H4.I

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	oth/un	25°C	0.0	U		K1=7.43	1965EHb (43068)	2107

****

C6H5OI HL 3-Iodophenol CAS 626-02-8 (3676)

3-Iodophenol; HO.C6H4.I

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	NaClO4	25°C	0.10M	U		K1=7.57	1966JMb (43070)	2108

```
**************************************************************************
C6H5OI                HL    4-Iodophenol     CAS 540-38-5  (3677)
4-Iodophenol; HO.C6H4.I
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe+++      sp  oth/un 25°C  0.0  U        K1=8.63        1965EHb (43072)2109
**************************************************************************
C6H6NO5P              H3L                    CAS 145432-83-3  (7384)
6-Phosphonopyridine-2-carboxylic acid; HOOC.C5H3N.PO3H2
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe+++      gl  KNO3   25°C 0.10M C        K1=15.97  B2=25.47  1998CMb (43222)2110
                                        K(Fe(OH)2L+H)=8.53
                                        K(Fe(OH)L+H)=3.25
                                        K(FeL2+H)=2.60
**************************************************************************
C6H6N2O               HL                     CAS 873-69-8  (1258)
Pyridine-2-aldoxime; C5H4N.CH:NOH
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe+++      sp  diox/w 21°C  40%  U  I     K1=12.19       1978GMd (43296)2111
--------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 0.50M U        K1=11.9   B2=23.3   1975CPc (43297)2112
                                        B3=32.6
                                        B(Fe2L)=14.2
                                        *K1=2.62
                                        *K2=3.15
*B(2,2)=3.20, *B(2,1)=5.77
--------------------------------------------------------------------------
Fe+++      gl  KNO3   24°C 0.10M U        K1=11.4   B2=21.70  1962BEa (43298)2113
                                        K3=8.4
--------------------------------------------------------------------------
Fe+++      gl  oth/un 25°C  0.0  U                  1962HIa (43299)2114
                                        K(FeL3+H)=3.5
**************************************************************************
C6H6N2O2              HL                      (8281)
3-Hydroxy-2-amidocarboxypyridine, Hydroxypicolinamide;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe+++      gl  KNO3   25°C 0.10M C        K1=8.70   B2=16.49  1990ARa (43375)2115
                                        K(FeL2+L)=6.39
**************************************************************************
C6H6N2O3              H2L                    CAS 2504-83-8  (1141)
Imidazolylpyruvic acid; C3H3N2.CH2.CO.COOH
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
```

```
------------------------------------------------------------------------------
Fe+++      gl  KCl    25°C 0.10M U        K1=8.7    B2=16.60  1975SDa (43452)2116
******************************************************************************
C6H6O                  HL    Phenol           CAS 108-95-2  (457)
Hydroxybenzene, phenol; C6H5.OH
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 0.10M U        K1=7.76        1969DMb (43535)2117
------------------------------------------------------------------------------
Fe+++      sp  KNO3   23°C 0.10M U                       1969LRa (43536)2118
                                        K(Fe+HL=FeL+H)=-2.17
------------------------------------------------------------------------------
Fe+++      sp  KNO3   23°C 0.50M U  I     K1=7.81        1968MCb (43537)2119
In 0.027 M NaClO4: K1=8.11
------------------------------------------------------------------------------
Fe+++      sp  oth/un 25°C  ->0  U        K1=8.20        1955MIa (43538)2120
******************************************************************************
C6H6O2                H2L    Catechol         CAS 120-80-9  (534)
1,2-Dihydroxybenzene, pyrocatechol; HO.C6H4.OH
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Fe+++      sp  KNO3   20°C 0.10M U        B2=35.0        1981NAc (43756)2121
                                        B3=44.2
------------------------------------------------------------------------------
Fe+++      gl  oth/un 27°C 0.08M M        K1=20.01  B2=34.70  1978ASa (43757)2122
                                        K3=9.06
------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 1.00M U T                     1973MPc (43758)2123
                                        K(Fe+H2L=FeL+2H)=-1.36
K(20 C)=-1.37, K(30 C)=-1.36
------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 0.10M U        K2=14.96       1969SZa (43759)2124
                                        K(FeL+H2L=FeL2+2H)=-7.65
                                        K(FeL2+H2L=FeL3+2H)=-13.8
                                        K3=9.5
******************************************************************************
C6H6O3                 HL    Maltol           CAS 118-71-8  (2442)
3-Hydroxy-2-methyl-4H-pyran-4-one;
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Fe+++      sp  NaClO4 26°C 0.10M C                       1987KOb (44083)2125
                                        B3=29.5
------------------------------------------------------------------------------
Fe+++      gl  NaClO4 25°C 2.00M U        K1=11.10  B2=20.40  1980GHa (44084)2126
                                        K3=8.05
                                        K(FeL(OH)+H)=3.8
                                        K(FeL(OH)2+2H)=3.9
```

K(2FeL+2OH=Fe2L2(OH)2)=24.0

Fe+++ sp NaClO4 20°C 0.10M U K1=11.5 B2=21.40 1968SHc (44085)2127
K3=8.3

****

C6H6O4 HL Kojic acid CAS 501-30-4 (1800)
5-Hydroxy-2-(hydroxymethyl)-4H-pyran-4-one;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	gl	KNO3	25°C	0.10M	U		K1=10.2	B2=19.0	1962MUb	(44211)2128
							K3=7.53			
							K((FeOHL)2+2H=2FeL)=3.92			
							K(Fe(OH)2L+2H=FeL)=7.40			
							K((Fe(OH)2L)2+4H=2FeL)=9.92			
							K(FeOHL+L=FeL)=3.16			
Fe+++	sp	oth/un	25°C	0.50M	U		K1=10.16	B2=18.45	1961MAa	(44212)2129
							K3=6.90			
Fe+++	sp	oth/un	20°C	0.0	U	I	B2=17.5		1961SLb	(44213)2130
							B3=24.6			
							K1=9.2(I=0.1), B2=16.8(I=0.2)			
Fe+++	EMF	KCl	21°C	0.10M	U		K1=9.2	B2=17.2	1959OKb	(44214)2131
							B3=24.4			
							Method: H electrode			

****

C6H6O4S H2L CAS 1333-39-7 (3686)
4-Hydroxybenzenesulfonic acid; HO.C6H4.SO3H

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	sp	KNO3	23°C	0.50M	U		K1=6.72		1968MCb	(44266)2132

****

C6H6O5S H3L CAS 7134-09-0 (3687)
3,4-Dihydroxybenzenesulfonic acid; (HO)2.C6H3.SO3H

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	gl	KNO3	30°C	0.10M	U		K1=>17	K2=14.0	1963MNa	(44282)2133
							K3=9.1			

****

C6H6O8S2 H4L Tiron CAS 149-45-1 (104)
4,5-Dihydroxybenzene-1,3-disulfonic acid; (HO)2.C6H2(SO3H)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	gl	KCl	25°C	0.20M	C	M	K1=18.61	B2=33.38	2002FCa	(44426)2134
							B3=44.44			

B(FeH-1L2)=27.4
B(FeAL)=28.21
B(FeA2L)=40.88
B(FeH-1AL)=23.68. A is acetohydroxamic acid.

Fe+++ sp NaClO4 25°C 1.00M U H 1996ZJa (44427)2135
K(FeL+H)=0.018
K(Fe+H2L=FeL+2H)=0.30
K(FeL2+H)<1.8
K(FeL+H2L=FeL2+2H)=-3.77
K(FeL3+H)=4.13, K(FeL2+H2L=FeL3+2H)=7.47. DH(Fe+H2L=FeL+2H)=-21 kJ mol-1, DS(Fe+H2L=FeL+2H)=-66 J K-1 mol-1.

Fe+++ kin NaClO4 25°C 1.00M U 1994CJa (44428)2136
K(Fe2(OH)2+H2L=Fe2(OH)2H2L)=3.81

Fe+++ sp NaClO4 22°C 0.30M C I K1=19.50 1993LCa (44429)2137
At I=1.0 M, K1=18.94; at I=2.0 M, K1=18.22.
Data for 0.1-2.9 M NaClO4 and 0-50% w/w EtOH/H2O.

Fe+++ sp NaClO4 25°C 0.10M C 1989KAb (44430)2138
K(FeL+H2L=FeL2+2H)=-5.29

Fe+++ oth NaClO4 RT 0.10M C 1989KAc (44431)2139
K(FeL+H2L=Fe(HL)L+H)=5.34
Method: electrophoresis. Medium pH 2.5.

Fe+++ sp NaClO4 25°C 1.00M U 1988XJa (44432)2140
K(Fe+H2L=FeL+2H)=3.15

Fe+++ sp KCl 25°C 0.10M U K1=20.4 B2=35.50 1986SOa (44433)2141
K3=10.8

Fe+++ sp NaClO4 25°C 0.00 M I K1=19.49 1985LYa (44434)2142

Fe+++ gl oth/un 27°C 0.15M M K2=15.12 1978ASa (44435)2143
K3=10.10

Fe+++ sp NaClO4 25°C 1.00M U K1=4.16 1976MPa (44436)2144
K(Fe+H2L=FeL+2H)=0.16

Fe+++ gl NaNO3 25°C 0.50M U K2=14.23 1972MSb (44437)2145
K3=10.28

Fe+++ sp NaNO3 25°C 0.50M U K1=18.74 1972MSb (44438)2146
B(FeHL)=20.86

Fe+++ sp NaClO4 ? 0.10M U K2=15.03 1969SZa (44439)2147
K3=10.7
K(FeL+H2L=FeL2+2H)=-5.23

```
                                        K(FeL2+H2L=FeL3+2H)=-9.55
--------------------------------------------------------------------------------
Fe+++      sp  KNO3   25°C  1.0M U  I M   K1=18.8   B2=33.50  1964MCa (44440)2148
                                        K3=11.6
K1=20.4(I=0.1),19.3(I=0.5); K2=15.1(0.1),15.1(0.5); K3=10.8(0.1),11.6(0.5)
In 0.1 M NaClO4:K1=20.4,K2=14.9,K2=10.1. Ternary complexes with TTHA
--------------------------------------------------------------------------------
Fe+++      gl  oth/un 25°C  0.0  U        K2=13.38       1956NVa (44441)2149
                                        K2=3.2
--------------------------------------------------------------------------------
Fe+++      sp  oth/un 18°C 0.10M U        K1=20.8   B2=36.20  1955VAa (44442)2150
                                        K3=11.5
--------------------------------------------------------------------------------
Fe+++      gl  KCl    20°C 0.10M U        K1=20.7   B2=35.90  1951WSa (44443)2151
                                        K3=11.0
                                        K(Fe+HL)=10.00
********************************************************************************
C6H6S                  HL    Thiophenol       CAS 108-98-5  (883)
Phenyl mercaptan, thiophenol; C6H5.SH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      kin non-aq 25°C 100%  U                         1993HOa (44546)2152
                                        K(L+Fe4S4A4--)=-0.54
                                        K(L+Fe4S4B4--)=-0.54
                                        K((MoFe3S4A3)2A3+L)=-0.39
                                        K((WFe3S4A3)2A3+L)=-0.14
Medium: MeCN. HA=ethanethiol; HB=tert-butylthiol
********************************************************************************
C6H7N                   L    gamma-Picoline   CAS 108-89-4  (325)
4-Methylpyridine; C5H4N.CH3
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      sp  non-aq 25°C 100%  U    M                   1991UHa (44823)2153
                                        K(FeAOCH3+2L=FeAOCH3L2)=-0.75
Medium: CH2Cl2. A=Octaethylporphine. With 3,4-dimethylpyridine K=-0.64
********************************************************************************
C6H7NO                  L                     CAS 7295-76-3  (3095)
3-Methoxypyridine; C5H4N.OCH3
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      kin NaClO4 25°C 0.10M U                        1998CWa (44993)2154
                                        K(Fe(CN)5(H2O)+L)=4.24
Medium: 0.1 M LiClO4, pH=5
********************************************************************************
C6H7NO                  L                     CAS 620-08-6  (3096)
4-Methoxypyridine; C5H4N.OCH3
--------------------------------------------------------------------------------
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```
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      kin NaClO4 25°C 0.10M U                          1998CWa (45017)2155
                                        K(Fe(CN)5(H2O)+L)=4.62
Medium: 0.1 M LiClO4, pH=7.
*************************************************************************
C6H7NO2                HL                    CAS 19365-01-6  (6771)
1-Methyl-3-hydroxy-2-pyridinone;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      gl  KCl    25°C 0.10M C        K1=11.8   B2=21.63  1992CMc (45025)2156
                                        B3=29.99
-------------------------------------------------------------------------
Fe+++      sp  NaClO4 26°C 0.10M C                          1987KOb (45026)2157
                                        B3=33.5
*************************************************************************
C6H7NO2                HL                    CAS 17184-19-9  (5888)
3-Hydroxy-2-methylpyridin-4(1H)-one;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      sp  KNO3   23°C 0.20M C        K2=12.027        1988TMa (45049)2158
                                        K3=9.734
*************************************************************************
C6H7NO3                HL                    CAS 99110-86-8  (8498)
1-Hydroxy-4-methoxy-2-pyridinone;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      sp  NaClO4 26°C 0.10M C                          1987KOb (45056)2159
                                        B3=29.3
*************************************************************************
C6H7O4As              H3L                    CAS 98-14-6  (219)
2-Hydroxyphenylarsonic acid; HO.C6H4.As(:O)(OH)2
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      sp  oth/un 25°C 0.04M U                          1974NUa (45203)2160
                                        K(Fe+HL)=11.99
*************************************************************************
C6H7O4P               H3L                    CAS 53104-46-4  (218)
2-Hydroxyphenylphosphonic acid; HO.C6H4.PO3H2
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      sp  oth/un 25°C 0.10M U  I                       1974NUa (45207)2161
                                        K(Fe+HL)=8.69
*************************************************************************
C6H8N2                  L                     CAS 108-50-9  (2531)
```

2,6-Dimethylpyrazine, 2,6-Dimethyl-1,4-diazine; C4H2N2(CH3)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	oth/un	25°C	0.00	U	T M		1985TSa	(45287)2162
							K(Fe(NH3)5L+H)=2.80		

****

C6H8O4 H2L CAS 5445-51-2 (69)
Cyclobutane-1,1-dicarboxylic acid; C4H6(COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	kin	NaClO4	25°C	0.50M	C		K1=7.46	1977CCb	(45507)2163
Fe+++	kin	NaClO4	25°C	0.50M	U		K1=7.46	1971CDa	(45508)2164

****

C6H8O6 H2L Ascorbic acid CAS 50-81-7 (285)
Ascorbic acid (Vitamin C);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	kin	NaCl	25°C	0.05M	C	T H		1987MZb	(45640)2165
							K(Fe+2HL)=6.36		

Medium buffered to pH 5.0. Data for 15-35 C.
DH(Fe+2HL)=30.1 kJ mol-1, DS=223 J K-1 mol-1.

****

C6H8O7 H3L Citric acid CAS 77-92-9 (95)
2-Hydroxypropane-1,2,3-tricarboxylic acid; HOOCCH2.CH(OH)(COOH).CH2COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	NaCl	25°C	1.0M	C		K1=9.50 B2=15.30	2000KKc	(46093)2166
							B(FeH-1L)=7.31		
							B(FeHL2)=19.12		
							B(FeH-1L2)=10.46		
Fe+++	cal	none	25°C	0.01M	U	H		1993CZa	(46094)2167

DH(K1)=-29 kJ mol-1, DS(K1)=117 J K-1 mol-1; DH(B2)=-18, DS(B2)=289;
DH(B(FeHL))=-260, DS=-636; DH(B(FeH-1L))=-350, DS=-1012.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	NaNO3	25°C	0.50M	M	M		1989MAa	(46095)2168
							K(Fe+H3L=FeH-1L+4H)=-8.0		
							K(2FeH-1L=Fe2H-2L2)=-20.1		

K(UO2+Fe+2H3L=FeUO2H-2L2 + 8H)=-2.45

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	NaNO3	25°C	0.50M	U		B2=16.73	1989RSd	(46096)2169
							B(FeHL)=11.97		
							B(FeH-1L)=7.85		
							B(FeH2L2)=22.56		
							B(FeHL2)=20.20		

B(FeH-1L2)=12.18, B(FeH-2L2)=6.58, B(FeH-3L2)=1.35.

Fe+++ vlt NaClO4 30°C 1.0M C K1=7.06 B2= 9.48 1988GMb (46097)2170
Method: polarography. Medium pH 5.0.

Fe+++ NaCl 25°C 0.15M U K1=11.2 B2=18.20 1986MAa (46098)2171
K(Fe+HL)=6.7
K(FeHL=FeL+H)=-1.3
K(FeL=FeH-1L+H)=-2.8
25-37 C. From a survey of literature data

Fe+++ sp NaClO4 20°C 1.0M C TI 1980MBb (46099)2172
K(Fe+H3L=FeL+3H)=-1.73
At 8C, K(Fe+H3L=FeL+3H)=-1.80. Also data for MeOH/H2O and n-PrOH/H2O mixtures.

Fe+++ sp oth/un 25°C >1.0 U K2=4.31 1978VKb (46100)2173
K(FeL+H)=1.18
K(FeH-1L+H)=2.11
Medium: 1 M (3H,3Na,Fe)L

Fe+++ ISE KNO3 25°C 0.50M C 1975VDa (46101)2174
K1eff=5.65 (pH 2.5)
Method: liquid phase Fe(III)-N-benzoyl-N-phenylhydroxylamine electrode.

Fe+++ EMF KNO3 25°C 0.10M U K1=11.21 1974FMa (46102)2175
B(FeHL)=12.38
B(FeH-1L)=8.60

Fe+++ gl NaClO4 25°C 0.10M U M K1=10.24 B2=15.94 1974RMc (46103)2176
Beff(Fe+L+fulvic acid)=16.45
K(Fe(fulvic acid)+L)=11.07
K(FeL+fulvic acid)=6.21
K(Fe+L+HPO4)=19.46
K(FeL+HPO4)=9,22; K(FeHPO4+L)=10.51

Fe+++ gl NaClO4 25°C 0.10M U K1=10.24 B2=15.94 1973RMb (46104)2177

Fe+++ sp oth/un ? ? U K1=17.29 1972GTc (46105)2178

Fe+++ sp oth/un 25°C 0.30M U M 1971BIc (46106)2179
K(Sn+Fe+3L=FeSnH-1L3+H)=24.82

Fe+++ sp NaClO4 ? 1.00M U 1971KEc (46107)2180
K(Fe+H3L=FeH2L+H)=-1.12
K(Fe+H3L=FeHL+2H)=-2.00
K(Fe+H3L=FeL+3H)=-2.14

Fe+++ gl NaClO4 20°C 0.10M U K1=11.40 1964TIb (46108)2181
K(Fe2H-2L2)=21.2

By spectrophotometry: K1=11.56

Fe+++ gl NaClO4 25°C 1.0M U K1=11.85 1954HSa (46109)2182
K(Fe+HL)=6.3
Polarography also used

Fe+++ gl NaNO3 24°C 0.10M U 1953WWa (46110)2183
K(FeL+3H=Fe+H3L)=1.82
K(FeH-1L+H)=1.92
K(Fe+L=FeH-1L+H)=9.46
K(Fe+H-1L)=25

Fe+++ EMF oth/un ? 0.10M U K1=11.7 1952BEb (46111)2184
By spectrophotometry K1=12.5

Fe+++ oth NaNO3 ? 1.0M U 1948LQa (46112)2185
K(Fe+HL)=6.31

****

C6H9NO6 H3L CAS 41035-84-1 (4367)
N-Carboxymethyl-L-aspartic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	KCl	25°C	0.10M	C		K(Fe+H2L)=4.19	1982MDb (46378)2186	

****

C6H9NO6 H3L NTA CAS 139-13-9 (191)
Nitrilotriethanoic acid; N(CH2.COOH)3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaClO4	20°C	0.10M	U		K1=16.72	1999PKb (46806)2187	
Fe+++	sp	NaClO4	20°C	0.10M	U	M	K1=16.72	1999PKb (46807)2188	
							B(Fe(OH)L)=22.97		
							K[Fe(OH)L+H)=3.8		
Fe+++	gl	KNO3	25°C	0.5M	C		K1=15.09 B2=22.94	1999SEb (46808)2189	
							B(FeHL)=16.13		
							B(FeH-1L)=11.18		
							B(FeH-2L)=3.64		
							B(Fe2L2)=30.92		
							B(Fe2H-2L2)=24.24, B(FeHL2)=26.47.		
Fe+++	kin	KNO3	25°C	0.10M	U	T M	K(FeL+Hbipy=FeL(bipy)+H)=-1.60	1997BBe (46809)2190	
Fe+++	EMF	KNO3	25°C	0.10M	C		K1=16.06	1997DFa (46810)2191	
							K[Fe(OH)L+H]=3.75		
							K[Fe(OH)2L+H]=7.4		

```
--------------------------------------------------------------------------------
Fe+++      gl  KCl    25°C 0.10M U        K1=15.9   B2=23.97  1994MMd (46811)2192
                                          *K(FeL(H2O))=-4.1
                                          *K(FeL(OH))=-7.58
                                          *K(FeL(OH)2)=-10.72
--------------------------------------------------------------------------------
Fe+++      dis NaClO4 35°C 0.10M U        K1=11.57       1994TEa (46812)2193
Methd: Paper electrophoresis; Medium: 0.1 HClO4.
--------------------------------------------------------------------------------
Fe+++      gl  NaClO4 25°C 1.00M U        K1=14.78       1986ANb (46813)2194
                                          B(FeHL)=15.67
--------------------------------------------------------------------------------
Fe+++      cal NaCl   25°C 0.10M C   H                   1982GLb (46814)2195
DH(K1)=-17.1 kJ mol-1, DS(K1)=246 J K-1 mol-1; DH(K2)=4.2, DS(K2)=175.
--------------------------------------------------------------------------------
Fe+++      gl  NaClO4 25°C 0.10M U    M   K1=11.70  B2=19.84  1974RMc (46815)2196
                                          Beff(Fe+L+fulvic acid)=18.14
                                          K(Fe(fulvic acid)+L)=12.76
                                          K(FeL+fulvic acid)=6.44
                                          K(Fe+L+HPO4)=21.09
K(FeL+HPO4)=9.39; K(FeHPO4+L)=12.4
--------------------------------------------------------------------------------
Fe+++      EMF NaNO3  25°C 0.50M U    M   K1=16.33       1973MSa (46816)2197
                                          K(Fe+L=FeL(OH)+H)=12.35
                                          B(FeLA)=30.80
                                          B(FeLB)=26.60
H4A=pyrocatechol-3,5-disulfonic acid. H3B=sulfosalicylic acid
--------------------------------------------------------------------------------
Fe+++      gl  NaClO4 25°C 0.10M U    M   K1=11.70  B2=19.84  1973RMb (46817)2198
                                          K(FeL+A)=8.08
                                          K(FeL+B)=7.84
                                          K(FeL+C)=7.28
                                          K(FeL+D)=7.89
H2A=malonic acid, H2B=succinic acid, H2C=glutaric acid, H2D=meso-tartaric
acid, K=(FeL+E)=9.69, H3E=citric acid. Other data also given
--------------------------------------------------------------------------------
Fe+++      EMF NaClO4 20°C 0.10M U      T K1=16.26       1967BAc (46818)2199
--------------------------------------------------------------------------------
Fe+++      gl  KNO3   20°C 0.10M U                       1964PCa (46819)2200
                                          K(FeL+H2A=FeLA+2H)=-4.28
                                          B(FeLA)=31.85
H2A=tiron
--------------------------------------------------------------------------------
Fe+++      gl  KCl    25°C  1.0M U                       1963GMc (46820)2201
                                          K(FeOHL+H)=5.0
                                          K(2FeL=(FeOHL)2+2H)=-6.0
                                          K(2FeOHL=(FeOHL)2)=4.0
--------------------------------------------------------------------------------
Fe+++      dis NaClO4 20°C 0.10M U      T K1=15.91  B2=24.61  1963STc (46821)2202
--------------------------------------------------------------------------------
```

```
Fe+++      gl  KNO3   20°C 0.10M U        K1=8.2         1958CGa (46822)2203
--------------------------------------------------------------------------------
Fe+++      EMF KCl    20°C 0.10M U      T K1=15.87  B2=24.32  1951SHa (46823)2204
                                          K(FeOHL+H)=4.08
                                          K(FeL(OH)2+H=FeLOH)=7.77
--------------------------------------------------------------------------------
Fe+++      gl  KCl    20°C 0.10M U        K1=>10         1948SBa (46824)2205
                                          K(FeLOH+H)=4
                                          K(FeL(OH)2+H)=9.0
********************************************************************************
C6H9N3O2               HL    Histidine        CAS 71-00-1  (1)
2-Amino-3-(4'-imidazolyl)propanoic acid; H2N.CH(CH2.C3H3N2)COOH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      sp  oth/un 25°C  1.0M C                        1985BKb (47557)2206
                                          K(Fe+HL=FeL+H)=1.0
Medium not stated.
--------------------------------------------------------------------------------
Fe+++      sp  oth/un 25°C    ?  U    M                 1982WPa (47558)2207
                                          K(FeA+2L)=4.40
                                          K(2FeA+4L=2FeAL2)=-8.82
A=Tetrakis(4-N-methylpyridyl)porphyrin
--------------------------------------------------------------------------------
Fe+++      gl  KCl    25°C .058M U T      K1=4.00        1961SMa (47559)2208
0 C, K1=4.21, 45 C, K1=3.72
--------------------------------------------------------------------------------
Fe+++      EMF oth/un 20°C 0.20M U        K1=4.7         1958PEd (47560)2209
********************************************************************************
C6H10N2O6             H3L                        (7019)
N,N-Bis(carboxymethyl)aminoacetohydroxamic acid; (HOOC.CH2)2N.CH2.CO.NHOH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      sp  NaClO4 20°C 0.10M U        K1=16.22       1977KJa (47863)2210
                                          K(Fe+HL)=10.30
                                          K(H+FeL)=3.50
********************************************************************************
C6H10N4O2              HL                      CAS 25486-00-4  (2554)
2-Amino-3-(4'-imidazolyl)propanehydroxamic acid, Histidine-hydroxamic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      gl  NaCl   25°C 0.15M C        K1=13.389 B2=18.984 1984BSd (47906)2211
                                          B3=21.606
                                          B(FeHL)=18.070
                                          B(FeHL2)=25.885
                                          B(FeH-1L3)=12.441
********************************************************************************
C6H10O2                HL                      CAS 3002-24-2  (2742)
```

2,4-Hexanedione; CH3.CO.CH2.CO.CH2.CH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaClO4	25°C	0.5M	C		K1=10.9	1998BLa (47929)	2212
Fe+++	gl	NaClO4	25°C	0.5M	U		K1=10.9	1990HMb (47930)	2213

C6H10O4S2 H2L CAS 7244-02-2 (438)
1,2-Bis(carboxymethylthio)ethane; HOOC.CH2.S.CH2.CH2.S.CH2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaClO4	25°C	0.10M	U		K(Fe+HL)=4.35	1971PPb (48242)	2214

C6H10O7 HL Galacturonic CAS 685-73-4 (290)
D-Galacturonic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	vlt	NaClO4	25°C	0.10M	U		B3=8.51 B(FeH-2L3)=1.54 B(FeH-3L3)=-2.03	1990DGa (48391)	2215
Fe+++	gl	NaClO4	25°C	1.0M	U		B3=8.51 B(FeH-3L3)=-2.03 B(FeH-2L3)=1.54	1989DGa (48392)	2216

C6H10O8 H2L Saccharic acid CAS 87-73-0 (1191)
D-2,3,4,5-Tetrahydroxy-1,6-hexanedioic acid, Glucaric acid; HOOC.(CHOH)4.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KNO3	25°C	1.00M	U		K(Fe+H2L=FeH-2L+4H)=-24.47 K(Fe+3H2L=FeL3+6H)=-9.2	1976VOa (48473)	2217
Fe+++	sp	KNO3	25°C	1.0M	C		B3=3.12	1975VOa (48474)	2218

C6H11NO4 H2L CAS 5336-17-4 (345)
N-Ethyliminodiethanoic acid; C2H5.N(CH2.COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KNO3	25°C	0.5M	C		K1=11.53 B2=21.45 B(FeHL)=12.72	1999SEb (48602)	2219

```
                                        B(FeH-1L)=8.19
                                        B(FeH-2L)=5.38
                                        B(Fe2L2)=24.5
B(Fe2H-2L2)=19.3.
*******************************************************************************
C6H11NO5              H2L    HIMDA            CAS 93-62-9  (192)
N-(2-Hydroxyethyl)iminodiethanoic acid; HO.CH2.CH2.N(CH2.COOH)2
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe+++      sp  NaClO4 20°C  0.1M C    M   K1=11.64       2000PKc (48726)2220
                                        K(Fe+OH+L)=22.97
-------------------------------------------------------------------------------
Fe+++      sp  NaClO4 20°C 0.10M U    M   K1=11.64       2000PKc (48727)2221
                                        B(Fe(OH)L)=22.97
                                        B(Fe(OH)2L)=31.17
-------------------------------------------------------------------------------
Fe+++      gl  NaClO4 25°C 1.00M U        K1=11.60       1986ANb (48728)2222
                                        B(FeHL)=13.80
                                        B(FeH-1L)=8.57
-------------------------------------------------------------------------------
Fe+++      sp  oth/un 20°C    ?  U                       1972KVa (48729)2223
                                        K(Fe+H2L)=4.18
                                        K(Fe+HL)=11.75
-------------------------------------------------------------------------------
Fe+++      vlt KNO3   25°C 0.10M U                       1965VFa (48730)2224
                                        B(FeL(OH))=24.94
                                        B(FeL(OH)2)=32.33
-------------------------------------------------------------------------------
Fe+++      gl  KCl    25°C  1.0M U                       1960GMa (48731)2225
                                        K(FeOHL+H)=4.11
                                        K(2FeL=(Fe(OH)L)2+2H)=-5.84
                                        K(2FeOHL=(Fe(OH)L)2)=2.38
-------------------------------------------------------------------------------
Fe+++      EMF KCl    20°C 0.10M U        K1=11.61       1955ASb (48732)2226
                                        K(FeLOH+H)=2.46
                                        K(FeL(OH)2+H)=5.70
*******************************************************************************
C6H12N2O4             H2L    EDDA             CAS 5657-17-0  (119)
1,2-Diaminoethane-N,N'-diethanoic acid; HOOC.CH2.NH.CH2.CH2.NH.CH2.COOH
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe+++      gl  NaClO4 25°C 0.10M U        K1=15.50       2001SGc (49239)2227
                                        *K(FeL)=-3.64
                                        *K(Fe(OH)L)=-7.18
*******************************************************************************
C6H12N2O4             H2L    N,N-EDDA         CAS 5835-29-0  (2333)
1,2-Diaminoethane-N,N-diethanoic acid; H2N.CH2.CH2.N(CH2.COOH)2
-------------------------------------------------------------------------------
```

```
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      EMF KCl    20°C 0.10M U        K1=16.92  B2=26.54  1955ASb (49301)2228
                                          K(FeLOH+H)=3.88
                                          K(FeL(OH)2+H)=7.61
*************************************************************************
C6H12N2O4             H2L                        (6926)
N,N'-Dihydroxy-N,N'-dimethylbutanediamide; CH3N(OH).CO.(CH2)2.CO.N(OH)CH3
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      kin NaClO4 25°C 2.00M C                      1994CCa (49318)2229
                                          K(Fe+H2L=FeHL+H)=5.08
                                          K(Fe2HL2+H=2FeHL)=-2.0
                                          K(Fe2L2+H=Fe2HL2)=-0.22
*************************************************************************
C6H12N2O4             H2L                     CAS 4726-83-4  (5911)
N,N-Dihydroxyhexanediamide; HN(OH).CO.(CH2)4.CO.NH(OH)
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      gl  NaNO3  25°C 0.10M C        K1=17.60       1989EHa (49333)2230
*************************************************************************
C6H12N2O5             H2L                        (4384)
N-(Carboxymethyl)-N-(2-hydroxyethyl)aminoacethydroxamic acid;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      sp  NaClO4 20°C 0.10M U        K1=14.31       1983KJb (49369)2231
-------------------------------------------------------------------------
Fe+++      sp  NaClO4 20°C 0.10M U        K1=18.54       1970MKa (49370)2232
                                          K(FeL+2OH)=22.87
-------------------------------------------------------------------------
Fe+++      gl  NaClO4 20°C 0.10M U        K1=18.50       1970MKa (49371)2233
                                          B(FeL(OH)2)=41.2
                                          B(FeL(OH)3)=50.5
*************************************************************************
C6H12N4O4              HL                         (6028)
Triglycine hydroxamic acid; H2N.CH2.CO.NH.CH2.CO.NH.CH2.CO.NHOH
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      gl  KCl    25°C 0.20M C        K1=11.63  B2=17.14  1989BMc (49393)2234
                                          B3=20.50,  B(Fe2L)=16.53
                                          B(FeH2L2)=29.99
                                          B(FeHL2)=24.37
                                          B(FeH-2L2)=0.668
B(FeH3L3)= 42.75,  B(FeH2L3)= 35.72
*************************************************************************
C6H12N4O6             H3L                        (2677)
```

Nitrilotriacetohydroxamic acid; N(CH2.CO.NH.OH)3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KCl	25°C	0.10M	M		K1=18.63 B(FeHL)=23.73 B(FeH-1L)=11.88 B(FeH-2L)=2.85	1980LSb	(49401)2235
Fe+++	gl	NaClO4	20°C	0.10M	U		K1=19.35 K(Fe+H2L)=9.35	1975KAe	(49402)2236

****

C6H12O5S HL (691)
1-Thio-beta-D-glucopyranose;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KNO3	37°C	0.15M	M		B2=7.25	1979ZJa	(49526)2237

Method: ligand competition.

****

C6H12O6 L D-Fructose CAS 57-48-7 (1561)
D-Fructose

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	oth/un	20°C	?	U		K(Fe+L=FeH-1L+H)=-2.8	1986ASa	(49547)2238

Alternative method: spectrophotometry (UV, CD).

****

C6H12O7 HL Gluconic acid CAS 526-95-4 (904)
D-Gluconic acid, 2,3,4,5,6-Pentahydroxyhexanoic acid; HO.CH2(CHOH)4.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KNO3	20°C	0.10M	C	M	K1=10.51 B2=22.23 B(FeH-1L)=9.03 B(FeH-2L)=6.35 B(FeH-3L)=1.78 B(FeH-4L)=-8.4	2002BBb	(49715)2239
Fe+++	sp	NaClO4	25°C	0.30M	C		K1=9.63 B(Fe2L)=19.08	1983ZGa	(49716)2240
Fe+++	oth	oth/un	?	0.10M	U		K[Fe+L=FeL(OH)3+3H)=-5.5 K(FeL=FeL(OH)2+2H)=-2.3 K(FeL(OH)2=FeL(OH)3+H)=-4.0 K(FeL(OH)3=FeL(OH)4+H)=-13.3	1955PSa	(49717)2241

B(FeH-1L2)=18.22, B(FeH-2L2)=15.30, B(FeH-3L2)=9.84, B(FeH-4L2)=-1.15, B(FeH-5L2)=-20.0, B(Fe2H-7L2)=-1.42. Also ternary Ca-Fe-L complexes.

****

C6H13NO2 HL Leucine CAS 61-90-5 (47)
2-Amino-4-methylpentanoic acid; H2N.CH(CH2.CH(CH3)2)COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	EMF	NaClO4	20°C	1.0M	U	T	K1=9.9	1958PEd	(50074)2242

****

C6H13NO2 HL CAS 4312-93-0 (4386)
Hexanohydroxamic acid; CH3.CH2.CH2.CH2.CH2.CO.NH.OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KCl	25°C	0.20M	C		K1=11.18 B2=20.65 B3=28.40 K(Fe+HL=FeL+H)=1.82	1998FKa	(50227)2243

****

C6H13NO4 HL Bicine CAS 150-25-4 (2124)
N,N-Bis(2-hydroxyethyl)glycine; (HO.CH2.CH2)2N.CH2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	NaClO4	25°C	1.00M	U		K1=7.35 B(FeHL)=9.68 B(Fe2H-2L2)=12.90	1986ANb	(50361)2244
Fe+++	gl	oth/un	25°C	0.01M	U		K(Fe+HL+H2O=Fe(OH)2L+3H)=-7.4	1964NBa	(50362)2245
Fe+++	vlt	NaClO4	25°C	0.50M	U		B2=5.9 B(FeL(OH)2)=30.1	1955TKb	(50363)2246

****

C6H13NO5 L D-Glucosamine CAS 3416-24-8 (565)
2-Amino-2-deoxyglucose;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	NaCl	37°C	0.15M	U		B(Fe(OH)L)=19.15 B(Fe(OH)2L)=30.05	1987IAa	(50461)2247
Fe+++	gl	NaNO3	25°C	0.10M	U	I	K1=8.47 B2=15.10	1984GMa	(50462)2248

****

C6H14N2O2 HL (5984)
Leucinehydroxamic acid; NH2.CH(CH2.CH(CH3)2).CO.NHOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KCl	25°C	0.50M	U		B2=22.89 B3=28.00	1991LNb	(50860)2249

B(FeHL)=16.65
B(FeHL2)=28.50
B(FeH2L2)=32.60
B(Fe2H-2L2)=21.48, B(FeHL3)=35.55, B(FeH2L3)=41.93,
B(FeH-1L2)=15.98, B(Fe2H-1L3)=35.40.
****
C6H14N2O4 HL CAS 31918-44-2 (4383)
N,N-Bis(2-hydroxyethyl)aminoacethydroxamic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp NaClO4 20°C 0.10M U 1971KMc (50875)2250
B(FeL(OH))=26.17
B(FeL(OH)2)=35.67
B(FeL(OH)3)=40.37
****
C6H14N4O2 HL Arginine CAS 74-79-3 (40)
2-Amino-5-guanidopentanoic acid; H2N.CH((CH2)3.NH.C(:NH)(NH2)COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl oth/un 25°C ? U K1=7.67 B2=15.20 1960PEd (51008)2251

Fe+++ EMF NaClO4 20°C 1.0M U K1=8.7 1958PEd (51009)2252
****
C6H14O6 L Glucitol CAS 50-70-4 (2878)
D-Sorbitol;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl KNO3 25°C 0.10M C 1999CMa (51102)2253
B(FeH-1L)=2.0
B(FeH-2L)=-2.8
B(FeH-3L)=-4.9
B(FeH-4L)=-14.0
B(Fe3H-9L)=-12.8, B(Fe3H-10L)=-23.1, B(Fe6H-6L)=3.1, B(Fe6H-18L)=-24.2,
B(Fe6H-24L)=-90.
****
C6H15NO3 Triethanolamine CAS 102-71-6 (447)
Tris-(2-hydroxyethyl)amine; L

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl NaClO4 25°C 1.00M U K1=<7 1986ANb (51290)2254
B(FeHL) < 9.4

Fe+++ sp oth/un ? ? U 1973KUa (51291)2255
K(FeOH+L)=3.5
B(FeL2(OH)4)=44.6
****

C6H15N3 L CAS 4730-54-5 (26)
1,4,7-Triazacyclononane; cyclo(-NH.CH2.CH2.NH.CH2.CH2.NH.CH2.CH2-)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KNO3	20°C	0.10M	U	T H	K1=13.24 B2=19.39	1997BAa	(51409)2256

At 32 C, K1=13.05. DH(K1)=-28.52 kJ mol-1. DS(K1)=94 J K-1 mol-1.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KNO3	25°C	0.10M	U			1988PWa	(51410)2257
							K(FeH-1L2+H)=11.4		

****

C6H15N3O2 HL CAS 52760-35-7 (6670)
Lysine hydroxamic acid; H2N.(CH2)4.CH(NH2)CO.NHOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KCl	25°C	0.20M	C			2002ECa	(51426)2258
							B(FeHL)=23.33		
							B(FeH3L2)=47.8		
							B(FeH2L2)=43.1		
							B(FeH4L3)=66.1		

B(FeH3L3)=59.7, B(FeH2L3)=52.0, B(Fe2HL2)=37.3.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaClO4	25°C	2.0M	C			2002WSb	(51427)2259
							K(Fe+H2L)=6.80		
							K(Fe+2H2L)=12.4		
							K(Fe+3H2L)=16.1		
							K(Fe+H+HL)=15.69		

K(Fe+2H+2HL)=30.2, K(Fe+3H+3HL)=42.8.

