

SC-Database

Software version = 5.81 Data version = 4.62

Experiment list contains 614 experiments for
(no ligands specified)

Metal : Y+++

(no references specified)

(no experimental details specified)

e- HL Electron (442)
Electron;

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

Y+++ oth none 25°C 0.0 U 1952LAb (1033) 1
K(Y+3e=Y(s))=-120.3(-2.37 V)

Method:combination of thermodynamic data

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

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

Y+++ sol none 25°C 0.0 C 1992FIa (1166) 2
Kso(YAsO4)=-22.60

Equilibrium monitored by EDTA and iodine titrations.

Br- HL Bromide CAS 10035-10-6 (19)
Bromide;

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

Y+++ cal mixed 25°C 50% C IH K1=1.7 B2= 2.00 1999IUa (2377) 3
Medium: 0.5 mole fraction DMA/DMF, 0.2 M Me4NCl. DH(K1)=5 kJ mol-1,
DH(B2)=53. Also data for 0.6-0.85 mole fraction.

Y+++ dis NaClO4 25°C 1.0M U K1=-0.15 1963Cub (2378) 4
Medium: HClO4

Y+++ EMF NaClO4 25°C 0.50M U T H K1=0.45 1962PAb (2379) 5
Method: Ag electrode. K1=0.49(15 C), 0.40(35 C); K1=1.32(25 C, I=0 corr.)
DH(K1)=-3.8 kJ mol-1, DS=-4.2 J K-1 mol-1.

CO3-- H2L Carbonate CAS 465-79-6 (268)
Carbonate;

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

Y+++ gl NaClO4 25°C 0.70M C K1=5.75 2004LBb (3439) 6
K(Y+HCO3=YHCO3)=1.27

Medium: 0.70 m NaClO4. Calculated for I=0, K1=7.48, B2=12.63,
 K(Y+HCO3=YHCO3)=2.32, K(Y+HL=YL+H)=-2.85, K(Y+2HL=YL2+2H)=-8.03

 Y+++ dis NaClO4 25°C 0.70M C I K1=5.75 B2=10.11 1998LBb (3440) 7
 Method: H2O/tributylphosphate distribution and ICP-mass spectrometry.
 Values calculated for I=0.0 M, K1=7.73, B2=13.19.

 Y+++ dis NaClO4 25°C 0.70M C 1995LBc (3441) 8
 B1eff=5.71
 B2eff=10.34
 Keff(Y+HL)=1.49

By solvent extraction from 0.7 M NaClO4 into tributylphosphate using 88Y.
 B1eff=[YL]/[Y]([L]+[NaL]). Keff=[YHL]/[Y]([HL]+[NaHL]).

 Y+++ sol NaClO4 25°C 0.0 C I 1992GSc (3442) 9
 *Kso=21.55

Extrap. from data for 0.01-3.0 M NaClO4, 0-1.0 M Y(ClO4)3, using SIT and
 Pitzer. *Kso: Y2(CO3)3+6H=2Y+3CO2+6H2O. At I=3.0 M: Kso=-28.56, *Kso=24.31

 Y+++ sol none 25°C 0.0 C 1986FMa (3443) 10
 Kso(Y2(CO3)3)=-31.52

 Y+++ sol none 25°C 0.0 C 1986HMa (3444) 11
 Kso(Y2(CO3)3)=-31.52

Method: spectrophotometry.

 Y+++ gl NaClO4 25°C 3.00M C K1=6.02 1985SPa (3445) 12
 B(Y2L)=6.98
 K(Y+HL)=1.29

 Y+++ sol oth/un 25°C 0.0 U 1966JHa (3446) 13
 Kso(Y2L3)=-30.6

 C6N6Co--- H3L Cyanocobaltate (5470)
 Hexacyanocobaltate; [Co(CN)6]---

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

 Y+++ con diox/w 25°C 10% U I K1=4.06 1960ATb (3507) 14
 Medium: 10% w/w dioxan/H2O; K1=3.83(0%), 4.43(20%)

 Cl- HL Chloride CAS 7647-01-0 (50)
 Chloride;

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

 Y+++ cal non-aq 25°C 100% U K1=2.20 B2=4.54 1980VCa (5950) 15
 Medium: dimethylacetamide

 Y+++ dis NaClO4 25°C 1.0M U K1=-0.03 1963CUB (5951) 16

Y+++ EMF NaClO4 25°C 2.0M U K1=-0.3 1963FDa (5952) 17
B(YCl(CH3CO2))=1.18

Method:quinhydrone electrode

Y+++ EMF NaClO4 25°C 0.50M U TIH K1=0.36 1962PAb (5953) 18
Method: Ag electrode. K1=0.38(15 C), 0.32(35). DH(K1)=-1.3 kJ mol⁻¹, DS=-4
At I=0 corr.: K1=1.26