****

C6H15N5O2 L CAS 5699-67-2 (6357)
2-Amino-5-((Aminoiminomethyl)amino)-N-hydroxypentanamide, Arginine hydroxamic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KCl	25°C	0.50M	C		B2=21.10	1991LNa	(51471)2260
							B(FeH2L2)=31.04		
							B(FeHL)=16.057		
							B(FeHL2)=26.69		
							B3=26.90		

B(Fe2H-2L2)=20.27; B(Fe2H-4L2)=7.53; B(FeHL3)=33.78; B(FeH-1L3)=18.35;
B(Fe2H-1L3)=33.34; B(FeH2L3)=39.75

****

C6H15O2PS2 HL (2059)
O,O'-Dipropyl dithiophosphoric acid; (C3H7O)2P(S)SH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	EMF	mixed	25°C	90%	U			1984GGa	(51487)2261
							B3=17.97		

Medium: 90% 2-propanol/H2O, 0.1 M NaClO4
****
C6H15O2PS2 HL CAS 25134-38-7 (4401)
Phosphorodithioic acid O,O-diisopropyl ester; (CH3.CH(CH3)O)2PS.SH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	EMF	mixed	25°C	90%	U			1984GGa	(51500)2262
							B3=18.97		

Medium: 90% 2-propanol/H2O, 0.1 M NaClO4
****
C6H18N2O6P2 H4L (1363)
N,N'-Dimethyldiaminoethane-N,N'-dimethylphosphonic acid;
CH3N(CH2PO3H2).CH2.CH2.N(CH2.PO3H2)CH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	oth/un	25°C	0.10M	U		K1=22.5	1976MDa	(51951)2263

****
C6H18N4 L Trien-tetramine CAS 112-24-3 (11)
1,4,7,10-Tetraazadecane; H2N.CH2.CH2.NH.CH2.CH2.NH.CH2.CH2.NH2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	NaNO3	25°C	0.10M	C	M		2002MDa	(52102)2264

K(Fe+L+B(OH)4=FeL(H2BO4)+2H)=21.89, K(2Fe+2L+B(OH)4=Fe2L2(BO4)+4H)=37.68

Fe+++	gl	NaNO3	25°C	0.10M	C		K1=21.77	2002MDa	(52103)2265
							B(FeH-1L)=15.47		
							B(FeH-2L)=10.85		
Fe+++	kin	oth/un	20°C	->0	U		K1=21.94	1958BGa	(52104)2266
Fe+++	sol	oth/un	20°C	->0	U		K1=21.7	1958BGa	(52105)2267

****
C6H18O24P6 HnL Phytic acid CAS 83-86-3 (745)
Cyclohexane-1,2,3,4,5,6-hexol-hexaphosphoric acid, Myo-inositol hexaphosphoric
acid; H12L

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	vlt	oth/un	25°C	0.7M	C			2000WHa	(52225)2268
							K1eff=22.3		

Competitive ligand (1-nitroso-2-naphthol) cathodic stripping voltammetry.
Medium: photo-oxidised seawater, pH 6.9. At pH 8 (kinetic): K1eff=22.4
****
C6H20N2O12P4 H8L EDTPA CAS 1429-50-1 (434)
Ethane-1,2-bis(iminobis(methylenephosphonic acid)); ((H2O3PCH2)2NCH2.)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo

```
--------------------------------------------------------------------------------
Fe+++      kin KNO3   35°C 0.10M U T                    1987RAa (52331)2269
                                      *K(FeL(H2O))=-10.09
--------------------------------------------------------------------------------
Fe+++      gl  KNO3   25°C 0.10M U       K1=19.6        1965WRa (52332)2270
                                      K(Fe+H2L)=13.2
                                      K(H+FeHL)=6.32
                                      K(H+FeL)=7.14
--------------------------------------------------------------------------------
Fe+++      gl  oth/un 25°C 0.10M U       K1=>10         1956WMe (52333)2271
********************************************************************************
C7H4N2O7              H2L                      CAS 609-99-4  (400)
3,5-Dinitrosalicylic acid; (O2N)2.C6H2(OH).COOH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      gl  KNO3   30°C 0.10M C       K1=9.81   B2=17.21  1996MMa (52477)2272
                                      K3=3.1
--------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 1.00M U                     1982MSe (52478)2273
                                      K(Fe+HL=FeL+H)=2.591
********************************************************************************
C7H4O3Br2             H2L                      CAS 3147-55-5  (1116)
3,5-Dibromosalicylic acid; C6H2(OH)(Br)2.COOH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      gl  NaClO4 25°C 0.10M U       K1=11.00  B2=19.71  1974JAa (52541)2274
                                      K3=5.60
********************************************************************************
C7H4O3Cl2             H2L                      CAS 320-72-9  (1117)
3,5-Dichlorosalicylic acid; C6H2(OH)(Cl)2.COOH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      gl  NaClO4 25°C 0.10M U       K1=10.81  B2=19.02  1974JAa (52554)2275
                                      K3=5.37
********************************************************************************
C7H4O7                H3L    Meconic acid      CAS 497-59-6  (3723)
3-Hydroxy-4-pyrone-2,6-dicarboxylic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      sp  oth/un 25°C 0.20M U                     1966HDa (52563)2276
                                      K(Fe+H2L)?=4.76
                                      K(Fe+2HL)?=7.29
--------------------------------------------------------------------------------
Fe+++      sp  oth/un 20°C  0.0  U  I    K1=15.0   B2=25.3   1961SLb (52564)2277
                                      B3=31.6
B3=30.9(I=0.03), K(Fe+H2L)=5.1(I=0.1). In 30% EtOH:K(Fe+H2L+FeHL+H)=5.2,
```

K(FeL+HL=FeL2+H)=0.4, K(FeL2+HL=FeL3+H)=-4.0

****

C7H5NO HL Salicylnitrile CAS 611-20-1 (3746)
2-Cyanophenol; H0.C6H4.CN

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	sp	NaClO4	25°C	0.10M	U		K1=5.52		1969DMb (52574)	2278

****

C7H5NO HL CAS 837-62-1 (4434)
3-Cyanophenol; HO.C6H4.CN

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	sp	NaClO4	25°C	0.10M	U		K1=6.29		1969DMb (52576)	2279

****

C7H5NO HL CAS 767-00-0 (1632)
4-Cyanophenol; HO.C6H4.CN

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	sp	NaClO4	25°C	0.10M	U		K1=5.78		1969DMb (52581)	2280

****

C7H5NO2 H2L CAS 67984-81-0 (1189)
4-Cyano-1,2-dihydroxybenzene; (HO)2.C6H3.CN

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	sp	NaClO4	25°C	1.00M	U				1976MPa (52593)	2281
							K(Fe+H2L=FeL+2H)=3.31			

****

C7H5NO4 H2L Quinolinic acid CAS 89-00-9 (567)
2,3-Pyridinedicarboxylic acid; C5H3N.(COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	gl	NaClO4	25°C	1.00M	U	T	K1=7.24		1984PHa (52627)	2282

****

C7H5NO4 H2L CAS 100-26-5 (2528)
2,5-Pyridinedicarboxylic acid, Isocinchomeronic acid; C5H3N.(COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	EMF	NaClO4	25°C	0.10M	U		K1=7.77	B2=13.17	1970OMa (52669)	2283
							B3=23.28			

****

C7H5NO4 H2L Dipicolinic aci CAS 449-83-2 (418)
2,6-Pyridinedicarboxylic acid; C5H3N.(COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo

```
--------------------------------------------------------------------------------
Fe+++      gl  NaClO4 25°C 1.00M U T      B2=16.77       1984PHa (52772)2284
                                          B(FeHL2)=17.26
--------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 1.00M U T H                   1982BPb (52773)2285
                                          K(Fe+H2L=FeL+2H)=2.36
Data also at 35, 50, 65, 80 C.  DH=14.2 kJ mol-1 (calculated).
--------------------------------------------------------------------------------
Fe+++      gl  NaClO4 20°C 0.10M U        B2=16.74       1964TIa (52774)2286
--------------------------------------------------------------------------------
Fe+++      EMF NaNO3  20°C 0.10M U        K1=10.91  B2=17.13  1960ANa (52775)2287
********************************************************************************
C7H5NO4                HL                     CAS 3084-13-7  (3751)
5-Nitrotropolone;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C  2.0M U        K1=6.57        1962OUa (52942)2288
********************************************************************************
C7H5NO5               H2L    Nitrosalicylic   CAS 85-38-1  (1416)
2-Hydroxy-3-nitrobenzoic acid; HO.C6H3(NO2).COOH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      gl  KNO3   30°C 0.10M C        K1=13.44  B2=22.94  1996MMa (52974)2289
                                          K3=7.3
--------------------------------------------------------------------------------
Fe+++      sp  oth/un 25°C  0.0  U        K1=14.193      1963EMd (52975)2290
********************************************************************************
C7H5NO5               H2L    Nitrosalicylic   CAS 96-97-9  (148)
2-Hydroxy-5-nitrobenzoic acid; HO.C6H3(NO2).COOH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      gl  KNO3   30°C 0.10M C        K1=13.88  B2=24.08  1996MMa (53045)2291
                                          K3=8.3
--------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 1.00M U                       1982MSe (53046)2292
                                          K(Fe+HL=FeL+H)=3.230
--------------------------------------------------------------------------------
Fe+++      oth oth/un   ?     ?  U        K1=5.84        1971KHb (53047)2293
--------------------------------------------------------------------------------
Fe+++      sp  oth/un 25°C  0.0  U        K1=14.339      1963EMd (53048)2294
********************************************************************************
C7H5NO5               H2L    Nitrosalicylic   CAS 601-99-0  (2682)
2-Hydroxy-6-nitrobenzoic acid; HO.C6H3(NO2).COOH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 0.10M U        K1=12.81       1974CSa (53061)2295
```

****

C7H5N3O HL CAS 35252-03-0 (3142)
2-Hydroxypyrido[3',4'-b]pyrazine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	oth/un	20°C	0.01M	U		K1=11.0	1954AHb (53090)	2296

****

C7H5O2Br HL CAS 4584-68-3 (2691)
3-Bromotropolone;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaClO4	25°C	2.0M	U		K1=9.25	1965OYa (53114)	2297

****

C7H5O2Br HL CAS 698-47-5 (3749)
4-Bromotropolone;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaClO4	25°C	2.0M	U		K1=10.04	1964OYc (53119)	2298

****

C7H5O2Br HL CAS 3172-00-7 (3750)
5-Bromotropolone;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaClO4	25°C	2.0M	U		K1=9.74	1962OUa (53134)	2299

****

C7H5O2Cl HL (3748)
5-Chlorotropolone;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaClO4	25°C	2.0M	U		K1=9.92	1962OUa (53227)	2300

****

C7H5O3Br H2L CAS 3883-95-2 (1111)
3-Bromosalicylic acid; Br.C6H3(OH).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	NaClO4	25°C	0.10M	U		K1=11.20 B2=20.43 K3=6.28	1974JAa (53289)	2301

****

C7H5O3Br HL CAS 85-55-4 (1194)
5-Bromosalicylic acid; Br.C6H3(OH).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	NaClO4	25°C	0.10M	U		K1=15.47 B2=27.70	1983LEb (53309)	2302

K3=10.64

Fe+++ sp oth/un 25°C 0.0 U K1=16.762 1963EMd (53310)2303

****

C7H5O3Cl H2L CAS 321-14-2 (1113)

5-Chlorosalicylic acid; Cl.C6H3(OH).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	gl	NaClO4	25°C	0.10M	U		K1=15.74	B2=28.12	1983LEb	(53339)2304
							K3=10.84			
Fe+++	sp	NaClO4	25°C	1.00M	U	T	K(Fe+HL=FeL+H)=2.803		1982MSe	(53340)2305
Fe+++	sp	NaClO4	25°C	0.10M	U		K1=15.42		1976CHa	(53341)2306
Fe+++	gl	NaClO4	25°C	0.10M	U		K1=12.17	B2=22.61	1974JAa	(53342)2307
							K3=8.03			
Fe+++	sp	oth/un	25°C	0.0	U		K1=16.842		1963EMd	(53343)2308

****

C7H5O3I H2L CAS 119-30-2 (1114)

2-Hydroxy-5-iodobenzoic acid, 5-Iodosalicylic acid; I.C6H3(OH).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	gl	NaClO4	25°C	0.10M	U		K1=15.35	B2=26.98	1983LEb	(53361)2309
							K3=9.36			
Fe+++	gl	NaClO4	25°C	0.10M	U		K1=12.30	B2=22.82	1974JAa	(53362)2310
							K3=8.41			

****

C7H6NO2Cl HL CAS 17512-69-5 (1918)

2-Chloro-benzohydroxamic acid; Cl.C6H4.CO.NH.OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaClO4	25°C	1.00M	U	H	K(Fe+HL=FeL+H)=1.07	1989DBa	(53380)2311

****

C7H6N2O4 H2L CAS 2683-49-0 (3753)

4-Aminopyridine-2,6-dicarboxylic acid (4-aminodipicolinic acid)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	EMF	KNO3	20°C	0.10M	U		K1=13.15	B2=22.89	1965ABa	(53508)2312

****

C7H6N2S HL CAS 583-39-1 (2043)

2-Mercaptobenzimidazole;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl alc/w 25°C 50% U K1=10.45 1978ZIa (53529)2313
****
C7H6O2 HL Salicylaldehyde CAS 90-02-8 (193)
2-Hydroxybenzaldehyde, Salicylaldehyde; HO.C6H4.CHO

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp NaClO4 25°C 1.0M C HM 1992DAb (53621)2314
K(Fe+HL=FeL+H)=3.73
Data for 25, 30 and 35 C. DH(K)=31.8 kJ mol-1, DS(K)=118 J K-1 mol-1.

Fe+++ gl oth/un 25°C 3.0M U H K1=8.75 B2=15.55 1956AGa (53622)2315
K1=8.70(15 C), 8,80(35 C). DH(K1)=8.4 kJ mol-1, DS=197 J K-1 mol-1

Fe+++ gl NaClO4 25°C 3.0M U K1=8.75 B2=15.55 1955AGa (53623)2316
****
C7H6O2 HL Tropolone CAS 533-75-5 (3129)
2-Hydroxycyclohepta-2,4,6-trien-1-one;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp NaClO4 25°C 2.0M U K1=10.50 1962OUa (53672)2317

Fe+++ sp oth/un ? ? U K1=11.0 1958OMa (53673)2318
****
C7H6O2 HL CAS 100-83-4 (3724)
3-Hydroxybenzaldehyde; HO.C6H4.CHO

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp oth/un 25°C 0.0 U K1=8.11 1965EHb (53704)2319
****
C7H6O2 HL CAS 123-08-0 (455)
4-Hydroxybenzaldehyde; HO.C6H4.CHO

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp oth/un 25°C 0.0 U K1=7.56 1965EHb (53709)2320
****
C7H6O2S H2L Thiosalicylic CAS 147-93-3 (236)
2-Mercaptobenzoic acid; HS.C6H4.COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ ISE KNO3 25°C 0.50M C 1975VDa (53905)2321
K1eff=5.04 (pH 2.5)
Method: liquid phase Fe(III)-N-benzoyl-N-phenylhydroxylamine electrode.

****

C7H6O3 H2L Salicylic acid CAS 69-72-7 (14)
2-Hydroxybenzoic acid, Salicylic acid; HO.C6H4.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	oth	NaClO4	RT	0.25M	U				1995ETa	(54197)2322
							K(Fe+HL=FeL+H)=3.31			

Method: flow injection analysis with spectrophotometric detection. pH 1.66.

Fe+++	gl	NaClO4	25°C	0.1M	U	T	K1=16.45	B2=29.12	1983LEb	(54198)2323
							K3=11.77			

Fe+++	sp	NaClO4	25°C	0.10M	U		K1=16.19		1982CHb	(54199)2324

Fe+++	sp	NaClO4	24°C	0.20M	U	M	K1=15.79	B2=23.47	1979DDa	(54200)2325

Fe+++	sp	oth/un	25°C	0.0	C		K1=17.73		1976PCa	(54201)2326

From data for self medium 0.006 M, pH 2.74. At 0.006 M, K1=17.37.

Fe+++	sp	NaClO4	25°C	0.10M	U		K1=16.17		1974CSa	(54202)2327

Fe+++	gl	NaClO4	25°C	0.10M	U		K1=16.36	B2=29.92	1973RMb	(54203)2328

Fe+++	sp	NaNO3	25°C	1.00M	U	TI	K1=14.13		1973VVa	(54204)2329

Temperature range 10-50C. Range of ionic strength 0-2.0
K1(10 C)(I=O)=17.80,(I=2.0)=14.17; K(50 C)(I=0)=17.18,(I=2.0)=13.37

Fe+++	sp	NaClO4	25°C	0.50M	U				1970MRa	(54205)2330
							K(Fe+HL=FeL+H)=2.85			
							K(Fe+H2L=FeL+2H)=0.03			

Fe+++	gl	oth/un	25°C	0.10M	U		K2=8.58		1969ZOb	(54206)2331
							K3=6.87			

Fe+++	sp	oth/un	23°C	0.05M	U		K1=15.35	B2=27.20	1966OTa	(54207)2332
							B3=36.27			

Fe+++	gl	NaClO4	25°C	0.10M	U				1966PAb	(54208)2333
							K(Fe+HL=FeL+H)=2.92			
							K(FeL+HL=FeL2+H)=1.2			
							K(FeL2+HL=FeL3+H)=-4.2			
							K(Fe+HL)=4.4			

2nd method: platinum electrode

Fe+++	sp	oth/un	25°C	0.0	U		K1=17.436		1963EMc	(54209)2334

Fe+++	sp	diox/w	18°C	50%	U	I	K1=17.42	B2=28.43	1961TSd	(54210)2335
							K3=8.09			

Medium: 50% EtOH, 0.1 M. In aqueous soln K1=16.44

```
--------------------------------------------------------------------------------
Fe+++      sp  oth/un 18°C 0.25M U        K1=16.48  B2=28.16  1960COb (54211)2336
                                         K3=8.68
--------------------------------------------------------------------------------
Fe+++      gl  KCl    20°C 0.10M U        K1=16.35  B2=28.25  1958PEe (54212)2337
--------------------------------------------------------------------------------
Fe+++      gl  oth/un 25°C  3.0M U T H    K1=15.81       1956AGa (54213)2338
K1=15.95(15 C), 15.69(35 C). DH1=-22 kJ mol-1, DS=230 J K-1 mol-1
--------------------------------------------------------------------------------
Fe+++      sol oth/un 25°C 0.20M U                      1956CFa (54214)2339
                                         K3=-0.07
--------------------------------------------------------------------------------
Fe+++      vlt NaClO4 25°C  3.0M U        K1=15.82  B2=27.49  1955AGa (54215)2340
                                         K3=7.82
--------------------------------------------------------------------------------
Fe+++      sp  oth/un 15°C  0.0  U        K1=16.35       1952BEa (54216)2341
--------------------------------------------------------------------------------
Fe+++      sp  oth/un   ?     ?  U        K1=16.4   B2=27.86  1947BAa (54217)2342
                                         K3=5.7
--------------------------------------------------------------------------------
Fe+++      sp  oth/un   ?  0.10M U        K1=16.4        1945BAb (54218)2343
********************************************************************************
C7H6O3                H2L                     CAS 99-96-7  (1371)
4-Hydroxybenzoic acid; HO.C6H4.COOH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      sp  oth/un 15°C  ->0  U        K1=15.2        1952BEb (54416)2344
********************************************************************************
C7H6O4                H3L                     CAS 303-38-8  (1398)
2,3-Dihydroxybenzoic acid; C6H3(OH)2.COOH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 1.00M U      T                1988XJa (54463)2345
                                         K(Fe+H2L=FeL+2H)=6.95
--------------------------------------------------------------------------------
Fe+++      gl  NaClO4 25°C 1.00M U      T                1987GNa (54464)2346
                                         K(FeHL+H2L=FeH2L2+H)=-2.2
                                         K(FeH2L3+H)=9.1
                                         K(FeHL3+H)=9.8
                                         K(FeL3+H)=10.9
K(FeH2L2+H2L=FeH3L3+H)=-4.5.  Alternative method: spectroscopy.
--------------------------------------------------------------------------------
Fe+++      gl  oth/un 27°C 0.10M M      T K1=7.3    B2=11.60  1978ASa (54465)2347
                                         B(FeHL)=23.5
--------------------------------------------------------------------------------
Fe+++      sp  alc/w    ?  0.10M U                      1962TSc (54466)2348
                                         K(Fe+H2L=FeLH+H)=4.21
                                         K(Fe+H2L=FeL+2H)=1.58
```

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C7H6O4 H3L Resorcylic acid CAS 89-86-1 (876)
2,4-Dihydroxybenzoic acid, b-Resorcylic acid; C6H3(OH)2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	NaClO4	25°C	1.00M	U	T	K(Fe+H2L=FeHL+H)=2.80 K(FeHL+H2L=FeH2L2+H)=-1.5 K(FeH2L3+H)=8.6 K(FeHL3+H)=9.0	1987GNa	(54522)2349
							K(FeHL3=FeL3+H)=-9.1. Alternative method: Spectrophotometry.		
Fe+++	gl	NaClO4	25°C	0.10M	U		K1=14.09 B2=26.09 K3=10.92	1974JAa	(54523)2350
Fe+++	gl	NaClO4	25°C	0.10M	U		K(Fe+H2L=FeHL+H)=3.135 K(FeHL+H2L=Fe(HL)2+H)=1.75 K(Fe(HL)2+H2L=Fe(HL)3+H)=-3.7 K(Fe+H2L)=4.8	1966PAb	(54524)2351
							2nd method: platinum electrode.		
Fe+++	vlt	KCl	30°C	0.10M	U		K1=15.05	1965GJb	(54525)2352
Fe+++	sp	oth/un	25°C	?	U		K(Fe+H2L=FeHL+H)=4.04	1964RSa	(54526)2353
Fe+++	sp	oth/un	?	0.10M	U	I	K(Fe+H2L=FeLH+H)=3.19 K(FeHL+H2L=FeH2L2+H)=1.61	1962TSc	(54527)2354
							In 50% EtOH, 0.1 M K(Fe+H2L=FeHL+H)=4.18, K(FeHL+H2L=FeH2L2+H)=2.23 K(FeH2L2+H2L=FeH3L3+H)=-4.61		

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C7H6O4 H3L CAS 409-79-9 (1115)
2,5-Dihydroxybenzoic acid; C6H3(OH)2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	NaClO4	25°C	0.10M	U		K1=13.65 B2=25.31 K3=9.66	1974JAa	(54585)2355
Fe+++	sp	oth/un	?	0.10M	U		K(FeHL+H2L=FeH2L2+H)=2.07 K(FeH2L2+H2L=FeH3L3+H)=-3.94	1962TSc	(54586)2356

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C7H6O4 H3L g-Resorcylic ac CAS 303-07-1 (1624)
2,6-Dihydroxybenzoic acid; C6H3(OH)2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	NaClO4	25°C	1.00M	U	T	K1=2.18 K(FeHL+H2L=FeH2L2+H)=-1.4 K(FeH2L3+H)=11.5 K(FeH2L2+H2L=FeH3L3+H)=-4.6	1987GNa	(54605)2357
Fe+++	sp	NaClO4	25°C	1.00M	U	T	K(Fe+HL=FeL+H)=2.348	1982MSe	(54606)2358
Fe+++	gl	NaClO4	25°C	0.10M	U		K(Fe+H2L=FeHL+H)=2.76 K(FeHL+H2L=Fe(HL)2+H)=1.2	1966PAb	(54607)2359

2nd method: platinum electrode

C7H6O4 H3L Protocatechuic CAS 99-50-3 (875)
3,4-Dihydroxybenzoic acid; C6H3(OH)2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	NaClO4	25°C	1.00M	U		K(Fe+H3L=FeHL+2H)=-0.70 K(FeHL+H3L=Fe(HL)2+2H)=-5.3 K(FeL2+2H)=5.70 K(FeL2+H2L=FeL3+2H)=-11.20	1987ABb	(54670)2360
Fe+++	sp	NaClO4	25°C	1.00M	U		K(Fe+H2L=FeL+2H)=3.01	1976MPa	(54671)2361
Fe+++	EMF	oth/un	?	0.25M	U		K1=19.00 B2=33.54 K3=10.85	1973MIb	(54672)2362
Fe+++	sp	oth/un	?	0.25M	U		K1=18.99 B2=33.26 K3=10.12	1973MIb	(54673)2363
Fe+++	sp	NaClO4	?	0.10M	U		K3=8.8 K(FeHL+HL)=15.5 K(FeHL+H3L=Fe(HL)2+2H)=-5.76 K(FeL2+H2L=FeL3+2H)=-12.51	1969SZa	(54674)2364

C7H6O5 H4L Gallic acid CAS 149-91-7 (446)
3,4,5-Trihydroxybenzoic acid; C6H2(OH)3.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KCl	25°C	0.10M	U		K1=22.28 B2=33.89 K3=8.26 K(Fe+HL)=18.05 K(FeHL+HL)=7.96 K(Fe(HL)2+HL)=7.15	1972LMb	(54751)2365

K(Fe+H2L)=10.50; K(FeH2L+H2L)=7.80; K(Fe(H2L)2+H2L)=6.50

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C7H6O5S H2L CAS 632-25-7 (4436)
2-Carboxybenzenesulfonic acid; HOOC.C6H4.SO3H

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	EMF	NaClO4	25°C	1.0M	U		K1=3.49	B2=5.57	1970PCc (54778)	2366

****

C7H6O5S H2L CAS 29848-93-9 (3151)
Salicylaldehyde-5-sulfonic acid; (5-Sulfosalicylaldehyde)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	sp	KCl	20°C	0.10M	U		K1=7.15		1972KEd (54797)	2367
Fe+++	EMF	KCl	20°C	0.10M	U		K2=5.44		1972KEd (54798)	2368
							K3=3.90			

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C7H6O5S H2L CAS 2745-13-3 (3755)
Tropolone-5-sulfonic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	sp	NaClO4	25°C	2.0M	U		K1=8.71	B2=16.14	1962OUa (54801)	2369
							K3=5.72			

****

C7H6O6S H3L CAS 5965-83-3 (399)
5-Sulfosalicylic acid, 2-Hydroxy-5-sulfobenzoic; HO3S.C6H3(OH).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	nmr	KNO3	25°C	1.00M	U		K1=13.44	B2=23.75	1993POa (54976)	2370
Fe+++	gl	NaNO3	25°C	0.50M	C		K1=17.05	B2=26.42	1990SRb (54977)	2371
							B(FeHL)=19.12			
							B(Fe2L3)=48.41			
							B3=32.76			
Fe+++	sp	NaClO4	25°C	0.10M	C				1989KAb (54978)	2372
							K(FeL+HL=FeL2+H)=-1.42			
Fe+++	oth	NaClO4	RT	0.10M	C				1989KAc (54979)	2373
							K(FeL+H2L=Fe(HL)L+H)=1.39			

Method: electrophoresis. Medium pH 2.2.

Fe+++	sp	NaClO4	24°C	0.20M	U	M	K1=13.78	B2=18.22	1979DDa (54980)	2374
Fe+++	sp	NaClO4	25°C	0.10M	U	M			1976CSb (54981)	2375
							B(FeAL)=15.28			

Protonation constants of A(3-mercuri-5-sulfosalicylate): K1=12.03, K2=2.43

Fe+++ sp NaClO4 25°C 0.10M U K1=14.96 1974CSa (54982)2376

Fe+++ gl NaClO4 25°C 0.10M U K1=11.65 B2=21.73 1974JAa (54983)2377
K3=6.57

Fe+++ EMF oth/un ? ? U K1=10.95 B2=20.91 1972BMa (54984)2378
K3=7.00

Fe+++ sp alc/w ? 40% U I 1972PDa (54985)2379
K(Fe+HL)=3.70
K(FeHL+HL)=-0.58
K(Fe(HL)2+HL)=-3.85

Medium: 40% MeOH, 0.1 M KNO3. In aqueous solution:
K(Fe+HL)(0%)=3.28, K(FeHL+HL)(0%)=-1.00, K(Fe(HL)2+HL)(0%)=-4.90

Fe+++ gl NaNO3 25°C 0.50M U K1=12.08 B2=23.22 1971MPa (54986)2380
K3=7.02

Fe+++ sp NaNO3 25°C 0.50M U K1=12.08 B2=23.22 1971MPa (54987)2381
K3=7.02

Fe+++ sp NaClO4 25°C 0.50M U 1970MRa (54988)2382
K(Fe+H2L=FeL+2H)=0.69

Fe+++ sp KNO3 25°C 0.50M U 1970MRa (54989)2383
K(Fe+H2L=FeL+2H)=0.49
K(FeL+H2L=FeL2+2H)=4.75
K(FeL2+H2L=FeL3+2H)=7.56

Fe+++ sp KNO3 25°C 0.50M U 1970MRa (54990)2384
K(Fe+HL=FeL+H)=2.79
K(FeL+HL=FeL2+H)=-0.94
K(FeL2+HL=FeL3+H)=-4.13

Fe+++ EMF NaClO4 25°C 1.0M U 1970NPa (54991)2385
K(Fe+HL)=4.30
K(FeHL+HL)=2.34

By spectrophotometry, values are 4.18, 2.14

Fe+++ sp oth/un 25°C 0.12M U K1=15.42 1969SMf (54992)2386

Fe+++ sp oth/un 27°C 0.05M U K1=14.05 B2=24.33 1966OTa (54993)2387
B3=33.10

Fe+++ sp oth/un 18°C 0.10M U K1=5.05 B2=15.76 1961TSd (54994)2388
K3=8.96

Fe+++ sp oth/un 18°C 0.25M U K1=15.02 B2=25.76 1960COb (54995)2389

K3=6.84

Fe+++ gl KCl 20°C 0.10M U K1=14.60 B2=25.15 1958PEe (54996)2390

Fe+++ sp oth/un ? 0.20M U I 1957NAa (54997)2391
*K(Fe+HL=FeL+H)=2.40
K=2.54(I=0.02),2.46(I=0.05). Recalculated values

Fe+++ gl oth/un 25°C 3.0M U H 1956AGa (54998)2392
DG(K1)=-82.8 kJ mol-1, DH=-11, DS=243 J K-1 mol-1

Fe+++ vlt R4N.X ? 0.60M U B2=10.60 1956ITa (54999)2393
Medium: NH4Cl

Fe+++ sp oth/un 18°C 0.25M U K1=14.64 B2=25.18 1955VAb (55000)2394
K3=6.94

Fe+++ gl NaClO4 25°C 3.0M U K1=14.42 B2=25.18 1954AGa (55001)2395
K3=7.06

Fe+++ vlt oth/un 25°C 1.0M U 1951BPa (55002)2396
B3=42

Fe+++ sp oth/un 25°C 0.06M U I K1=4.89 1948FAa (55003)2397
At I=0.153 M K1=3.68

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C7H7NO2 H2L Salicylaldoxime CAS 94-67-7 (1486)
2-Hydroxybenzaldehyde oxime; HO.C6H4.CH:N.OH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo

---

Fe+++ sp oth/un 20°C 0.26M U 1967MAj (55309)2398
K(Fe+H2L)=3.89

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C7H7NO2 HL Salicylamide CAS 65-45-2 (3155)
2-Hydroxybenzamide; HO.C6H4.CO.NH2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo

---

Fe+++ gl oth/un 15°C 3.00M U T K1=9.99 1956AGa (55327)2399
K1=10.00(35 C)

Fe+++ gl oth/un 25°C 3.00M U K1=10.02 B2=17.32 1956AGa (55328)2400

Fe+++ gl NaClO4 25°C 3.0M U K1=10.02 B2=16.26 1955AGa (55329)2401

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C7H7NO2 HL CAS 30659-61-1 (3757)
4-Aminotropolone;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo

```
--------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C  2.0M U        K1=12.58       1964OYc (55399)2402
********************************************************************************
C7H7NO2                HL                      CAS 495-18-1  (184)
Benzohydroxamic acid; C6H5.CO.NH.OH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      gl  KCl    25°C  0.2M C        K1=11.08  B2=21.20  1998FKa (55497)2403
                                        B3=28.80
                                        K(Fe+HL=FeL+H)=2.39
--------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 1.00M U   H                  1989DBa (55498)2404
                                        K(Fe+HL=FeL+H)=2.12
--------------------------------------------------------------------------------
Fe+++      dis NaClO4 25°C  1.0M U        K1=12.18       1965BGa (55499)2405
Medium: HClO4
--------------------------------------------------------------------------------
Fe+++      EMF NaClO4 20°C 0.10M U        K1=11.06  B2=20.43  1963ANe (55500)2406
                                        K3=7.4
********************************************************************************
C7H7NO3               H2L    B-Resorcylamide  CAS 5399-68-8  (3758)
2,4-Dihydroxybenzoic acid amide; (HO)2.C6H3.CO.NH2
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 0.10M U        K1=3.58        1966DEb (55535)2407
********************************************************************************
C7H7NO3               H2L                     CAS 89-57-6  (2675)
2-Hydroxy-5-aminobenzoic acid, 5-Aminosalicylic acid; H2N.C6H3(OH).COOH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      sp  KCl    37°C 0.15M C                       1993WWa (55549)2408
                                        B(FeHL2)=21.83
--------------------------------------------------------------------------------
Fe+++      sp  NaClO4 20°C 0.10M U                       1962TSc (55550)2409
                                        K(FeL+H)=2.36
                                        K(Fe+HL)=6.00
                                        K(Fe+H2L)=2.27
--------------------------------------------------------------------------------
Fe+++      sp  oth/un 20°C 0.25M U        K1=16.4   B2=29.4   1960COb (55551)2410
                                        K3=8.2
--------------------------------------------------------------------------------
Fe+++      gl  oth/un 25°C 3.00M U        K1=16.92  B2=29.01  1956AGa (55552)2411
                                        B3=36.1
--------------------------------------------------------------------------------
Fe+++      gl  NaClO4 25°C  3.0M U        K1=16.97  B2=29.01  1955AGa (55553)2412
                                        K3=7.04
********************************************************************************
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C7H7NO3 H2L CAS 89-73-6 (204)
2-Hydroxybenzohydroxamic acid (salicylhydroxamic acid); HO.C6H4.CO.NHOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaClO4	25°C	1.00M	U	H	K(Fe+H2L=FeHL+H)=2.33	1989DBa (55594)	2413
Fe+++	gl	KCl	25°C	0.15M	C		K1=17.22 B2=29.55 B3=38.80 B(FeHL)=19.36 B(FeH2L)=19.23 B(FeH-1L)=10.39 B(FeH-2L2)=7.41, B(Fe2H-2L)=11.40, B(FeHL2)=31.09, B(Fe2H-3L2)=15.89	1989SEa (55595)	2414
Fe+++	sp	NaClO4	20°C	1.00M	U		B(FeHL)=9.09	1987SHb (55596)	2415

C7H7NO3 H2L (1112)
4-Aminosalicylic acid; H2N.C6H3(OH).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	NaClO4	25°C	0.10M	U		K1=14.14 B2=26.46 K3=10.00	1974JAa (55638)	2416
Fe+++	sp	NaClO4	25°C	0.50M	U		K(Fe+H2L=FeL+2H)=0.40 K(FeL+H2L=FeHL2+H)=3.03 K(FeL2+H2L=FeL3+2H)=10.65	1970MRa (55639)	2417
Fe+++	sp	NaClO4	25°C	0.50M	U		K(Fe+HL=FeL+H)=4.06 K(FeL+HL=FeL2+H)=-0.97 K(FeL2+HL=FeL3+H)=-5.70	1970MRa (55640)	2418
Fe+++	sp	oth/un	30°C	0.20M	U	I	K(Fe+HL=FeL+H)=-3.66 K=-3.43(I=0),-3.51(I=0.02),-3.59(I=0.05),-3.63(I=0.10)	1960DAa (55641)	2419

C7H7N3O2 H2L CAS 4463-97-2 (1654)
2,6-Pyridinedialdoxime;C5H3N.(CH:NOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	EMF	KCl	25°C	.025M	U		K(FeHL+H)=2.299 K(FeL+H)=5.903	1977HMa (55741)	2420

C7H7N3O3 L CAS 606-26-8 (2643)

2-Nitrobenzoic acid hydrazide; O2N.C6H4.CO.NH.NH2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaClO4	25°C	0.10M	U			1981BPc (55747)	2421
							B3=13.27		
							K(Fe+3(H-1L))=38.80		

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C7H7N3O3 L CAS 618-94-0 (2644)

3-Nitrobenzoic acid hydrazide; O2N.C6H4.CO.NH.NH2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	oth/un	25°C	0.10M	U			1981BPc (55752)	2422
							B3=12.60		
							K(Fe+3(H-1L))=36.45		

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C7H7N3O3 L CAS 636-97-5 (2645)

4-Nitrobenzoic acid hydrazide; O2N.C6H4.CO.NH.NH2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaClO4	25°C	0.10M	U			1981BPc (55757)	2423
							B3=11.97		
							K(Fe+3(H-1L))=35.38		

****

C7H8N2O HL CAS 88-68-6 (4438)

Benzamide oxime; C6H5.C(:N.OH)NH2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	oth	non-aq	?	100%	U		B2=6.68	1967MAa (55821)	2424

Method: freezing point depression. Medium: nitrobenzene

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C7H8N2O HL Salicylaldazone CAS 3291-00-7 (3760)

Salicylaldehyde-hydrazone; 2-(OH).C6H4.CH:N.NH2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	mixed	25°C	20%	U	I	K1=10.563 B2=16.09	1985RRf (55848)	2425
							B(FeHL)=12.168		

40% DMF, K1=11.005, K2=5.732, B(FeHL)=12.355,
In 60% DMF/H2O: K1=11.825, K2=5.990, B(FeHL)=12.879

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C7H8N2O2 HL CAS 5623-04-1 (1917)

2-Amino-benzohydroxamic acid; H2N.C6H3.CO.NH.OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaClO4	25°C	1.00M	U	H		1989DBa (55854)	2426

K(Fe+HL=FeL+H)=1.47

****

C7H8N2O2 HL Salicylic hydra CAS 936-02-7 (2646)
2-Hydroxybenzoic acid hydrazide; HO.C6H4.CO.NH.NH2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaClO4	25°C	0.10M	U		K1=15.83 B2=29.70 B3=42.84	1981BPc (55874)	2427

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C7H8N2O2 HL CAS 59393-77-0 (3158)
4-Aminosalicylamide (4-amino-2-hydroxybenzamide); H2N.C6H3(OH).CO.NH2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	NaClO4	25°C	3.0M	U	T H	K1=10.70	1956AGa (55911)	2428

DH(K1)=1.7 kJ mol-1, DS=213 J K-1 mol-1. K1=10.67(15 C), 10.65(35 C)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	NaClO4	25°C	3.0M	U		B2=18.00	1956AGa (55912)	2429

****

C7H8O HL m-Cresol CAS 108-39-4 (1494)
3-Methylphenol, 3-Methylhydroxybenzene; CH3.C6H4.OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	oth/un	25°C	0.0	U		K1=8.51	1965EHb (56039)	2430

****

C7H8O HL p-Cresol CAS 106-44-5 (471)
4-Methylphenol, 4-Methylhydroxybenzene; CH3.C6H4.OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	KNO3	23°C	0.50M	U	I	K1=8.33	1968MCb (56050)	2431

In 0.027 NaClO4: K1=8.73

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	oth/un	25°C	->0	U		K1=8.20	1955MIa (56051)	2432

****

C7H8O2 H2L Methylcatechol CAS 452-86-8 (525)
1,2-Dihydroxy-4-methylbenzene; CH3.C6H3(OH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaClO4	25°C	1.00M	U		K(Fe+H2L=FeL+2H)=2.45	1976MPa (56066)	2433

****

C7H8O8P2 H4L (6892)
1,2-((Phenylenedioxo)methylene)diphosphonic acid); C6H4O2C(PO3H2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo

Fe+++ gl R4N.X 25°C 0.50M U K1=15.0 1985GMb (56167)2434
Medium: 0.5 M Me4NCl

****

C7H9NO2 HL CAS 30652-11-0 (2458)
3-Hydroxy-1,2-dimethylpyridin-4(1H)-one; (OH)(CH3)(O:)C5H2N.CH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	gl	KNO3	25°C	0.10M	C		K1=15.10	B2=26.61	2004SGc (56429)	2435
							B3=35.88			
Fe+++	gl	KCl	25°C	0.10M	C		K1=15.10	B2=26.61	1994MRa (56430)	2436
							K3=9.27			
Fe+++	gl	KCl	25°C	0.10M	C		K1=15.10	B2=26.61	1992CMb (56431)	2437
							K3=9.27			
Fe+++	gl	KCl	25°C	0.10M	C		K1=15.14	B2=26.68	1991MMb (56432)	2438
							B3=35.92			
Fe+++	sp	oth/un	25°C	?	U		K1=14.92	B2=27.15	1990HTa (56433)	2439
							K3=9.79			
							B3=36.94			
							K(FeLOH+H)=4.23			
Fe+++	sp	NaClO4	26°C	0.10M	C		B3=34.5		1987KOb (56434)	2440

****

C7H9O4P H3L (7127)
Hydroxybenzene-2-(methylphosphonic acid); HO.C6H4CH2PO3H2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	KNO3	20°C	1.0M	U		K(Fe+HL)=8.64	1995AAa (56524)	2441

****

C7H10N2 L CAS 1122-58-3 (492)
4-(N,N-Dimethylamino)pyridine; C5H4N.N(CH3)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	non-aq	25°C	100%	U	M	K(FeAOCH3)+2L=FeAOCH3L2)=1.96	1991UHa (56633)	2442

Medium: CH2Cl2. A=Octaethylporphine

****

C7H10N2O2S HL (560)
2-(Methanesulfonamidomethyl)pyridine; C5H4N.CH2S(:O)2NHCH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo

Fe+++ gl diox/w 30°C 45% U K1=11.70 B2=22.94 1982MYb (56684)2443
Medium: 45% v/v dioxan/H2O, 0.01 M KNO3
****
C7H10O2 L CAS 1670-46-8 (4416)
2-Acetylcyclopentanone;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp NaClO4 10°C 0.50M C 1994BSf (56712)2444
K(Fe+HL=FeL+H)=2.34
****
C7H10O3 H2L (793)
Heptane-2,4,6-trione; CH3.CO.CH2.CO.CH2.CO.CH3

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp alc/w 25°C 70% C 1991HKd (56717)2445
B(FeHL)=12.24
K(Fe+HL+2H2O=FeH-3L+2H)=5.28
Medium: 70% v/v MeOH/H2O, 0.5 M NaClO4
****
C7H10O4 H2L CAS 5802-62-3 (71)
Cyclopentane-1,1-dicarboxylic acid; C5H8.(COOH)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ kin NaClO4 25°C 0.50M C K1=7.62 1977CCb (56732)2446
****
C7H10O7P2 H4L CAS 2809-26-9 (8731)
1-Phenyl-1-hydroxymethylene-1,1-diphosphonic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl KNO3 25°C 0.10M C 2002GKc (56763)2447
B(Fe2H-1L2)=42.21
B(Fe2H-2L2)=33.60
B(FeH3L2)=45.31
B(Fe2L2)=46.20
****
C7H11NO6P2 H4L CAS 4712-06-5 (4470)
Amino(phenyl)methylenediphosphonic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl KCl 25°C 0.10M U K1=20.15 B2=27.52 1969DMd (56942)2448
K(Fe+HL)=15.08
K(Fe+HL+L)=22.75
****
C7H11O9P H5L (5041)
2-Phosphonobutane-1,2,4-tricarboxylic acid; HOOCCH2CH2C(PO3H2)(COOH).CH2COOH

```
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Fe+++      gl  NaNO3  25°C 0.50M C                         1999SEa (57024)2449
                                        B(FeH-3L2)=51.44
                                        B(FeH-6L2)=41.57
                                        B(FeH-12L2)=12.41
******************************************************************************
C7H12O2                HL                      CAS 7424-54-6  (4421)
Heptane-3,5-dione; CH3.CH2.CO.CH2.CO.CH2.CH3
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C  0.5M C        K1=11.8          1998BLa (57244)2450
------------------------------------------------------------------------------
Fe+++      gl  NaClO4 25°C 0.50M U        K1=11.8          1990HMb (57245)2451
******************************************************************************
C7H12O4               H2L                      CAS 534-59-8  (480)
Butylpropanedioic acid (Butylmalonic acid); HOOC.CH(C4H9).COOH
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Fe+++      kin NaClO4 25°C 0.50M C        K1=7.30          1977CCb (57336)2452
------------------------------------------------------------------------------
Fe+++      gl  NaClO4 30°C 0.10M U        K1=7.07   B2=12.88  1976DGd (57337)2453
                                        K3=3.54
------------------------------------------------------------------------------
Fe+++      kin NaClO4 25°C 0.50M U        K1=7.30          1971CDa (57338)2454
******************************************************************************
C7H12O4               H2L                      CAS 510-20-3  (482)
Diethylpropanedioic acid (Diethylmalonic acid); HOOC.C(C2H5)2.COOH
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Fe+++      kin NaClO4 25°C 0.50M C        K1=7.86          1977CCb (57363)2455
******************************************************************************
C7H13NO4              H2L                      CAS 16578-07-5  (341)
N-Propyliminodiethanoic acid; CH3.CH2.CH2.N(CH2.COOH)2
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Fe+++      gl  KNO3   25°C  0.5M C         K1=12.09  B2=22.73  1999SEb (57530)2456
                                        B(FeHL)=13.39
                                        B(FeH-1L)=8.27
                                        B(FeH-2L)=6.02
                                        B(Fe2L2)=25.39
B(Fe2H-2L2)=19.86
******************************************************************************
C7H14N2O4              HL                      CAS 38937-65-4  (1661)
Pimelyldihydroxamic acid; HONH.CO.(CH2)5.CO.NHOH
```

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	vlt	KCl	25°C	0.15M	U		K1=17.30	B2=25.78	1987MCa (57820)	2457
							B(Fe2L3)=41.06			

****

C7H15NO2 HL (7023)

Heptanoic acid hydroxyamide, enantihydroxamic acid; C6H13.CO.NHOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	EMF	NaClO4	25°C	0.10M	U		K1=11.49	1979SRb (57916)	2458

****

C7H21N2O10P3 H6L (7004)

N-(2-Hydroxyethyl)-1,2-diaminoethane-N,N'N'-trimethylenephosphonic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	gl	KCl	25°C	0.10M	U		K1=19.6		1974KRd (58373)	2459
							K(Fe+HL)=12.7			

****

C8H4N2O4 HL (4495)

3-Nitrophthalimide;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	gl	alc/w	30°C	100%	U		K1=5.19	B2=9.57	1970MSf (58395)	2460
							K3=3.57			
							K4=2.76			

Medium: MeOH

****

C8H5NO2 HL (3811)

3-Cyanotropolone;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaClO4	25°C	2.0M	U		K1=7.28	1965OYa (58411)	2461

****

C8H5NO2 HL (3812)

5-Cyanotropolone;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaClO4	25°C	2.0M	U		K1=7.53	1964OYa (58413)	2462

****

C8H5O2F3S HL TTA CAS 326-91-0 (165)

4,4,4-Trifluoro-1-(2-thienyl)butane-1,3-dione; F3C.CO.CH2.CO.C4H3S

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo

```
Fe+++      sp  NaClO4 25°C  0.5M C        K1=7.02        1998BLa (58620)2463
--------------------------------------------------------------------------------
Fe+++      sp  oth/un 25°C  1.0M U                       1971JFa (58621)2464
                                        K(Fe+HL=FeL+H)=0.65
--------------------------------------------------------------------------------
Fe+++      sp  oth/un 25°C 0.10M U        K1=6.9         1964PCa (58622)2465
********************************************************************************
C8H6N2O                HL                     CAS 5423-54-1  (3217)
4-Hydroxy-1,5-naphthyridine;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      gl  oth/un 20°C 0.01M U        K1=11.0        1954AHb (58738)2466
                                        B3=27.8
********************************************************************************
C8H6N2O                HL                     CAS 17056-99-4  (3220)
5-Hydroxyquinoxaline;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      gl  oth/un 20°C 0.01M U        K1=9.3         1954AHb (58747)2467
                                        B3=25.8
********************************************************************************
C8H6N2O                HL                     CAS 17057-00-0  (3218)
8-Hydroxy-1,6-naphthyridine;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      gl  oth/un 20°C 0.01M U        K1=10.3        1954AHb (58753)2468
                                        B3=25.9
********************************************************************************
C8H6N2O                HL                     CAS 70730-36-8  (3219)
8-Hydroxy-1,7-naphthyridine;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      gl  oth/un 20°C 0.01M U        K1=12.2        1954AHb (58758)2469
********************************************************************************
C8H6N2O                HL                       (6290)
8-Hydroxycinnoline, (2-Hydroxybenzo)pyrimidine;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      gl  oth/un 20°C 0.01M U        K1=9.6         1954AHb (58768)2470
********************************************************************************
C8H6N2O                HL    8-Quinazolinol   CAS 7757-02-2  (3221)
8-Hydroxyquinazoline;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
```

```
Fe+++      gl  oth/un 20°C 0.01M U        K1=10.6        1954AHb (58778)2471
                                         B3=27.7
**************************************************************************
C8H7NO4                HL                      CAS 24195-03-7  (4498)
4-Methylpyridine-2,4-dicarboxylic acid,4-methyl ester; CH3.C5H2N(COOH)(COOCH3)
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe+++      EMF NaClO4 25°C 0.10M U        K1=6.11   B2=11.11  1970OMa (59146)2472
                                         B3=23.00
**************************************************************************
C8H7NO6               H3L                      CAS 42050-90-8  (4500)
N-Glycylcomenamic acid, 2-carboxy-5-hydroxy-4-oxo-1(4H)-Pyridineethanoic acid;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe+++      sp  NaClO4   ?  0.10M U        K1=11.30       1973AOa (59167)2473
**************************************************************************
C8H8O2                 HL    2-Acetylphenol   CAS 118-93-4  (1888)
2-Hydroxyacetophenone; HO.C6H4.CO.CH3
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C  1.0M C   HM                  1992DAb (59461)2474
                                         K(Fe+HL=FeL+H)=0.88
Data for 25, 30 and 35 C. DH(K)=39.8 kJ mol-1, DS(K)=132 J K-1 mol-1.
--------------------------------------------------------------------------
Fe+++      gl  diox/w 27°C  75%  U        K1=11.56  B2=20.76  1973KDc (59462)2475
Medium: 75% dioxan, 0.1 M NaClO4
--------------------------------------------------------------------------
Fe+++      gl  oth/un 25°C  3.0M U   H                   1956AGa (59463)2476
DG(K1)=-60.3 kJ mol-1, DH(K1)=3.4, DS=21.4 J K-1 mol-1
**************************************************************************
C8H8O2                 HL    3-Acetylphenol   CAS 121-71-1  (3795)
3-Hydroxyacetophenone; HO.C6H4.CO.CH3
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe+++      sp  oth/un 25°C  0.0  U        K1=8.36        1965EHb (59478)2477
**************************************************************************
C8H8O2                 HL    4-Acetylphenol   CAS 99-93-4  (3796)
4-Hydroxyacetophenone; HO.C6H4.CO.CH3
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe+++      sp  oth/un 25°C  0.0  U        K1=7.20        1965EHb (59487)2478
**************************************************************************
C8H8O2                 HL                      CAS 583-80-2  (3191)
beta-Methyltropolone;
--------------------------------------------------------------------------
```

```
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      sp  diox/w   ?   40%  U        K1=11.88  B2=22.82  1966SDa (59596)2479
                                         K3=9.6
Medium: 40% dioxan, 0.1 M NaClO4
*************************************************************************
C8H8O2S                HL    2-Thenoylaceton  CAS 3151-27-2  (3224)
2-Thenoylacetone, 1-(2'-Thienyl)butane-1,3-dione; C4H3S.CO.CH2.CO.CH3
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      gl  NaClO4 25°C 0.50M U        K1=10.0        1990HMb (59638)2480
*************************************************************************
C8H8O2S                HL    3-Thenoylaceton  CAS 21808-13-9  (2736)
3-Thenoylacetone, 1-(3'-Thienyl)butane-1,3-dione; C4H3S.CO.CH2.CO.CH3
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C  0.5M C        K1=10.0        1998BLa (59646)2481
*************************************************************************
C8H8O3               H2L                      CAS 89-84-9  (4477)
2,4-Dihydroxyacetophenone   (4-acetylresorcinol)
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      sp  NaClO4   ?  0.10M U                         1968GDa (59666)2482
                                         K(?)=2.90
*************************************************************************
C8H8O3               H2L    o-Cresotic acid  CAS 83-40-9  (2338)
2-Hydroxy-3-methylbenzoic acid; CH3.C6H3(OH).COOH
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      EMF NaClO4 25°C 0.10M U                         1966PAb (59700)2483
                                         K(Fe+HL=FeL+H)2.58
                                         K(FeL+HL=FeL2+H)=0.5
                                         K(FeL2+HL=FeL3+H)=-3.7
                                         K(Fe+HL)=4.6
-------------------------------------------------------------------------
Fe+++      sp  oth/un 25°C  0.0  U        K1=18.130      1963EMd (59701)2484
*************************************************************************
C8H8O3               H2L    p-Cresotic acid  CAS 89-56-5  (3797)
2-Hydroxy-5-methylbenzoic acid, (5-methylsalicylic acid)
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      EMF NaClO4 25°C 0.10M U                         1966PAb (59709)2485
                                         K(Fe+HL=FeL+H)=2.98
                                         K(FeL+HL=FeL2+H)=1.2
                                         K(Fe+HL)=4.4
```

****
C8H8O3 H2L CAS 567-61-3 (3798)
2-Hydroxy-6-methylbenzoic acid, (6-methylsalicylic acid)

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ EMF NaClO4 25°C 0.10M U 1966PAb (59711)2486
K(Fe+HL=FeL+H)=2.58
K(FeL+HL=FeL2+H)=0.6
K(FeL2+HL=FeL3+H)=-3.0
****
C8H8O3 HL Mandelic Acid CAS 611-72-3 (80)
2-Phenyl-2-hydroxyethanoic acid; C6H5.CH(OH).COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp none 30°C 0.0 U 1976GCa (59829)2487
K1eff=3.69
Measured at pH 3.0

Fe+++ gl NaClO4 25°C 0.10M U 1973RMb (59830)2488
K(Fe+H-1L)=18.01
K(FeH-1L+H-1L)=15.89

Fe+++ sp oth/un 25°C ? U K1=3.71 1961BBa (59831)2489
****
C8H8O3 H2L m-Cresotic acid CAS 50-85-1 (1244)
4-Methylsalicylic acid; CH3.C6H3(OH).COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ EMF NaClO4 25°C 0.10M U 1966PAb (59997)2490
K(Fe+HL=FeL+H)=2.99
K(FeL+HL=FeL2+H)=1.3
K(Fe+HL)=4.7

Fe+++ sp oth/un 35°C 0.20M U I 1963KCa (59998)2491
Keff=5.00, 4.67, 3.68
At I=0 corr: Keff=6.01, 5.65, 4.64. Apparent constants varying with pH

Fe+++ oth oth/un ? 0.10M U I 1962POb (59999)2492
K(Fe+HL=FeL+H)=3.02
In 12% EtOH K(Fe+2HL=FeL2+2H)=2.44, K(Fe+HL=FeL+H)=3.95.
In 50% EtOH: K(Fe+2HL=FeL2+2H)=1.66, K(Fe+3HL=FeL3+3H)=-4.62
****
C8H8O3 HL CAS 119-36-8 (3196)
Methyl salicylate; 2-(OH)C6H4.COOCH3

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---

```
Fe+++      gl  oth/un 15°C 3.00M U T      K1=9.77        1956AGa (60015)2493
At 35 C: K1=9.85
--------------------------------------------------------------------------------
Fe+++      gl  oth/un 25°C 3.00M U   H    K1=9.79        1956AGa (60016)2494
DH(K1)=6.7 kJ mol-1, DS=213 J K-1 mol-1
--------------------------------------------------------------------------------
Fe+++      gl  NaClO4 25°C  3.0M U        K1=9.74        1955AGa (60017)2495
********************************************************************************
C8H8O4               H3L                     CAS 102-32-9  (1826)
3,4-Dihydroxyphenylethanoic acid; C6H3(OH)2.CH2COOH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      gl  oth/un 27°C 0.06M M        K1=20.1   B2=34.9   1978ASa (60069)2496
                                          K3=9.0
********************************************************************************
C8H8O4                HL                     CAS 520-45-6  (4478)
3-Acetyl-2-hydroxy-6-methylpyran-4-one, Dehydroethanoic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      gl  diox/w 35°C  50%  U        K1=6.06   B2=11.55  1971MAa (60088)2497
Medium: 50% dioxan, 0.1 M NaClO4
********************************************************************************
C8H9NO2               HL                     CAS 17512-73-1  (1916)
2-Methyl-benzohydroxamic acid; CH3.C6H4.CO.NH.OH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 1.00M U   H                    1989DBa (60220)2498
                                          K(Fe+HL=FeL+H)=1.72
********************************************************************************
C8H9NO2               HL                     CAS 2446-50-6  (8185)
N-Methyl-benzohydroxamic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      vlt non-aq 25°C 100%  C                      1992SSe (60267)2499
                                          B3=38.4
Medium: acetonitrile, 0.20 M Et4NPF6. Method: cyclic voltammetry.
********************************************************************************
C8H9NO2               HL                       (2591)
N-Phenyl-N-acetohydroxamic acid; CH3.CO.N(OH)C6H5
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      gl  KCl    25°C 0.20M C        K1=10.92  B2=20.12  1998FKa (60283)2500
                                          B3=28.87
                                          K(Fe+HL=FeL+H)=2.45
--------------------------------------------------------------------------------
```

```
Fe+++      EMF NaClO4 25°C 1.00M U        K1=10.83       1979SRb (60284)2501
--------------------------------------------------------------------------
Fe+++      gl  NaClO4 25°C 1.00M U        K1=10.82  B2=20.48  1978SSe (60285)2502
**************************************************************************
C8H9NO3                HL    Pyridoxal        CAS 65-22-5  (110)
3-Hydroxy-5-(hydroxymethyl)-2-methyl-4-pyridinecarboxaldehyde;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe+++      gl  NaCl   37°C 0.15M U        K1=9.90        1986AIa (60425)2503
                                        B(Fe(OH)L))=20.53
                                        B(Fe(OH)2L)=28.90
Equilibria est. ca.1 hour:point titration used.
--------------------------------------------------------------------------
Fe+++      gl  NaCl   37°C 0.15M U        K1=9.90        1986AId (60426)2504
                                        K(Fe+L+OH)=20.53
                                        K(Fe+L+2OH)=28.90
**************************************************************************
C8H9NO4                H2L                      (4520)
Dehydroethanoic acid oxime;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe+++      gl  diox/w 35°C  50%  U                        1971MAa (60494)2505
                                        K(Fe+HL)=5.78
                                        K(Fe+2HL)=10.82
Medium: 50% dioxan, 0.01 M NaClO4
**************************************************************************
C8H10O9                H4L                      CAS 137172-86-2  (6612)
SS-Oxydisuccinic acid; O(CH(COOH)CH2.COOH)2
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe+++      gl  KCl    25°C 0.10M C        K1=11.43       1992MMa (60903)2506
                                        K(FeL+H)=2.49
                                        *K(FeL)=-3.87
                                        *K(FeH-1L)=-5.37
                                        K(Fe+HL)=7.95
**************************************************************************
C8H10O9                H4L                      CAS 84852-72-2  (6611)
meso-Oxydisuccinic acid; O(CH(COOH)CH2.COOH)2
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe+++      gl  KCl    25°C 0.10M C        K1=12.01       1992MMa (60915)2507
                                        K(FeL+H)=2.37
                                        *K(FeL)=-3.96
                                        *K(FeH-1L)=-5.49
                                        K(Fe+HL)=8.41
**************************************************************************
```

C8H10O10 H4L (5894)
1-Hydroxy-3-oxapentane-1,2,4,5-tetracarboxylic acid;
HO.CH(COOH).CH(COOH).O.CH(COOH).CH2(COOH)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KCl	25°C	0.10M	C		K1=10.70 K(FeL+H)=2.11 K(FeH-1L+H)=3.67 K(FeH-2L+H)=5.36	1989MMd	(60927)2508

****
C8H11NO2 H2L Dopamine CAS 579-59-9 (251)
2-(3',4'-Dihydroxyphenyl)ethylamine; (HO)2.C6H3.CH2.CH2.NH2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	kin	KNO3	25°C	0.10M	C		K(Fe+HL)=21.14 K(FeHL+H)=1.52	1997EHa	(61079)2509
HL is the ligand form with both phenolic groups ionized.									
Fe+++	sp	NaClO4	25°C	1.00M	C		B3=43.72 B(FeHL3)=55.25 B(FeH2L3)=65.86 B(FeH3L3)=76.08	1994GCa	(61080)2510
B(FeH2L2)=55.92, B(FeH2L)=34.56, B(FeHL)=30.71. Combined pH-metric and spec.									
Fe+++	gl	KNO3	20°C	1.00M	C		K(Fe+H3L=FeL+3H)=-7.96 K(Fe+H3L=FeHL+2H)=-3.4 K(Fe+2H3L=FeL2+6H)=-29.0 K(Fe+2H3L=FeHL2+5H)=-19.96	1983CLd	(61081)2511
K(Fe+H3L=FeH2L+H)=-1.5, K(Fe+H3L=FeL(OH)+4H)=-15.3									

****
C8H11NO3 HL Vitamin B6 CAS 65-23-6 (254)
5-Hydroxy-6-methyl-3,4-pyridinedimethanol, Pyridoxine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaCl	25°C	0.15M	C		K1=10.64 B(FeHL)=13.02 B(FeH-1L)=7.60 B(FeH-1L2)=16.47 B(Fe2H-3L)=7.80	1988EHa	(61115)2512
B(Fe2H-2L2)=20.95, B(Fe2H-2L3)=29.65.									
Fe+++	gl	NaCl	37°C	0.15M	U		K(Fe+HL)=4.69 K(Fe+OH+HL)=15.73	1984ABd	(61116)2513

```
                                        K(Fe+2OH+HL)=25.48
                                        K(Fe+2OH+2HL)=27.89
--------------------------------------------------------------------------------
Fe+++      sp  KCl    25°C 0.50M U                      1977ESa (61117)2514
                                        K(Fe+HL)=4.47
--------------------------------------------------------------------------------
Fe+++      sp  oth/un 20°C 0.25M U                      1960COb (61118)2515
                                        K(Fe+HL=FeL+H)=4.30
                                        K(1/2HL+FeL=FeL3/2+1/2H)=-0.7
********************************************************************************
C8H11NO4S             H2L                        (6643)
N-Ethyl-3,4-dihydroxybenzene sulphonamide;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      gl  NaClO4 25°C 1.00M U                      1992AGa (61175)2516
                                        K(Fe+H2L=FeL+2H)=-0.36
                                        K(FeL+H2L=FeL2+2H)=-5.29
                                        K(FeL2+H2L=FeL3+2H)=-9.18
K1 from spectrophotometry
********************************************************************************
C8H11NO8              H4L                      CAS 7408-20-0  (2608)
Amino-di(butanedioic acid);HN(CH(COOH)CH2.COOH)2
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      gl  KCl    25°C 0.10M U   H    K1=14.70  B2=22.48  2002NKa (61207)2517
                                        B(FeHL)=18.66
                                        B(Fe(OH)L)=24.50
                                        B(FeH2L)=20.10
                                        B(Fe(OH)2L)=31.40
********************************************************************************
C8H12N2O2              HL    Pyridoxamine     CAS 85-87-0  (1175)
4-(Aminomethyl)-5-hydroxy-6-methyl-3-pyridinemethanol;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      gl  KNO3   25°C 0.10M U        K1=>15         1957GMa (61420)2518
********************************************************************************
C8H12N2O7             H3L                      CAS 43101-36-6  (669)
Glycylglycine-N,N-diethanoic acid; (HOOC.CH2)2N.CH2.CO.NH.CH2.COOH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      gl  KNO3   25°C 0.10M C        K1=10.56       1974MMb (61477)2519
                                        K(FeL+H)=1.6
                                        K(FeH-1L+H)=6.62
********************************************************************************
C8H12O2                HL                       CAS 874-23-7  (3203)
2-Acetylcyclohexanone;
```

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaClO4	25°C	0.5M	C		K1=11.9	1998BLa	(61670)2520
Fe+++	sp	NaClO4	25°C	0.50M	C		K1=11.65	1998BRb	(61671)2521
							K(Fe+HL=FeL+H)=1.39		
Fe+++	gl	NaClO4	25°C	0.50M	U		K1=11.9	1990HMb	(61672)2522

C8H12O7P2 H4L (7244)
1-Hydroxy-2-phenylethane-1,1-diphosphonic acid; HO.C(PO(OH)2)2.CH2C6H5

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KNO3	25°C	0.10M	C			2002GKc	(61739)2523
							B(Fe2L2)=45.22		
							B(Fe2H-1L2)=41.47		
							B(Fe2H-2L2)=32.50		
							B(Fe2H-3L2)=22.04		
							B(FeH3L2)=46.61		

C8H13NO6S H3L (5675)
2-Mercapto-1-aminoethane-N,N,S-triethanoic acid; HOOC.CH2.S.CH2.CH2.N(CH2COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	con	NaClO4	25°C	0.10M	U		K1=13.3	1975POa	(61824)2524
							K(Fe+HL)=3.02		
By potentiometry: K(FeL+OH)=7.01									

C8H14O2 HL CAS 3002-23-1 (4485)
6-Methylheptane-2,4-dione; CH3.CO.CH2.CO.CH2.CH(CH3)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaClO4	25°C	0.5M	C		K1=11.1	1998BLa	(62052)2525
Fe+++	gl	NaClO4	25°C	0.5M	U		K1=11.1	1990HMb	(62053)2526

C8H14O2 HL CAS 14090-87-0 (4486)
Octane-2,4-dione; CH3.CO.CH2.CO.CH2.CH2.CH2.CH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaClO4	25°C	0.5M	C		K1=11.3	1998BLa	(62061)2527

C8H14O4S3 H2L (2526)
3,6,9-Trithiaundecanedioic acid; HOOC.CH2.S.C2H4.S.C2H4.S.CH2.COOH

```
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 0.10M U                      1971PPc (62123)2528
                                        K(Fe+HL)=5.26
*************************************************************************
C8H15NO2               HL                    CAS 6051-21-4  (8043)
Cyclohexylacetohydroxamic acid;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      sp  NaNO3  25°C 0.10M C                      1996NWa (62165)2529
                                        B3=34.22
*************************************************************************
C8H15N3O4              HL    Gly-Ala-Ala      CAS 6491-25-4  (6783)
Glycyl-alanyl-alanine;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      gl  KNO3   25°C 0.10M C        K1=26.32       1983IMb (62250)2530
*************************************************************************
C8H16N2O4              H2L                   CAS 13288-40-9  (3237)
1,2-Diaminoethane-N,N'-di(3-propanoic acid); (HOOCCH2CH2NHCH2.)2
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      gl  KCl    30°C 0.10M U        K1=13.1        1953CCb (62502)2531
                                        K(FeLOH=FeL+OH)=10.0
                                        K(FeL(OH)2=FeL(OH)+OH)=7.0
*************************************************************************
C8H16N2O4              H2L                     (6925)
N,N'-Dihydroxy-N,N'-dimethylhexanediamide; CH3N(OH).CO.(CH2)4.CO.N(OH)CH3
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      kin NaClO4 25°C 2.00M C                      1994CCa (62513)2532
                                        K(Fe+H2L=FeHL+H)=4.89
                                        K(Fe2HL2+H=2FeHL)=-1.47
                                        K(Fe2L2+H=Fe2HL2)=-0.027
*************************************************************************
C8H16N2O4              H2L                   CAS 38937-66-5  (5912)
N,N-Dihydroxyoctanediamide; HN(OH).CO.(CH2)6.CO.NH(OH)
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      gl  NaNO3  25°C 0.10M C        K1=18.01       1989EHa (62539)2533
*************************************************************************
C8H16N2O6              H2L                   CAS 50730-95-5  (4548)
Ethylenediiminobis(3-hydroxy-2-propanoic acid);
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
```

```
------------------------------------------------------------------------------
Fe+++      EMF oth/un 20°C 0.10M U    M                 1972DKa (62586)2534
                                        K(FeOH+L)=14.26
                                        K(FeOHL+OH)=7.72
******************************************************************************
C8H16N4O4            H2L                    CAS 56199-16-7  (8363)
Piperazine-N,N'-diacetohydroxamic acid;
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Fe+++      sp  NaClO4 20°C 0.10M C        K1=17.56       1975KAf (62604)2535
                                        B(Fe2L4)=50.9
                                        K(Fe+HL)=12.18
                                        K(Fe+H2L)=9.63
                                        K(Fe+H3L=FeH2L+H)=1.25
K(2Fe+2HL+2L=Fe2H2L4)=48.8
******************************************************************************
C8H16O2S2            H3L    Dihydrolipoic      (6750)
6,8-Dimercapto-octanoic acid, dihydrolipoic acid; HSCH2.CH2.CH(SH).(CH2)4.COOH
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Fe+++      gl  none   25°C  0.0  C        K1=16.81       1992BPa (62629)2536
                                        B(FeHL)=24.52
                                        B(FeH2L)=28.51
                                        B(Fe2H4L4)=62.96
******************************************************************************
C8H17NO2              HL                      (7022)
Octanoic acid hydroxyamide, caprylhydroxamic acid; C7H15.CO.NHOH
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Fe+++      EMF NaClO4 25°C 1.00M U        K1=11.24       1979SRb (62751)2537
******************************************************************************
C8H18N2O10P2         H6L    EDDADPO          CAS 2310-83-0  (2436)
1,2-Diaminoethane-N,N'-diethanoic-N,N'-dimethylphosphonic acid;
(-CH2.N(CH2.COOH)(CH2.PO3H2))2
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Fe+++      gl  KCl    25°C 0.10M U        K1=>12         1965DKb (62900)2538
******************************************************************************
C8H18N2O10P2         H6L                    CAS 2310-83-0  (5667)
1,2-Diaminoethane-N,N-diethanoic-N',N'-dimethylphosphonic acid;
(HOOC.CH2)2NCH2CH2N(CH2.PO3H2)2
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Fe+++      gl  KNO3   25°C 0.10M U                       1976TIa (62919)2539
                                        K(Fe+H2L)=10.41
```

****
C8H19O2PS2 HL CAS 2253-44-3 (2060)
O,O'-Dibutyl dithiophosphoric acid; (C4H9O)2P(S)SH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	EMF	mixed	25°C	90%	U		B3=18.00	1984GGa	(63155)2540

Medium: 90% 2-propanol/H2O, 0.1 M NaClO4
****
C8H19O2PS2 HL CAS 107-55-1 (4585)
O,O-Di-sec-butyldithiophosphoric acid; (CH3.CH2.CH(CH3)O)2P(S)SH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	EMF	mixed	25°C	90%	U		B3=19.55	1984GGa	(63170)2541

Medium: 90% 2-propanol/H2O, 0.1 M NaClO4
****
C8H22N2O6P2 H4L CAS 13516-59-1 (3850)
2,2'-(Ethylenedi-imino)bis(propylphosphonic acid);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KCl	25°C	0.10M	U		K(Fe+HL) > 10	1965DKb	(63338)2542

****
C8H22N2O8P2 H4L CAS 55703-43-0 (1354)
N,N'-Di-(2-hydroxyethane)ethylenediamine-N,N'-dimethylphosphonic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	oth/un	25°C	0.10M	M		K1=22.1	1976MRa	(63370)2543

****
C9H6NOBr HL CAS 1198-14-7 (3281)
5-Bromo-8-hydroxyquinoline;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	EMF	diox/w	25°C	75%	U		B3=35.6	1958TWb	(63644)2544

Medium: 75% dioxan, 0.3 M NaCl
****
C9H6NOCl HL CAS 130-16-5 (1268)
5-Chloro-8-hydroxyquinoline;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	diox/w	25°C	60%	U		B3=34.38	1973SCd	(63662)2545

Medium: 60% dioxan, 0.1 M NaClO4

****

C9H6NOF HL CAS 387-97-3 (3283)
5-Fluoro-8-hydroxyquinoline;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	diox/w	25°C	50%	U			1958TWb	(63673)2546
							B3=35.6		

Medium: 50% dioxan, 0.3 M NaCl

****

C9H6NOI HL CAS 15207-63-1 (3282)
5-Iodo-8-hydroxyquinoline;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	EMF	diox/w	25°C	75%	U			1958TWb	(63683)2547
							B3=34.2		

Medium: 75% dioxan, 0.3 M NaCl

****

C9H6NO4BrS H2L CAS 3062-38-2 (4688)
5-Bromo-8-hydroxyquinoline-7-sulfonic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	oth/un	25°C	dil	U		K1=12.02	1970BBd	(63687)2548

****

C9H6NO4BrS H2L CAS 3062-37-1 (3889)
7-Bromo-8-hydroxyquinoline-5-sulfonic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaClO4	20°C	0.10M	U		K1=9.28	1970ABd	(63695)2549

****

C9H6NO4ClS H2L CAS 3244-71-1 (4687)
5-Chloro-8-hydroxyquinoline-7-sulfonic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	oth/un	25°C	dil	U		K1=11.67	1970BBd	(63710)2550
Fe+++	sp	oth/un	25°C	?	U			1968BBc	(63711)2551
							K(Fe+HL=FeL+H)=3.5		

****

C9H6NO4IS H2L CAS 3075-21-6 (4689)
5-Iodo-8-hydroxyquinoline-7-sulfonic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	oth/un	25°C	dil	U		K1=12.22	1970BBd	(63717)2552

****
C9H6NO4IS H2L Ferron CAS 547-91-1 (275)
7-Iodo-8-hydroxyquinoline-5-sulfonic acid; (HO)(HO3S)C9H4NI

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp NaClO4 45°C 1.0M C H K1=0.78 1994DAb (63793)2553
Data for 40-50 C. DH(K1)=37.7 kJ mol-1, DS(K1)=133.5 J K-1 mol-1.
By kinetics at 45 C, K1=0.77

Fe+++ gl KNO3 25°C 0.10M C K1=11.79 B2=21.20 1985ZHa (63794)2554
K3=5.62

Fe+++ sp KCl 25°C 0.10M U I K1=11.5 B2=22.00 1982GTa (63795)2555
K3=9.7
In Fe(III)-ferron-CTMAC solution K1=11.5, K2 < 9.7, K3 > 12.2

Fe+++ sp oth/un 20°C 0.0 U I K1=3.22 B2=7.74 1972PBc (63796)2556
K3=4.25
Medium: 10% EtOH, I=0. B3=12.3, 30% EtOH: B3=11.8, 50% EtOH: B3=11.1

Fe+++ gl KCl 25°C 0.10M U K1=8.9 B2=17.3 1961SLa (63797)2557
K3=7.9

Fe+++ sp oth/un 30°C 0.30M U H B2=7.46 1960SDa (63798)2558
Medium: 0.3 M K2SO4. DG(K1)=-43.30 kJ mol-1. By glass electrode B2=7.64

Fe+++ EMF diox/w 25°C 50% U 1958TWb (63799)2559
B3=31.5
Medium: 50% dioxan, 0.3 M NaCl
****
C9H6N2O3 HL CAS 5437-99-0 (3865)
5-Nitro-8-hydroxyquinoline;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl diox/w 25°C 60% U 1973SCd (63863)2560
B3=25.89
Medium: 60% dioxan, 0.1 M NaClO4
****
C9H6O3 HL CAS 3952-69-0 (3852)
5-Hydroxybenzo[b]-4-pyrone (5-hydroxychromone);

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp alc/w 20°C 10% U K1=12.74 B2=23.25 1968MIa (63940)2561
K(Fe+HL=FeL+H)=1.99
K(FeL+HL=FeL2+H)=-0.24
Medium: 10% MeOH, 0.1 M (H,Na)ClO4

```
Fe+++      sp  alc/w  20°C  10%  U        K1=12.74  B2=23.25  1968MIa (63941)2562
Medium: 10% MeOH, 0.1 M NaClO4
********************************************************************************
C9H6O7               H4L                    CAS 609-98-3  (4591)
2-Hydroxybenzene-1,3,5-tricarboxylic acid; HO.C6H2(COOH)3
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      sp  oth/un   ?     ?  U                        1969MPf (64005)2563
                                       K(FeOH+HL)=3.85
********************************************************************************
C9H6O7               H4L                    CAS 54176-76-0  (4592)
5-Hydroxybenzene-1,2,4-tricarboxylic acid; HO.C6H2(COOH)3
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      sp  oth/un   ?     ?  U                        1969MPf (64009)2564
                                       K(FeOH+HL)=3.75
********************************************************************************
C9H7NO                HL    Oxine          CAS 148-24-3  (504)
8-Hydroxyquinoline (8-quinolinol);
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 1.00M C T HM                   1992DAa (64262)2565
                                       K(Fe+H2L=FeL+2H)=-0.84
By calorimetry: DH(K1)=44.7 kJ mol-1, DS=127 J K-1 mol-1
--------------------------------------------------------------------------------
Fe+++      gl  KNO3   25°C 1.00M U  I     K1=13.41  B2=25.44  1987VZa (64263)2566
                                       B3=36.93
For 0.313 mol fraction dioxan/H2O K1=14.01; B2=26.77; B3=38.33. Also data
for other dioxan fractions.
--------------------------------------------------------------------------------
Fe+++      gl  diox/w 25°C  60%  U                      1973SCd (64264)2567
                                       B3=37.74
Medium: 60% dioxan, 0.1 M NaClO4
--------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 0.10M U        K1=13.69  B2=26.3   1968TSa (64265)2568
                                       B3=36.9
                                       Kso=-43.51
--------------------------------------------------------------------------------
Fe+++      EMF diox/w 25°C  50%  U                      1958TWb (64266)2569
                                       B3=38.00
Medium: 50% dioxan, 0.3 M NaClO4
--------------------------------------------------------------------------------
Fe+++      EMF diox/w 25°C  75%  U                      1958TWb (64267)2570
                                       B3=37.20
Medium: 75% dioxan, 0.3 M NaClO4
--------------------------------------------------------------------------------
Fe+++      gl  oth/un 20°C 0.01M U        K1=12.3   B2=23.6   1954AHb (64268)2571
```

B3=33.9

Fe+++ sp oth/un 25°C 0.0 U K1=14.52 1949SSa (64269)2572

****

C9H7NO2 HL CAS 1127-45-3 (4614)

8-Hydroxyquinoline-N-oxide;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	diox/w	30°C	50%	U		K1=11.0 B2=21.10	1970GMb (64404)	2573

Medium: 50% dioxan, 0.3 M NaClO4

****

C9H7NO4S H2L Sulfoxine CAS 84-88-8 (448)

8-Hydroxyquinoline-5-sulfonic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaClO4	25°C	1.00M	C		K1=12.07 B2=23.24	1994GCa (64538)	2574
							K3=9.42		
							B3=32.66		
Fe+++	sp	NaClO4	25°C	1.00M	C T HM			1992DAa (64539)	2575
							K(Fe+H2L=FeL+2H)=-0.63		

By calorimetry: DH(K1)=44.0 kJ mol-1, DS=128 J K-1 mol-1

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	oth/un	25°C	?	U			1968BBd (64540)	2576
							K(?)=3.80		
Fe+++	gl	KNO3	25°C	0.10M	U		K1=11.6 B2=22.8	1959RGa (64541)	2577
							K(FeLOH+H)=3.02		
							K(FeL(OH)2+H)=3.94		
							K(FeL2OH+H)=5.02		
							K(FeL2(OH)2+2H)=5.45		
Fe+++	EMF	diox/w	25°C	50%	U			1958TWa (64542)	2578
							B3=35.65		

Medium: 50% dioxan, 0.3 M NaCl

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	oth/un	20°C	0.01M	U		K1=12.0	1953ALa (64543)	2579

****

C9H7NO4S H2L CAS 3062-35-9 (4676)

8-Hydroxyquinoline-7-sulfonic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	oth/un	25°C	dil	U		K1=11.57	1970DBb (64595)	2580

****

C9H8N2 L CAS 578-66-5 (503)

8-Aminoquinoline;

```
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      gl  KCl    20°C 0.10M U        K1=3           1957WSa (64782)2581
*************************************************************************
C9H8N2O3S             H2L                      CAS 148292-08-4  (7219)
Nordesferriferrithiocin; (HO)C5NH3.C3NSH3(COOH)
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      sp  KCl    25°C 0.10M C        B2=29.09       1996LHa (64815)2582
*************************************************************************
C9H8O3                 HL                       CAS 1738-16-5  (3854)
4-Acetyltropolone;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C  2.0M U        K1=9.60        1964OYc (64880)2583
*************************************************************************
C9H8O4                 H2L                      CAS 97652-17-0  (3855)
3-Carboxy-4-methyltropolone;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      sp  NaClO4   ?  0.10M U        K1=11.65  B2=21.90  1966SDa (64939)2584
                                         K3=6.90
*************************************************************************
C9H8O4                 H2L                      CAS 2613-89-0  (1145)
Phenylmalonic acid; HOOC.CH(C6H5).COOH
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      gl  NaClO4 30°C 0.10M U        K1=6.65   B2=12.35  1976DGd (64994)2585
                                         K3=3.28
*************************************************************************
C9H9NO4                H2L    Salicylglycine   CAS 487-54-7  (3869)
N-(2-Hydroxybenzoyl)glycine, 2-hydroxyhippuric acid; HO.C6H4.CO.NH.CH2.COOH
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      EMF NaClO4 25°C 0.10M U                         1966PAb (65094)2586
                                         K(Fe+HL=FeL+H)=2.09
                                         K(FeL+HL=FeL2+H)=0.57
                                         K(FeL2+HL=FeL3+H)=-4.1
                                         K(Fe+HL)=3.9
*************************************************************************
C9H9N3O2S2              HL    Sulfathiazole    CAS 72-14-0  (8357)
4-Amino-N-2-thiazolyl-benzenesulfonamide;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
```

Fe+++ gl alc/w 25°C 50% C K2=8.30 1999GAa (65133)2587
Medium: 50% EtOH/H2O, 0.10 M NaNO3.
****
C9H10NO3Br H2L (6645)
N-Ethyl-5-bromo-3,4-dihydroxybenzamide;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl NaClO4 25°C 1.00M U 1992AGa (65185)2588
K(Fe+H2L=FeL+2H)=-0.33
K(FeL+H2L=FeL2+2H)=-4.37
K(FeL2+H2L=FeL3+2H)= -8.20
K1 from spectrophotometry. Data also for 5-nitro- and 5-fluoro- analogues
****
C9H10O2 HL CAS 6921-64-8 (4595)
2-Hydroxy-4-methylacetophenone; HO(CH3).C6H3.CO.CH3

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl diox/w 27°C 75% U K1=9.76 B2=17.38 1973KDc (65327)2589
Medium: 50% v/v dioxan, 0.5 M NaClO4
****
C9H10O2 HL CAS 1450-72-2 (4596)
2-Hydroxy-5-methylacetophenone; HO(CH3).C6H3.CO.CH3

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl diox/w 27°C 75% U K1=7.90 B2=14.73 1973KDc (65334)2590
Medium: 50% v/v dioxan, 0.5 M NaClO4
****
C9H10O2 HL CAS 610-99-1 (4597)
2-Hydroxypropiophenone;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl diox/w 27°C 75% U K1=9.69 B2=17.12 1973KDc (65344)2591
Medium: 75% dioxan, 0.1 M NaClO4
****
C9H10O3 H2L CAS 5792-36-9 (4599)
2,4-Dihydroxypropiophenone; (OH)2.C6H3.CO.C2H5

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp NaClO4 ? 0.10M U 1968GDa (65424)2592
K(?)=3.11
****
C9H10O3 H2L CAS 1643-34-0 (4598)
2,6-Dihydroxy-4-methylacetophenone; (HO)2(CH3).C6H2.CO.CH3

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo

```
------------------------------------------------------------------------------
Fe+++      gl  diox/w 27°C  75%  U                      1973KDc (65430)2593
                                      K(Fe+HL)=7.80
                                      K(FeHL+HL)=16.07
Medium: 75% dioxan, 0.1 M NaClO4
******************************************************************************
C9H10O3                HL    Phenyllactic     CAS 828-01-3  (1190)
2-Hydroxy-3-phenylpropanoic acid, b-Phenyllactic acid; C6H5.CH2.CH(OH).COOH
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Fe+++      sp  none   30°C  0.0  U                      1976GCa (65449)2594
                                      K1eff=3.69
Measured at pH 3.0
******************************************************************************
C9H11NO2               HL    Phenylalanine    CAS 63-91-2  (2)
2-Amino-3-phenylpropanoic acid; H2N.CH(CH2.C6H5)COOH
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Fe+++      gl  NaClO4 25°C  3.0M U      T K1=10.39  B2=19.11  1972WYa (65937)2595
                                      B3=26.0
                                      K(2Fe+2L=Fe2(OH)2L2+2H)=16.9
------------------------------------------------------------------------------
Fe+++      EMF NaClO4 20°C  1.0M U        K1=8.9         1958PEd (65938)2596
******************************************************************************
C9H11NO2             H2L                      CAS 18265-75-3  (4651)
2-Hydroxypropiophenone oxime; HO.C6H4.C(:N.OH).CH2.CH3
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Fe+++      sp  NaClO4   ?  0.10M U                      1968GDa (65993)2597
                                      K(?)=3.19
******************************************************************************
C9H11NO3             H2L                        (2260)
2,3-Dihydroxy-N,N-dimethylbenzamide; (HO)2.C6H3.CO.N(CH3)2
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Fe+++      gl  KNO3   25°C 0.10M C        K1=17.77  B2=31.73  1979HCb (66047)2598
                                      K3=8.51
By spec. K1=17.95, K2=13.97, K3=8.90
******************************************************************************
C9H11NO3             H2L                        (3874)
3-2',4'-Dihydroxypropiophenone oxime;
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Fe+++      sp  NaClO4   ?  0.10M U                      1967GDa (66273)2599
                                      K(?)=3.20
```

****

C9H11NO4 HL CAS 95215-59-1 (8724)
1-(2'-Carboxyethyl)-2-methyl-3-hydroxy-4-pyridinone;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KNO3	25°C	0.10M	C		K1=18.41 B2=29.42 B3=37.97 B(FeH2L2)=35.60	2002SGb (66303)	2600

****

C9H11NO4 H3L DOPA CAS 59-92-7 (5)
2-Amino-3-(3,4-dihydroxyphenyl)propanoic acid;H2NCH(CH2C6H3(OH)2)COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	NaCl	25°C	0.12M	U		K1=18.39 K(Fe+H2L)=10.28 K(FeL+2H)=13.53	1978RMc (66397)	2601
Fe+++	sp	NaClO4	25°C	1.00M	U		K(Fe+H3L=FeHL+2H)=2.71	1976MPa (66398)	2602

****

C9H11NO6S H3L CAS 73487-23-7 (5467)
N,N-Dimethyl-2,3-dihydroxy-5-sulfonatobenzamide; HSO3.C6H2(OH)2.CONMe2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KNO3	25°C	0.10M	U		K1=18.7 B2=32.0 B3=40.3	1982PWa (66461)	2603
Fe+++	gl	KNO3	25°C	0.10M	C		K1=ca.41 K(Fe+HL=FeL+H)=7.23 K(FeL+HL=FeL2+H)=1.81 K(FeL2+HL=FeL3+H)=-3.21	1981HRa (66462)	2604

By spectrophotometry: K(FeL+HL=FeL2+H)=1.87, K(FeL2+HL=FeL3+H)=-3.13

****

C9H12N2O HL (6765)
N-(2-Aminoethyl)salicylideneimine; HO.C6H4.CH:NCH2CH2NH2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	mixed	25°C	80%	C		K1=19.0	1991LMa (66563)	2605

Medium: 80% w/w DMSO/H2O, 0.1 M KClO4

****

C9H12N2O4S H2L CAS 42197-15-9 (4685)
N-(5-Sulfo)salicylidenediaminoethane; HO3S.C6H3(OH).CH:N.CH2.CH2.NH2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KCl	20°C	0.10M	U		B2=29.9	1972KEd (66626)	2606

****
C9H13NO2 L (7151)
1,2-Diethyl-3-hydroxy-4-pyridinone

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl KCl 25°C 0.10M C K1=15.21 B2=26.97 1994MRa (66794)2607
K3=9.78
****
C9H13NO2 HL CAS 116407-52-4 (5869)
3-Hydroxy-1-butylpyridin-2(1H)-one;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp KCl 25°C 0.10M C 1988SRc (66803)2608
K(FeL2+L=FeL3)=8.7
K(FeL3=FeL(OH)2+2L+2H)=-25.1
****
C9H13NO3 H2L (-)Adrenaline CAS 51-43-4 (252)
4-(1-Hydroxy-2-(methylamino)ethyl)-1,2-dihydroxybenzene,
Epinephrine;CH3NHCH(OH)C6H3(OH)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp NaClO4 25°C 1.00M U 1976MPa (66862)2609
K(Fe+H2L=FeL+2H)=2.84
****
C9H14O7P2 H5L CAS 147608-61-5 (7128)
Hydroxy-4-methylbenzene-2,6-di(methylphosphonic acid);

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp KNO3 20°C 1.0M U 1995AAa (67368)2610
K(Fe+H2L)=12.05
****
C9H14O7P2 H2L CAS 445253-97-4 (8732)
[(Dimethoxyphosphinyl)hydroxyphenylmethyl]phosphoric acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl KNO3 25°C 0.10M C B2=18.90 2002GKc (67376)2611
B(FeH-3L)=-5.59
B(FeH-1L2)=13.38
B(FeH-2L2)=6.68
****
C9H15NO6S H3L DCMM CAS 72306-91-3 (8239)
Dicarboxymethyl-N,N-methionine acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---