Y+++ sol none 25°C 0.0 U 1960ASd (5954) 19
Kso(Y(OH)2.5Cl0.5)=-21.9
Kso(Y(OH)2Cl)=-16.6

Y+++ dis NaClO4 20°C 3.0M U 1960PBa (5955) 20
B6=-0.87
Bn=-0.145n + 0.019n(6-n)

F- HL Fluoride CAS 7644-39-3 (201)
Fluoride;

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

Y+++ ix oth/un 25°C 0.02M C T H K1=3.97 B2= 6.35 2004LMa (7335) 21
Medium: 0.025 M HNO3. Applying Pitzer parameters: at I=0, K1=10.24.
Data for 5 to 45 C. DH(K1)=9.8 kJ mol⁻¹, DH(B2)=20.8.

Y+++ ISE NaClO4 25°C 0.0 C I K1=4.46 2000LBa (7336) 22
Method: Fluoride ISE. Values calc. from data for I=0.015-0.70 M NaClO4.
At I=0.70 M, K1=3.538

Y+++ ix KNO3 25°C 0.02M C K1=3.89 B2= 6.50 1999SBc (7337) 23
Medium: 0.025 M HNO3. Additional method: ICP-MS.
Assumed K1(HF) = 3.03, derived from literature values.

Y+++ cal NaClO4 25°C 1.00M C H 1988GBa (7338) 24
DH(K1)=9.27 kJ mol⁻¹; DS(K1)= 100 J mol⁻¹ K⁻¹

Y+++ ISE KNO3 25°C 0.10M C M K1=3.76 1987YHa (7339) 25
K(YA+F)=2.62(H3A=NTA), 1.8(H3A=HEDTA), 1.5(H4A=EDTA), 1.6(H4A=CDTA)

Y+++ gl KCl 25°C 1.00M U M 1981KTb (7340) 26
K(YEDTA+F)=1.89
K(Y(EDTA)F+F)=0.48

Y+++ oth NaClO4 25°C 0.10M U K1=3.43 1973MSg (7341) 27
method:electromigration or transference number

Y+++ dis NaClO4 25°C 0.50M C K1=7.89 B2= 7.11 1970ALc (7342) 28
Method: extraction of 91Y from 0.50 M NaClO4 medium into toluene/
di-(2-ethylhexyl)phosphoric acid. Medium pH 3.6.

Y+++ ISE NaClO4 25°C 0.50M U T H K1=3.91 B2=7.16 1969ALa (7343) 29
DH(K1)=5.2 kJ mol-1,DH(B2)=-5.0. K1=3.88,B2=7.19(15 C);K1=3.94,B2=7.16(35 C)

Y+++ dis NaClO4 25°C 0.50M U K1=3.89 B2=7.11 1969ALd (7344) 30
B3=10.30

Y+++ EMF NaClO4 25°C 0.50M U H 1967APa (7345) 31
DH(K1)=9.2 kJ mol-1, DS=104 J K-1 mol-1. At I=0 corr:DH(K1)=9.6, DS=125

Y+++ EMF NaClO4 25°C 1.0M U H K1=3.60 1967WCa (7346) 32
By calorimetry: DH(K1)=34.8 kJ mol-1, DS=186.0 J K-1 mol-1

Y+++ EMF NaClO4 25°C 0.50M U T H K1=3.93 B2=7.1 1961PGa (7347) 33
K3=3.2
K(Y+HF=YF+H)=1.00
K(YF+HF=YF2+H)=0.3
K(YF2+HF=YF3+H)=0.3

At 15 C: *K1=1.02,*K2=0.0,*K3=0. At 35 C:*K1=0.98,*K2=0.7,*K3=0.5
At I=0 corr: K1=4.81,K2=3.73,K3=3.60. DH(*K1)=-4 kJ mol-1,DS=4 J K-1 mol-1

Y+++ EMF NaClO4 25°C 0.50M U K1=3.88 1959SEa (7348) 34

I03- HL Iodate CAS 7782-68-5 (1257)
Iodate;

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

Y+++ sol oth/un 25°C 0.0 U 1966FPb (8574) 35
Kso=-9.96

I04- HL Periodate CAS 13444-71-8 (6063)
Periodate;

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

Y+++ sol oth/un 25°C dil U 1974LOa (8619) 36
Kso(Y(H2IO6)(H2O)3)=-10.22

Mo12042U----- H8L (2922)
Uranium-12-molybdate;

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

Y+++ gl oth/un 20°C 0.10M U K1=3.88 1989SBb (8784) 37
B(YHL)=7.97
B(YH2L)=10.34

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

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

Y+++ gl R4N.X 25°C 5.00M U K1=0.4 1985MMa (9222) 38

NO3- HL Nitrate CAS 7697-37-2 (288)
Nitrate;