```
Fe+++      gl  NaCl   25°C 0.50M C                        1980MFc (67471)2612
                                          K(Fe+HL)=10.98
Addditional methods: conductivity, spectrophotometry
**************************************************************************
C9H16O2                HL                       CAS 18362-64-6  (1134)
2,6-Dimethyl-3,5-heptanedione; (CH3)2.CH.CO.CH2.CO.CH(CH3)2
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C  0.5M C        K1=12.7        1998BLa (67744)2613
**************************************************************************
C9H16O2                 L                       CAS 107803-05-4  (1437)
Nonane-2,4-dione; CH3COCH2CO(CH2)4CH3
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C  0.5M C        K1=11.5        1998BLa (67753)2614
**************************************************************************
C9H18N2O4             H2L                      CAS 18992-11-5  (5913)
N,N-Dihydroxynonanediamide; HN(OH).CO.(CH2)7.CO.NH(OH)
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe+++      gl  KCl    25°C 0.20M C        K1=19.13       1999FEa (67938)2615
                                          B(Fe2L3)=56.0
--------------------------------------------------------------------------
Fe+++      gl  NaNO3  25°C 0.10M C        K1=20.08       1989EHa (67939)2616
**************************************************************************
C9H24N3O9P3           H6L    NOTPH            CAS 83843-39-3  (224)
1,4,7-Triazacyclononane-N,N',N"-tris(methylenephosphonic acid);
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe+++      gl  KNO3   25°C 1.00M U        K1=29.6        1990BSd (68318)2617
--------------------------------------------------------------------------
Fe+++      gl  KCl    25°C  1.0M U        K1=29.6        1984KMa (68319)2618
**************************************************************************
C10H6N2O               HL                       CAS 6759-78-0  (3316)
5-Cyano-8-hydroxyquinoline;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe+++      EMF diox/w 25°C  50%  U                        1958TWb (68439)2619
                                          B3=29.8
Medium: 50% dioxan, 0.3 M NaCl
**************************************************************************
C10H7NO2               HL                       CAS 2598-30-3  (3317)
5-Formyl-8-hydroxyquinoline;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
```

```
--------------------------------------------------------------------------------
Fe+++      gl  diox/w 25°C  50%  U        K1=11.7   B2=21.7   1958JPa (68672)2620
                                         K3=8.3
Medium: 50% dioxan, 0.3 M NaCl
--------------------------------------------------------------------------------
Fe+++      EMF diox/w 25°C  50%  U                      1958TWb (68673)2621
                                         B3=29.5
Medium: 50% dioxan, 0.3 M NaCl
********************************************************************************
C10H7NO2               HL    Quinaldic acid   CAS 93-10-7  (2209)
Quinoline-2-carboxylic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      sp  oth/un 20°C .077M U        B2=7.58        1952WMa (68709)2622
********************************************************************************
C10H7NO5S             H2L                    CAS 23525-13-6  (1813)
2-Nitroso-1-hydroxynaphthalene-5-sulfonic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      EMF oth/un 25°C  0.0  U        K1=5.01   B2=8.21   1972MSi (68910)2623
********************************************************************************
C10H7NO5S             H2L                    CAS 31005-79-9  (1814)
2-Nitroso-1-hydroxynaphthalene-8-sulfonic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      EMF oth/un 25°C  0.0  U        K1=6.78   B2=10.33  1972MSi (68944)2624
********************************************************************************
C10H7NO8S2            H3L                    CAS 26276-77-7  (4767)
1-Hydroxy-2-nitrosonaphthalene-4,8-disulfonic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      EMF oth/un 25°C  0.0  U        K1=7.35   B2=10.41  1972MSi (68964)2625
********************************************************************************
C10H7O2F3              HL                     CAS 326-06-7  (196)
3-Benzoyl-1,1,1-trifluoroacetone; CF3.CO.CH2.CO.C6H5
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      gl  alc/w  25°C  75%  C        K1=6.16   B2=12.46  1998ERa (69146)2626
                                         B3=14.6
                                         B(FeH-1L2)=-1.25
Medium: 75% v/v EtOH/H2O, 0.10 M KCl
--------------------------------------------------------------------------------
Fe+++      dis NaClO4 25°C  4.0M C  I                    1986SIc (69147)2627
                                         K(Fe+3L=FeL3(org))=29.3
Method: distribution from 4.0 M NaClO4 into CCl4.
```

Using MIBK,K(Fe+3L=FeL3(org))=25.9

Fe+++ dis NaClO4 25°C 4.0M C K1=7.7 B2=14.40 1985IIa (69148)2628
B3=19.8

Method: extraction into CCl4; analysis by spectrophotometry.
K(Fe+3HL(org)=FeL3(org)+3H)=2.3. Values for K1, B2, B3 are approximate.

****

C10H8N2 L 2,2'-Bipyridyl CAS 366-18-7 (25)
2,2'-Bipyridine; (C5H4N)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	gl	NaNO3	25°C	0.10M	C	M			2002MDa	(69572)2629

K(Fe+L+B(OH)4=FeL(H2BO4)+2H)=14.39, K(2Fe+2L+B(OH)4=Fe2L2(BO4)+4H)=24.06,
K(Fe+2L+B(OH)4=FeL2(H2BO4)+2H)=21.28, K(2Fe+4L+B(OH)4=Fe2L4(BO4)+4H)=36.78

Fe+++	gl	NaNO3	25°C	0.10M	C		K1=9.13	B2=18.11	2002MDa	(69573)2630
							B(FeH-1L)=6.96			
							B(FeH-2L)=5.11			
							B(FeH-1L2)=14.74			
							B(FeH-2L2)=10.76			

Fe+++	sp	KNO3	22°C	2.8M	U	T	K1=-0.43		1976RAa	(69574)2631

Fe+++	gl	oth/un	20°C	var	U				1962ANc	(69575)2632
							K(2Fe+4L=Fe2(OH)2L4+2H)=16.29			

****

C10H8N2O2 HL (3318)
8-Hydroxyquinoline-5-carbaldehyde oxime

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	EMF	diox/w	25°C	50%	U				1958TWb	(69685)2633
							B3=34.0			

Medium: 50% dioxan, 0.3 M NaCl

****

C10H8O2 H2L CAS 92-44-4 (1658)
2,3-Dihydroxynaphthalene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	sp	NaClO4	?	0.10M	U		K1=20.85	B2=36.15	1969ZSb	(69769)2634
							K3=9.8			
							K(Fe+H2L=FeL+2H)=-1.15			
							K(FeL+H2L=FeL2+2H)=-6.5			
							K(FeL2+H2L=FeL3+2H)=-12.0			

****

C10H8O5S H2L CAS 16223-97-7 (2392)
1,2-Dihydroxynaphthalene-4-sulfonic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	NaClO4	25°C	0.10M	C		K1=19.84 B2=34.95 K(FeL+L+2H)=19.3 K(FeL2+OH)=6.4	1977BMd (69808)	2635

****

C10H8O5S H3L DHNSA (877)
2,3-Dihydroxynaphthalene-6-sulfonic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	NaClO4	25°C	0.10M	C		K1=18.10 B2=30.50 K3=8.00	1980NSe (69843)	2636
Fe+++	sp	NaClO4	?	0.10M	U		K1=19.5 B2=33.65 K3=9.8 K(Fe+H2L=FeL+2H)=-0.75 K(FeL+H2L=FeL2+2H)=-6.05 K(FeL2+H2L=FeL3+2H)=-10.5	1969ZSb (69844)	2637
Fe+++	sp	KCl	20°C	0.10M	U		K1=19.88 B2=34.35 B3=44.22	1952HSb (69845)	2638

****

C10H8O7S2 H3L CAS 1330-52-5 (3904)
2-Hydroxynaphthalene-3,6-disulfonic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	oth/un	25°C	?	U		K(?)=8.8	1962BAa (69878)	2639

****

C10H8O8S2 H4L Chromotropic ac CAS 148-25-4 (1875)
1,8-Dihydroxynaphthalene-3,6-disulfonic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaClO4	20°C	0.2M	M	IH	K1=17.01	1995LHa (69944)	2640
In 50% EtOH: K1=19.70									
Fe+++	gl	NaNO3	25°C	0.10M	U		K1=20.6 B2=33.50	1990HWa (69945)	2641
K1 by spectrophotometric methods.									
Fe+++	sp	oth/un	25°C	0.10M	U		K(FeOH+L)=3.31 K(FeOH+2HL)=3.33	1969NBc (69946)	2642
Fe+++	vlt	oth/un	?	1.0M	U		K1=22.8	1960BEa (69947)	2643
Fe+++	sp	oth/un	20°C	0.20M	U		K1=23.10 B2=36.86	1959SOd (69948)	2644
Medium: 0.2 M hexamethylenetetramine									

```
-------------------------------------------------------------------------------
Fe+++      gl  oth/un 20°C 0.10M U    M                  1951HSa (69949)2645
                                        K(FeA+2L)=17.0
H3A=NTA
*******************************************************************************
C10H9NO                HL                     CAS 5541-67-3  (999)
5-Methyl-8-hydroxyquinoline;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe+++      EMF diox/w 25°C  50%  U                        1958TWb (70065)2646
                                        B3=39.5
Medium: 50% dioxan, 0.3 M NaCl
*******************************************************************************
C10H9NO2               HL                     CAS 87-51-4  (891)
Indole-3-ethanoic acid;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe+++      oth none     ?   0.0  U        K1=6.0         1958RHb (70135)2647
*******************************************************************************
C10H9NO3               HL                     CAS 24618-19-7  (1133)
8-Amino-7-hydroxy-4-methyl coumarin;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe+++      sp  alc/w  30°C  50%  U        K1=10.34       1975PTa (70149)2648
*******************************************************************************
C10H9NO3S             H2L                     CAS 49608-51-7  (8280)
4,5-Dihydro-2-(2-hydroxyphenyl)-4-thiazolecarboxylic acid,
Deazademethyldesferrithiocin;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe+++      gl  KNO3   25°C 0.10M C        B2=31.4        1990ARa (70169)2649
*******************************************************************************
C10H9NO4               HL                     CAS 21659-48-3  (4719)
alpha-Furoinoxime, Furoylfuryloxime;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe+++      sp  alc/w  25°C 100%  U                        1968ADb (70184)2650
                                        B3=8.17
*******************************************************************************
C10H9NO7S2             H3L                     CAS 82-47-3  (6247)
8-Amino-1-hydroxynaphthalene-3,6-disulfonic acid;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe+++      sp  oth/un 25°C    ?  U                        1963RSb (70221)2651
```

K(Fe+HL=FeL+H)=3.67(?)

****

C10H9N3OS HL CAS 1823-44-5 (4780)
2-(2'-Thiazolylazo)-4-methylphenol; CH3.C6H3(OH).N:N.C3H3NS

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	vlt	oth/un	25°C	0.7M	C		B2eff=22.4	2000CJa (70347)2652	

Method: cathodic stripping voltammetry. Medium: seawater buffered to pH 8.0 (5 mM EPPS). B2eff: Fe+2L'=Fe(L')2. K(Fe'+2L')=12.4.

****

C10H10NO2Cl HL CAS 6144-11-0 (247)
Acetoacet-2-chloroacetanilide; CH3.CO.CH2.CO.NH.C6H4.Cl

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	diox/w	30°C	50%	U	I	K1=11.46	1972TSe (70492)2653	

75% dioxan: K1=13.27

****

C10H10N2O3S H2L CAS 76045-30-2 (7218)
Desferriferrithiocin,
2-(3-Hydroxypyridin-2-yl)-4-methyl-4,5-dihydrothiazole-4-carboxylic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	KCl	25°C	0.10M	C		B2=31.04	1996LHa (70560)2654	
Fe+++	gl	KNO3	25°C	0.10M	C		B2=29.6	1990ARa (70561)2655	

****

C10H10O2 HL Benzoylacetone CAS 93-91-4 (197)
1-Phenylbutane-1,3-dione; C6H5.CO.CH2.CO.CH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	alc/w	25°C	75%	C		K1=11.14 B2=20.08 B3=22.8	1998ERa (70726)2656	

Medium: 75% v/v EtOH/H2O, 0.10 M KCl

Fe+++	dis	NaClO4	25°C	4.0M	C	I	K(Fe+3L=FeL3(org))=36.0	1986SIc (70727)2657	

Method: distribution from 4.0 M NaClO4 into CCl4.
Using MIBK, K(Fe+3L=FeL3(org))=37.7

Fe+++	dis	NaClO4	25°C	4.0M	C		K1=11.4 B2=20.80 B3=26.7	1985IIa (70728)2658	

Method: extraction into CCl4; analysis by spectrophotometry.
K(Fe+3HL(org)=FeL3(org)+3H)=0.3. Values for K1, B2, B3 are approximate.

Fe+++	vlt	non-aq	25°C	100%	U		K1=13.8 B2=26.50	1969INb (70729)2659	

K3=10.9

Medium: 0.1(C2H5)4NCl, HCON(CH3)2

****

C10H10O3 HL Mellein CAS 1200-93-7 (7616)

Mellein;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaClO4	25°C	0.10M	C			1998AGa (70804)	2660

K1eff=3.93

Method: fluorescence. pH=2.6.

****

C10H10O4 H2L CAS 616-75-1 (4700)

Benzylmalonic acid; HOOC.CH(CH2.C6H5).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	kin	NaClO4	25°C	0.50M	C		K1=7.26	1977CCb (70820)	2661
Fe+++	kin	NaClO4	25°C	0.50M	U		K1=7.26	1971CDa (70821)	2662

****

C10H11NOS L (2831)

Acetothioacetanilide; CH3.CO.CH2.CS.NH.C6H5

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	alc/w	25°C	60%	U		K1=4.39	1984FNa (70881)	2663

Medium: 60% v/v EtOH/H2O. Data also for 4-Cl-, 4-Br- and 3-Me- analogues

****

C10H11NO2 L CAS 102-01-2 (250)

Acetoacetanilide; CH3.CO.CH2.CO.NH.C6H5

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	diox/w	30°C	50%	U	I	K1=12.82	1971TSg (70910)	2664

Medium: 50% dioxan, 0.002 M FeCl3

In 0.002 FeCl3, 75% dioxan: K1=12.90

****

C10H11NO4 H2L CAS 1137-73-1 (2567)

N-Phenyliminodiethanoic acid; C6H5.N(CH2.COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	KNO3	20°C	0.10M	U		K1=6.78	1975KOa (71002)	2665

****

C10H11NO5 H3L CAS 100844-86-8 (2108)

N-(2-Hydroxyphenyl)iminodiethanoic acid; HO.C6H4.N(CH2.COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo

Fe+++ EMF oth/un ? ? U K1=15.18 1968TRc (71041)2666
****
C10H12N2O4 HL (6004)
N-Benzyloxycarbonylglycyl hydroxamic acid; C6H5.CH2.O.CO.NH.CH2.CO.NHOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl KNO3 25°C 0.10M U K1=11.4 B2=21.5 1987CSb (71301)2667
B3=30.2
B3 obtained by spectrophotometric method.
****
C10H12O2 HL CAS 7624-24-2 (4702)
2-Hydroxy-4-methylpropiophenone; HO.C6H3(CH3).CO.CH2.CH3

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl diox/w 27°C 75% U K1=9.79 B2=15.68 1973KDc (71527)2668
Medium: 75% dioxan, 0.1 M NaClO4
****
C10H12O2 HL CAS 1946-74-3 (202)
3-Isopropyltropolone;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ dis oth/un 25°C 1.0M U K1=13.0 1971MMa (71581)2669
B3=24.77

Fe+++ sp diox/w ? 40% U K1=11.80 B2=22.76 1966SDa (71582)2670
K3=9.54
Medium: 40% dioxan, 0.1 M NaClO4
****
C10H12O2 HL CAS 499-44-5 (3303)
4-Isopropyltropolone;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp NaClO4 25°C 2.00M U K1=11.55 1964OYc (71631)2671
****
C10H12O2 HL CAS 672-76-4 (3893)
5-Isopropyltropolone;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp NaClO4 25°C 2.00M U K1=10.64 1962OUa (71639)2672
****
C10H12O3 H2L CAS 829-20-9 (4703)
2,4-Dihydroxybutyrophenone; (HO)2.C6H3.CO.CH2.CH2.CH3

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---

Fe+++ sp NaClO4 ? 0.10M U 1968GDa (71642)2673
K(?)=2.83
****
C10H12O3 H2L CAS 7053-88-5 (3894)
3-Isopropylsalicylic acid; (CH3)2.CH.C6H3(OH).COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ EMF NaClO4 25°C 0.10M U 1966PAb (71647)2674
K(Fe+HL=FeL+H)=2.56
****
C10H12O4 HL CAS 90-24-4 (4704)
2-Hydroxy-4,6-dimethoxyacetophenone; (HO)(CH3O)2.C6H2.CO.CH3

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl diox/w 27°C 75% U K1=11.49 B2=22.47 1973KDc (71664)2675
K3=9.84
Medium: 75% dioxan, 0.1 M NaClO4
****
C10H13NO2 H2L CAS 39775-68-5 (4744)
2-Hydroxybutyrophenone oxime; HO.C6H4.C(:N.OH).CH2.CH2.CH3

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp NaClO4 ? 0.10M U 1968GDa (71714)2676
K(?)=3.09
****
C10H13NO3 H3L (4745)
2,4-Dihydroxybutyrophenone oxime; (HO)2.C6H3.C(:N.OH).CH2.CH2.CH3

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp NaClO4 ? 0.10M U 1968GDa (71723)2677
K(?)=3.04
****
C10H13NO3 H2L Salicyl-alanine CAS 57471-91-7 (6944)
2-(N-(2-Hydroxybenzyl))aminopropanoic acid; HO.C6H4.CH2.NH.CH(CH3)COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp NaClO4 25°C 0.10M U K1=18.56 1994OIa (71736)2678
****
C10H13NO4 HL CAS 137528-47-3 (8725)
1-(3'-Carboxypropyl)-2-methyl-3-hydroxy-4-pyridinone;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl KNO3 25°C 0.10M C B2=28.60 2002SGb (71756)2679
B3=36.78

B(FeHL)=19.83
B(FeHL2)=32.69
B(FeH2L2)=35.89
****
C10H14N2O L CAS 7006-13-5 (4746)
N,N-Diethylpicolinamide; C5H4N.CO.N(CH2.CH3)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ oth oth/un 0°C ? U K1=1.0 B2=1.80 1971KAc (72069)2680
Method: freezing point depression
****
C10H14N2O3 H2L CAS 157198-10-2 (6943)
2-(N-(2-Hydroxybenzoyl))-amino-N'-hydroxypropanamide, salicyl-alanine hydroxamic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp NaClO4 25°C 0.10M U K1=23.17 1994OIa (72076)2681
K(Fe+HL)=10.29
K(Fe+H3L=FeH2L+H)=1.50
****
C10H14O2 H2L CAS 58979-61-8 (1188)
4-Butyl-1,2-dihydroxybenzene; (C4H9).C6H3.(OH)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp NaClO4 25°C 1.00M U K1=2.36 1976MPa (72612)2682
K(Fe+H2L=FeL+2H)=-1.64
****
C10H15NO L Ephedrine CAS 299-42-3 (1836)
(1-Methylaminoethyl)benzyl alcohol; C6H5.CH(OH)CH(CH3)NHCH3

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl KCl 25°C .058M U T K1=3.68 B2=6.87 1961SMa (72644)2683
At 0 C: K1=4.00, B2=7.46; 45 C: K1=3.37
****
C10H15N3O8 H3L CAS 43068-75-3 (2463)
Triglycine-N,N-diethanoic acid; (HOOC.CH2)2N.CH2.CO-Gly-Gly-OH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl KNO3 25°C 0.10M C K1=10.01 1974MMb (72717)2684
K(FeL+H)=2.00
****
C10H16N2O8 H4L EDDS CAS 52759-67-8 (1100)
1,2-Diaminoethane-N,N'-di-1,4-butanedioic acid; (CH2.NH.CH(COOH)CH2.COOH)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo

```
--------------------------------------------------------------------------------
Fe+++      gl  NaCl   25°C 0.10M C        K1=20.6        2002OHa (73131)2685
                                          K(Fe(OH)L+H)=7.9
                                          K(Fe(OH)2L+H)=9.9
Ligand is [S,S] isomer.
--------------------------------------------------------------------------------
Fe+++      EMF NaClO4 25°C 0.10M U        K1=22.7        1985PLb (73132)2686
                                          K(Fe+HL)=15.0
--------------------------------------------------------------------------------
Fe+++      gl  KNO3   30°C 0.10M U        K1=15.45       1971TSc (73133)2687
--------------------------------------------------------------------------------
Fe+++      oth KNO3   20°C 0.10M U        K1=21          1968MJa (73134)2688
--------------------------------------------------------------------------------
Fe+++      sp  KNO3   20°C 0.10M U        K1=22.0        1966MSg (73135)2689
********************************************************************************
C10H16N2O8            H4L    EDTA             CAS 60-00-4  (120)
1,2-Diaminoethane-N,N,N',N'-tetraethanoic acid, Sequestric acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      oth oth/un 20°C  0.7M C T                       2003SHb (73766)2690
                                          K1eff=7.08 (pH=8.2)
                                          K1eff=5.46 (pH=8.8)
Medium: Uv-treated seawater. Method: adsoprtion of 59Fe-labelled Fe(OH)n
species from EDTA solution onto C18/silica. At 10 C, K1eff=7.14 (pH 8.11).
--------------------------------------------------------------------------------
Fe+++      cal NaNO3  25°C  0.5M U                       2000KPb (73767)2691
                                          K1(FeL+ox=FeLox)=2.44;
                                          DH1=-13.47 kJ/mol
Ox - oxalate
--------------------------------------------------------------------------------
Fe+++      gl  NaNO3  25°C  0.5M U                       2000PKb (73768)2692
                                          K(FeL+ox=FeLox)=2.44
Ox - oxalate
--------------------------------------------------------------------------------
Fe+++      EMF KNO3   25°C 0.10M C        K1=25.10       1997DFa (73769)2693
                                          K(FeL+H)=1.88
                                          K(Fe(OH)L+H)=7.53
--------------------------------------------------------------------------------
Fe+++      gl  R4N.X  25°C 0.10M C        K1=24.95       1997DQa (73770)2694
                                          K(Fe(OH)L+H)=7.41
Medium: Me4NNO3
--------------------------------------------------------------------------------
Fe+++      sp  alc/w  25°C  75%  U        K1=26.3        1991CMc (73771)2695
                                          K(FeL+H)=1.49
                                          *K(FeL)=-7.42
Medium: 75% v/v EtOH/H2O
--------------------------------------------------------------------------------
Fe+++      gl  NaCl   25°C  3.0M C                       1989MDa (73772)2696
                                          *K(FeL)=-7.20
```

```
--------------------------------------------------------------------------------
Fe+++      gl  NaClO4 25°C 1.00M C                      1983AHa (73773)2697
                                        K(FeL+H)=0.52
--------------------------------------------------------------------------------
Fe+++      sp  KCl    25°C 0.10M C                      1983BMd (73774)2698
                                        *K(Fe(edta)H2O)=-7.6
Additional method: spectrophotometry.
--------------------------------------------------------------------------------
Fe+++      cal NaClO4 25°C 0.10M C   H                  1978DOe (73775)2699
DH(K1)=-11.5 kJ mol-1, DS(K1)=440 J K-1 mol-1.
--------------------------------------------------------------------------------
Fe+++      sp  NaClO4 20°C 0.10M U       B2=19.34       1977KSa (73776)2700
--------------------------------------------------------------------------------
Fe+++      gl  NaClO4 25°C  1.0M M                      1977KSc (73777)2701
                                        K(2FeL(H2O)=LFeOFeL+2H)=-12.21
                                        K(2FeL(OH)=LFeOFeL+H2O)=2.53
--------------------------------------------------------------------------------
Fe+++      ISE KNO3   25°C 0.50M C                      1975VDa (73778)2702
                                        K1eff=12.80 (pH 2.5)
Method: liquid phase Fe(III)-N-benzoyl-N-phenylhydroxylamine electrode.
--------------------------------------------------------------------------------
Fe+++      vlt oth/un 20°C 0.20M U T     K1=25.42       1972BOa (73779)2703
K1(10 C)=25.75, K1(30 C)=25.11, K1(40 C)=24.85
--------------------------------------------------------------------------------
Fe+++      sp  oth/un   ?     ?  U                      1968BLb (73780)2704
                                        K(FeL(OH)+HO2)=4.0
--------------------------------------------------------------------------------
Fe+++      EMF NaClO4 20°C 0.10M U  I    K1=25.1        1967BAc (73781)2705
                                        K(FeL+H)=1.2
                                        K(FeL+OH)=6.50
K1=25.15(I=1)
--------------------------------------------------------------------------------
Fe+++      sp  KNO3     ?     ?  U                      1967LUa (73782)2706
                                        K(FeL+H+SCN)=1.20
--------------------------------------------------------------------------------
Fe+++      sp  oth/un 19°C 0.10M U       K1=23.75       1967ZAa (73783)2707
                                        K(Fe+HL)=14.59
                                        K(Fe+H6L=FeHL+5H)=1.35
                                        K(Fe+H5L=FeL+5H)=1.30
--------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C  1.0M U                      1965BRc (73784)2708
                                        K(Fe+HL)=15.2
                                        K(FeL+OH)=7.1
--------------------------------------------------------------------------------
Fe+++      gl  KCl    25°C  1.0M U T H                  1963GMc (73785)2709
                                        K(FeLOH+H)=7.58
                                        K(2(FeLOH)=(FeLOH)2)=2.95
                                        K((FeLOH)2+2H=2FeL)=12.21
K(FeLOH+H)=7.97(0.4 C),7.80(13.7 C),7.11(42.4 C),DH=-42 kJ mol-1, DS=8;
K(dimer)=3.23, 3.24, 2.18; DH=-63, DS=-151; K(FeL(OH)2+2H)=12.71,12.37,12.04
```

```
--------------------------------------------------------------------------------
Fe+++      dis NaClO4 20°C 0.10M U                      1963STc (73786)2710
                                        K(Fe+L+OH)=34.0
Medium: KClO4
--------------------------------------------------------------------------------
Fe+++      sp  none   20°C  0.0  U        K1=24.23       1960BGd (73787)2711
                                        K(Fe+HL)=15.26
                                        K(Fe+H2L)=8.72
--------------------------------------------------------------------------------
Fe+++      sp  oth/un 20°C  0.0  U        K1=24.23       1959BGa (73788)2712
                                        K(Fe+H2L)=8.70
--------------------------------------------------------------------------------
Fe+++      gl  KNO3   25°C 0.10M U        K1=25.1        1959SCc (73789)2713
                                        K(FeLOH+H)=7.4
                                        K(FeLOH+OH)=4.53
                                        K(FeL(OH)2+OH)=1.5
--------------------------------------------------------------------------------
Fe+++      ix  oth/un 25°C  1.0M U        K1=24          1952JLa (73790)2714
--------------------------------------------------------------------------------
Fe+++      vlt NaNO3  25°C  1.0M U        K1=25.7        1952KAa (73791)2715
--------------------------------------------------------------------------------
Fe+++      EMF KCl    20°C 0.10M U      T K1=25.1        1951SHa (73792)2716
                                        K(Fe+HL)=16.2
                                        K(FeLOH+H)=7.49
                                        K(FeL(OH)2+H)=9.41
********************************************************************************
C10H17NO5             H2L                       CAS 6243-06-7  (3326)
N-(2-Hydroxycyclohexyl)iminodiethanoic acid; HO.C6H10.N(CH2.COOH)2
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      EMF KCl    20°C 0.10M U        K1=12.94       1964PCa (74988)2717
                                        K(Fe(OH)L+H)=2.43
                                        K(Fe(OH)2L+H)=5.95
********************************************************************************
C10H17N3O6S           H3L    Glutathione      CAS 70-18-8  (333)
Glutamyl-cysteinyl-glycine;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      kin NaClO4 25°C 0.10M C                      1976KLb (75119)2718
                                        Keff(Fe(OH)+H3L)=3.49
Method: stopped flow spectrophotometry. Medium pH 1-3.
By spectrophotometry, Keff=3.48.
********************************************************************************
C10H18N2O4            H2L                       CAS 124125-60-6  (914)
1,5-Diazacyclooctane-N,N'-diethanoic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
```

```
Fe+++      gl  NaNO3  25°C 0.10M U        K1=14.43       1990HNa (75203)2719
**************************************************************************
C10H18N2O7            H3L    HEDTA            CAS 150-39-0  (392)
N-(Hydroxyethyl)diaminoethane-N,N',N'-triethanoic acid;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe+++      gl  NaClO4 25°C  1.0M M                        1977KSc (75390)2720
                                      K(2FeL(H2O)=LFeOFeL+2H)=-5.84
                                      K(2FeL(OH)=LFeOFeL+H2O)=2.38
--------------------------------------------------------------------------
Fe+++      sp  none   25°C  0.0  U    M                  1977YOa (75391)2721
                                      K(FeL+SCN)=1.2
                                      K(FeL+CH3COO)=1.7
                                      K(FeL+Cl)=0.2
                                      K(FeL+Br)<0.2
--------------------------------------------------------------------------
Fe+++      sp  oth/un 20°C    ?  U        K1=19.06       1967KAe (75392)2722
--------------------------------------------------------------------------
Fe+++      gl  KCl    25°C  1.0M U                       1963GMc (75393)2723
                                      K(Fe(OH)L+H)=4.11
                                      K(2FeL=(Fe(OH)L)2+2H)=-5.84
                                      K(2Fe(OH)L=(Fe(OH)L)2)=-2.38
                                      K(Fe(OH)2L+H)=8.69
--------------------------------------------------------------------------
Fe+++      gl  KNO3   25°C 0.10M U        K1=19.8        1959SCc (75394)2724
                                      K(FeLOH+H)=3.88
                                      K(FeLOH+OH)=4.95
                                      K(FeL(OH)2+OH)=3.78
**************************************************************************
C10H18N4O6            H2L                      (4504)
Hexanoic acid bis(3-hydroxycarbamoyl-methyl)amide; HONHCOCH2NHCO(CH2)4CONHCH2CONHOH
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe+++      gl  KCl    25°C 0.20M C        K1=17.9        1999FEa (75568)2725
                                      B(Fe2L3)=51.6
**************************************************************************
C10H18N4O8            H4L                   CAS 35048-92-5  (4751)
Ethylenedinitrilo-N,N'-diacetohydroxamic-N,N'-diethanoic acid;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe+++      gl  KNO3   25°C 0.10M U                       1971MMe (75583)2726
                                      K(Fe+H2L)=10.80
                                      K(FeL+H)=4.60
                                      K(FeHL+H)=2.98
                                      K(Fe(OH)L+H)=8.07
**************************************************************************
C10H20N2O4            H2L                   CAS 58534-57-9  (2113)
```

Hexamethylenediamine-N,N-diethanoic acid; H2N(CH2)6.N(CH2.COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KNO3	25°C	0.10M	U		K1=18.79	1977TIa	(75776)2727

****

C10H20N2O4 H2L (6924)

N,N'-Dihydroxy-N,N'-dimethyloctanediamide; CH3N(OH).CO.(CH2)6.CO.N(OH)CH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	kin	NaClO4	25°C	2.00M	C			1994CCa	(75789)2728
							K(Fe+H2L=FeHL+H)=4.85		
							K(FeL+H=FeHL)=1.3		
							K(Fe2HL2+H=2FeHL)=1.80		
							K(Fe2L2+H=Fe2HL2)=-0.097		

****

C10H20N2O4 H2L CAS 5578-84-7 (5914)

N,N-Dihydroxydecanediamide; HN(OH).CO.(CH2)8.CO.NH(OH)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	kin	NaClO4	25°C	2.00M	C			1994CCa	(75799)2729
							K(Fe+H2L=FeHL+H)=6.23		
							K(FeL+H=FeHL)=0.11		
Fe+++	gl	NaNO3	25°C	0.10M	C		K1=20.30	1989EHa	(75800)2730

****

C10H20N2O6 H2L CAS 96817-35-5 (4755)

1,2-Diaminoethane-N,N'-bis(4-hydroxy-2-butanoic acid);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	oth/un	20°C	0.10M	U			1972DKa	(75846)2731
							K(FeOH+L)=14.12		
							K(FeOHL+OH)=7.60		

****

C10H20N2O6 H2L CAS 5616-21-7 (570)

N,N'-Bis(2-hydroxyethyl)diaminoethane-N,N'-diethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	oth/un	30°C	0.10M	U		K1=<15	1953CBa	(75856)2732
							K(FeLOH+H)=2.2		

****

C10H20N4O4 H2L CAS 475984-27-1 (6717)

Piperazine-1,4-bis(N-methylacetohydroxamic acid); C4H8N2(CH2.CO.N(OH)CH3)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo

```
Fe+++      sp  KNO3   25°C 0.10M U                        1993SEa (75895)2733
                                        B(Fe2L3)=61.7
By competition with EDTA. By voltammetry, for Fe(II): B(Fe2HL3)=32.6.
**************************************************************************
C10H20N6O8            H4L                    CAS 38932-78-4  (4756)
1,2-Diaminoethane-N,N,N',N'-tetraacethydroxamic acid;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe+++      sp  NaClO4 20°C 0.10M U        K1=25.6        1972KMc (75901)2734
                                        K(Fe+HL)=20.5
                                        K(Fe+H3L)=12.67
                                        K(Fe+H4L)=9.92
                                        K(FeL+OH)=4.90
K(FeLOH+OH)=3.30
**************************************************************************
C10H20O5               L    15-Crown-5       CAS 33100-27-5  (576)
1,4,7,10,13-Pentaoxacyclopentadecane; cyclo(-(O.CH2.CH2)5-)
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe+++      con mixed  25°C  90%  C        K1=2.78        2003ISa (76002)2735
Medium: 90% v/v DMSO/H2O.
**************************************************************************
C10H22N2O3             L    Cryptand 2,1     CAS 31249-95-3  (835)
4,7,13-Trioxa-1,10-diazacyclopentadecane (Trioxa(2,1)cryptand);
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe+++      gl  R4N.X  25°C 0.05M U        K1=13.0        1999BDb (76316)2736
Medium: Et4NClO4
**************************************************************************
C10H24N4               L    Cyclam           CAS 295-37-4  (8)
1,4,8,11-Tetraazacyclotetradecane; cyclo(-(HN.CH2.CH2.NH.(CH2)3)2-)
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe+++      gl  KCl    25°C 0.50M M        K1=24.1        2001BYb (76665)2737
**************************************************************************
C10H25N5               L    15-Ane-N5        CAS 295-64-7  (99)
1,4,7,10,13-Pentaazacyclopentadecane; cyclo(-(HN.CH2.CH2)5-)
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe+++      gl  none    RT     0  U                        1998ZBb (76733)2738
                                        *K1(FeLCl2)=-3.46
                                        *K2(FeLCl2)=-7.31
**************************************************************************
C10H25N5               L                    CAS 155115-12-1  (8660)
12-Methyl-1,4,7,10-tetraazacyclotridecan-12-amine;
```

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl KCl 25°C 0.50M M K1=27.6 2001BYb (76744)2739
****
C10H26N2O12P4 H8L CAS 28698-30-8 (3342)
N,N,N',N'-Tetra(phosphomethyl)cyclohexane-1,2-diamine;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp oth/un 25°C 0.10M U K1=23.31 1959BYa (76758)2740
****
C11H7NO5 H2L CAS 14461-79-1 (4825)
4-Nitro-2-hydroxy-3-naphthoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp alc/w 25°C ? U 1968ACa (76903)2741
K(Fe+3HL)=7.54
****
C11H7O3Br H2L CAS 2208-15-3 (4824)
4-Bromo-3-hydroxy-2-naphthoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp alc/w 25°C 100% U 1968ACa (76910)2742
K(Fe+3HL)=8.33
****
C11H8O3 H2L CAS 86-48-6 (1129)
1-Hydroxy-2-naphthoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp alc/w 20°C 50% U T K1=4.27 1971PSb (77010)2743
Medium: 50% EtOH. 0.1 M NaClO4. K1(25 C)=4.20, K1(30 C)=4.15, K1(40 C)=4.02
I=0: K1=4.47
****
C11H8O3 H2L CAS 2083-08-1 (1131)
2-Hydroxy-1-naphthoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp NaClO4 30°C 0.10M U T 1972PSa (77061)2744
K(Fe+2HL)=7.83
K(20 C)=8.01, K(40 C)=7.67, K(50 C)=7.51. I=0: K(Fe+2HL)=8.02
****
C11H8O3 H2L CAS 92-70-6 (1130)
2-Hydroxy-3-naphthoic acid (3-Hydroxy-2-naphthoic acid);

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo

```
------------------------------------------------------------------------------
Fe+++      sp  oth/un 30°C    ?  U                      1966GSf (77122)2745
                                          K(Fe+HL=FeL+H)=5.01(?)
******************************************************************************
C11H8O4                HL                     CAS 7555-37-5  (4812)
3-Acetyl-4-hydroxycoumarin
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Fe+++      gl  diox/w 35°C  50%  U        K1=5.11   B2=9.70   1971MAa (77176)2746
Medium: 50% dioxan, 0.01 M NaClO4
******************************************************************************
C11H8O5              H2L                     CAS 5112-55-0  (1132)
7-Hydroxy-4-methyl-coumarin-6-carboxylic acid;
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Fe+++      sp  alc/w  30°C  50%  U        K1=10.43       1975PTa (77216)2747
******************************************************************************
C11H8O6S             H3L                     CAS 66695-90-7  (1996)
1-Hydroxy-4-sulfo-2-naphthoic acid;
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Fe+++      gl  NaClO4 25°C 0.10M U        K1=15.85  B2=26.81  1981LAa (77225)2748
                                          B3=34.05
------------------------------------------------------------------------------
Fe+++      gl  NaClO4 25°C 0.10M C        K1=14.04  B2=24.92  1979LPd (77226)2749
                                          B3=32.29
K1 measured by spectrophotometry
******************************************************************************
C11H8O6S             H3L                     CAS 6407-91-6  (1994)
1-Hydroxy-7-sulfo-2-naphthoic acid;
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 0.10M U        K1=15.85  B2=27.43  1981LAa (77239)2750
                                          B3=34.11
Using pH titrations, K1=14.69, B2=24.40
******************************************************************************
C11H8O6S             H3L                     CAS 15509-36-1  (2658)
3-Hydroxy-7-sulfo-2-naphthoic acid;
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 0.10M C        K1=14.57  B2=25.24  1981LAb (77251)2751
                                          B3=33.58
******************************************************************************
C11H8O9S2            H4L                     CAS 67097-84-1  (1995)
1-Hydroxy-4,7-disulfo-2-naphthoic acid;
```

```
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 0.10M U        K1=14.69  B2=24.74  1981LAa (77279)2752
******************************************************************************
C11H8O9S2             H4L                    CAS 67097-83-0  (1618)
3-Hydroxy-5,7-disulfo-2-naphthoic acid;
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 0.10M C        K1=14.05  B2=23.77  1981LAb (77295)2753
                                          B3=32.03
******************************************************************************
C11H9NO2               HL                     CAS 92609-55-3  (4827)
5-Acetyl-8-hydroxyquinoline;
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Fe+++      gl  diox/w 25°C  60%  U                        1973SCd (77330)2754
                                          B3=31.38
Medium: 60% dioxan, 0.1 M NaClO4
******************************************************************************
C11H9NO4               H2L                    CAS 4321-82-7  (4829)
3-Acetyl-4-hydroxycoumarin oxime;
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Fe+++      gl  diox/w 35°C  50%  U                        1971MAa (77419)2755
                                          K(Fe+HL)=4.82
                                          K(Fe+2HL)=8.79
Medium: 50% dioxan, 0.01 M NaClO4
******************************************************************************
C11H11NO6              H3L                    CAS 1147-65-5  (425)
N-(2'-Carboxyphenyl)iminodiethanoic acid; HOOC.C6H4.N(CH2.COOH)2
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Fe+++      sp  NaNO3  20°C 0.10M U                        1960DSa (77827)2756
                                          K(?)=9.62
******************************************************************************
C11H11N2O2Br           HL                      (9228)
3-[4-Bromophenylazo]penta-2,4-dione;
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Fe+++      gl  alc/w  25°C  0.1M U        K1=8.53         2004GMc (77875)2757
Medium: 0.1 mol/L KCl in 3:7 EtOH/H2O mixture
******************************************************************************
C11H11N2O2Cl           HL                      (9229)
3-[4-Chlorophenylazo]penta-2,4-dione;
```

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl alc/w 25°C 0.1M U K1=8.37 2004GMc (77888)2758
Medium: 0.1 mol/L KCl in 3:7 EtOH/H2O mixture
****
C11H11N2O2I HL (9227)
3-[4-Iodophenylazo]penta-2,4-dione;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl alc/w 25°C 0.1M U K1=8.67 2004GMc (77899)2759
Medium: 0.1 mol/L KCl in 3:7 EtOH/H2O mixture
****
C11H11N3O4 HL (9230)
3-[4-Nitrophenylazo]penta-2,4-dione;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl alc/w 25°C 0.1M U K1=8.02 2004GMc (77959)2760
Medium: 0.1 mol/L KCl in 3:7 EtOH/H2O mixture
****
C11H12N2O2 HL Tryptophan CAS 73-22-3 (3)
2-Amino-3-(3-indolyl)propanoic acid; H2N.CH(CH2.C8H6N)COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ EMF NaClO4 20°C 1.0M U T K1=9.0 1958PEd (78205)2761
****
C11H12N2O2 HL (9226)
3-[Diphenylazo]penta-2,4-dione;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl alc/w 25°C 0.1M U K1=9.10 2004GMc (78250)2762
Medium: 0.1 mol/L KCl in 3:7 EtOH/H2O mixture
****
C11H12N2O5S HL CAS 56475-09-3 (8410)
3-(4'-Sulfophenylhydrazo)-pentane-2,4-dione;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl KCl 25°C 0.10M U T K1=8.43 2005ACa (78319)2763
For 35 C K1=8.20; for 45 C K1=7.96
****
C11H13NOS L CAS 67077-39-8 (6233)
Aceto-4-methylphenylthioamide; CH3.CO.CH2.CS.NH.C6H4.CH3

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---

Fe+++ sp alc/w 25°C 60% U K1=4.53 1984FNa (78444)2764
****
C11H13NO2 HL CAS 3026-99-1 (249)
Acetoacet-2-toluidide; CH3.CO.CH2.CO.NH.C6H4.CH3

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp diox/w 30°C 50% U K1=12.56 1972TSe (78465)2765
In 75% dioxan: K1=14.18
****
C11H13NO2S L CAS 72369-82-5 (6232)
Aceto-4-methoxyphenylthioamide; CH3.CO.CH2.CS.NH.C6H4.OCH3

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp alc/w 25°C 60% U K1=4.65 1984FNa (78479)2766
****
C11H13NO3 HL CAS 91099-10-4 (246)
Acetoacet-2-anisidide; CH3.CO.CH2.CO.NH.C6H4.OCH3

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp diox/w 30°C 50% U K1=12.43 1972TSe (78521)2767
In 75% dioxan: K1=14.35
****
C11H13NO5 H3L HBIDA CAS 7372-13-6 (1603)
N-(2-Hydroxybenzyl)iminodiethanoic acid; HO.C6H4.CH2.N(CH2.COOH)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl KNO3 25°C 0.10M C K1=22.4 1975HMb (78624)2768
****
C11H13NO6 H4L CAS 1911-59-2 (4852)
2,3-Dihydroxybenzyliminodiethanoic acid; (HO)2.C6H3.CH2.N(CH2.COOH)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ EMF oth/un ? ? U 1975DTa (78662)2769
K(Fe+HL)=17.6
****
C11H13NO6 H4L CAS 59036-09-8 (2111)
2,5-Dihydroxybenzyliminodiethanoic acid; (HO)2.C6H3.CH2.N(CH2.COOH)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl oth/un 25°C 0.0 U 1970TTb (78677)2770
K(Fe+HL)=17.7
****
C11H13NO6 H4L CAS 31477-66-7 (4853)
2,6-Dihydroxybenzyliminodiethanoic acid; (HO)2.C6H3.CH2.N(CH2.COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	EMF	oth/un	?	?	U			1975DTa (78691)	2771
							K(Fe+HL)=17.0		

C11H15NO4 HL CAS 480436-59-7 (8726)
1-(4'-Carboxybutyl)-2-methyl-3-hydroxy-4-pyridinone;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KNO3	25°C	0.10M	C		B2=28.79	2002SGb (79036)	2772
							B3=37.01		
							B(FeHL)=19.62		
							B(FeHL2)=33.12		
							B(FeH2L2)=36.45		

C11H18N2O8 H4L PDTA CAS 4408-81-5 (1655)
1,2-Diaminopropane-N,N,N',N'-tetraethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KNO3	20°C	1.0M	U			1986HZa (79284)	2773
							K(FeL+H)=1.25		
							K(FeL+OH)=6.95		

C11H18N2O8 H4L CAS 4408-81-5 (923)
1,3-Diaminopropane-N,N,N',N'-tetraethanoic acid; ((HOOC.CH2)2N.CH2.)2.CH2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	EMF	NaClO4	20°C	0.10M	U		K1=21.4	1967BAc (79442)	2774
							K(FeL+H)=2.4		
Fe+++	gl	KNO3	20°C	0.10M	U			1964LAa (79443)	2775
							K(FeL+H)=2.45		

By redox: K1=21.61

C11H18N2O9 H4L HDPTA CAS 3148-72-9 (431)
1,3-Diamino-2-hydroxypropane-N,N,N',N'-tetraethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KNO3	25°C	0.10M	U		K1=17.2	1971KRa (79551)	2776
Fe+++	sp	oth/un	25°C	?	U		K1=16.6	1971KRa (79552)	2777
Fe+++	gl	KNO3	25°C	0.10M	U			1971KRa (79553)	2778
							K(Fe(OH)L+H)=4.55		
							K(Fe(OH)2L+H)=9.30		

```
--------------------------------------------------------------------------------
Fe+++      sp  oth/un 25°C    ?  U                      1971KRa (79554)2779
                                        B(Fe2L)=21.3
--------------------------------------------------------------------------------
Fe+++      sp  KNO3   20°C 0.10M U        K1=19.68       1967SMf (79555)2780
--------------------------------------------------------------------------------
Fe+++      oth KNO3   20°C 0.10M U        K1=>18         1965JMb (79556)2781
Method: electrophoresis
********************************************************************************
C11H20O2               HL    Dipivaloylmeth.  CAS 1118-71-4  (363)
2,2,6,6-Tetramethyl-3,5-heptanedione; (CH3)3C.CO.CH2.CO.C(CH3)3
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C  0.5M C        K1=14.1        1998BLa (79747)2782
--------------------------------------------------------------------------------
Fe+++      gl  NaClO4 25°C 0.50M U        K1=14.1        1990HMb (79748)2783
********************************************************************************
C11H21N3O5            H2L                     CAS 499238-77-6  (8837)
N-Hydroxy-N'-[4-(hydroxymethylamino)-4-oxobutyl]-N-methylpentanediamide;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      gl  KCl    25°C 0.20M C        K1=19.84       2002FBb (79794)2784
                                        B(Fe2L3)=58.99
K1 determined by spectrophotometry.
********************************************************************************
C11H22N2O4              L                      CAS 90149-53-4  (5532)
N,N'-Dihydroxy-N,N'-diisopropylpentanediamide;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      gl  KNO3   25°C 0.10M C        K1=22.84       1984BHa (79828)2785
                                        B(Fe2L3)=62.1
********************************************************************************
C11H22N2O4            H2L                       (6923)
N,N'-Dihydroxy-N,N'-dimethylnonanediamide; CH3N(OH).CO.(CH2)7.CO.N(OH)CH3
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      kin NaClO4 25°C 2.00M C                        1994CCa (79829)2786
                                        K(Fe+H2L=FeHL+H)=4.30
                                        K(FeL+H=FeHL)=0.85
********************************************************************************
C11H22N4O4            H2L                       (6756)
1,4-Diazacycloheptane-N,N'-bis(N-methyl-acetohydroxamic acid);
C5H10N2(CH2.CO.N(OH)CH3)2
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
```

Fe+++ sp KNO3 25°C 0.10M C 1993SEb (79843)2787
B(Fe2L3)=65.4
Method: competitive reaction with EDTA
****
C12H6O2Cl4S H2L CAS 97-18-7 (4944)
Bithionol; Cl2.C6H2(OH).S.C6H2(OH).Cl2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl alc/w 25°C 75% U K2=11.1 1970FGa (80099)2788
Medium: 75% EtOH, 1.0 M NaClO4
****
C12H7N3O2 L CAS 4199-88-6 (449)
5-Nitro-1,10-phenanthroline;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp oth/un 25°C 0.0 U 1964LAe (80175)2789
B3=7.46

Fe+++ oth oth/un ? ? U B2=9 1944SRa (80176)2790
****
C12H8N2 L Phenanthroline CAS 66-71-7 (144)
1,10-Phenanthroline;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl NaNO3 25°C 0.10M C M 2002MDa (80445)2791
K(Fe+L+B(OH)4=FeL(H2BO4)+2H)=14.78, K(2Fe+2L+B(OH)4=Fe2L2(BO4)+4H)=25.02,
K(Fe+2L+B(OH)4=FeL2(H2BO4)+2H)=22.82, K(2Fe+4L+B(OH)4=Fe2L4(BO4)+4H)=39.91

Fe+++ gl NaNO3 25°C 0.10M C K1=10.41 B2=19.92 2002MDa (80446)2792
B(FeH-1L)=8.54
B(FeH-2L)=6.43
B(FeH-1L2)=16.43
B(FeH-2L2)=12.52

Fe+++ sp R4N.X 25°C 0.10M U 1988SKb (80447)2793
Kout(FeL3+A)=0.15
Kout(FeL3+B)=1.26
Kout(FeL3+C)=1.85
Kout(FeL3+D)=1.92
A=PF6, B=BF4, C=ClO4, D=CF3SO3. Medium: 0.05-0.2M Bu4N(X) (X=A,B,C,D).

Fe+++ kin alc/w 25°C 80% U I M 1983TYa (80448)2794
Kout(FeL3+ClO4)=1.02
Kout(FeL3+Cl)=1.26
Kout(FeL3+SCN)=1.40
Medium: 80% MeOH. In DMSO, O.1 KCl: Kout(FeL3+Cl)=1.72, Kout(FeL3+ClO4)=1.59
In H2O: Kout(FeL3+Cl)=0.176, Kout(FeCl3+SCN)=0.414

```
--------------------------------------------------------------------------------
Fe+++      sp  KNO3   22°C  2.8M U T      K1=-1.02       1976RAa (80449)2795
--------------------------------------------------------------------------------
Fe+++      sol oth/un 25°C 100%  U   H                  1974ARb (80450)2796
                                       Kout(FeA2P+L)=2.43
Medium: CH2Cl2. DH(Kout)=-32.0 kJ mol-1 and DS(Kout)=-63.0 J mol-1 K-1.
A=imidazole, P=deuteroprotoporphin(IX) dimethyl ester
--------------------------------------------------------------------------------
Fe+++      sp  oth/un 35°C  0.0  U   H                  1964LAe (80451)2797
DH(B3)=-41.4 kJ mol-1, DS=121 J K-1 mol-1
--------------------------------------------------------------------------------
Fe+++      EMF oth/un   ?     ?  U        K1=6.5    B2=11.4   1962ANc (80452)2798
                                       B3=23.5
--------------------------------------------------------------------------------
Fe+++      kin none   25°C  0.0  U                     1951CLa (80453)2799
                                       B3=21.1
--------------------------------------------------------------------------------
Fe+++      EMF oth/un 25°C 0.10M U                     1948LKa (80454)2800
                                       B3=14.10
--------------------------------------------------------------------------------
Fe+++      EMF oth/un 25°C  1.0M U  I                  1948LKa (80455)2801
                                       B3=15.00
Method: redox. Medium: 1 M H2SO4. In 8 M H2SO4 B3=20
********************************************************************************
C12H10N2O2S            HL                    CAS 104969-73-5  (6086)
2'-Thienylmethylene-2-iminobenzohydroxamic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      oth mixed  25°C  40%  U        K1=17.45       1986SEa (80715)2802
Medium: 40% DMF/H2O
********************************************************************************
C12H10N4O2             HL                    CAS 90357-70-3  (6767)
3-Hydroxyisonicotinaldehyde isonicotinoyl hydrazone
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      sp  KNO3   25°C 0.10M U        B2=30.0        1990VHa (80772)2803
                                       K(Fe+H2L=FeH2L)=10.43
                                       K(Fe+2H2L=FeH4L2)=17.4
                                       K(Fe+HL=FeHL)=15.7
                                       K(Fe+2HL=FeH2L2)=23.6
********************************************************************************
C12H11N2O4As          H3L                    CAS 54435-90-4  (1105)
5-Phenylazo-2-hydroxyphenylarsonic acid; C6H5.N:N.C6H3(OH).AsO3H2
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      sp  oth/un 25°C 0.04M U  I                  1974NUb (80859)2804
                                       K(Fe+HL)=11.43
```

K(Fe+HL)=11.31 at 0.08mol dm-3
K(Fe+HL)=11.99 at 0.0

****

C12H11N3O4S H2L (4003)
3-Hydroxy-3-phenyl-1-(4'-sulfonyl)triazene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	oth/un	20°C	?	U			1960MSa (80939)	2805
							K(?)=11.62		

****

C12H12O3 H2L CAS 39113-56-9 (794)
1-Phenylhexane-1,3,5-trione; C6H5.CO.CH2.CO.CH2.CO.CH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	alc/w	25°C	70%	C			1991HKd (81156)	2806
							B(FeHL)=12.30		

Medium: 70% v/v MeOH/H2O, 0.5 M NaClO4

****

C12H13O10S H5L (8082)
3-Bis(N,N-carboxymethyl)aminomethyl-2-hydroxy-5-sulphobenzoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KCl	25°C	0.1M	U		K1=19.5	1978TZa (81326)	2807

****

C12H14N2O6 H2L (4919)
5-Hydroxy-5-(2-hydroxy-4,4-dimethyl-6-oxo-1-cyclohexenyl)barbituric acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	KCl	20°C	0.10M	U			1968KUa (81345)	2808
							K(Fe+H2L=FeHL+H)=2.69		

****

C12H14N4O2S L Sulfadimidine CAS 57-68-1 (6167)
2-(4-Aminobenzolsulfamido)-4,6-dimethylpyrimidine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	alc/w	25°C	50%	C		K1=8.57 B2=16.55	1999GAa (81367)	2809

Medium: 50% EtOH/H2O, 0.10 M NaNO3.

****

C12H14O14 H6L CAS 111451-17-3 (5895)
3,6-Dioxaoctane-1,2,4,5,7,8-hexacarboxylic acid; (CH2(COOH).CH(COOH).O.CH(COOH)-)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KCl	25°C	0.10M	C		K1=20.96	1989MMd (81416)	2810
							K(FeL+2H)=7.78		

K(FeH-1L+H)=7.01
B(Fe2H-1L)=22.98
B(Fe2H-2L)=20.26
B(Fe2H-3L)=16.22, B(Fe2H-4L)=11.02, B(Fe2H-5L)=5.06

****

C12H16N2O4 H2L (5872)
2,3-Dihydroxy-N,N'-dimethylterephthalamide; C6H2(OH)2(CO.N(Me2))2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	sp	KCl	25°C	0.10M	C		K1=16.4	B2=30.90	1989GMb (81583)	2811
							K3=10.9			

****

C12H18N2O5S H2L CAS 80459-15-0 (1595)
2-Nitroso-5-(N-propyl-3-sulfopropylamino)phenol;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	gl	KNO3	25°C	0.10M	C		K1=9.30	B2=17.29	1988YSc (81810)	2812

****

C12H18N4O9 H3L CAS 43101-37-7 (2935)
Tetraglycine-N,N-diethanoic acid; (HOOC.CH2)2N.CH2.CO.Gly-Gly-Gly-OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	gl	KNO3	25°C	0.10M	C		K1=9.99		1974MMb (81951)	2813
							K(FeL+H)=1.89			

****

C12H20N2O2 H2L CAS 6310-76-5 (3387)
4,4'-Ethylenedi-iminodi(pentan-2-one);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	gl	alc/w	25°C	0.2M	U		K1=9.83		1999MTc (82006)	2814

Medium: 0.2 M KCl in 3:7 v/v H2O/EtOH

****

C12H20N2O8 H4L CAS 40623-42-5 (1101)
1,2-Diaminoethane-N,N'-di(2-pentane-1,5-dioic acid); (CH2NHCH(COOH)CH2CH2COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	gl	KNO3	30°C	0.10M	U		K1=15.7		1971TSc (82070)	2815

****

C12H20N2O8 H3L Mugineic acid CAS 69199-37-7 (9036)
2-Carboxy-a-[(3-carboxy-3-hydroxypropyl)amino]-b-hydroxy-1-azetidinebutanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	gl	KNO3	20°C	0.10M	U		K1=18.1		1981STc (82247)	2816

****

C12H20N2O8 H4L BDTA CAS 868-43-9 (1742)
DL-2,3-Diaminobutane-N,N,N',N'-tetraethanoic acid;
(HOOC.CH2)2N.CH(CH3).CH(CH3).N(CH2.COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	EMF	KCl	25°C	0.10M	U		K1=28.05 K(FeL(OH)+H)=6.45	1971ISa	(82300)2817
Fe+++	sp	KNO3	20°C	0.50M	U		K1=28.4	1968SKb	(82301)2818

****

C12H20N2O8 H4L CAS 22968-57-6 (3992)
meso-2,3-Diaminobutane-N,N,N',N'-tetraethanoic acid;
(HOOC.CH2)2N.CH(CH3).CH(CH3).N(CH2.COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	EMF	KCl	25°C	0.10M	U		K1=25.65 K(FeL(OH)+H)=6.17	1971ISa	(82395)2819
Fe+++	sp	KNO3	20°C	0.50M	U		K1=25.0	1968SKb	(82396)2820

****

C12H20N2O8S H4L TEDTA CAS 923-74-0 (3394)
2,2'-Thiobis(ethyliminodiethanoic acid); S(CH2.CH2.N(CH2.COOH)2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	EMF	NaClO4	20°C	0.10M	U		K1=20.41	1967BAc	(82455)2821
Fe+++	sp	oth/un	19°C	dil	U		K1=20.67 K(Fe+HL)=13.19	1966ZAb	(82456)2822

****

C12H20N2O9 H4L EEDTA CAS 923-73-9 (2112)
Oxa-bis(ethyleneimino)diethanoic acid; ((HOOC.CH2)2N.CH2.CH2)2O

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	EMF	NaClO4	20°C	0.10M	U		K1=24.7	1967BAc	(82533)2823
Fe+++	sp	oth/un	19°C	?	U		K1=23.03	1965ZAa	(82534)2824

****

C12H20N2O10 H4L CAS 10258-50-1 (3993)
(2,3-Dihydroxytetramethylenedinitrilo)tetraethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	oth	oth/un	?	?	U		B(Fe2L)=32.42	1967LDa	(82587)2825

Method: high-frequency titration

****

C12H21N3O6 H3L NOTA (5589)
1,4,7-Triazacyclononane-N,N',N"-triethanoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl KCl 25°C 0.10M C K1=28.3 1991CMd (82733)2826
****
C12H22O11 L alpha-Lactose CAS 5989-81-1 (2486)
4-D-Beta-D-Galactopyranosyl-alpha-D-glucose;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp NaClO4 25°C 0.30M C K1=2.40 1983ZGa (82874)2827
****
C12H22O12 HL Lactobionic acd CAS 96-82-2 (2487)
4-O-Beta-D-Galactopyranosyl-D-gluconic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl NaNO3 20°C 0.10M C 1994EOa (82928)2828
B(FeH-1L)=2.03
K(FeH-1L=FeH-2L+H)=-3.89
K(FeH-2L=FeH-3L+H)=-9.93

Fe+++ sp NaClO4 25°C 0.30M C K1=4.63 1983ZGa (82929)2829
B(FeHL)=8.49
B(Fe2L)=13.02
****
C12H23N3O5 H2L CAS 499238-78-7 (8836)
N-Hydroxy-N'-[5-(hydroxymethylamino)-5-oxopentyl]-N-methylpentanediamide;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl KCl 25°C 0.20M C K1=19.87 2002FBb (82984)2830
B(Fe2L3)=57.53
K1 by spectrophotometry.
****
C12H23N3O5 H2L CAS 499238-79-8 (8835)
N-Hydroxy-N'-[6-(hydroxymethylamino)-6-oxohexyl]-N-methylbutanediamide;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl KCl 25°C 0.20M C K1=21.05 2002FBb (82994)2831
B(Fe2L3)=61.01
K1 determined by spectrophotometry.
****
C12H24N2O4 L CAS 73586-25-1 (5533)
N,N'-Dihydroxy-N,N'-diisopropylhexanediamide;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo

```
--------------------------------------------------------------------------------
Fe+++      gl  KNO3   25°C 0.10M C        K1=22.83       1984BHa (83050)2832
                                          B(Fe2L3)=62.2
********************************************************************************
C12H24N2O4           H2L                      (6922)
N,N'-Dihydroxy-N,N'-dimethyldecanediamide; CH3N(OH).CO.(CH2)8.CO.N(OH)CH3
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      kin NaClO4 25°C 2.00M C                         1994CCa (83051)2833
                                          K(Fe+H2L=FeHL+H)=4.70
                                          K(FeL+H)=1.04
********************************************************************************
C12H24O6               L    18-Crown-6       CAS 17455-13-9  (577)
1,4,7,10,13,16-Hexaoxacyclooctadecane;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      con mixed  25°C  90%  C        K1=2.54        2003ISa (83361)2834
Medium: 90% v/v DMSO/H2O.
--------------------------------------------------------------------------------
Fe+++      dis non-aq 25°C 100%  U    M                  1996BSa (83362)2835
                                          K((A+,B-)+L=(A+,L,B-))=3.80
Medium: CHCl3; 0.1 M picrate. Host-guest complex. A=ferrioxamine,
B=(O2N)3C6H2O. Also data for host-guest with other crown ethers.
********************************************************************************
C12H26N2O4             L    Cryptand 2,2     CAS 23978-55-4  (925)
4,7,13,16-Tetraoxa-1,10-diazacyclooctadecane;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      gl  R4N.X  25°C 0.05M U        K1=13.0        1999BDb (83839)2836
Medium: Et4NClO4
********************************************************************************
C12H26O4S             HL    SDS              CAS 151-21-3  (2522)
Dodecyl sulfate; CH3(CH2)11.OSO3H
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      dis NaNO3  25°C 0.10M C    M                   1994BSb (83981)2837
                                          Kout(FeA+L=FeAL)=1.93
At pH 4.80. A=Ferrioxamine B.
********************************************************************************
C12H27N3O3             L                        (6685)
1,3,5-Trideoxy-1,3,5-tris(dimethylamino)-cis-inositol;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      gl  KCl    25°C 0.10M U        K1=18.8   B2=32.6   1992KHa (84070)2838
                                          B(FeHL2)=37.1
```

****
C12H27N5O2 HL CAS 188985-14-0 (8661)
13-Amino-13-methyl-1,4,8,11-tetraazacyclotetradecane-6-carboxylic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KCl	25°C	0.50M	M		K1=26.8	2001BYb	(84107)2839

****
C12H27P L CAS 998-40-3 (170)
Tri-n-butylphosphine; (CH3.(CH2)3)3P

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	nmr	non-aq	25°C	100%	U			1992LSa	(84135)2840
							K(FePAL+L=FePL2+A)=0.70		
							K(FePBL+L=FePL2+B)=0.70		

Medium: CHCl3. P=5,10,15,20-tetraphenylporphyrin dianion. A=imidazole.
B=N-methylimidazole. In acetone, K(FePAL+L=FePL2+A)=0.90
****
C12H28N4O2 L CAS 296-36-6 (2472)
1,10-Dioxa-4,7,13,16-tetraazacyclooctadecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	dis	non-aq	25°C	100%	C	I		2004CCa	(84233)2841
							K(Fe+A+L(org)=FeAL(org))=19.65		

Distribution of FeA3 from H2O into CH2Cl2. A is nitrate. For the N-tetra-
benzyl- derivative, K'=22.71. Distribution into CHCl3, K=19.96; K'=18.38
****
C12H29N5 L CAS 155115-12-1 (7505)
10-Methyl-10-amino-1,4,8,12-tetraazacyclopentadecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KCl	25°C	0.50M	M		K1=25.1	2001BYb	(84267)2842

****
C12H32N4O12P4 H8L DOTPH CAS 91987-74-5 (229)
1,4,7,10-Tetraazacyclododecane-N,N',N",N"'-tetramethylenephosphonic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KNO3	25°C	1.0M	U		K1=23.7	1984KMb	(84410)2843
							K(Fe+HL)=19.4		

****
C13H8O3 HL CAS 719-41-5 (3397)
1-Hydroxyxanthone (1-Hydroxy-9-xanthenone)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	alc/w	25°C	50%	U		K1=13.05	1968GDb	(84496)2844

Medium: 50% EtOH, 0.1 M NaClO4

****

C13H10N2 L CAS 3003-78-6 (2752)
5-Methyl-1,10-phenanthroline;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	sp	oth/un	25°C	0.0	U			1967LAe	(84814)	2845
							B3=16.77			

****

C13H10N2O6S H2L MordentYellow10 CAS 21542-82-5 (1390)
5-(4'-Sulfophenylazo)salicylic acid; HO3S.C6H4.N:N.C6H3(OH).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	gl	KNO3	25°C	0.10M	U		K2=10.70	1964MTc	(84939)	2846

****

C13H11NO2 HL CAS 304-88-1 (181)
N-Phenylbenzohydroxamic acid; C6H5.CO.N(C6H5).OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	vlt	non-aq	25°C	100%	C			1992SSe	(85147)	2847
							B3=35.3			

Medium: acetonitrile, 0.20 M Et4NPF6. Method: cyclic voltammetry.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values			Reference	ExptNo
Fe+++	sp	alc/w	25°C	75%	U		K1=4.63	B2=6.33	1967BMa	(85148)	2848
							B3=5.33				

Medium: 75% EtOH, conditional constants

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values			Reference	ExptNo
Fe+++	sp	NaClO4	25°C	?	U		K1=11.38	B2=20.65	1967PKa	(85149)	2849
							B3=29.09				
Fe+++	sp	oth/un	?	?	U		K1=5.28		1957ARa	(85150)	2850

****

C13H11N2O3F3 HL (5563)
3-(2-Acetylphenylhydrazone)-1,1,1-trifluoropentane-2,4-dione;
CF3.CO.C(CO.CH3):N.HN.C6H4.COCH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values			Reference	ExptNo
Fe+++	gl	diox/w	25°C	75%	U		K1=12.50	B2=24.18	1990ASb	(85245)	2851

****

C13H11N3O2 HL (4984)
1-Isonicotinyl-2-salicylidene hydrazone; C5H4N.CO.NH.N:CH.C6H4.OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	sp	KNO3	25°C	0.10M	U		B2=56	1990VHa	(85268)	2852
							K(Fe+HL)=38.3			

K(Fe+2HL)=48.8
K(Fe+HL+L)=54
****
C13H11N3O4S2 HL Tenoxicam CAS 59804-37-4 (8393)
4-Hydroxy-2-methyl-N-2'-pyridinyl-2H-thien[2,2-e]-1,2-thiazine-3-carboxamide-1,1-di
oxide;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl mixed 25°C 50% C K2=9.4 2002MWa (85289)2853
K3=8.9
Medium: 50% v/v CH3CN/H2O, 0.05 M NaNO3.
****
C13H11N3O6S H2L (2811)
1-(2-Carboxy-5-sulfonatophenyl)-3-hydroxy-phenyltriazene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp none 25°C 0.0 U K1=7.22 1974CHa (85303)2854
****
C13H12N2O HL CAS 69067-12-5 (4986)
Benzanilidoxime; C6H5.C(:N.OH).NH.C6H5

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp NaClO4 25°C 0.10M U 1969MKd (85335)2855
K(Fe+HL)=4.03
K(FeHL+HL)=4.15
****
C13H14NO3P H2L CAS 19316-85-7 (1466)
2-Hydroxyphenyl-N-phenylaminomethylphosphinic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl NaClO4 20°C 0.10M U K1=7.55 1985SIb (85563)2856
****
C13H14N2O L CAS 87413-05-6 (6300)
1-Benzyl-1,4-dihydronicotinamide;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp non-aq 25°C 100% U 1989FKb (85579)2857
K(FeP+L)=3.90
K(FePL+L)=2.83
Medium: CH2Cl2. FeP=tetraphenylporphyrinatoiron(III) perchlorate. For FePCl,
K(FeP+L=FePL)=1.41
****
C13H14N2O3 HL (4940)
3-(2-Acetylphenylhydrazone)pentane-2,4-dione;(CH3.CO)2C:N.NH.C6H4(CO.CH3)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	gl	diox/w	25°C	75%	U		K1=14.50	B2=28.15	1990ASb (85608)	2858

C13H14N3O5P H2L CAS 80767-75-5 (1467)
2-Hydroxy-4-nitrophenyl-N-(2-pyridylmethyl)aminemethylphosphinic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	NaClO4	20°C	0.10M	U		K1=8.15	1985SIb (85641)	2859

C13H14N3O5P H2L CAS 80767-76-6 (1468)
2-Hydroxy-4-nitrophenyl-N-(3-pyridylmethyl)aminemethylphosphinic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	NaClO4	20°C	0.10M	U		K1=8.12	1985SIb (85654)	2860

C13H15NO2S L (6235)
Diaceto-4-methylphenylthioamide; (CH3.CO)2CH.CS.NH.C6H4.CH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	alc/w	25°C	60%	U		K1=4.40	1984FNa (85706)	2861

C13H15NO3S L (6234)
Diaceto-4-methoxyphenylthioamide; (CH3.CO)2CH.CS.NH.C6H4.OCH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	alc/w	25°C	60%	U		K1=4.48	1984FNa (85709)	2862

C13H15N2O3P H2L CAS 80767-72-2 (1460)
2-Hydroxyphenyl-(N-2-pyridylmethylamino)methylphosphinic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	NaClO4	20°C	0.10M	U		K1=9.75	1985SIa (85781)	2863

C13H15N2O3P H2L CAS 80767-73-3 (1461)
2-Hydroxyphenyl-(N-3-pyridylmethylamino)methylphosphinic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	NaClO4	20°C	0.10M	U		K1=10.10	1985SIa (85794)	2864

C13H15N2O3P H2L CAS 80767-74-4 (1462)
2-Hydroxyphenyl-(N-4-pyridylmethylamino)methylphosphinic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo

```
--------------------------------------------------------------------------------
Fe+++      gl  NaClO4 20°C 0.10M U        K1=10.23       1985SIa (85807)2865
********************************************************************************
C13H15N2O4P           H3L                      CAS 80767-78-8  (1463)
2-Hydroxyphenyl-(N-2-pyridylmethylamino)methylphosphonic acid;
C6H4(OH)CH(PO3H2).NH.CH2.C5H4N
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      gl  NaClO4 20°C 0.10M U        K1=16.72       1985SIa (85820)2866
********************************************************************************
C13H15N2O4P           H3L                      CAS 85946-85-6  (1464)
2-Hydroxyphenyl-(N-3-pyridylmethylamino)methylphosphonic acid;
C6H4(OH)CH(PO3H2).NH.CH2.C5H4N
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      gl  NaClO4 20°C 0.10M U        K1=16.80       1985SIa (85833)2867
********************************************************************************
C13H15N2O4P           H3L                      CAS 85946-86-7  (1465)
2-Hydroxyphenyl-(N-4-pyridylmethylamino)methylphosphonic acid;
C6H4(OH)CH(PO3H2).NH.CH2.C5H4N
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      gl  NaClO4 20°C 0.10M U        K1=17.80       1985SIa (85846)2868
********************************************************************************
C13H20NO4P            H3L                        (1471)
2-Hydroxyphenyl-N-(cyclohexylamino)methylphosphonic acid;
C6H4(OH)CH(PO3H2).NH.C6H11
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      gl  NaClO4 20°C 0.10M U        K1=14.60       1985SIb (86091)2869
********************************************************************************
C13H26N2O4             L                        CAS 90149-54-5  (5534)
N,N'-Dihydroxy-N,N'-diisopropylheptanediamide;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      gl  KNO3   25°C 0.10M C        K1=22.76       1984BHa (86453)2870
                                         B(Fe2L3)=62.4
********************************************************************************
C14H8N3O8S2F3          HL                       (9231)
1-(2-Thenoyl),4-trifluoro,2-[2-hydroxy-2-sulpho-5-nitrophenylazo]butadi-1,3-one;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      gl  KCl    25°C  0.1M U        K1=8.67   B2=15.60  2004ACa (86610)2871
********************************************************************************
```

C14H8O4 H2L Quinizarin CAS 81-64-1 (1060)
1,4-Dihydroxyanthraquinone;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	alc/w	25°C	43%	U			1991MJa (86664)	2872
							K(Fe+H2L=FeHL+H)=1.66		
							K(FeHL+Fe=Fe2L+H)=1.56		
In 42.8% v/v MeOH/H2O, 0.50 M NaClO4									
Fe+++	sp	alc/w	20°C	50%	U			1982KMd (86665)	2873
							K(Fe+HL)=10.9		
Medium: 50% v/v EtOH/H2O									

****

C14H8O7S H3L (4037)
1,4-Dihydroxyanthraquinone-2-sulfonic acid, quinizarin-2-sulfonic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaClO4	25°C	0.50M	U			1991MJa (86778)	2874
							K(Fe+H2L=FeHL+H)=1.29		
							K(FeHL+Fe=Fe2L+H)=0.91		
Fe+++	sp	oth/un	25°C	0.10M	U			1971TAa (86779)	2875
							K(Fe+H2L=FeHL+H)=1.48		
							K(4Fe+3H2L=Fe4L+6H)=11.14		
Fe+++	sp	NaCl	29°C	0.10M	U			1964JJa (86780)	2876
							K(Fe+H2L=FeHL+H)=3.73(?)		

****

C14H10NO2F3 HL CAS 530-28-9 (2574)
N-(3-Trifluoromethylphenyl)-2-aminobenzoic acid; HOOC(C6H4)NH(C6H4)CF3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	mixed	22°C	90%	U		K1=5.17	1982GKb (86897)	2877
Medium: 90% DMF/H2O									

****

C14H11O2NF2S HL CAS 51679-49-3 (2928)
N-((3-Difluoromethylthio)phenyl)anthranilic acid;HOOC(C6H4).NH.(C6H4).S.CHF2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	mixed	22°C	90%	U		K1=5.42	1982GKb (87027)	2878
Medium: 90% DMF/H2O									

****

C14H11O2NF2S HL CAS 51679-50-4 (2929)
N-((4-Difluoromethylthio)phenyl)anthranilic acid;HOOC(C6H4).NH.(C6H4).S.CHF2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo

```
------------------------------------------------------------------------------
Fe+++      gl  mixed  22°C  90%  U        K1=5.27        1982GKb (87032)2879
Medium: 90% DMF/H2O
******************************************************************************
C14H12N2                L                       CAS 3002-81-1  (451)
5,6-Dimethyl-1,10-phenanthroline;
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Fe+++      sp  oth/un 25°C  0.0  U                        1968LAa (87161)2880
                                          B3=18.55
Medium: acetate and phosphate buffers
******************************************************************************
C14H12N4O2Br2          HL                      CAS 72833-87-5  (2533)
2-(2-(3,5-Dibromopyridyl)azo)-5-dimethylaminobenzoic acid;
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Fe+++      sp  diox/w 25°C  40%  C        K1=7.85        1986KHa (87318)2881
******************************************************************************
C14H13N                 L                       CAS 4217-54-3  (6299)
10-Methyl-9,10-dihydroacridine;
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Fe+++      sp  non-aq 25°C 100%  U                        1989FKb (87359)2882
                                        K(FeP+L)=3.32
                                        K(FePL+L)=2.38
Medium: CH2Cl2. FeP=tetraphenylporphyrinatoiron(III) perchlorate
******************************************************************************
C14H14N2O3            H2L                       (7146)
N-Pyridoxyl-2-hydroxyaniline; HO.C6H4.NH.CH2.C7H6NO2
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 0.10M U        K1=21.35  B2=45.8   1995OJa (87662)2883
******************************************************************************
C14H14N4O3             HL                      CAS 82845-52-1  (6626)
Pyridoxal isonicotinoylhydrazone;
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Fe+++      sp  KNO3   25°C 0.10M U         B2=34.0        1990VHa (87700)2884
                                        K(Fe+H2L=FeH2L)=8.93
                                        K(Fe+2H2L=FeH4L2)=15.89
                                        K(Fe+2HL=FeH2L2)=24.80
                                        K(Fe+HL+L=FeHL2)=29.0
Medium: succinic-succinate buffer
******************************************************************************
C14H15N2O8Cl          H4L                       (1903)
```

4-Chloro-1,2-diaminobenzene-N,N,N',N'-tetraethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KNO3	25°C	0.50M	C	H	K1=20.99 K(Fe+HL)=16.30 B(FeL(OH))=26.69	1997SDa (87748)	2885

DH(K1)=2.5 kJ mol-1, DS(K1)=408 J K-1 mol-1

****

C14H16NO3P H2L CAS 25881-35-0 (1469)
Phenyl-N-(benzylamino)methylphosphonic acid; C6H5.CH(PO3H2).NH.CH2.C6H5

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	NaClO4	20°C	0.10M	U		K1=11.80	1985SIb (87810)	2886

****

C14H16NO4P H3L CAS 61146-25-6 (1470)
2-Hydroxyphenyl-N-(benzylamino)methylphosphonic acid; C6H4(OH)CH(PO3H2).NH.CH2.C6H5

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	NaClO4	20°C	0.10M	U		K1=14.95	1985SIb (87823)	2887

****

C14H16N2O8 H4L CAS 40774-59-2 (1901)
1,2-Diaminobenzene-N,N,N',N'-tetraethanoic acid; C6H4(N(CH2.COOH)2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KNO3	25°C	0.50M	C	H	K1=21.82 K(Fe+HL)=16.45 B(FeL(OH))=26.98	1997SDa (87951)	2888

DH(K1)=3.24 kJ mol-1, DS(K1)=420 J K-1 mol-1

****

C14H17NO9 HL CAS 95594-32-4 (7504)
2,4-Dihydroxy-2H-1,4-benzoxazin-3-(4H)-on-glucoside;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KCl	25°C	0.20M	C		K1=7.41 B2=13.52 B(FeH-1L2)=8.80 K(Fe+HL=FeL+H)=0.56	1998FKa (88033)	2889

****

C14H17N2O4P H3L (1472)
2-Hydroxyphenyl-N-(2-(2'-pyridyl)ethylamino)methylphosphonic
acid;C6H4(OH)CH(PO3H2)NHCH2CH2C5H4N

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	NaClO4	20°C	0.10M	U		K1=16.31	1985SIb (88043)	2890

****

C14H18N2O2 HL (7898)
1-(2-Hydroxyphenyl)-2,5-diaza-8-oxonona-1,5-diene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	alc/w	25°C	0.2M	U		1999MTc (88064)		2891
							K(Fe+L)=8.48		

Medium: 0.2 M KCl in 3:7 v/v H2O/EtOH

****

C14H18O8 L (7000)
1.2-Dihydroxy-3,4,5-triethoxycarbonylcyclopenta-2,5-diene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	KNO3	20°C	0.10M	U	I	K1=12.43 B2=21.48	1977KKd (88142)	2892
							K3=7.28		
							K(FeL2+H)=3.42		

Data also for 70% w/w MeOH/H2O

****

C14H20O5 L Benzo15-crown-5 CAS 14098-44-3 (608)
2,3-Benzo-1,4,7,10,13-pentaoxacyclopentadeca-2-ene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	con	mixed	25°C	90%	C		K1=3.15	2003ISa (88268)	2893

Medium: 90% v/v DMSO/H2O.

****

C14H22N2O8 H4L CDTA CAS 482-54-2 (200)
trans-1,2-Diaminocyclohexane-N,N,N',N'-tetraethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaClO4	25°C	0.10M	U			1998Va (88649)	2894
							K(FeL+H)=1.10		
							*K(Fe(H2O)L)=-6.9		
Fe+++	EMF	KNO3	25°C	0.10M	C		K1=28.70	1997DFa (88650)	2895
							K(FeL+H)=1.91		
							K[Fe(OH)L+H]=9.51		
Fe+++	vlt	oth/un	18°C	0.20M	U	T	K1=29.49	1972BOa (88651)	2896

K1(28 C)=29.15, K1(35 C)=28.90, K1(40 C)=28.75

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	EMF	NaClO4	20°C	0.10M	U		K1=28.05	1967BAc (88652)	2897
							K(FeL+OH)=9.70		
Fe+++	gl	KCl	25°C	1.0M	U	T H		1963GMc (88653)	2898
							K(Fe(OH)L+H)=9.32		
							K(2FeLOH=(FeLOH)2)=1.01		

K(FeLOH+H)=9.95(1.0 C), 8.90(42.3 C), DH=-41.8 kJ mol-1(25 C), DS=-114

K(dimer)=1.31(0 C), 0.89(42.3 C). DH=-16, DS=-40

Fe+++	sp	oth/un	30°C	1.0M	U	K1=26.93	1963RSa (88654)2899

Fe+++	dis	NaClO4	20°C	0.10M	U		1963STc (88655)2900
						B(FeL(OH))=36.6	

Medium: KClO4

Fe+++	sp	oth/un	?	?	U		1960BCb (88656)2901
						K(FeL+HO2)=2.87	

Fe+++	sp	oth/un	20°C	?	U	K1=27.48	1960BGa (88657)2902
						K(Fe+H2L)=10.95	
						K(Fe+HL)=17.0	

****

C14H22N4O10 H3L CAS 29725-87-9 (5074)
Ethylenedinitrilo-N,N'-bis(methylenecarbonyliminoethanoic)-N,N'-diethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KNO3	25°C	0.10M	U			1970MMc	(88933)2903
							K(FeH-1L+H)=2.95		
							K(FeH-2L+H)=3.57		

****

C14H22N4O10 H4L DGENTA CAS 29725-86-8 (2371)
N,N-Diglycyldiaminoethane-tetraethanoic acid;(-CH2.HNCOCH2N(CH2COOH)2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KNO3	25°C	0.10M	U		K1=14.0	1970MMc	(88950)2904

****

C14H23N3O10 H5L DTPA CAS 67-43-6 (238)
Diethylenetriamine-pentaethanoic acid; HOOC.CH2.N(CH2.CH2.N(CH2.COOH)2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	NaClO4	25°C	0.10M	C		K1=28.0	2001CCa	(89238)2905
							K(Fe(OH)L+H)=9.66		
							K(FeL+H)=3.56		

K1 from competition with DTPA using LC-MS.

Fe+++	EMF	NaClO4	20°C	1.00M	C		2000BMa (89239)2906
						K(Fe+CrL)=8.15	

Method: Pt/Fe+++/Fe++ and glass electrodes.

Fe+++	EMF	KNO3	25°C	0.10M	C	K1=27.74	1997DFa (89240)2907
						K(FeL+H)=3.37	

Fe+++	EMF	NaClO4	25°C	1.00M	U	K1=28.7	1985PLb (89241)2908
						K(Fe+HL)=21.4	

```
                                        K(Fe+H2L)=14.3
-------------------------------------------------------------------------------
Fe+++      sp  oth/un 25°C 0.10M U                      1974MBa (89242)2909
                                        B(FeH4L)=34.27
-------------------------------------------------------------------------------
Fe+++      sp  NaClO4 20°C 0.10M U                      1973KBc (89243)2910
                                        K(Fe+HL)=19.5
-------------------------------------------------------------------------------
Fe+++      EMF NaClO4 20°C 0.10M U       K1=27.3        1967BAc (89244)2911
                                        K(FeL+H)=3.58
                                        K(FeL+OH)=3.9
-------------------------------------------------------------------------------
Fe+++      EMF oth/un 20°C 0.10M U       K1=27.50       1959ANd (89245)2912
                                        K(Fe+HL)=19.48
-------------------------------------------------------------------------------
Fe+++      gl  KNO3   25°C 0.10M U       K1=28.6        1959VCa (89246)2913
                                        K(FeL+H)=3.56
                                        K(FeL+OH)=4.12
*******************************************************************************
C14H24N2O7            H3L                          (3440)
N-(2-Hydroxycyclohexyl)ethylenediamine-N,N',N'-triethanoic acid;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe+++      EMF oth/un 25°C 0.10M U       K1=21.46       1960SAc (89494)2914
                                        K(FeL(OH)2+H)=8.00
*******************************************************************************
C14H24N2O8            H4L    HMDTA            CAS 1633-00-7  (920)
1,6-Diaminohexane-N,N,N',N'-tetraethanoic acid; ((HOOC.CH2)2N.CH2.CH2.CH2)2
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe+++      sp  KNO3   20°C 0.10M U       K1=16.50       1977KKc (89575)2915
-------------------------------------------------------------------------------
Fe+++      sp  oth/un 19°C    ?  U                      1965ZAa (89576)2916
                                        K(Fe+HL)=10.3
*******************************************************************************
C14H24N2O8            H4L    EDTP             (2936)
Diaminoethane-N,N,N',N'-tetrapropanoic acid; (HOOC.CH2CH2)2N.CH2CH2.N(CH2CH2.COOH)2
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe+++      gl  KCl    30°C 0.10M U       K1=14.4        1953CCb (89682)2917
                                        K(FeL+OH)=9.9
                                        K(FeLOH+OH)=7.1
*******************************************************************************
C14H24N2O10                EGTA             CAS 67-42-5  (349)
Ethyleneglycol-O,O'-bis(2-aminoethyl ether)-N,N,N',N'-tetraethanoic acid; H4L
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
```

```
-------------------------------------------------------------------------------
Fe+++      sp  oth/un 19°C  dil  U        K1=20.38       1971CAg (89864)2918
-------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 0.10M U        K1=20.5        1963SCa (89865)2919
*******************************************************************************
C14H25N3O7            H3L                          (5397)
1-Oxa-4,7,10-triazacyclododecane-4,7,10-triethanoic acid;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe+++      gl  KCl    25°C 0.10M C        K1=26.8        1993DSa (90083)2920
                                         K(FeL+H)=2.17
                                         K(Fe(OH)L+H)=7.75
*******************************************************************************
C14H26N4O6            H2L                          (4690)
Hexanoic acid bis(3-hydroxycarbamoyl-propyl)amide;
HONHCO(CH2)3NHCO(CH2)4CONH(CH2)3COHNOH
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe+++      gl  KCl    25°C 0.20M C        K1=19.1        1999FEa (90264)2921
                                         B(Fe2L3)=55.6
*******************************************************************************
C14H28N2O4              L    Cryptand 2,1,1   CAS 31250-06-3  (836)
1,10-Diaza-4,7,13,18-tetraoxabicyclo[8,5,5]eicosane (2,1,1);
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe+++      gl  R4N.X  25°C 0.05M U        K1=17.3        1999BDb (90365)2922
Medium: Et4NClO4
*******************************************************************************
C14H28N2O4              L                     CAS 73586-26-2  (5535)
N,N'-Dihydroxy-N,N'-diisopropyloctanediamide;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe+++      gl  KNO3   25°C 0.10M C        K1=22.63       1984BHa (90466)2923
                                         B(Fe2L3)=62.3
*******************************************************************************
C14H36N4O12P4         H8L                     CAS 107446-90-2  (2015)
1,4,7,11-Tetraazacyclotetradecane-N,N',N",N"'-tetramethylphosphonic acid;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe+++      nmr none   25°C    0  U        K1=33.5        1992MNa (90872)2924
                                         B(FeHL)=42.7
                                         B(FeH2L)=50.7
                                         B(FeH3L)=57.3
                                         B(FeH-1L)=20.7
Calculated from protonation constants reported by S A Pisareva et al.
```

Izv Akad Nauk SSSR Ser Khim,1987,413

Fe+++	nmr	none	25°C	0	U	K1=30.6 B(FeHL)=38.7 B(FeH2L)=45.2 B(FeH3L)=50.5 B(FeH-1L)=21.2	1992MNa	(90873)2925

Calculated from protonation constants reported by R Delgado et al.
Helv. Chim. Acta,1990,73,140.

****

C15H10O3 HL CAS 491-78-1 (3444)
5-Hydroxyflavone;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	alc/w	20°C	50%	U		K1=14.12	1973MTb	(90983)2926

Medium: 50% MeOH, 0.1 M

****

C15H10O3 HL CAS 6486-96-8 (5098)
5-Hydroxyisoflavone;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	alc/w	20°C	50%	U		K1=13.83	1973MTb	(90985)2927

Medium: 50% MeOH, 0.1 M

****

C15H10O7 H5L Quercetin CAS 117-39-5 (5101)
3,5,7-Trihydroxy-2-(3',4'-dihydroxyphenyl)-1-benzopyran-4-one;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	non-aq	25°C	100M	C		K1eff=-1.59	2001ADb	(91022)2928

Medium: MeOH, 0.2 M acetate buffer, pH 5.0. K1eff: Al+HnL=AlL

Fe+++	gl	NaNO3	20°C	0.10M	C	K(Fe+2OH+L)=44.2 K(Fe(OH)2L+H)=8.88 K(Fe(OH)L+H)=6.76 K(Fe2(OH)2L+H)=5.50	1991ESa	(91023)2929

K(FeHL+H)=4.95, K(Fe(OH)2L+Fe=Fe2(OH)6L+4H)=-17.16, K(Fe2(OH)6L+H)=9.35
K(Fe2(OH)5L+H)=8.24, K(Fe2(OH)4L+H)=6.73,K(Fe2(OH)3L+H)=6.08,K(FeL+H)=6.29

****

C15H11NO2 HL (5109)
2-Benzofuran phenyl ketoxime; C8H5O.C(:N.OH).C6H5

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	oth	alc/w	30°C	80%	U		K(FeOH+L)=11.0	1972SMb	(91068)2930

K(FeOH+2L)=19.50

****

C15H12NO2Br L (1202)

3-Bromo-benzoylacetanilide; Br.C6H4.CO.CH2.CO.NH.C6H5

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	sp	alc/w	25°C	60%	U		K1=8.44	B2=13.52	1981SNa	(91406)2931
Fe+++	sp	alc/w	25°C	60%	U		K1=8.90	B2=15.07	1976SEa	(91407)2932
							B3=18.06			

****

C15H12NO2Br L (1200)

4-Bromo-benzoylacetanilide; Br.C6H4.CO.CH2.CO.NH.C6H5

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	sp	alc/w	25°C	60%	U		K1=9.16	B2=15.54	1976SEa	(91409)2933
							B3=18.75			

****

C15H12NO2Cl L (1201)

3-Chloro-benzoylacetanilide; Cl.C6H4.CO.CH2.CO.NH.C6H5

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	sp	alc/w	25°C	60%	U		K1=8.43	B2=13.66	1981SNa	(91413)2934
Fe+++	sp	alc/w	25°C	60%	U		K1=9.07	B2=15.25	1976SEa	(91414)2935
							B3=18.50			

****

C15H12NO2Cl L (1199)

4-Chloro-benzoylacetanilide; Cl.C6H4.CO.CH2.CO.NH.C6H5

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	sp	alc/w	25°C	60%	U		K1=8.88	B2=14.65	1981SNa	(91417)2936
Fe+++	sp	alc/w	25°C	60%	U		K1=9.24	B2=15.76	1976SEa	(91418)2937
							B3=18.82			

****

C15H12O2 HL Diphenylacac CAS 120-46-7 (362)

1,3-Diphenylpropane-1,3-dione, Dibenzoylmethane; C6H5.CO.CH2.CO.C6H5

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	dis	NaClO4	25°C	4.0M	C		K1=11.4	B2=20.80	1985IIa	(91548)2938
							B3=26.7			

Method: extraction into CCl4; analysis by spectrophotometry.

K(Fe+3HL(org)=FeL3(org)+3H)=-2.1. Values for K1, B2, B3 are approximate.

****

C15H13NO2 HL CAS 959-66-0 (245)
Benzoyl-acetanilide; C6H5.CO.CH2.CO.NH.C6H5

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	sp	alc/w	25°C	60%	U		K1=9.52	B2=16.02	1981SNa (91628)	2939
Fe+++	sp	alc/w	25°C	60%	U		K1=9.52 B3=19.05	B2=16.02	1976SEa (91629)	2940
Fe+++	sp	alc/w	35°C	60%	U		K1=6.92		1971TSg (91630)	2941

Medium: 60% EtOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	oth/un	35°C	0.10M	U	T	K1=8.61	1971TSg (91631)	2942

K1(20 C)=8.70, K1(25 C)=8.67, K1(30 C)=8.64

****

C15H13N5O2 HL BIAAP CAS 385824-97-5 (8021)
2-(2-Benzimidazolylazo)-4-acetamidophenol;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	none	25°C	0.0	C		K1=5.35	2001MEa (91678)	2943

****

C15H14N2O5S HL (9232)
3-(5-Sulphonylnaphthylazo)penta-2,4-dione;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KCl	25°C	0.1M	U	H	K1=7.76	2004ACb (91735)	2944

for 35 C K1=7.55; for 45 C K1=7.33

****

C15H14N2O6S H2L (6312)
2-Carboxy-2'-hydroxy-3',5'-dimethylazobenzene-4-sulfonic acid;
(CH3)2(OH)C6H2.N:N.C6H4.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	gl	alc/w	25°C	50%	U	T	K1=14.30	B2=24.75	1976BDb (91741)	2945

At 35 C:K1=14.20, K2=10.30. 45 C:14.05, 10.20. Data also for 3',5'-dichloro-analogue. K1=10.60, K2=8.15 at 25 C

****

C15H14O3 HL (5102)
2-Hydroxy-4-benzyloxy acetophenone; C6H5.CH2.O.C6H3(OH).CO.CH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	gl	diox/w	27°C	75%	U		K1=9.07	B2=15.53	1973KDc (91780)	2946

Medium: 75% dioxan, 0.1 M NaClO4

****

C15H14O7 H5L CAS 970-73-0 (1796)

Epigallocatechin;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	none	20°C		U			1998JSa (91820)	2947
							K1eff=27.4		
							K(Fe+LH3=FeLH2+H)=4.90		
							K(FeLH2+LH2=FeLH+LH3)=8.60		

K1eff by competition with EDTA at pH 7.

****

C15H15NO2 HL CAS 61-68-7 (2927)
N-(2,3-Dimethylphenyl)anthranilic acid; HOOC(C6H4).NH.(C6H3)(CH3)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	mixed	22°C	90%	U		K1=5.66	1982GKb (91830)	2948

Medium: 90% DMF/H2O

****

C15H15N3O3 H2L CAS 72343-06-7 (6768)
Pyridoxal benzoylhydrazone;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	KNO3	25°C	0.10M	U		B2=48.0	1990VHa (91905)	2949
							K(Fe+HL=FeHL)=27.2		
							K(Fe+2HL=FeH2L2)=38.5		
							K(Fe+HL+L=FeHL2)=44.3		

Medium: succinic-succinate buffer

****

C15H16N4O6 H2L CAS 97570-39-3 (8600)
N,N'-1,3-Propanediylbis[1,6-dihydro-1-hydroxy-6-oxo]-2-pyridinecarboxamide;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaClO4	25°C	0.10M	C			1985SWb (91951)	2950
							B(Fe2L3)=52.3		

Method: competition with edta.

****

C15H17N4OBr HL CAS 14357-53-2 (712)
2-(5-Bromo-2-pyridylazo)-5-diethylaminophenol; BrC5H3N.N:N.C6H3(OH)N(CH3)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	KCl	25°C	?	U		B2=10.41	1988WSa (91980)	2951

****

C15H18N2O8 H4L CAS 101455-18-9 (1902)
1-Methyl-3,4-diaminobenzene-N,N,N',N'-tetraethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo

```
Fe+++      gl  KNO3   25°C 0.50M C   H    K1=22.05       1997SDa (92083)2952
                                          K(Fe+HL)=16.57
                                          B(FeL(OH))=27.16
DH(K1)=-1.7 kJ mol-1, DS(K1)=416 J K-1 mol-1
**************************************************************************
C15H20N2O7            H4L    HBET              (6954)
N-(Hydroxobenzyl)diaminoethane-N,N',N'-triethanoic acid;
HO.C6H4.CH2.N(CH2COOH)CH2CH2.N(CH2COOH)2
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe+++      gl  KCl    25°C 0.10M C        K1=32.02       1995MMa (92167)2953
                                          B(FeHL)=33.59
**************************************************************************
C15H21NO6             H3L    Domic acid       CAS 14277-97-5  (8625)
2-Carboxy-4-[5-carboxy-1-methyl-1,3-hexadienyl]-3-pyrrolidinethanoic acid;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe+++      vlt oth/un 25°C 0.70M C        K1=18.7        2001RBa (92197)2954
                                          K1eff=8.7
Method: adsorptive cathodic stripping voltammetry using salicylaldoxime.
Medium: UV seawater, 6.5 mM HEPES, pH 8.0.
**************************************************************************
C15H27N3O7            H3L                    (7396)
4,7,11-Tris(carboxymethyl)-1-oxa-4,7,11-triazacyclotridecane;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe+++      gl  R4N.X  25°C 0.10M C        K1=21.24       1997CCa (92479)2955
                                          K(FeL+H)=3.02
Medium: Me4NNO3
**************************************************************************
C15H35N5               L                    CAS 158523-84-3  (7630)
2R,5S,8R,11S,14S-Pentamethyl-1,4,7,10,13-pentaazacyclopentadecane;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe+++      gl  none   25°C    0  U                        1998ZBb (92600)2956
                                          *K1(FeLCl2)=-3.6
                                          *K2=(FeLCl2)=-7.4
**************************************************************************
C16H11NO3              HL    HPBI             CAS 41836-94-6  (7740)
3-Phenyl-4-benzoyl-5-isoxazolone;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe+++      dis non-aq 30°C 100%  U                        1999SPa (92685)2957
                                          Kd=5.57
Kd: Fe+3HL(org)=FeL3(org)+3H.
```

Method: Solvent extraction, H2O/xylene.
****
C16H12N2O8S2 H4L Chromotrope 2R CAS 4197-07-3 (2604)
2-(Benzeneazo)-chromotropic acid, Acid Red 29

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	oth/un	25°C	?	U			1967PMb	(93063)2958
							K(?)=4.4		
Fe+++	oth	KCl	20°C	0.10M	U		K1=22.41	1964PCa	(93064)2959

****
C16H13NO4S HL (5182)
N-4-Toluenesulfonyl-benzofur-2-yl-carboxamide;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	EMF	alc/w	?	70%	U		B2=7.02	1971MSc	(93159)2960

Medium: 70% MeOH
****
C16H14NO4Cl H2L CAS 197517-41-2 (7615)
5-Chloro-2-hydroxy-N-L-phenylalaninebenzamide;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaClO4	25°C	0.10M	C			1998AGa	(93402)2961
							K1eff=3.71		

Method: fluorescence. pH=2.6.
****
C16H14N2O HL CAS 38214-71-0 (8453)
3-(2-Hydroxy-5-methylphenyl)-5-phenylpyrazole;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	diox/w	27°C	70%	C		K1=11.65 B2=21.35	1994SNa	(93420)2962
							K3=5.25		

Medium: 70% v/v dioxane/H2O, 0.10 M NaClO4.
****
C16H14O6 H2L CAS 20210-97-3 (8309)
Ethylene disalicylate;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	alc/w	25°C	61%	C		K1=21.54	1995SDa	(93593)2963

Medium: 61.1 wt % EtOH/H2O, I=0.50 M LiCl.
Data for the propyl- and higher analogues.
****
C16H14O6 H2L Hematoxylin CAS 517-28-2 (1381)
Hematoxylin

```
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      gl  KCl    25°C 0.10M U        K1=3.54        1982MHa (93600)2964
*************************************************************************
C16H15NO2               L                     CAS 31844-90-3  (1198)
3-Methylbenzoylacetanilide; CH3.C6H4.CO.CH2.CO.NH.C6H5
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      sp  alc/w  25°C  60%  U        K1=9.80   B2=17.05  1981SNa (93608)2965
-------------------------------------------------------------------------
Fe+++      sp  alc/w  25°C  60%  U        K1=9.71   B2=15.91  1976SEa (93609)2966
                                         B3=19.19
*************************************************************************
C16H15NO2               L                       (1197)
4-Methylbenzoylacetanilide; CH3.C6H4.CO.CH2.CO.NH.C6H5
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      sp  alc/w  25°C  60%  U        K1=9.91   B2=16.39  1976SEa (93611)2967
                                         B3=19.23
*************************************************************************
C16H15NO3              HL                       (1196)
4-Methoxybenzoylacetanilide; CH3O.C6H4.CO.CH2.CO.NH.C6H5
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      sp  alc/w  25°C  60%  U        K1=10.25  B2=18.03  1981SNa (93614)2968
-------------------------------------------------------------------------
Fe+++      sp  alc/w  25°C  60%  U        K1=10.10  B2=16.88  1976SEa (93615)2969
                                         B3=19.41
*************************************************************************
C16H15NO7              H4L                      (4082)
N-(3-Carboxy-2-hydroxynaphthy-1-ylmethyl)iminodiethanoic acid;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      gl  KCl    25°C 0.10M U        K1=20.6        1975TRb (93631)2970
*************************************************************************
C16H16N2O2             H2L                     CAS 94-93-9  (2101)
N,N'-Bis(salicylidene)ethylenediamine;(HO(C6H4)CH:NCH2-)2
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      gl  alc/w  25°C  0.2M U                          1999MTc (93679)2971
                                         K(Fe+HL)=5.53
Medium: 0.2 M KCl in 3:7 v/v H2O/EtOH
-------------------------------------------------------------------------
Fe+++      gl  mixed  25°C  80%  C        K1=22.85       1991LMa (93680)2972
Medium: 80% w/w DMSO/H2O, 0.1 M KClO4
```

Fe+++ gl mixed 25°C 80% C K1=25.85 1983LMa (93681)2973
In 80% w/w DMSO-H2O; 0.10 M KClO4.

Fe+++ gl mixed 25°C 80% C 1983LMb (93682)2974
K(FeL+A)=14.68
K(2FeL+H2O=(FeL)2O+2H)=-12.30
In 80% w/w DMSO-H2O; 0.10 M KClO4. H2A=catechol.
****
C16H16N2O4 H2L CAS 6345-72-8 (6729)
N,N'-Ethylenebis(salicylamide), N,N'-1,2-Ethanediylbis(2-hydroxybenzamide);

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp alc/w 25°C 61% C K1=20.80 1995SDa (93703)2975
Medium: 61.1 wt % EtOH/H2O, I=0.50 M LiCl.
Data for the N,N'-propyl- (K1=20.77) and N,N'-butyl- (K1=21.19) compounds
****
C16H17NO3 H2L N-Salycyl-Phe CAS 23847-75-8 (6938)
2-(N-(2-Hydroxybenzyl))amino-3-phenylpropanoic acid;
HO.C6H4.CH2.NH.CH(CH2.C6H5)COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp NaClO4 25°C 0.10M U K1=17.71 1994OJa (93728)2976
****
C16H18N2O3 HL (5564)
2-(2-Acetylphenylhydrazone)-5,5-dimethyl-1,3-cyclohexanedione;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl diox/w 25°C 75% U K1=13.07 B2=24.77 1990ASb (93777)2977
****
C16H18N2O5S HL Penicillin V CAS 87-08-1 (943)
Phenoxymethylpenicillinic acid, 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic
acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl KNO3 25°C 0.10M M T H K1=7.10 B2=10.60 1983SBc (93817)2978
Also data for 35 C. DH(B2)=2.85 kJ mol-1, DS(B2)=303 J K-1 mol-1.
****
C16H18O9 HL Chlorogenic acd CAS 327-97-9 (2844)
3-(3',4'-Dihydroxycinnamoyl)-1,3,4,5-tetrahydroxycyclohexane carboxylic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl KNO3 20°C 1M U K1=17.64 1996AAa (93899)2979
B(FeHL)=22.20
****

C16H20N2O10 H6L (704)
1,2-Dihydroxy-3,6-di-(methyleneiminodiethanoic acid)-benzene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	gl	KNO3	25°C	0.10M	C		K1=22.0		1988ZHa	(94065)2980
							K(Fe+H2L)=12.84			
							K(Fe+HL)=19.02			
							K(FeHL+H)=4.95			
							K(FeL+H)=8.87			

****
C16H22N2O6P2 H4L CAS 85425-45-2 (5193)
2,2'-(Ethylenedi-imino)bis(2-hydroxybenzylphosphinic acid);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	EMF	KCl	?	0.10M	U		K1=31.0		1968MRc	(94141)2981

****
C16H22N2O6P2 H4L CAS 86857-07-0 (5192)
2,2'-(Ethylenedi-imino)bis(benzylphosphonic acid);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	EMF	KCl	?	0.10M	U		K1=15.90		1968MRc	(94151)2982
							K(Fe+H2L)=8.43			

****
C16H22N4O L (3471)
2-(N-(2-Dimethylaminoethyl)-N-(4-methoxybenzyl)amino)pyrimidine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	gl	KCl	25°C	0.06M	U	T	K1=3.14	B2=6.19	1961SMa	(94198)2983

K1=3.17(0 C), 3.10(45 C)

****
C16H24N2O4 H2L (5873)
2,3-Dihydroxy-N,N'-diethylterephthalamide; C6H2(OH)2(CO.NEt2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	sp	KCl	25°C	0.10M	C		K1=16.3	B2=30.70	1989GMb	(94307)2984
							K3=11.5			

Data for propyl (K1=16.0, K2=15.2, K3=11.9) and butyl (K1=11.0) analogues

****
C16H24N2O12 H4L (7217)
Rhizoferrin; (CH2CH2NHCOCH2C(OH)(COOH)CH2COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	sp	NaClO4	25°C	2.00M	C		K1=25.3		1996CDc	(94323)2985
							B(FeHL)=30.8			

B(FeH2L)=35.1
B(FeH3L)=36.9
****
C16H24O6 L Benzo18-crown-6 CAS 14098-24-9 (513)
2,3-Benzo-1,4,7,10,13,16-hexaoxacyclooctadeca-2-ene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	dis	non-aq	25°C	100%	U			1998BJa	(94399)2986
							Keff(FeA(ClO4)+L)=3.17		

Medium: Chloroform, 0.1 m Mg(ClO4)2, pH=8.1. A: desferrioxamine B.
****
C16H25NO4 L (7444)
1-Aza-4,7,10,13-tetraoxa-1-phenyl-cyclopentadecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	con	mixed	25°C	80%	C	IH		1999MFa	(94516)2987
							K(Fe(NO3)3+L)=2.22		
							K(Fe(ClO4)3+L)=2.33		

Medium: 80% acetonitrile/H2O. Data for 70-95% acetonitrile/H2O, and for
20-35 C. DH(K)=24.84 kJ mol-1, DS(K)=512.2 J K-1 mol-1.
****
C16H28N4O8 H4L DOTA CAS 60239-18-1 (1017)
1,4,7,10-Tetraazacyclododecane-1,4,7,10-tetraethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	EMF	KCl	25°C	0.10M	C		K1=29.4	1991CMb	(94894)2988
							K(FeL+H)=3.23		

K1 by competitive reaction with EDTA
****
C16H28N4O8 H2L Alcaligin CAS 117959-43-0 (7649)
1,8,11,18-Tetrahydroxy-1,6,11,16-tetraazacycloeicosane-2,5,12,25-tetrone;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KCl	25°C	0.10M	C		K1=23.5	1998HRa	(94942)2989
							B(Fe2L3)=64.7		
							B(FeH-1L)=17.2		
							B(Fe2H-4L2)=16.7		

****
C16H29N3O7 H3L (7395)
4,8,12-Tris(carboxymethyl)-1-oxa-4,8,12-triazacyclotetradecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	R4N.X	25°C	0.10M	C		K1=21.93	1997CCa	(94951)2990
							K(FeL+H)=2.63		
							K(Fe(OH)L+H)=3.8		

Medium: Me4NNO3

****

C16H29N3O8 H3L (6699)

1,7-Dioxa-4,10,13-triazacyclopentadecane-N,N',N"-triethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KCl	25°C	0.10M	C		K1=19.82 K(FeL+H)=2.65 K(Fe(OH)L+H)=6.15	1993DSa (94972)	2991

****

C16H30N4O8 H4L CAS 111557-57-4 (5834)

Diaminoethane-N,N'-diethanoic-N,N'-di(N-2-propyl-acetohydroxamic)acid;(CH2N(CH2COOH)CH2CON(OH)Pr

---

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaCl	25°C	0.10M	U		K1=30.2 B(FeH2L)=39.1 K(FeL=FeLOH+H)=-10.27 K(FeL+H)=4.26 K(FeHL+H)=4.71	1988TRa (95077)	2992

****

C16H30N6O6 H2L DOCYDMAHA CAS 221003-26-5 (7588)

1,4,8,11-Tetraazacyclotetradecane-12,14-dioxo-4,8-bis(N-methylacetohydroxamic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KNO3	25°C	0.10M	C		K1=21.33 B(FeHL)=24.50 B(FeH2L)=27.94 B(FeH-2L)=5.07 B(Fe2L3)=60.50	1998SGa (95095)	2993

****

C16H32N2O5 L Cryptand 2,2,1 CAS 31364-42-8 (837)

1,10-Diaza-4,7,13,16,21-pentaoxabicyclo[8,8,5]tricosane (2,2,1);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	R4N.X	25°C	0.05M	U		K1=16.2	1999BDb (95206)	2994

Medium: Et4NClO4

****

C17H12N2O3 H2L (2040)

1-(2-Carboxyphenylazo)-2-hydroxynaphthalene; HOOC.C6H4.N:N.C10H6.OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	NaClO4	25°C	0.01M	U		K1=8.57	1981GMe (95703)	2995

****

C17H14N2O2 L CAS 4551-69-3 (698)

4-Benzoyl-3-methyl-1-phenyl-2-pyrazolin-5-one;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ dis NaClO4 ? 0.10M U K1=3.60 B2=6.60 1972NIa (95881)2996
In 0.1 H2SO4, K1=2.90
****
C17H14O3 H2L CAS 1467-40-9 (795)
1,5-Diphenylpentane-1,3,5-trione; C6H5.CO.CH2.CO.CH2.CO.C6H5

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp alc/w 25°C 70% C 1991HKd (95977)2997
B(FeHL)=11.84
Medium: 70% v/v MeOH/H2O, 0.5 M NaClO4
****
C17H16N2O2 HL CAS 65840-98-4 (8454)
3-(2-Hydroxy-5-methyphenyl)-5-(4-methoxyphenyl)pyrazole;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl diox/w 27°C 70% C K1=11.50 B2=22.40 1994SNa (96029)2998
K3=7.25
Medium: 70% v/v dioxane/H2O, 0.10 M NaClO4.
****
C17H17N3O HL (5218)
alpha-Cyano-4-hydroxyphenacylidene-4-dimethylaminoaniline;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp alc/w 30°C 100% U 1970GSe (96195)2999
K(Fe+2HL)=6.95
Medium: MeOH
****
C17H18N2O4 H3L (5874)
N-(2-(Salicylideneamino)ethyl)-(2-hydroxyphenyl)glycine;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp KNO3 25°C 0.10M U M K1=33.3 1989SCb (96209)3000
K(FeL=FeLOH+H)=-6.7
K(FeL+A)=10.6
H2A=catechol. Constants determined by competition with EDTA
****
C17H18N3O3F HL Ciprofloxacin CAS 189257-90-7 (7142)
1-Cyclopropyl-6-fluoro-1,4-dihydro-4-oxo-7[1-piperazinyl]-3-quinoline carboxylic
acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---

```
Fe+++      gl  KNO3   20°C  0.1M C  I     K1=15.91  B2=26.55  2000DSa (96224)3001
                                          B(FeH-1L)=11.76
In 0.05 M KNO3: K1=15.20, B2=26.45, B(FeH-1L)=10.25
**************************************************************************
C17H19N3                L    Antazoline       CAS 91-75-8  (3486)
2-(N-(Benzyl)-N-phenylaminomethyl)-1,4,5H-1,3-diazole, antistine;
C3H5N2.CH2.N(C6H5)CH2.C6H5
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe+++      gl  KCl    25°C 0.06M U T      K1=3.80   B2=7.15   1961SMa (96265)3002
K1=4.09(0 C), 3.63(45 C); K2=3.36(0 C), 3.31(45 C)
**************************************************************************
C17H21NO                L    Benadryl         CAS 58-73-1  (3492)
N,N-Dimethyl-2-(diphenylmethoxy)ethylamine;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe+++      gl  KCl    25°C 0.06M U T      K1=4.05   B2=7.40   1961SMa (96372)3003
At 0 C: K1=4.22, K2=3.42; 45 C: K1=3.82, K2=3.31(45C)
**************************************************************************
C17H24N4O6            H3L                    (7349)
3,6,9,15-Tetraazabicyclo[9.3.1]pentadeca-1(15),11,13-triene-3,6,9-triethanoic acid;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe+++      gl  R4N.X  25°C 0.10M C        K1=21.77       1997DQa (96454)3004
                                          K(FeL+H)=1.74
                                          K(Fe2(OH)L2+H=2FeL)=1.8
Medium: Me4NNO3
**************************************************************************
C17H26N4O4            H2L                    CAS 205595-08-0  (8972)
3,11-Bis(carboxymethyl)-3,7,11,17-tetraazabicyclo[11.3.1]heptadeca-1(17),13,15-trie
ne;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe+++      gl  R4N.X  25°C 0.10M C        K1=20.49       1998CDa (96503)3005
                                          *K(FeL)=-5.03
Medium: 0.10 M Me4NNO3.
**************************************************************************
C17H30N4O8            H4L    TRITA           CAS 60239-20-5  (1018)
1,4,7,10-Tetraazacyclotridecane-1,4,7,10-tetraethanoic acid;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe+++      gl  KCl    25°C 0.10M C        K1=27.46       1991CMb (96648)3006
                                          K(FeL+H)=2.64
K1 by competitive reaction with NTA
**************************************************************************
```

C17H33N3O9 L CAS 132259-53-1 (6558)
1,1,1-Tris((2-((N-methylhydroxyamino)carbonyl)ethoxy)methyl)ethane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KCl	25°C	0.10M	C		K1=28.11 K(FeL+H)=3.72	1991MSa (96736)	3007

****
C18H16N2O3 HL (5560)
2-(2-Acetylphenylhydrazone)-1-phenyl-but-1,3-dione;
C6H5.CO.C(CO.CH3):N.NH.C6H4.COCH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	diox/w	25°C	75%	U		K1=14.00 B2=26.70	1990ASb (97170)	3008

****
C18H19NO5 H3L (6939)
2-N-Carboxymethyl-N-2-hydroxybenzylamino-3-phenylpropanoic acid;
HOC6H4CH2N(CH2COOH)CH(CH2Ph)COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaClO4	25°C	0.10M	U		K1=21.61	1994OJa (97307)	3009

****
C18H20N2O6 H4L CAS 10328-28-6 (3501)
Ethylenedinitrilo-N,N'-bis(2'-hydroxyphenyl)-N,N'-diethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KCl	25°C	0.10M	C		K1=31.8 K(FeL+H)=1.0	1993MMa (97395)	3010
Fe+++	sp	KNO3	25°C	0.10M	C		K1=40.1	1992GVa (97396)	3011
Fe+++	EMF	oth/un	?	?	U		K1=20.0	1968TRc (97397)	3012
By polarography: K1=20.2									
Fe+++	sp	KNO3	20°C	0.10M	U		K1=33.91	1964ALa (97398)	3013
Fe+++	gl	KNO3	25°C	0.10M	U		K1=33	1964PCa (97399)	3014
Fe+++	sp	NaClO4	25°C	0.10M	U		K1=33.9	1964SCc (97400)	3015

****
C18H20N2O6 H4L EHPG CAS 10328-28-6 (429)
N,N'-Ethylene-bis-(2-(2'-hydroxyphenyl))glycine; (HOOCCH(C6H4OH)NHCH2.)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaCl	25°C	1.0M	U		K1=39.3 K(Fe(OH)L+H)=12.67	1990ADb (97425)	3016

```
--------------------------------------------------------------------------------
Fe+++      gl  KCl    25°C 0.10M C        K1=35.54       1989BMd (97426)3017
                                          K(FeLOH+H)=11.78
                                          K1=33.28 (meso ligand)
                                          K(FeLOH+H)=10.45 (meso ligand)
                                          K(FeL+H)=2.72 (meso ligand)
********************************************************************************
C18H20N2O12S2         H6L                          (5478)
1,6-Bis(2,3-dihydroxy-5-sulfobenzoyl)-1,6-diazahexane;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      gl  KNO3   25°C 0.10M C        K1=27.4        1982KRb (97450)3018
                                          B(FeHL2)=51.1
                                          B(FeH2L2)=58.3
                                          B(Fe2L3)=76
********************************************************************************
C18H21NO2              HL                           (683)
trans-5-(3-Methylbutyl)-2-hydroxy-diphenylketoxime;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      gl  KNO3   35°C 0.10M C        K1=14.52  B2=28.01  1978JIa (97489)3019
********************************************************************************
C18H21N3O4            H2L                       CAS 76218-93-4  (9124)
1,5-Bis-(2-hydroxybenzamido)-3-azapentane;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      sp  alc/w  25°C 2.5%  C        K1=23.3        2004DRa (97494)3020
                                          *K(FeL(H2O))=-5.2
                                          *K(FeH-1L(H2O))=-7.0
                                          *K(FeH-1L(OH))=-9.2
                                          K(FeL+H)=2.2
Medium: 2.5% v/v MeOH/H2O, 0.5 M NaClO4. K(Fe+H3L=FeH2L+H)=0.55.
********************************************************************************
C18H22N4O4            H2L                       CAS 2444-14-6  (3502)
N,N'-Bis(2-pyridylmethyl)diaminoethane-N,N'-diethanoic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      gl  oth/un 25°C 0.10M U        K1=28.8        1965LCa (97541)3021
********************************************************************************
C18H26N2O6P2          H4L                       CAS 53431-86-0  (5266)
Ethylenebis(imino(2-hydroxyphenyl)methylene(methyl)phosphinic acid);
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      EMF oth/un   ?     ?  U        K1=31.25       1970DMc (97674)3022
********************************************************************************
```

C18H28N4O4 H2L (7378)
7-Methyl-3,7,11,17-tetraazabicyclo[11.3.1]heptadeca-1(17),13,15-triene-3,11-diethan
oic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	R4N.X	25°C	0.10M	C		K1=20.64	1997CDb	(97784)3023
							K(FeL)=2.84		
							K(Fe(OH)L+H)=ca 5.9		

Medium: NMe4NO3

****

C18H30N4O12 H6L TTHA CAS 869-52-3 (694)
Triethylenetetraaminehexaethanoic acid;((HOOC.CH2)2N.CH2.CH2.N(CH2.COOH).CH2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	EMF	KNO3	25°C	0.10M	C		K1=27.66	1997DFa	(98030)3024
							K(FeL+H)=7.49		
							K(FeL+Fe)=12.13		
							K(FeHL+H)=2.05		
							K[Fe2(OH)L+H]=2.11		

K[Fe2(OH)2L+2H]=5.91

Fe+++	EMF	KNO3	25°C	0.10M	U		K1=26.8	1970HAa	(98031)3025
							B(Fe2L)=40.5		

By glass electrode, K(FeL+H)=7.60, K(FeHL+H)=2.75, K(Fe2L+2OH)=21.0

Fe+++	gl	KNO3	25°C	0.10M	U	M		1967BMe	(98032)3026
							K(Fe2(OH)2L+2H)=6.6		
							K(Fe2(OH)2L+2HA)=5.05		
							K(Fe2L+2A)=23.5		
							K(Fe2L+2B)=18.10		

H4A=1,2-dihydroxybenzene-3,5-disulfonic acid, H2B=oxine-5-sulfonic acid

Fe+++	EMF	NaClO4	25°C	0.10M	U		K1=29.4	1965SCb	(98033)3027
							K(FeL+H)=7.51		
							K(FeHL+H)=2.60		
							K(FeL+OH)=4.20		
							K(FeLOH+OH)=3.50		

K(Fe2LOH+OH)=2.9

****

C18H32N4O6 H2L Bisucaberin CAS 112972-60-8 (7650)
6,17-Dihydroxy-1,6,12,17-tetraazacyclodoccasane-2,5,13,16-tetrone;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KCl	25°C	0.10M	C		K1=23.5	1998HRa	(98138)3028
							B(Fe2L3)=64.3		

****

C18H32N4O8 H4L TETA CAS 60239-22-7 (1019)

1,4,8,11-Tetraazacyclotetradecane-1,4,8,11-tetraethanoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl KCl 25°C 0.10M C K1=26.53 1991CMb (98202)3029
K(FeL+H)=3.53
K1 by competitive reaction with NTA
****
C18H32N4O9 H4L CAS 189282-31-3 (8974)
4,7,10,13-Tetrakis-(carboxymethyl)-1-oxa-4,7,10,13-tetraazacyclopentadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl R4N.X 25°C 0.10M C K1=23.82 1999CDb (98256)3030
K(FeL+H)=3.03
K(FeL+Fe)=6.87
Medium: 0.10 M NMe4NO3.
****
C18H32N6O8 H2L CAS 204185-67-1 (7978)
1,1-Bis(10-hydroxy-2,5,10-triaza-1,6,9-trioxoundecanyl)ethane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp NaClO4 25°C 0.10M C K1=20.03 2001NGa (98263)3031
K(2FeL(H2O)2+L=Fe2L3)=19.52
K(2Fe+3L)=59.45
K(2Fe+3L) from EDTA competition experiment.
****
C18H32N6O8 H2L CAS 380230-89-7 (7977)
1,1-Bis(9-hydroxy-2,5,9-triaza-1,6,10-trioxoundecanyl)ethane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp NaClO4 25°C 0.10M C K1=19.85 2001NGa (98265)3032
K(2FeL(H2O)2+L=Fe2L3)=19.39
K(2Fe+3L)=59.22
K(2Fe+3L) from EDTA competition experiment.
****
C18H33N3O9 H3L (6700)
1,7,13-Trioxa-4,10,16-triazacyclooctadecane-N,N',N"-triethanoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl KCl 25°C 0.10M C K1=22.5 1993DSa (98296)3033
K(FeL+H)=3.65
****
C18H34N4O9 H3L DO3A-B (7301)
10-[2,3-Dihydroxy-(1-hydroxymethyl)-propyl]-1,4,7,10-tetraazacyclododecane-1,4,7-tr
iethanoic ac.;

```
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      gl  KCl    25°C 0.10M C        K1=25.7        1996TKa (98378)3034
                                          K(Fe+HL)=2.7
*************************************************************************
C18H34N6O8            H4L                    CAS 253273-56-2  (5455)
2,2',2",2"'-(1,2-Cyclohexanediyldinitrilo)tetrakis[N-hydroxy-N-methyl] acetamide;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      sp  KNO3   25°C 0.10M C                        2000ARa (98388)3035
                                          B(FeH3L)=46.39
                                          B(FeH4L)=48.2
                                          B(Fe2H3L2)=78.4
*************************************************************************
C18H36N2O6              L    Cryptand 2,2,2   CAS 23978-09-8  (514)
1,10-Diaza-4,7,13,16,21,24-hexaoxabicyclo[8.8.8]hexacosane;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      gl  R4N.X  25°C 0.05M U        K1=13.3        1999BDb (98574)3036
Medium: Et4NClO4
*************************************************************************
C18H37N5                L                      CAS 160964-42-1  (7629)
2R,3R,8S,9S-Dicyclohexano-1,4,7,10,13-pentaazacyclopentadecane;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      gl  none   25°C    0  U                        1998ZBb (98813)3037
                                          *K1(FeLCl2)=-3.7
                                          *K2(FeLCl2)=-7.50
-------------------------------------------------------------------------
Fe+++      gl  none   25°C    0  U                        1998ZBb (98814)3038
                                          *K1(FeLCl2)=-4.1
                                          *K2=(FeLCl2)=-7.73
*************************************************************************
C18H38N4O8            H2L                    CAS 98902-93-3  (5580)
7,24-Dihydroxy-1,4,14,17-tetraoxa-7,11,20,24-tetraazahexacosa-8,23-dione;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      gl  KNO3   25°C 0.10M C                        1985SMb (98863)3039
                                          K(FeL+H)=15.78
                                          K(FeHL+H)=10.58
*************************************************************************
C19H14O7S             H4L    Pyrocatechol Vi  CAS 369596-29-2  (709)
Pyrocatechol Violet,
3-[3,4-Dihydroxyphenyl-3-hydroxy-4-oxo-2,5-cyclohexadien-1-ylidenemethyl-b.;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
```

```
--------------------------------------------------------------------------------
Fe+++      sp  KCl    25°C 0.50M U                        1974CMc (99105)3040
                                        K(Fe+H3L=FeH2L+H)=0.25
                                        K(FeH2L+H3L=FeH3L2+2H)=-5.82
                                        K(FeH3L2+H2L=FeH4L3+H)=-1.91
                                        K(2Fe+H3L=Fe2HL+2H)=4.65
K(Fe+H2L)=7.5, K(Fe+H2L+HL)=19.3, K(Fe+H2L+2HL)=27.2, K(Fe2+HL)=22.2
K(Fe+H2L+2HL=Fe(H4L3))=27.2,K(2Fe+HL=Fe2HL)=22.2. Ligand: Pyrocatechol sulf.
--------------------------------------------------------------------------------
Fe+++      sp  KNO3     ?  0.50M U                        1972YVa (99106)3041
                                        K(FeOH+2H2L)=13.80
********************************************************************************
C19H15NO8             H4L    Alizarin Comp.   CAS 3952-78-1  (671)
(3,4-Dihydroxy-2-anthraquinonyl-methyl)iminodiethanoic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      sp  diox/w       20%  U                        1973INa (99132)3042
                                        K(Fe+HL)=19.6
Medium: 20% dioxan, 0.1 M
********************************************************************************
C19H19N3O4            H2L                    CAS 75281-26-4  (1604)
N-Pyridoxylidene-L-tryptophan;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      gl  NaCl   25°C 0.50M C                        1989KOb (99267)3043
                                        K(Fe+HL)=9.65
                                        K(Fe+2HL)=18.38
********************************************************************************
C19H22N2O6            H4L                    CAS 102165-09-3  (9199)
Propylenediamine-N,N'-bis(2-hydroxyphenylethanoic acid);
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      gl  NaCl   25°C 0.10M C        K1=33.54       2004SGb (99327)3044
                                        B(FeHL)=35.84
                                        B(FeH-1L)=21.74
Additional method: UV-visible spectrometry
********************************************************************************
C19H24N2O2              L                      (1564)
1,5-Diaza-7,8:13,14-dibenzo-9,12-dioxacyclopentadecan-7,13-diene;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      con non-aq 25°C 100%  C T H    K1=4.93        2000MTc (99362)3045
Medium: acetonitrile. Data for 20-35 C. DH(K1)=-4.50 kJ mol-1, DS(K1)=
79.2 J K-1 mol-1.
********************************************************************************
C19H28N4O6            H3L                    CAS 106967-44-6  (8973)
```

3,7,11-Tris(carboxymethyl)-3,7,11,17-tetraazabicyclo[11.3.1]heptadeca-1(17),13,15-t
riene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	R4N.X	25°C	0.10M	C		K1=19.21 *K(FeL)=-5.46	1998CDa	(99407)3046

Medium: 0.10 M Me4NNO3.

****

C19H39N7O6 H3L TETMAHA (7468)
1,4,8,11-Tetraazacyclotetradecane-N,N',N"-tris(N-methylacetohydroxamic acid);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KNO3	25°C	0.10M	C		K1=25.5 B(FeHL)=37.8 B(FeH2L)=41.6	1999GGa	(99502)3047

****

C20H14N4 L CAS 63283-05-6 (4146)
2,2':6',2'':6'',2'''-Quaterpyridine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	KNO3	25°C	0.02M	U	H	K1=11.40	1964BOa	(99741)3048

Medium: HNO3. DH(K1)=-38 kJ mol-1, DS=92 J K-1 mol-1

****

C20H16N2O2 H2L CAS 3946-91-6 (2733)
N,N'-Bis(2'-hydroxybenzylidene)-1,2-diaminobenzene; (HOC6H4CH:N)2.C6H4

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	mixed	25°C	80%	C		K1=17.80 B(FeHL)=21.52 B(FeH-1L)=12.99	1997HMc	(99773)3049

Medium: 80% w/w DMSO/H2O, 0.5 M NaClO4.

****

C20H18NO6Cl H2L Phe-OTA CAS 303-47-9 (7614)
Ochratoxin A;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaClO4	25°C	0.10M	C		K1eff=3.34	1998AGa	(99822)3050

Method: fluorescence. pH=2.6. For Ochratoxin B, K1eff=3.49.

****

C20H18N4O2 HL (5917)
Pyruvic monohydrazone-3-hydrazino-4-benzyl-6-phenylpyridazine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo

Fe+++ gl diox/w 30°C 75% U B2=24.51 1985RSb (99832)3051
K(Fe+HL)=6.05
K(Fe+2HL)=12.06
K(Fe+L+HL)=18.77

****

C20H24N2O4 H2L CAS 39556-13-3 (8593)
N,N'-1,2-Ethanediylbis[N-(phenylmethyl)]glycine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	NaClO4	25°C	0.10M	U		K1=15.20	2001SGc (99947)	3052
							*K(FeL)=-3.52		
							*K(Fe(OH)L)=-7.27		

****

C20H24N2O5 H3L CAS 219686-81-4 (8594)
N-[2-[(Carboxymethyl)[(2-hydroxyphenyl)methyl]amino]ethyl]-N-(phenylmethyl)glycine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaClO4	25°C	0.10M	C		K1=27.00	2001SGc (99955)	3053
							*K(FeL)=-5.76		

****

C20H24N2O6 H4L CAS 115538-91-5 (9198)
Butylenediamine-N,N'-bis(2-hydroxyphenylethanoic acid);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	NaCl	25°C	0.10M	C		K1=29.69	2004SGb (99960)	3054
							B(FeHL)=33.66		
							B(FeH-1L)=18.75		

Additional method: UV-visible spectrometry

****

C20H24N2O6 H4L (6591)
Diaminoethanebis(2-hydroxy-4-methyl-phenyl)ethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaCl	25°C	1.0M	U		K1=39.0	1990ADb (99962)	3055
							K(Fe(OH)L+H)=13.45		
							K(FeL+H)=1.9		

Data listed refer to meso-form of L
For racemic form: K1=37.9; K(Fe(OH)L+H)=11.86;K(FeL+H)=2.5

****

C20H24N2O6 H4L HBED CAS 3625-89-6 (2208)
N,N'-Di-(2-hydroxybenzyl)-diaminoethane-N,N'-diethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KCl	25°C	0.10M	U		K1=39.01	1994MMe (99993)	3056
							K(FeL+H)=1.51		

```
--------------------------------------------------------------------------------
Fe+++      sp  KCl    25°C 0.10M M        K1=39.68       1990MMa (99994)3057
--------------------------------------------------------------------------------
Fe+++      gl  KNO3   25°C 0.10M U        K1=39.68       1967LMd (99995)3058
********************************************************************************
C20H24N2O12S2         H6L                     CAS 3625-85-3  (5755)
N,N'-Bis(2-hydroxy-5-sulfobenzyl)-diaminoethane-N,N'-diethanoic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      sp  KCl    25°C 0.10M M        K1=36.87       1990MMa (100027)3059
                                          K(Fe(OH)L+H=FeL+H2O)=10.57
--------------------------------------------------------------------------------
Fe+++      gl  KCl    25°C 0.10M C        K1=36.87       1989MSc (100028)3060
                                          K(FeH-1L+H)=10.56
--------------------------------------------------------------------------------
Fe+++      gl  KCl    25°C 0.10M C        K1=38.30       1984TMb (100029)3061
********************************************************************************
C20H24O6               L    DiBz-18-Crown-6  CAS 14187-32-7  (604)
2,3:11,12-Dibenzo-1,4,7,10,13,16-hexaoxacyclooctadeca-2,11-diene
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      con mixed  25°C  90%  C        K1=2.76        2003ISa (100120)3062
Medium: 90% v/v DMSO/H2O.
********************************************************************************
C20H26N4O6            H4L    ENDA-HP            (6746)
N,N'-Bis(3-hydroxy-6-methyl-2-pyridylmethyl)diaminoethane-N,N'-diethanoic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      sp  KCl    25°C 0.10M C        K1=35.08       1992MSa (100329)3063
                                          K(FeL+H)=5.86
                                          K(FeHL+H)=4.84
Additional method: Pt/Fe(III),Fe(II) electrode
********************************************************************************
C20H30N2O8P2          H4L                     CAS 112827-88-0  (8105)
N,N'-Bis(2-hydroxybenzyl)diaminoethane-N,N'-bis(methylenephosphonic acid monomethyl
ester);
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      gl  KCl    25°C 0.10M C        K1=28.21       1984TMd (100413)3064
                                          K(FeOHL+H)=6.72
********************************************************************************
C20H34N4Fe              L                       (7287)
1,1-Bis(5-methyl-2,5-diazahexyl)ferrocene;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
```

Fe+++ gl KNO3 25°C 0.10M C 1996TBb (100510)3065
K(FeL+H)=9.5
K(FeHL+H)=7.7
K(FeH2L+H)=4.2
K(FeH3L+H)=3.8
****
C20H36N6O8 H2L CAS 204185-70-6 (7979)
1,1-Bis(11-hydroxy-2,5,11-triaza-1,6,10-trioxododecanyl)ethane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp NaClO4 25°C 0.10M C K1=19.69 2001NGa (100589)3066
K(2FeL(H2O)2+L=Fe2L3)=19.53
K(2Fe+3L)=58.91
K(2Fe+3L) from EDTA competition experiment.
****
C20H36O6 L DiCy-18-crown-6 CAS 16069-36-6 (1653)
2,3:11,12-Dicyclohexyl-1,4,7,10,13,16-hexaoxacyclooctadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ con mixed 25°C 90% C K1=2.96 2003ISa (100646)3067
Medium: 90% v/v DMSO/H2O.

Fe+++ dis non-aq 25°C 100% U 1995BSa (100647)3068
K(Fe(HA)X+L=Fe(HA),L,X)=4.25
K(Fe(HA)Y+L=Fe(HA),L,Y)=2.21
Medium:CHCl3. Data for host-guest associations. H3A: desferrioxamine. X=ClO4
Y=NO3. L: cis-syn-cis and cis-anti-cis mixture. Also data for syn-L, anti-L
****
C20H37N5O10 H5L CAS 111557-58-5 (5835)
Diethylenetriamine-N,N',N"-triethanoic-N,N"-di(N-2-propyl-acetohydroxamic) acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp NaCl 25°C 0.10M U K1=29.7 1988TRa (100731)3069
B(FeH2L)=4
K(FeL=FeLOH+H)=-9.93
K(FeL+H)=8.10
K(FeHL+H)=6.15
****
C20H39N3O9 L CAS 132234-45-8 (6559)
1,1,1-Tris((3-(hydroxy(methylcarbonyl)amino)propoxy)methyl)ethane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl KCl 25°C 0.10M C K1=26.42 1991MSa (100761)3070
K(FeL+H)=3.74
****
C20H39N5O2 HL CAS 333309-52-7 (8662)

16-Aminodocosahydro-16-methyl-dibenzo[b,i][1,4,8,11]tetraazacyclotetradecine-7-carb
oxylic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KCl	25°C	0.50M	M		K1=25.3	2001BYb (100768)	3071
							K(Fe+L+OH)=7.1		
							B(FeHL)=4.8		

****

C21H18O5S H3L o-Cresol red CAS 1733-12-6 (1634)
2-Cresolsulfonephthalein;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	kin	NaClO4	25°C	0.10M	C			1975NFb (101131)	3072
							K(Fe(OH)HL+H)=2.25		
							K(Fe+HL)=1.47		

Medium: 0.10 M NaClO4/HClO4.

****

C21H20O6 H3L Curcumin CAS 458-37-7 (8774)
1,7-Bis(4-hydroxy-3-methoxyphenyl)-1,6-heptadiene-3,5-dione;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	alc/w	25°C	50%	C		K1=22.06	2002BFb (101156)	3073
							B(FeH2L)=29.13		
							K(Fe+H2L)=9.14		
							K(Fe+H2L=FeL+2H)=2.07		
							K(Fe+H2L+2OH=FeH2L(OH)2)=29.1		

Medium: 50% v/v MeOH/H2O, 0.10 M NaNO3. B(FeH-1L)=12.51

****

C21H21NO3 L CAS 6393-39-1 (7647)
Tris(2-hydroxybenzyl)amine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	alc/w	25°C	70%	C		K1=37.0	1998MMa (101159)	3074
							K(FeL+H)=7.40		

Medium: 70% (v/v) EtOH/H2O, 0.1 M KCl.

****

C21H22O10 L G-Rubrofusarin CAS 63174-98-1 (7067)
2-Methyl-5,6-dihydroxy-6-O-B-D-galactosyl-8-methoxy-naphtho-pyrone;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaClO4	25°C	1.00M	C			1995PDa (101214)	3075
							B(Fe2L2)=29.38		

****

C21H25N3O7 H4L (6563)
N-(2-Hydroxybenzyl)-N'-(pyridoxyl)ethylenediamine-N,N'-diethanoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp KCl 25°C 0.10M C K1=31.01 1991MSb (101272)3076
K(FeL+H)=6.86
K(FeHL+H)=3.38
****
C21H26N2O6 H4L BHTDA CAS I4 (6592)
N,N'-Bis(2-hydroxybenzyl-trimethylenedinitrilo-N,N'-diethanoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp NaCl 25°C 1.0M U K1=37.8 1990ADb (101276)3077
K(FeL+H)=3.7
K(Fe(OH)L+H) is about 12.75 as far as L decomposes at pH>12.75
****
C21H27N3O6 H4L CAS 54135-84-1 (8822)
1,10-Bis(2,3-Dihydroxybenzoyl)-1,5,10-triazadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp KCl 25°C 0.20M C K1=31 2001CBc (101289)3078
K(FeL+H)=5.15
K(FeHL+H)=3.65
K(FeH2L+H)=1.50
****
C21H27N3O6 H4L Pistallarin CAS 89647-69-8 (8821)
1,10-Bis(3,4-Dihydroxybenzoyl)-1,5,10-triazadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp KCl 25°C 0.20M C K1=29 2001CBc (101291)3079
K(FeL+H)=6.05
K(FeHL+H)=4.25
K(FeH2L+H)=1.80
****
C21H29N7O14P2 H2L alpha-NAD CAS 7298-93-3 (2775)
Nicotinamide adenine dinucleotide, Diphosphopyridine nucleotide;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp oth/un 25°C 0.10M U 1973GEa (101362)3080
K1eff=3.86
K2eff=4.60
Medium: glycine buffer. pH=2.0
****
C21H38N6O8 H2L CAS 204185-69-3 (7980)
1,1-Bis(10-hydroxy-2,5,10-triaza-1,6,9-trioxoundecanyl)pentane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo

---
Fe+++ gl NaClO4 25°C 0.10M C K1=19.85 2001NGa (101439)3081
K(2FeL(H2O)2+L=Fe2L3)=18.81
K(2Fe+3L)=58.46
K(2Fe+3L) from EDTA competition experiment.
****
C22H14O9 H5L CAS 4431-00-9 (3513)
Aurintricarboxylic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp oth/un 25°C ? U 1965SAb (101497)3082
K(Fe+HL)=4.5(?)

Fe+++ sp oth/un 25°C ? U K1=4.68 1958MDa (101498)3083
****
C22H18O10 H7L CAS 1257-08-5 (2128)
Epicatechin gallate;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp none 20°C U 1998JSa (101678)3084
K1eff=27.3
K(Fe+LH3=FeLH2+H)=4.30
K(FeLH2+LH2=FeLH+LH3)=7.30
K1eff by competition with EDTA at pH 7.
****
C22H18O11 H8L CAS 989-51-5 (2270)
Epigallocatechin gallate;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp none 20°C U 1998JSa (101681)3085
K1eff=27.6
K(Fe+LH3=FeLH2+H)=4.40
K(FeLH2+LH2=FeLH+LH3)=7.40
K1eff by competition with EDTA at pH 7.
****
C22H21N4OS L CAS 51134-29-3 (5319)
4-(6-Methoxy-3-methylbenzothiazolylazo)-N-methyldiphenylamine;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ dis non-aq ? 100% U 1972KKg (101709)3086
K(FeCl4+HL)=7.47
Medium: 5:1 benzene:cyclohexanone.
****
C22H23N2O8Cl H2L Aureomycin CAS 56235-18-8 (3515)
Chlorotetracycline;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	gl	oth/un	20°C	0.01M	U		K1=9.4 K3=5.6	B2=16.60	1956ARd (101760)	3087

****

C22H24N2O8 H2L Tetracycline CAS 60-54-8 (2201)
Tetracycline;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	gl	NaNO3	25°C	0.10M	C		K1=13.4		1992GAa (101815)	3088
Fe+++	gl	oth/un	20°C	0.01M	U		K1=9.9 K3=6.8	B2=18.50	1956ARd (101816)	3089

****

C22H24N2O9 H2L Oxotetracycline CAS 79-57-2 (2202)
Oxytetracycline, 5-Hydroxy-tetracycline;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	gl	oth/un	20°C	0.01M	U		K1=9.6 K3=5.7	B2=16.80	1956ARd (101883)	3090

****

C22H26N4O8 H4L (5526)
N,N'-Dipyridoxylethylenediamine-N,N'-diethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Fe+++	sp	KCl	25°C	0.10M	M		K1=30.78 K(FeL+H)=6.93 K(FeHL+H)=6.02		1990MMa (101950)	3091
Fe+++	gl	KCl	25°C	0.10M	C		K1=30.78 K(FeL+H)=6.93 K(FeHL+H)=6.02		1989MSc (101951)	3092
Fe+++	nmr	none	15°C	0.0	U		K1=36.88 K(FeL+H)=7.49 K(FeHL+H)=6.59		1985TMa (101952)	3093
Fe+++	gl	KCl	25°C	0.10M	C		K1=36.91 K(FeL+H)=7.49 K(FeHL+H)=6.59		1984TMb (101953)	3094
Fe+++	gl	KCl	25°C	0.10M	C		K1=36.91 K(FeL+H)=7.49 K(FeHL+H)=6.59		1984TMc (101954)	3095

****

C22H28N2O6 H4L (8056)
N,N'-Bis(2-hydroxybenzyl)ethylenediamine-,N,N'-dipropanoic acid;

```
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe+++      gl  KNO3   25°C 0.10M U        K1=31.16       1992GKa (102014)3096
*******************************************************************************
C22H31N5O6           H2L                     CAS 813432-03-0  (9200)
Imino-bis(acetyl(1-(3'-aminopropyl)-3-hydroxy-2-methyl-4-pyridinone);
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe+++      gl  KNO3   25°C 0.10M C        K1=26.16       2004SGc (102191)3097
                                         B(FeHL)=31.16
                                         B(FeH3L)=33.59
                                         B(Fe2L3)=74.26
                                         B(Fe2HL3)=79.90
B(Fe2H2L3)=85.54, B(Fe2H3L3)=89.53, B(Fe2H-2L2)=44.00
*******************************************************************************
C22H32N4O14P2        H6L    DPDP             CAS 118248-91-2  (5896)
N,N'-Dipyridoxyldiaminoethane-N,N'-diethanoic acid 5,5'-diphosphoric acid;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe+++      gl  NaCl   25°C 0.10M C        K1=33.52       1989RCa (102203)3098
                                         K(FeL+H)=7.88
                                         K(FeHL+H)=6.85
                                         K(FeH2L+H)=6.08
                                         K(FeH3L+H)=5.31
*******************************************************************************
C22H34N2O8P2         H4L                     CAS 92278-41-6  (8106)
N,N'-Bis(2-hydroxybenzyl)diaminoethane-N,N'-bis(methylenephosphonic acid monoethyl
ester);
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe+++      gl  KCl    25°C 0.10M C        K1=28.19       1984TMd (102216)3099
                                         K(FeOHL+H)=6.70
*******************************************************************************
C22H34O9              HL                     CAS 205057-99-4  (7637)
5-[11'-(Oxymethyl)-2',3'-benzo-18-crown-6]pentanoic acid;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Fe+++      dis non-aq 25°C 100%  U                         1998BJa (102245)3100
                                         K(FeA(ClO4)+HL)=3.38, pH=3.2
                                         Keff(FeA(ClO4)+L)=4.29, pH=9.3
Medium: Chloroform, 0.1 m Mg(ClO4)2.  A: desferrioxamine B.
*******************************************************************************
C22H35N5O7           H2L                     CAS 132149-21-4  (7606)
N,N'-Bis(3-(acetylhydroxamino)propyl)-4-pentyloxy-2,6-pyridinedicarboxamide;
-------------------------------------------------------------------------------
```

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaNO3	25°C	0.10M	C		K1=21.3	1994CDc (102259)	3101

At pH 1.0, K1eff=2.32.

****

C22H36N4O13 H5L Aerobactin CAS 26198-65-2 (2258)

Aerobactin; ((CH3.CO.NOH.(CH2)4)(CO2H)CH.NH.CO.CH2)2.C(CO2H)(OH)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KNO3	25°C	0.10M	C		K1=23.06	1979HCa (102288)	3102
							B(FeH3L)=31.74		
							B(FeH2L)=29.70		
							B(FeHL)=26.68		
							B(FeH-1L)=18.48		

****

C22H40N4O12 H4L CAS 98902-95-5 (5581)

7,24-Dihydroxy-1,4,14,17-tetraoxa-7,11,20,24-tetraazahexacosa-8,23-dione-7,24-dieth
anoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KNO3	25°C	0.10M	C		K1=24.45	1985SMb (102368)	3103
							K(FeL+H)=4.73		
							K(FeHL+H)=3.67		
							K(FeH2L+H)=2.70		

****

C23H16O9Cl2S H4L Chrome azurol S CAS 1667-99-8 (711)

Chromazurol S;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaNO3	20°C	0.10M	C		K1=16.85	1996ZLa (102550)	3104
							B(Fe2L)=22.61		
Fe+++	sp	KCl	25°C	0.10M	U			1987WZa (102551)	3105
							B(Fe2L2)=16.63		
Fe+++	sp	NaCl	25°C	0.10M	U	M		1971NIc (102552)	3106

Medium: 0.1(Na,NH4),(Cl,OH). K(Fe+2H2LA2=Fe(HLA)2+2H+2A)=-2.05

A=zephiramine.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	KCl	25°C	0.10M	U			1969KLb (102553)	3107
							B(Fe2L2)=37.6		
Fe+++	sp	oth/un	?	?	U			1968ATa (102554)	3108
							K(Fe+2HL)=6.40		
Fe+++	sp	KCl	20°C	0.10M	U		K1=15.6	1963LKa (102555)	3109
							B(Fe2L2)=36.2		

```
                                        B(Fe2L)=20.2
--------------------------------------------------------------------------------
Fe+++      sp  oth/un 25°C 0.10M U                      1962SDb (102556)3110
                                        K(?)=4.8
********************************************************************************
C23H18N2O3             HL                        (5561)
2-(2-Acetylphenylhydrazone)-1,3-diphenyl-prop-1,3-dione;
C6H5.CO.C(CO.C6H5):N.NH.C6H4.COCH3
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      gl  diox/w 25°C  75%  U        K1=12.42  B2=23.96  1990ASb (102593)3111
********************************************************************************
C23H18O9S              H4L    Eriochrome cyan  CAS 3564-18-9  (433)
4'-Hydroxy-3,3'-dimethyl-2''-sulfofuchsone-5,5'-dicarboxylic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      sp  KNO3   20°C 0.10M U        K1=5.07        1993ZZa (102628)3112
                                        B(Fe2L)=10.07
--------------------------------------------------------------------------------
Fe+++      sp  KCl    20°C 0.10M U        K1=17.9        1965LSa (102629)3113
                                        B(Fe2L)=22.5
                                        B(Fe2L2)=37.9
********************************************************************************
C23H30N2O6             H4L                      CAS 132750-98-2  (6543)
N,N'-Trimethylenebis(2-(2-hydroxy-3,5-dimethylphenyl)glycine);
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      sp  KCl    25°C 0.10M C        K1=34.22       1991BMa (102755)3114
                                        K(FeL+H)=2.71
                                        K(FeOHL+H)=11.31
For racemic ligand. For meso form: K1=34.83, K(FeL+H)=2.98, K(FeOHL+H)=12.03
********************************************************************************
C23H33N3O2               L    OenN(CH3)ditnH4  CAS 85735-82-6  (5583)
1,12,16-Triaza-3,4:9,10-dibenzo-12-methyl-5,8-dioxacyclononadeca-3,9-diene;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      sp  NaNO3  25°C 0.10M M                      1988MWa (102807)3115
                                        *K(FeL(H2O)2)=-5.79
                                        *K(FeLH2O(OH))=-11.71
********************************************************************************
C24H24N2O6             H4L                      CAS 385439-50-9  (9197)
p-Xylylenediamine-N,N'-bis(o-hydroxyphenyl)ethanoic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      gl  NaCl   25°C 0.10M C        K1=30.13       2004SGb (102945)3116
```

B(FeHL)=34.12
Additional method: UV-visible spectrometry
****
C24H31N3O8 H3L CAS 35369-55-2 (6972)
N,N"-Bis(2-hydroxybenzyl)-2,5,8-triazanonane-N,N',N"-triethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KCl	25°C	0.10M	C		K1=30.44	1994MMf	(103056)3117
							K(FeL+H)=8.81		
							K(FeHL+H)=4.89		
							K(FeH2L+H)=1.20		

****
C24H32N2O6 H3L Me4-HBED (6507)
N,N'-Bis(2-hydroxy-3,5-dimethylbenzyl)ethylenediamine-N,N'-diethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	KCl	25°C	0.10M	M		K1=37.41	1990MMa	(103061)3118

****
C24H32O8 L DiBz-24-Crown-8 CAS 14174-09-5 (580)
2,3:14,15-Dibenzo-1,4,7,10,13,16,19,22-octaoxacyclotetracosa-2,14-diene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	con	mixed	25°C	90%	C		K1=3.45	2003ISa	(103128)3119

Medium: 90% v/v DMSO/H2O.
****
C24H33N5O8 H5L (6747)
N,N"-Bis(3-hydroxy-6-methyl-2-pyridylmethyl)diethylenetriamine-N,N'.N"-triethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	KCl	25°C	0.10M	C		K1=32.7	1992MSa	(103202)3120
							K(FeL+H)=7.8		
							K(FeHL+H)=5.6		
							K(FeH2L+H)=4.3		
							K(FeH3L+H)=3.0		

Additional method: Pt/Fe(III),Fe(II) electrode
****
C24H34N2O5 H3L (6509)
N,N'-Bis(2-hydroxy-3,5-dimethylbenzyl)-N-(2-hydroxyethyl)-diaminoethane-N'-ethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	KCl	25°C	0.10M	M		K1=31.21	1990MMa	(103213)3121
							K(FeL+H)=3.43		

****

C24H34N3O6 H3L CAS 134627-54-6 (6564)
N-(2-Hydroxy-3,5-dimethylbenzyl)-N'-((3-hydroxy-1,2,5-trimethyl-4-pyridinyl)methyl)
EDDA;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	KCl	25°C	0.10M	C		K1=32.97	1991MSb (103217)	3122

****
C24H34N4O12 H6L (5480)
1,4-Bis(2,5,5-tris(carboxymethyl)-2,5-diazapentyl)benzene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KNO3	25°C	0.10M	C			1983NMa (103226)	3123
							B(FeHL)=31.53		
							K(FeHL+H)=4.91		
							K(FeH2L+H)=2.34		
							K(FeH3L+H)=1.5		

****
C24H36N4O8 H2L CAS 134653-17-1 (6565)
N,N'-Bis(1,2-dimethyl-3-hydroxy-5-hydroxymethyl)-4-pyridinyl)-methyl)diaminoethaned
iethanoic acid

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	KCl	25°C	0.10M	C		K1=27.2	1991MSb (103269)	3124

****
C24H44O8 L Dicy-24-crown-8 CAS 17455-23-1 (2401)
2,3,14,15-Dicyclohexyl-1,4,7,10,13,16,19,22-octaoxacyclotetracosane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	con	mixed	25°C	90%	C		K1=3.63	2003ISa (103429)	3125

Medium: 90% v/v DMSO/H2O.
****
C25H20O9 H5L CAS 2947-64-0 (4166)
4',3''-Dihydroxy-3,3',4''-trimethylfuchsone-5,5',5''-tricarboxylic acid, Chromoxane
violet R

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	oth/un	?	0.10M	U		K1=12.53	1967LMf (103604)	3126

****
C25H22O10 H3L Silybin CAS 22888-70-6 (8699)
3,5,7-Trihydroxy-2-[3-(4-hydroxy-3-methoxyphenyl)-2-hydroxymethyl-1,4-benzodioxan-6
-yl]-4chroman;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	alc/w	25°C	100%	C	M		2001BGa (103643)	3127

B(FeH3L)=37.03
B(FeH3LA)=41.53
B(FeH3LA2)=46.91
Medium: MeOH, 0.10 M NaNO3. A is methoxide ion.
****
C25H24O8 HL CAS 19697-86-0 (8775)
1,7-Bis[4-(acetyloxy)-3-methoxyphenyl]-1,6-heptadiene-3,5-dione;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl alc/w 25°C 50% C K1=11.44 2002BFb (103650)3128
B(FeH-2L)=3.06
K(Fe+2OH+L=Fe(OH)2L)=30.1
B(FeH-3L)=-5.00
Medium: 50% v/v MeOH/H2O, 0.10 M NaNO3.
****
C25H32N6 L CAS 132177-84-5 (536)
3,11-Bis(2-pyridylmethyl)-3,7,11,17-tetraazabicyclo[11.3.1]heptadeca-1(17),13,15-tr
iene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl KNO3 25°C 0.10M C K1=15.87 1999CDa (103744)3129
K(FeL+H)=3.31
****
C25H40O9 HL CAS 205058-00-0 (7638)
8-[11'-Oxymethyl)-2',3'-benzo-18-crown-6]octanoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ dis non-aq 25°C 100% U 1998BJa (103773)3130
K(FeA(ClO4)+HL)=3.18, pH=3.2
Keff(FeA(ClO4)+L)=4.55, pH=9.3
Medium: Chloroform, 0.1 m Mg(ClO4)2. A: desferrioxamine B.
****
C25H48N6O8 H3L Desferrioxamine CAS 70-51-9 (2488)
Desferrioxamine B; NH2.((CH2)5.NOH.CO.C2H4.CO.NH)2.(CH2)5.NOH.CO.CH3

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp KNO3 25°C 0.10M C I M 2001OHa (103804)3131
K(FeL+H+phen)=6.96
In 0.10 M KNO3/0.16 M sodium dodecyl sulfate, K=8.64.

Fe+++ vlt oth/un 25°C 0.7M C 2000WHa (103805)3132
K1eff=21.6
Competitive ligand (1-nitroso-2-naphthol) cathodic stripping voltammetry.
Medium: photo-oxidised seawater, pH 6.9. At pH 8 (kinetic): K1eff=22.1

Fe+++ gl KCl 25°C 0.20M C K1=30.4 1999FEa (103806)3133

```
                                        B(FeHL)=41.01
--------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 0.10M C                      1994BSb (103807)3134
                                        K(Fe+HL)=28.30
                                        K(Fe+H+HL)=30.60
In 0.04 M sodium dodecyl sulfate.
--------------------------------------------------------------------------------
Fe+++      gl  KCl    25°C 0.10M C       K1=30.99       1989EHa (103808)3135
                                        K(FeL+H)=10.40
--------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 2.00M U                      1987BBb (103809)3136
                                        K(FeHL+H)=0.57
                                        K(Fe+H4L=FeH3L+H)=4.10
                                        K(FeH2L+Fe=Fe2HL+H)=2.72
--------------------------------------------------------------------------------
Fe+++      kin NaCl   25°C 1.00M U                      1984BBc (103810)3137
                                        K(FeH2L+Fe=Fe2HL+H)=1.76
--------------------------------------------------------------------------------
Fe+++      sp  NaCl   25°C 1.00M U                      1983BBd (103811)3138
                                        K(Fe+H4L=FeH3L+H)=2.64
                                        K(Fe+H4L=FeH2L+2H)=3.40
                                        K(Fe+H4L=FeHL+3H)=2.28
                                        K(2Fe+H4L=Fe2HL+3H)=5.43
--------------------------------------------------------------------------------
Fe+++      cal NaCl   25°C 0.10M C   H                  1982GLb (103812)3139
DH(Fe+HL)=-84 kJ mol-1, DS(Fe+HL)=303 J K-1 mol-1; DH(Fe+H2L)=-43.1,
DS(Fe+H2L)=274.
--------------------------------------------------------------------------------
Fe+++      kin NaCl   25°C  1.0M U                      1981BBf (103813)3140
                                        K(FeL+Fe)=2.72
--------------------------------------------------------------------------------
Fe+++      EMF NaClO4 20°C  0.1M U                      1963AEa (103814)3141
                                        K(Fe+HL)=30.60
                                        K(Fe+H2L)=21.84
                                        K(FeL+H) > 10
********************************************************************************
C26H36N2O10           H2L                    CAS 158069-81-9  (8592)
N,N'-1,2-Ethanediylbis[N-[(3,4,5-trimethoxyphenyl)methyl]glycine;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      gl  NaClO4 25°C 0.10M U        K1=13.95       2001SGc (104160)3142
                                        *K(FeL)=-3.34
                                        *K(Fe(OH)L)=-7.34
********************************************************************************
C26H38N2O4              L                    CAS 80757-23-9  (2450)
N,N'-Bis(benzyl)-1,10-diaza-4,7,13,16-tetraoxacyclooctadecane;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
```

Fe+++ con non-aq 25°C 100% C T H K1=4.28 2000MTc (104184)3143
Medium: acetonitrile. Data for 20-35 C. DH(K1)=0.0 kJ mol-1, DS(K1)=
80.4 J K-1 mol-1.
****
C26H42N6O2 H2L BDBPH CAS 226714-05-2 (7225)
13,27-Dimethyl-3,6,9,17,20,23-hexaazatricyclo[23.3.1]triacontahexaene-29,30-diol;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl NaCl 25°C 0.10M C K1=33.85 2000SMi (104261)3144
K(FeL+H)=9.75
K(FeHL+H)=6.50
*K(FeL)=-15.19
K(FeL+Fe)=15.03
*K(Fe2L)=-3.03, *K(Fe2H-1L)=-6.70, *K(Fe2H-2L)=-9.36, *K(Fe2H-3L)=-10.50,
*K(Fe2H-4L)=-11.06.
****
C26H48N6O10 H4L CAS 207388-25-8 (7648)
Triethylenetetramine-N,N,N',N",N"',N"'-hexaethanoic acid NN-bis(butanamide);

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl R4N.X 25°C 0.10M C K1=23.92 1998ACc (104305)3145
K(FeL+H)=4.97
K(FeHL+H)=1.86
K(FeL+Fe)=7.02
K(Fe2L(OH)+H)=2.16
Medium: N(CH3)4NO3. K(Fe2L(OH)2+2H)=4.38.
****
C27H29NO10 H2L Daunorubicine CAS 23541-50-6 (5660)
Daunomycin;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp NaClO4 25°C 0.50M U 1991MJa (104439)3146
K(Fe+H2L=FeHL+H)=1.36
K(FeHL+Fe=Fe2L+H)=0.30
Full name is 10-[(3-Amino-2,3,6-trideoxy-alfa-L-lyxo-hexopyranosyl)oxyl]-7,8
,9,10-tetrahydro-6,8,11-trihydroxy-8-acetyl-1-methoxy-5,12-naphthacenedione
---
Fe+++ gl KCl 25°C 0.05M U 1985BGb (104440)3147
K(Fe+3HL)=28.40

Fe+++ sp oth/un 20°C 0.15M U 1982KMd (104441)3148
K(Fe+HL)=11.0
****
C27H29NO11 L Adriamycin CAS 25316-40-9 (2407)
Doxorubicin;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo

```
------------------------------------------------------------------------------
Fe+++      gl  KCl    25°C 0.05M U                      1985BGb (104456)3149
                                        K(Fe+3HL)=28.40
------------------------------------------------------------------------------
Fe+++      gl  NaCl   37°C 0.15M C        K1=17.985 B2=29.034 1980MWa (104457)3150
                                        B3=33.413
                                        B(FeH-1L)=14.693
******************************************************************************
C27H30N4O6            H3L                     CAS 150164-08-2  (8763)
Tris-[(2-Hydroxybenzoyl)-2-aminoethyl]amine;
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Fe+++      gl  KCl    25°C 0.10M C        K1=25.34       1998CMc (104471)3151
******************************************************************************
C27H30N4O9            H6L    Trencam            (5754)
2,2',2"-Tri(2,3-dihydroxybenzamidoethyl)amine; N(C2H4.NH.CO.C6H3(OH)2)3
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Fe+++      sp  KNO3   25°C 0.10M C        K1=43.6        1987RLa (104474)3152
                                        K(FeL+H)=5.59
K1 determined from competition experiments with EDTA
******************************************************************************
C27H30N4O18S3         H9L    TRENCAMS         CAS 252906-93-7  (7599)
3,3',3"-[Nitrilotris(2,1-ethanediyliminocarbonyl)]tris(4,5-dihydroxybenzenesulfonic
acid);
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Fe+++      gl  NaClO4 25°C 0.10M C        K1=43.6        1999TBa (104480)3153
                                        K(Fe+H7L=FeH3L+4H)=-5.9
                                        K(Fe+H7L=FeH5L+2H)=0.95
                                        *K(FeHL)=-5.49
                                        K(FeH3L=FeHL+2H)=-8.34
Additional method: spectrophotometry. K(FeH5L=FeH3L+2H)=-6.60
******************************************************************************
C27H30O16             H4L    Rutin            CAS 153-18-4  (4169)
3,3',4',5,7-Pentahydroxyflavone-3-beta-rutinoside;
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Fe+++      sp  non-aq 25°C  100M C                        2001ADb (104507)3154
                                        K1eff=-1.62
Medium: MeOH, 0.2 M acetate buffer, pH 5.95.  K1eff: Al+HnL=AlL
------------------------------------------------------------------------------
Fe+++      gl  NaNO3  20°C 0.10M C                        1991ESa (104508)3155
                                        K(Fe+2OH+L)=44.1
                                        K(Fe(OH)2L+H)=9.28
                                        K(Fe(OH)L+H)=7.34
```

K(Fe2(OH)2L+H)=5.50
K(FeHL+H)=3.84, K(Fe(OH)2L+Fe=Fe2(OH)6L+4H)=-17.08, K(Fe2(OH)6L+H)=10.63
K(Fe2(OH)5L+H)=9.02, K(Fe2(OH)4L+H)=7.32,K(Fe2(OH)3L+H)=6.35,K(FeL+H)=6.20

****

C27H36N6O3 H3L TACN-HP (6748)
N,N',N"-Tris(3-hydroxy-6-methyl-2-pyridylmethyl)-1,4,7-triazacyclononane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	KCl	25°C	0.10M	C		K1=49.98 K(FeL+H)=6.14 K(FeHL+H)=5.09 K(FeH2L+H)=4.51 K(Fe+H3L)=33.04	1992MSa	(104571)3156
						*K(FeL)=-10.45. Additional method: Pt/Fe(III),Fe(II) electrode			
Fe+++	gl	KCl	25°C	0.10M	U		K1=49.98 K(FeL+H)=6.14 K(FeHL+H)=5.09 K(FeH2L+H)=4.51 K(Fe+H3L)=33.04	1990MMg	(104572)3157
						*K(FeL)=-10.45.			

****

C27H45N9O12 H3L CAS 34787-28-5 (3518)
Desferri-ferrichrome;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	KNO3	25°C	0.01M	C		K1=28.3 K(FeL+H)=4.62	1996HAa	(104619)3158
Fe+++	gl	NaNO3	20°C	0.1M	U		K1=29.07 K(Fe+HL)=20.7	1963AEa	(104620)3159

****

C27H48N6O10 H3L Nocardamin (3519)
Desferri-ferrioxamin E;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KNO3	25°C	0.10M	C		K1=32.21	1992KJb	(104636)3160
						Ligand:1,12,23-Trihydroxy-1,6,12,17,23,28-hexaazacyclotritriaconta-2,5,13, 16,24,27-hexa-one. Data also for other desferrioximes			
Fe+++	gl	NaNO3	20°C	0.1M	U		K1=32.49	1963AEa	(104637)3161

****

C27H50N6O9 H3L CAS 5722-48-5 (3520)
N-Acetyl-desferrioxamin B;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo

Fe+++ gl NaNO3 20°C 0.1M U K1=30.76 1963AEa (104641)3162
K(Fe+HL)=21.6
****
C28H31N3O18S3 H9L 3,4-LICAMS CAS 71659-79-5 (5469)
N,N',N''-Tris(2,3-dihydroxy-5-sulfonatobenzoyl)-1,5,10-triazadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl KNO3 25°C 0.10M C K1=ca.41 1981HRa (104743)3163
K(Fe+H3L=FeL+3H)=6.40
K(FeL+H)=6.16
K(FeHL+H)=5.3
K(FeH2L+H)=3.10
By spectrophotometry: K(FeL+H)=5.85, K(FeHL+H)=5.32, K(FeH2L+H)=3.05
****
C28H34N6O12 H6L DA-BDHT(26)N6 CAS 105103-80-8 (5712)
4,7-Bis(carboxymethyl)-10,11,23,24-tetrahydroxy-9,10:22,35-dibenzohexaazacyclotrico
ntatetraone;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl KNO3 25°C 0.10M C K1=37.6 1986SMa (104757)3164
K(FeL+H)=10.20
K(FeHL+H)=7.54
K(FeH2L+H)=4.86
****
C28H46O9 HL (7639)
11-[11'-(Oxymethyl)-2',3'-benzo-18-crown-6]-undecanoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ dis non-aq 25°C 100% U 1998BJa (104966)3165
K(FeA(ClO4)+HL)=3.26, pH=3.2
Keff(FeA(ClO4)+L)=4.85, pH=9.3
Medium: Chloroform, 0.1 m Mg(ClO4)2. A: desferrioxamine B.
****
C28H47N9O13 H3L CAS 37279-99-5 (8259)
Deferricrocin;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl KNO3 25°C 0.10M U K1=30.4 1983WKb (104970)3166
K(FeL+H)=0.53
K(Fe+H3L=FeL+3H)=3.3
****
C28H51N3O12 L CAS 123074-29-3 (6560)
7,19,30-Trihydroxy-1,13-dimethyl-3,11,15,23,26,34-hexaoxa-7,19,30-triazabicyclopent
atricontatrien

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo

```
--------------------------------------------------------------------------------
Fe+++      gl  KCl    25°C 0.10M C        K1=29.12       1991MSa (104981)3167
                                          K(FeL+H)=4.05
********************************************************************************
C29H37N3O6            H2L    Calcimycin       CAS 52665-69-7  (461)
Calcium Ionophore A23187, Calcimycin;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 0.10M U        K1=5.34        1969DMb (105124)3168
********************************************************************************
C29H49N9O14           H3L                    CAS 34787-29-6  (3523)
Desferrichrysin;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      sp  KNO3   25°C 0.01M C        K1=27.4        1996HAa (105166)3169
                                          K(FeL+H)=3.16
--------------------------------------------------------------------------------
Fe+++      gl  NaNO3  20°C  0.1M U        K1=29.96       1963AEa (105167)3170
********************************************************************************
C30H27N3O9            H6L                    CAS 71353-09-8  (8601)
1,3,5-Tris[(2,3-dihydroxybenzyl)carbamoyl]benzene;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      sp  KCl    25°C 0.10M C                        1988ELa (105183)3171
                                          K(FeL+H)=7.8
********************************************************************************
C30H27N3O9            H6L                      (6548)
N,N',N"-Tris(2,3-dihydroxybenzoyl-1,3,5-tris(aminomethyl)benzene);
C6H3(N(CH3)CO.C6H3(OH)2)3
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      sp  KCl    25°C 0.10M C                        1991LRa (105185)3172
                                          K(FeL+H)=7.2
                                          K(FeHL+H)=6.03
                                          K(FeH2L+H)=4.5
                                          K(FeH3L+H)=3.8
--------------------------------------------------------------------------------
Fe+++      cal KNO3   25°C 0.10M C   H                  1991SEa (105186)3173
DH(Fe+H3L=FeL+3H)=-18.4 kJ mol-1. DS(Fe+H3L=FeL+3H)=62.7 J K-1 mol-1
********************************************************************************
C30H27N3O15           H6L    Enterobactin     CAS 28384-96-5  (2259)
Enterobactin; cyclo-((OH)C6H3(OH).CO.NH.CH.CO.CH2)3
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      sp  KCl    25°C 0.10M C                        1991LRa (105191)3174
```

K(FeL+H)=4.95
K(FeHL+H)=3.52
K(FeH2L+H)=2.5

Fe+++ cal KNO3 25°C 0.10M C H 1991SEa (105192)3175
DH(Fe+H3L=FeL+3H)=-27.2 kJ mol-1. DS(Fe+H3L=FeL+3H)=146.4 J K-1 mol-1

Fe+++ sp KNO3 25°C 0.10M U K1=52 1979HCb (105193)3176
K(Fe+H6L=FeL+6H)=-9.7
K(FeL+H)=4.80
K(FeHL+H)=3.15

****

C30H27N3O18S3 H9L TRIMCAMS CAS 77069-63-7 (5468)
1,3,5-Tris(2,3-dihydroxy-5-sulfobenzoyl)carbamido)benzene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo

---

Fe+++ gl KNO3 25°C 0.10M C K1=ca.41 1981HRa (105204)3177
K(Fe+H3L=FeL+3H)=4.43
K(FeL+2H)=13.1

****

C30H27N3O18S3 H9L MECAMS CAS 71353-06-5 (8172)
1,3,5-Tris[((2,3-dihydroxy-5-sulfobenzoyl)amino)methyl]benzene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo

---

Fe+++ gl KNO3 25°C 0.10M C K1=ca.41 1981HRa (105209)3178
K(Fe+H3L=FeL+3H)=6.57
K(FeL+H)=5.74
K(FeHL+H)=4.10
K(FeH2L+H)=3.46
By spectrophotometry: K(FeL+H)=5.19

****

C30H29N3O16 H6L (6549)
N-(2,3-Dihydroxybenzoyl)serine linear trimer; H-(N(COC6H3(OH)2)).CH(CH2OH).CO)3-OH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo

---

Fe+++ sp KNO3 25°C 0.10M C H 1991SEa (105211)3179
K(FeL+H)=5.81
K(FeHL+H)=4.82
K(FeH2L+H)=4.32
K(FeH3L+H)=2.38
K(Fe+H6L=FeL+6H)=-15.6. K(Fe+H3L=FeL+3H)=6.5. DH(Fe+H3L)=-14.2 kJ mol-1
DS(Fe+H3L)=75.3 J K-1 mol-1

****

C30H30N4O4 H4L Deuteroporphrin CAS 68929-05-5 (6220)
Deuteroporphyrin IX, Dihydrogen-2,7,12,17-tetramethyl-3,18-porphinedipropanoic
acid;

```
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      sp  NaCl   25°C 0.10M U                         1974JPb (105212)3180
                                          K(2FeL=Fe2H-1L2+H)=-1.47
*************************************************************************
C30H44N2O6            H3L                        (6508)
N,N'-Bis(2-hydroxy-3-methyl-5-tert-butylbenzyl)diaminoethane-N,N'-diethanoic acid;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      sp  KCl    25°C 0.10M M        K1=38.52         1990MMa (105314)3181
*************************************************************************
C30H50N6O2              L                     CAS 380446-61-7  (8002)
3,7,11,19,23,27-Hexaaza-33,34-dihydroxy-15,31-dimethyltricyclotetratriaconta-1,13,1
5,17,29,30-hex
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      gl  KCl    25°C 0.10M U        K1=30.61         2001WMa (105370)3182
                                          K(FeL+H)=8.02
                                          K(FeHL+H)=5.19
                                          K(FeL+Fe)=14.06
                                          K(Fe2L+H)=11.51
*K(FeL)=-10.42, *K(Fe(OH)L)=-11.71, *K(Fe2L)=-2.89, *K(Fe2(OH)L)=-6.17,
*K(Fe2(OH)2L)=-8.78, *K(Fe2(OH)3L)=-10.71, *K(Fe2(OH)4L)=-11.67.
*************************************************************************
C31H32N2O13S          H6L    Xylenol orange   CAS 63721-85-5  (432)
5,5'-Bis-N,N-bis(carboxymethyl)aminomethyl-4'-hydroxy-3,3'-dimethylfuchsone-2"-sulf
onic acid;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 0.10M U                         1979YMa (105462)3183
                                          K(Fe+HL)=18.8
                                          B(2Fe+L)=31.3
                                          K(Fe(OH)HL+H)=6.3
                                          K(Fe(OH)L+H)=8.7
K((FeOH)2L+2H)=11.6. Potentiometry also used
-------------------------------------------------------------------------
Fe+++      sp  oth/un   ?  0.50M U                         1971KNc (105463)3184
                                          K(Fe+H3L)=8.85
                                          K(Fe+H2L)=14.16
                                          K(Fe+H4L+H3L)=13.87
                                          K(Fe+2H3L)=15.55
-------------------------------------------------------------------------
Fe+++      sp  NaNO3  20?°C 0.20M U                         1962BUa (105464)3185
                                          B(Fe2L)=39.80
-------------------------------------------------------------------------
Fe+++      sp  NaClO4   ?  0.05M U                         1960CHa (105465)3186
                                          K(?)=5.7
```

****
C31H35N3O18S3 H9L 3,3,4-CYCAMS CAS 77069-62-6 (8173)
1,5,9-Tris(2,3-dihydroxy-5-sulfobenzoyl)-1,5,9-triazacyclotridecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KNO3	25°C	0.10M	C		K1=ca.38	1981HRa	(105530)3187
							K(Fe+H3L=FeL+3H)=3.44		
							K(FeL+H)=6.92		
							K(FeHL+H)=5.82		
							K(FeH2L+H)=5.46		

K(FeH3L+H)=2.4. By spectrophotometry: K(FeL+H)=6.78, K(FeHL+H)=5.74,
K(FeH2L+H)=5.54, FeH3L+H)=2.3
****
C31H37N7 L CAS 259259-40-0 (537)
3,7,11-Tris(2-pyridylmethyl)-3,7,11,17-tetraazabicyclo[11.3.1]heptadeca-1(17),13,15
-triene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KNO3	25°C	0.10M	C		K1=15.70	1999CDa	(105537)3188
							K(FeL+H)=2.75		
							K(Fe(OH)L+H)=4.11		
****
C32H37N3O11 H7L CAS 252906-99-3 (8802)
5-[(2,3-Dihydroxybenzoyl)amino]-2,2-bis[3-[(2,3-dihydroxybenzoyl)amino]propyl]penta
noic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	alc/w	25°C	2%	U		K1=42.5	2000ITa	(105667)3189
							K(FeHL+H)=5.15		
							K(FeL+H)=6.59		

Medium: 2% MeOH/H2O, 0.10 M NaClO4.
K1 determined spectrophotometrically by competition with edta.
****
C32H38N6O2 H2L CAS 185675-92-7 (7485)
15,31-Dimethyl-3,11,19,27,33,35-hexaazapentacyclohexatriacontadodeca-34,36-diol;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KCl	25°C	0.10M	C	M	K1=33.04	2000HMa	(105695)3190
							B(FeH2L)=48.91		
							B(FeHL)=41.91		
							B(FeH-1L)=22.53		
							B(FeCuL)=45.92		

B(FeCuH-1L)=39.12, B(FeCuH-2L)=29.24, B(FeCdH-1L)=32.85, B(FeCdH-2L)=23.01
B(FeZnH-1L)=32.46, B(FeZnH-2L)=24.57, B(FeMnH-1L)=29.50, B(FeMnH-2L)=20.41

Fe+++	gl	KCl	25°C	0.10M	C		K1=32.02	1999WMa	(105696)3191

B(FeHL)=41.08
B(FeH2L)=47.99
B(FeH-1L)=22.06
B(Fe2L)=44.9
B(Fe2H-1L)=41.99; B(Fe2H-2L)=34.65; B(Fe2H-3L)=25.64
B(Fe2H-4L)=15.37. Also data for mixed Fe(II)-Fe(III)-L systems.
****
C32H42N6O12 H6L DA-BDHT(30)N6 CAS 105103-79-5 (5713)
5,20-Bis(carboxymethyl)-12,13,27,28-tetrahydroxydibenzahexaazacyclotriconta-10,15,25,30-tetraone;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl KNO3 25°C 0.10M C K1=36.0 1986SMa (105750)3192
K(FeL+H)=9.69
K(FeHL+H)=6.76
K(FeH2L+H)=3.32
****
C32H48N12O12 H2L CAS 219992-86-6 (7437)
Tris(2[2(1-hydroxy-2-oxo-1,2-dihydropyrimidinylamino)ethylaminocarbonyl]ethoxymethyl)ethane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp none RT 0 U K1=25.1 1998KHa (105806)3193
By competition with EDTA. Data for Fe+++ complexes of similar ligands also
****
C32H52N6O11 H6L CAS 84010-59-3 (7188)
N-(2,3-Dihydroxybenzoyl)desferrioxamine B;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl KCl 25°C 0.10M C K1=35.4 1994HWb (105821)3194
K(FeL+H)=9.47
K(FeHL+H)=5.56
K1 by spectrophotometry. Data also for other desferrioxamines
****
C33H33N3O9 H6L MECAM-Me CAS 79087-35-7 (6163)
1,3,5-Tris(((4-methyl-2,3-dihydroxybenzoyl)amino)methyl)benzene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp KCl 25°C 0.10M C 1989CGc (105872)3195
K(FeL+H)=7.98
****
C33H33N3O9 H6L EMECAM (7326)
1,3,5-Tris(2,3-dihydroxybenzamidomethyl)-2,4,6-trimethylbenzene;
Me3C6(CH2NHCO(C6H3(OH)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo

---
Fe+++ sp KCl 25°C 0.10M U K1=45.8 1997HSa (105874)3196
B(FeHL)=51.3
B(FeH2L)=55.9
****
C33H33N3O18S3 H9L CAS 78261-77-5 (2945)
1,3,5-Tris(N-methyl-N-(2,3-dihydroxysulfobenzoyl)aminomethyl)benzene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl KNO3 25°C 0.10M C K1=40.6 1981PWb (105877)3197
K(H3L+Fe=FeL+3H)=5.21
****
C33H36O7 HL Morellin CAS 1183-12-6 (3524)
Morellin;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp oth/un 25°C ? U 1957TPa (105899)3198
K(2Fe+3L)=16.31
****
C33H44N3O14P H6L CAS 193901-91-6 (7981)
(4,4-Diphenylcyclohexyl)(methylene-2-dien pentaethanoic acid) phosphoric acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl NaClO4 25°C 0.10M C K1=26.66 2001CCa (105937)3199
K(Fe(OH)L+H)=9.88
K(FeL+H)=3.57
K(FeHL+H)=1.28
K1 from competition with DTPA using LC-MS.
****
C33H45N3O3 H3L (6764)
N,N',N''-Tris(3,5-dimethyl-2-hydroxybenzyl)-1,4,7-triazacyclononane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp alc/w 25°C 75% U K1=51.3 1991CMc (105956)3200
Medium: 75% v/v EtOH/H2O. Competitive reaction with EDTA
****
C33H54N8O9 H2L AKPTYK (6948)
Ala-Lys-Pro-Thr-Tyr-Lys;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ vlt NaCl 25°C 0.10M U 1994TLa (105994)3201
Keff(Fe+L)=38.0
At pH 7.0 in 5 mM Bis(2-hydroxyethyl)iminotris(hydroxymethyl)methane.
Data also for 6 other related polypeptides
****

C34H34N4O4 H4L Protoporphyrin9 CAS 553-12-8 (1242)
3,18-Divinyl-2,7,12,17-tetramethylporphine-2,18-dipropanoic acid, Protoporphyrin IX

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	vlt	oth/un	25°C	0.7M	C		K1eff=22.4	2000WHa (106005)	3202

Competitive ligand (1-nitroso-2-naphthol) cathodic stripping voltammetry.
Medium: photo-oxidised seawater, pH 6.9. At pH 8 (kinetic): K1eff=21.9.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	mixed	25°C	0.0	U	M	K(FeLCl+2A)=8.55 K(FeLCl+2B)=8.77 K(FeLCl+2C)=6.27 K(FeLCl+2D)=5.65	1978HKb (106006)	3203

A=poly(N-vinylimidazole); B=poly(4(5)-vinylimidazole (9:1 MeOH/DMF).
C=imidazole; D=N-ethylimidazole (DMF).

****

C34H43N3O18S3 H9L DiP-3,4-LICAMS CAS 96649-34-2 (5595)
Diisopropyl-N,N',N"-tris(5-sulfonato-2,3-dihydroxybenzoyl)-1,5,10-triazadecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KNO3	25°C	0.10M	C		K1=40 K(Fe+H3L=FeL+3H)=5.36	1985KPb (106064)	3204

****

C34H54O8 H2L Lasalocid CAS 25999-20-6 (2335)
Lasalocid acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	dis	non-aq	25°C	100%	C		K(FeA+HL=FeAL+H)=-3.8	1998CCe (106134)	3205

Medium: CHCl3/H2O (pH=9, 0.1 M Mg(ClO4)2). A: desferrioxamine B.
K: FeA(aq)+HL(org) = FeA(org)+H(aq).

****

C34H55N7O12 H5L CAS 153502-63-7 (7187)
N-(2,3-Dihydroxy-4-(methylamido)benzoyl)desferrioxamine B;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KCl	25°C	0.10M	C		K1=34.8 K(FeL+H)=9.21 K(FeHL+H)=4.0	1994HWb (106164)	3206

K1 by spectrophotometry. Data also for other desferrioxamines

****

C35H56N6O13 H3L CAS 30315-65-2 (8261)
Deferricoprogen;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo

---
Fe+++ gl KNO3 25°C 0.10M U K1=30.2 1983WKb (106209)3207
K(FeL+H)=0.50
K(Fe+H3L=FeL+3H)=4.6
****
C36H33N7O15S3 H6L N-TRENSOX CAS 195306-10-6 (7371)
Tris-N-(2-aminoethyl-(8-hydroxyquinoline-5-sulphonato-2-carboxamido))amine;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp NaClO4 25°C 0.10M C K1=25.3 1997SBa (106234)3208
****
C36H33N7O15S3 H6L O-TRENSOX CAS 169209-69-2 (7370)
Tris-N-(2-aminoethyl-(8-hydroxyquinoline-5-sulphonato-7-carboxamido))amine;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp NaClO4 25°C 0.10M C K1=30.9 1997SBa (106241)3209
B(FeHL)=36.5
B(FeH5L)=42.2
****
C36H36N24O12 L Cucurbituril CAS 283175-97-3 (6744)
Cucurbit[6]uril;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sol none 25°C 0.0 C K1=1.60 2001BCe (106258)3210
Method: total organic carbon analysis of dissolved species.
For the homologous cucurbit[5]uril, K1=1.88.
****
C36H38N4O8 H6L CAS 531-14-6 (7709)
3,8,13,18-Tetramethylporphine-2,7,12,17-tetrapropanoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp KCl 25°C 0.10M U 2000HSb (106287)3211
K(FeL+His)=-1.60
K(FeL+Im)=-0.74
K(FeL+SSHA)=-0.92
SSHA is serylserylhistidylserine. Also data for other poly and
oligopeptides.
****
C36H39N3O9 H6L MMECAM (7325)
1,3,5-Tris(2,3-dihydroxybenzamidomethyl)-2,4,6-triethylbenzene;
Et3C6(CH2NHCO(C6H3(OH)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp KCl 25°C 0.10M U K1=47.1 1997HSa (106290)3212
B(FeHL)=52.62

B(FeH2L)=57.12
****
C36H39N3O18S3 H9L CAS 79087-39-1 (2946)
1,3,5-Tris(N-acetyl-N-(2,3-dihydroxysulfobenzyl)aminomethyl)benzene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl KNO3 25°C 0.10M C K1=40.3 1981PWb (106292)3213
K(Fe+H3L=FeL+3H)=4.0
****
C36H46N4 H2L Octaethylporph. CAS 2683-82-1 (1794)
2,3,7,8,12,13,17,18-Octaethyl-21H,23H-porphine;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp non-aq 25°C 100% U M 1990UHa (106368)3214
K(FeLA+H)=15.5
K(FeLA+4methyl-ph)=3.49
K(FeLA+ph)=3.50
K(FeLA+4-chloro-ph)=4.35
Medium: methylene chloride. A=OCH3, ph=phenol. K(FeLA+4-cyano-ph)=4.98,
K(FeLA+4-nitro-ph)=5.15, and other subst.phenols and acetic acids.

Fe+++ vlt R4N.X 23°C 0.10M U K1=7.0 B2=12.5 1982BKb (106369)3215

Fe+++ nmr non-aq 25°C 100% U M 1976SMa (106370)3216
K(FeLCl+2A)=2.82
Medium: CDCl3. A=1-Methylbenzimidazole
****
C36H53N11O18 H4L Alterobactin A CAS 153888-52-9 (8504)
Alterobactin A;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ vlt oth/un 25°C 0.7M C 2000WHa (106401)3217
K1eff=23.9
Competitive ligand (1-nitroso-2-napthol) cathodic stripping voltammetry.
Medium: photo-oxidised seawater, pH 6.9. At pH 8 (kinetic): K1eff=22.3
****
C36H55N11O19 H5L Alterobactin B CAS 153888-53-0 (8038)
Alterobactin B;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ vlt oth/un 25°C 0.7M C 2000WHa (106429)3218
K1eff>24.0
Competitive ligand (1-nitroso-2-naphthol) cathodic stripping voltammetry.
Medium: photo-oxidised seawater, pH 6.9. At pH 8 (kinetic): K1eff=22.5

Fe+++ vlt NaCl 25°C 0.10M C 1995LHb (106430)3219

```
                                        K1eff=43.6 (pH 8.2)
                                        K1eff=37.6 (pH 6.0)
Method: square wave voltammetry. Medium: 0.1 M NaCl, 5 mm BISTRIS.
**************************************************************************
C36H60N8O8              L                     CAS 121925-84-6  (7152)
Cyclo(Gly-eLL-Gly)2 (eLL=N,N'-ethylene-bridged (S)-leucyl-(S)-leucine
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe+++      sp  non-aq 25°C 100%  U        K1=5.76        1994MKa (106454)3220
                                        K(ML+M)=4.50
Medium: MeCN
**************************************************************************
C36H66N6O24             L    a-Cyclodextrin   CAS 207395-12-8  (7800)
Hexakis(2-amino)-alpha-cyclodextrin;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe+++      vlt oth/un 25°C 0.10M C                        1996GLa (106544)3221
                                        K(Fe(CN)6+L)=3.30
Medium: 0.1 M aminoacetonitrile buffer, pH 5.3. Method: cyclic voltammetry
Also data for the heptamer and octamer aminocyclodextrin.
**************************************************************************
C37H44N2O13S          H6L    MeThymol Blue      (428)
3,3'-Bis(N,N-di(carboxymethyl)aminomethyl)thymolsulfonephthalein;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Fe+++      sp  oth/un 25°C 0.10M C                        1997ASa (106595)3222
                                        K1eff=7.48
                                        K2eff=5.12
Medium: 0.10 M acetate buffer, pH 5.0.
--------------------------------------------------------------------------
Fe+++      gl  NaClO4 25°C 0.10M U        K1=17.7        1979YMa (106596)3223
                                        B(2Fe+L)=29.8
                                        K(Fe(OH)HL+H)=6.5
                                        K(Fe(OH)L+H)=9.3
                                        K((FeOH)2L+2H)=12.4
Spectrophotometry also used
--------------------------------------------------------------------------
Fe+++      sp  NaClO4   ?  0.10M U                       1968KKe (106597)3224
                                        K(Fe+H2L)=20.56
                                        B(FeH2L)=43.29
                                        K(FeH2L+H4L)=6.66
**************************************************************************
C37H47N3O15           H6L                      (7966)
Methyl-2,3,4-tris-O-{N-[2,3-di(hydroxy)benzoyl]-aminopropyl}-1-D-glucopyranoside;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
```

Fe+++ gl NaClO4 25°C 0.10M U K1=46.38 2001DHa (106630)3225
K(FeL+H)=10.12
K(FeHL+H)=9.12
K(FeH2L+H)=7.59
K(FeH3L+H)=5.72
K(FeH4L+H)=5.25. K1 by spectrophotometry.

****

C39H42N6O9 L (5718)
1,3,5-Tri(2,6-diaza-6-hydroxy-7-phenylheptane-3,7-dione)benzene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	mixed	25°C	?	U		K1=28	1987MWa	(106712)3226

Medium: DMF/H2O 3:1

****

C39H45N3O18S3 H9L TiP-MECAMS CAS 96649-36-4 (5599)
Triisopropyl-tris(5-sulfonato-2,3-dihydroxybenzoyl)-1,3,5-tris(aminoethyl)benzene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KNO3	25°C	0.10M	C		K1=40	1985KPb	(106714)3227
							K(Fe+H3L=FeL+3H)=4.15		

****

C39H51N7O9 H3L TRENDROX CAS 120385-15-1 (5887)
N,N',N"-(Nitrilotris-2,1-ethenyl)tris(N-hydroxy-N-(4-methylphenyl)butanediamide;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KNO3	25°C	0.10M	C		K1=32.9	1989NRa	(106725)3228
							K(FeL+H)=2.38		
							K(FeHL+H)=0.7		

****

C40H47N3O10 H7L CAS 86728-01-0 (5503)
Bis(3-(((2-hydroxy-5-methylbenzyl)amino)methyl)-2-hydroxy-5-methylbenzyl)amine-trie
thanoic acid

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	oth/un	25°C	0.10M	U		K1=25.00	1983YMa	(106786)3229
							K(FeH-1L+H)=4.54		
							K(FeH-2L+H)=7.54		
							K(FeH-3L+H)=9.87		
							K(FeL+H)=1.70		

****

C40H49N7O11 H5L CAS 128393-06-6 (7655)
Amonabactin T 789;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	KCl	25°C	0.10M	C		K1=34.5	1998TRa	(106800)3230

B(Fe2L3)=86.4
K(Fe2L3+2H)=18.9
B(Fe2H2L3)=105.3
EDTA used as a competitive ligand. Also data for amonabactin T 732,
amonabactin P 750 and amonabactin P 693.
****
C40H51N3O18S3 H9L DC-3,4-LICAMS CAS 96649-27-2 (5598)
Dicyclohexyl-N,N'N"tris(5-sulfonato-2,3-dihydroxybenzoyl)-1,5,10-triazadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl KNO3 25°C 0.10M C K1=40 1985KPb (106818)3231
K(Fe+H3L=FeL+3H)=4.85
****
C42H39N7O15S3 H2L CAS 252906-94-8 (7766)
3,3',3"-[Nitrilotris(2,1-ethanediyliminocarbonyl)]tris[4-hydroxy-5-(2-pyridinyl)ben
zeneHSO3;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp NaClO4 25°C 0.10M C K1=30.1 2000BBe (106909)3232
K(Fe+H7L=FeH5L+2H)=1.79
Method: UV/vis spectrophotometry.
****
C42H50N6O12 H9L (7434)
1,4,10,13-Tetrakis(2,3-dihydroxybenzoyl)-7,16-dimethyl-1,4,7,10,13,16-hexaazacycloo
ctadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl mixed 25°C 50% C 1998BBa (106945)3233
K(H2L+2H)=26.35
K(H2L+3H)=37.24
K(H2L+4H)=47.71
K(H2L+5H)=57.14
Medium: 50% v/v DMSO/H2O, 0.1 M NMe4Cl. K(H2L+6H)=65.92
K(H2L+7H)=70.78, K(H2L+8H)=75.37.

Fe+++ gl mixed 25°C 50% C 1998BBa (106946)3234
K(Fe+H2L+3H)=63.26
K(FeH5L+H)=4.48
K(FeH6L+H)=3.57
K(Fe+H5L)=26.02
Medium: 50% v/v DMSO/H2O, 0.1 M NMe4Cl. K(Fe+H6L)=20.03, K(Fe+H7L)=14.16.
K(2Fe+H2L)=58.08, K(2Fe+H2L+H)=62.0. Many other di-nuclear species.
****
C43H56N6O18 H6L (7965)
Methyl-2,3,4-tris-O-{N-[2,3-di(hydroxy)benzoyl-glycyl]-aminopropyl}-1-D-glucopyrano
side;

```
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      gl  NaClO4 25°C 0.10M U        K1=41.38       2001DHa (107012)3235
                                        K(FeL+H)=9.31
                                        K(FeHL+H)=8.16
                                        K(FeH2L+H)=7.05
                                        K(FeH3L+H)=3.49
K(FeH4L+H)=3.56. K1 by spectrophotometry.
*************************************************************************
C44H26N4Cl4           H2L                    CAS 22112-77-2  (1783)
5,10,15,20-4-Tetra-(4-chlorophenyl)porphine;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      sp  non-aq 25°C 100%  U    M                  1976WLa (107041)3236
                                        K(FeLCl+N-MeImidazole)=1.3
                                        K(FeLCl+2(N-MeImidazole))=2.85
Medium: CHCl3
*************************************************************************
C44H26N4F4            H2L                    CAS 37095-43-5  (1782)
5,10,15,20-Tetra-(4-fluorophenyl)porphine;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      sp  non-aq 25°C 100%  U    M                  1976WLa (107046)3237
                                        K(FeLCl+N-MeImidazole)=1.1
                                        K(FeCl+2(N-MeImidazole))=3.00
Medium: CHCl3
*************************************************************************
C44H30N4              H2L    Tetraphenylpor.  CAS 917-23-7  (1781)
5,10,15,20-Tetraphenyl-21H,23H-porphine;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      vlt non-aq 25°C 100%  U    M                  1996NSa (107063)3238
                                        K(FeL+2py=FeL(py)2)=2.2
                                        K(FeL+2A=FeLA2)<-0.8
                                        K(FeL+2B=FeLB2)=2.4
                                        K(FeL+2C=FeLC2)=7.2
Method: cyclic voltammetry. Medium: DMF. A=4-Cyanopyridine,
C=3,4-Dimethylpyridine. D=N-Methylimidazole. Also data for other porphyrins.
-------------------------------------------------------------------------
Fe+++      kin non-aq 25°C 100%  U        K1=3.1         1985FTa (107064)3239
Medium: pyridine. In 3,5-dichloropyridine K1=-2.6
-------------------------------------------------------------------------
Fe+++      nmr non-aq -25°C 100%  U    M                  1976SMa (107065)3240
                                        K(FeClL+2py)=0.97
                                        K(FeClL+2A)=1.73
py=pyridine, A=4-Methylpyridine. Medium=CDCl3.  Reference also contains many
data on ternary complexes of porphin with Fe(III) and other N-donor ligands
```

Fe+++ sp non-aq 25°C 100% U M 1976WLa (107066)3241
K(FeLCl+N-MeImidazole)=1.00
K(FeLCl+2(N-MeImidazole))=3.18
K(FeLCl+2(4-PhImidazole))=5.10
K(FeLCl+2(4-MeImidazole))=6.00
Medium: CHCl3

Fe+++ sp non-aq 25°C 100% U M 1976WLa (107067)3242
K(FeLCl+py)=-0.7
K(FeLCl+2py)=-0.3
K(FeLCl+2A)=5.5
Medium: CHCl3. A=N-Methylimidazole. Also data from ternary complexes with other ligands and in other solvents
---
Fe+++ sp non-aq 25°C 100% U M 1976WLa (107068)3243
K(FeLCl+A)=0.6
K(FeLCl+2A)=1.4
K(FeLCl+C)=1.71
K(FeLCl+2C)=3.42
Medium: CHCl3. A=2,3-Dimethypyridine, C=4-Dimethylaminopyridine. Also data for ternary complexes with other ligands and in other solvents
---
Fe+++ sp non-aq 25°C 100% U M 1976WLa (107069)3244
K(FeLCl+A)=1.20
K(FeLCl+2A)=3.52
K(FeLCl+A)=1.34(in CH2Cl2)
K(FeLCl+2A)=3.57 (in CH2Cl2)
Medium: CHCl3. A=2-Methylimidazole. Also data for ternary complexes with other ligands and in other solvents
---
Fe+++ sp non-aq 30°C 100% U M 1973CRa (107070)3245
K(FeLCl+2A)=5.68
Medium: CH2Cl2. A=imidazole
****
C44H38N8 H2L CAS 48242-70-2 (6629)
5,10,15,20-Tetrakis(1-methylpyridinium-4-yl)porphine;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp NaNO3 25°C 0.10M U M 1993MFa (107102)3246
Keff(FeL+2CN)=13.00
At pH 8.81. At pH 9.28 Keff(FeL+2CN)=13.03; at pH 10.03 Keff=13.31, at pH 10.4 Keff=13.56.

Fe+++ sp KCl 25°C 0.10M C 1988SRc (107103)3247
K(FeL2+L=FeL3)=8.1
*K(FeL3)=-9.2
*K(FeH-1L3)=-10.5
*K(FeH-2L3)=-12.0

```
--------------------------------------------------------------------------------
Fe+++      sp  NaNO3  25°C 0.05M U                      1977PLa (107104)3248
                                        *K1(FeL(H2O)2)=-4.7
                                        *B2(FeL(H2O)2)=-11.2
                                        K(2FeL=O(FeLOH)2)=5.95
********************************************************************************
C45H42N4O36S9         15L    TBPAS            CAS 156820-73-4  (9076)
5',5'",5""-[Nitrilotris(2,1-ethanediyliminocarbonyl)]tris[2,6'-dihydroxy-1,1'-biphe
ny]-3,3',5-trH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 0.10M C        K1=28.8        1994SMc (107216)3249
                                        K(Fe+H7L=FeH6L+H)=20.0
                                        K(Fe+H7L=FeH4L+3H)=49.0
                                        *K(FeH4L)=-2.4
                                        *K(FeH3L)=-4.3
*K(FeH2L)=-6.3; *K(FeHL)=-7.2. By competition with edta, K1=28.6.
********************************************************************************
C45H42N4O36S9         15L                    CAS 208399-32-0  (7755)
N,N',N"-Nitrilotris(2,1-ethanediyliminocarbonyl)tris[2,6'-dihydroxy-1,1'-biphenyl-3
,3',5triHSO3]H
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      gl  NaClO4 25°C 0.10M C        K1=30.03       1998BBg (107218)3250
                                        B(FeHL)=39.11
                                        B(FeH2L)=46.26
                                        B(FeH3L)=51.86
                                        B(FeH4L)=56.49.
B(FeH-1L)=20.26.  Data also determined spectrophotometrically:
B(FeH3L)=51.8, B(FeH5L)=60.0, B(FeH6L)=61.9.
********************************************************************************
C45H48N4O33S9                TBPANS           CAS 156820-75-6  (9077)
5',5'",5""-[Nitrilotris(2,1-ethanediyliminomethylene)]tris[2,6'-dihydroxy-1,1'-biph
enyl]-3,3',5-
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      sp  NaClO4 25°C 0.10M C        K1=31.6        1994SMc (107229)3251
                                        K(Fe+H10L=FeH9L+H)=18.2
                                        K(Fe+H10L=FeH8L+2H)=83.55
                                        *K(FeH8L)=-4.3
                                        *K(FeH7L)=-4.67
*K(FeH5L)=-4.75; *K(FeH4L)=-7.86, *K(FeH3L)=-9.1, *K(FeH2L)=-10.1,
*K(FeHL)=-11.1.  By competition with edta, K1=31.9.
********************************************************************************
C48H38N4              H2L                    CAS 14527-51-6  (1780)
5,10,15,20-Tetrakis-(4-methylphenyl)-21H,23H-porphine;
--------------------------------------------------------------------------------
```

```
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      nmr non-aq 25°C 100%  U T  M                 1976SMa (107349)3252
                                       K(FeClL+2A)=3.5
                                       K(FeBrL+2A) > 6.0
                                       K(FeIL+2A) > 6.0
Medium: CDCl3. A=1-Methyl-benzimidazole. At -34 C: K(FeBr2L+2A)=3.4
-------------------------------------------------------------------------
Fe+++      sp  non-aq 25°C 100%  U    M                 1976WLa (107350)3253
                                       K(FeLCl+N-MeImidazole)=1.3
                                       K(FeLCl+2(N-MeImidazole))=3.42
Medium: CHCl3
*************************************************************************
C48H38N4O4           H2L                     CAS 22122-78-3  (1788)
5,10,15,20-Tetra-(4-Methoxyphenyl)porphine;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      sp  non-aq 25°C 100%  U    M                 1976WLa (107355)3254
                                       K(FeLCl+N-MeImidazole)=1.6
                                       K(FeLCl+2(N-MeImidazole))=3.6
Medium: CHCl3
*************************************************************************
C51H40N6O              L    ImTPP           CAS 164173-28-8  (7949)
5-[2-(4-(1-Imidazolyl)butoxyl)phenyl]-10,15,20-triphenylporphyrin;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      sp  non-aq 25°C 100%  C T HM                1995JHa (107467)3255
                                       K(FeLCl+Im)=5.41
                                       K(FeLCl+2Im)=9.88
                                       K(FeLCl+2,3-(CH3)2py)=0.587
                                       K(FeLCl+3,5-(CH3)2py)=1.54
Medium: CHCl3. Data for 25-44 C. K(FeLClpy)=1.25, K(FeLCl+4-CH3py)=1.50.
DH(FeLCl+Im)=-137 kJ mol-1, DS=-356 J K-1 mol-1; DH(FeLCl+2Im)=-184.
*************************************************************************
C51H48S9             H3L                       (6818)
Tris((4,6-dimethyl-3-mercaptophenyl)thiol)-2,4,6-tris(p-tolylthio)benzene;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Fe+++      nmr non-aq 24°C 100%  U   HM                1990WSa (107468)3256
                                       K(Fe4S4LCl+3A)=2.58
Medium: CD3CN. DH=-95.0 kJ mol-1. DS=-280 J K-1 mol-1.
A: MeCN.
-------------------------------------------------------------------------
Fe+++      nmr non-aq 24°C 100%  U    M                1990WSa (107469)3257
                                       K(Fe4S4LCl+3A)=3.15
Medium: CD3CN. A=EtCN. For A=t-BuCN:K=4.15,DH=-110 kJ mol-1,DS=310 J K-1 m-1
For A=C6H11CN: K=4.48; 2,6-Me2C6H3CN: K=5.69
```

****
C52H46N4O12S4 H4L (6861)
5,10,15,20-Tetrakis(2,6-dimethyl-3-sulfonatophenyl)porphin;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ vlt NaNO3 ? 0.20M C 1991KZa (107477)3258
*K(FeL)=-6.55
*K(FeL(OH))=-10.55
****
C54H54N6O18 H9L (7435)
1,4,7,10,13,16-Hexakis(2,3-dihydroxybenzoyl)-1,4,7,10,13,16-hexaazacyclooctadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ gl diox/w 25°C 50% C 1998BBa (107530)3259
K(H3L+3H)=39.78
K(H3L+4H)=51.40
K(H3L+5H)=62.42
K(H3L+6H)=72.69
K(H3L+7H)=82.25, K(H3L+8H)=90.8, K(H3L+9H)=98.7.
Medium: 50% v/v DMSO/H2O, 0.1 M NMe4Cl.

Fe+++ gl mixed 25°C 50% C 1998BBa (107531)3260
K(Fe+H3L+2H)=67.75
K(Fe+H3L+3H)=74.65
K(Fe+H3L+4H)=82.46
K(Fe+H3L+5H)=89.08
Medium: 50% v/v DMSO/H2O, 0.1 M NMe4Cl. K(Fe+H3L+6H)=93.60,
K(Fe+H3L+7H)=96.95. K(2Fe+H3L=Fe2H2L+H)=64.4. Other di-nuclear complexes.
****
C55H74N4O5 H2L Phaeophytin a CAS 603-17-8 (8503)
3-Phorbinepropanoic acid...;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ vlt oth/un 25°C 0.7M C 2000WHa (107564)3261
K1eff=22.2
Competitive ligand (1-nitroso-2-napthol) cathodic stripping voltammetry.
Medium: photo-oxidised seawater, pH 6.9. At pH 8 (kinetic): K1eff=21.0
****
C55H83N17O22 H6L CAS 104022-79-9 (6918)
Pyoverdin PaA;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Fe+++ sp NaClO4 25°C 0.10M C K1=30.8 1994ABb (107573)3262
B(FeHL)=43.0
B(FeH2L)=47.8
****

C63H102N12O24 L CAS 341035-19-6 (8787)
1,3,5-Benzenetris[carbonylimino(1-oxo-hexanediyl)]tris[N-hydroxyalanyl-6-aminohexanoyl-N-hydroxy-

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	KNO3	25°C	0.10M	C		2001TSa (107728)		3263
							K(FeL+H)=2.36		
							K(Fe2L+H)=3.11		

K(FeL+H2edta+H=Fe(edta)+H3L)=7.18.
Also data for homologous hydroxamate ligands.

C70H89N15O18S2Fe H4L CAS 122801-25-6 (7667)
N-Acetylmicroperoxidase-8;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaCl	25°C	0.10M	C	HM		1999MMa (107841)	3264
							K(FeL+imidazole)=4.076		
							K(FeL+CN)=6.76		
							K(FeL+py)=2.62		
							K(FeL+gly)=3.44		

Data for addition of many substituted pyridines, imidazoles, amines and aminoacid esters. DH and DS values for alkyl- and cyanopyridines.

C72H58N12O4 H2L (5854)
meso-5,10,15,20-Tetrakis(2-(N-methylnicotinamido)phenyl)-21H,23H-porphin;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaNO3	25°C	0.10M	U	M		1993MFa (107843)	3265
							Keff(FeL+2CN)=14.6		

At pH 9.61. At pH 10.2 Keff(FeL+2CN)=14.7

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	NaNO3	25°C	0.10M	M	I		1988MWa (107844)	3266
							*K(FeL(H2O)2)=-6.09		
							*K(FeLH2O(OH))=-10.28		

Data also for I=0.05, 0.25, 0.50, and 1.0 mol L-1 NaNO3
and for (a)4 isomer at I=0.01 mol L-1

Polymer DNA (4185)
Deoxyribonucleic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	kin	oth/un	25°C	0.0	U	H		1965KYb (108149)	3267
							K'=5.11(rat intestine & liver)		

DH=0 kJ mol-1, DS=96 J K-1 mol-1. See reference for definitions

Polymer Fulvic acid (1523)

Fulvic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	KNO3	25°C	0.10M	U		1998DMb (108179)		3268
							K1eff=5.0		

Method: fluorescence quenching. Medium: pH 4.0.
Fulvic acid extracted from sewage sludge.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	NaClO4	25°C	0.10M	U		1974RMc (108180)		3269
							K1eff=5.38		

****

Polymer L (3532)
Human transferrin;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	KNO3	25°C	0.10M	C		1994HCa (108209)		3270
							Keff(Fe+HCO3L)=21.44		
							Keff(FeHCO3L+Fe)=20.34		
							Keff(Fe+L)=11.4		

At pH 7.4 in 0.1M N-(2-hydroxyethyl)piperazine-N'-2-ethanesulfonic acid, (HEPES) and 5mM HCO3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	kin	KCl	25°C	0.20M	U		1993CFa (108210)		3271
							K(Fe(NTA)+L)=-5.0		
							*K(Fe(NTA)L)=-6.35		

For binding at the C-terminal site of transferrin.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	sp	oth/un	25°C	0.10M	U		1987MSc (108211)		3272
							Keff1=22.7		
							Keff2=22.1		

Medium: 0.1 M Tris buffer, pH 7.4; 0.027 M HCO3-. By competition with the Fe-NTA complex.

****

Polymer Hyaluronic acid CAS 9004-61 9 (7143)
Hyaluronic acid, copoly(b-glucuronic acid - b-N-acetylglucosamine); (C18H28NO11)n

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Fe+++	gl	KNO3	25°C	0.10M	C		2002MCa (108252)		3273
							K(Fe+H-1L)=8.2		
							K(Fe+2H-1L)=16.1		
							B(Fe2L2)=6.7		

****

Polymer (6949)
Mytilis edulis foot protein 1;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo

```
Fe+++      vlt NaCl   25°C 0.10M U                        1994TLa (108263)3274
                                          Keff(Fe+L)=40.1
At pH 7.0 in 5 mM Bis(2-hydroxyethyl)iminotris(hydroxymethyl)methane.
Dala also for many component polypeptides
********************************************************************************
Polymer               H3L    Cox2000          CAS 400078-81-1  (9021)
Polyether-polymer;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      gl  NaClO4 25°C 0.10M C        K1=32.12       2002IBb (108327)3275
                                          B(FeHL)=34.24
                                          B(FeH4L)=38.98
********************************************************************************
Polymer                                          (6896)
Polymaleic acid-methacrylic acid copolymer; (-C4H2O3.CH2.C(CH3)COOH-)n
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Fe+++      dis NaCl   25°C 0.10M U                        1993KHa (108348)3276
                                          K1eff=9.5
Method: dialysis; pH=8  [Fe]=0.00005 M
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EXPLANATORY NOTES

DATA Flags are :-

T Data at other TEMPERATURES
I Data with various BACKGROUNDS
H Data for THERMOCHEMICAL quantities
M Data for TERNARY Complexes

EVALUATION Flags are :-

T or IUP=T signifies EVALUATION RATING = Tentative by IUPAC
R or IUP=R signifies EVALUATION RATING = Recommended by IUPAC

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