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

Y+++ cal NaClO4 25°C 2.0M C H K1=-0.92 1998BMb (10009) 39
DH(K1)=9.2 kJ mol-1

Y+++ dis NaClO4 20°C 3.0M U B6=-0.46 1960PBa (10010) 40
Bn=-0.77n-0.01n(6-n), n=1 to 6. Kd(Y+3L+3TBP(CCl4))=YL3T3(CCl4)=0

OH- HL Hydroxide (57)
Hydroxide;

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

Y+++ gl NaClO4 25°C 0.0 C IH *K1=-7.80 2000KBa (12494) 41
In 0.7 M NaClO4, *K1=-8.11. DH(*K1)=46 kJ mol-1.

Y+++ gl NaClO4 25°C 3.00M U *B2=-17.0 1973AKa (12495) 42
*B(2,2)=-14.04
Medium: LiClO4

Y+++ gl NaClO4 25°C 3.00M U *B2=-17.0(-16.8?) 1973AKb (12496) 43
*B(2,2)=-14.75
Medium: D2O containing LiClO4. *K2: YOD+D2O=Y(OD)2+D; *B(2,2): 2Y+2D2O=
Y2(OD)2 + 2D

Y+++ gl oth/un 25°C 3.0M U *B2=-16.04 1972MAa (12497) 44
*B(2,2)=-14.08
Medium: LiClO4

Y+++ gl oth/un 25°C 3.0M U *B2=-16.20 1972MAa (12498) 45
*B(2,2)=-14.93
Medium: D2O, 3 M LiClO4

Y+++ oth KNO3 25°C 0.01M U K1=10.5 B2=19.8 1972SSf (12499) 46
Method: electrical migration or transference number

Y+++ EMF alc/w 25°C 25% U I 1972USa (12500) 47
 *K1=-7.94
 Medium: 25% v/v EtOH/H2O, 0.05 M NaClO4. *K1=-8.03(0%), -7.49(50%),
 -7.71(0%,I=0)

Y+++ sol oth/un 25°C U 1970IEb (12501) 48
 K(YL3(s)=L=YL4)=-6.2
 K(YL3(s)+2L=YL5)=-7.8
 K(YL3(s)+3L=YL6)=-9.3

Y+++ oth oth/un rt 10% U 1967PBb (12502) 49
 Kso=-27.4
 K(YL3(s)=YL3)=-4.8
 Medium: 10% sea water. Method: Tyndall scattering

Y+++ gl NaClO4 25°C 0.30M U 1966FKa (12503) 50
 *K1=-8.34

Y+++ oth oth/un 20°C dil U 19660Sa (12504) 51
 Kso=-25.7
 Method: Tyndall scattering

Y+++ gl oth/un 25°C 3.00M U 1964BCa (12505) 52
 *B(2,2)=-14.30
 *B(3,5)=-33.8
 *K1=-9.1

Y+++ EMF none 25°C 0.0 M 1962AEa (12506) 53
 Kso=-24.5
 Method: H electrode

Y+++ sol none 22°C 0.0 U 1962KGa (12507) 54
 Kso(Y(OH)3)=-24.2

Y+++ gl oth/un 25°C ? U 1960ASd (12508) 55
 Kso=-24.5(aged)
 Kso=-23.3(fresh)(see also Cl-)
 Kso: K(Y(OH)3(s)=Y+3OH); method:also solubility

Y+++ EMF NaCl 25°C 4.0M C I 1959SEb (12509) 56
 *Kso=16.46
 *Kso: K(Y(OH)3(s)+3H=Y+3H2O); *Kso=17.01(I=3),17.44(I=2). Method:H electrode

Y+++ gl NaClO4 25°C var U 1951MFb (12510) 57
 Kso(Y(OH)3)=-22.80

Y+++ gl oth/un 25°C var U 1946MOa (12511) 58
 *K1=ca.-7
 Medium: SO4-- at various concentrations

Y+++ gl oth/un 25°C var U 1944MKa (12512) 59
Kso(Y(OH)3)=-22.1

Y+++ gl oth/un 25°C dil U 19380Ka (12513) 60
Kso(Y(OH)3)=-21.45

Method: also solubility

O2-- H2L Peroxide CAS 7772-84-1 (2813)
Peroxide; -0.0-

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

Y+++ gl NaNO3 25°C 0.10M C 2002MYb (12759) 61
K(2Y+3H2O2=Y2(O2)2(OH)2+6H)=-32.04; K(2Y+2H2O2=Y2(O2)2+4H)=-19.66.

P04--- H3L Phosphate CAS 7664-38-2 (176)
Phosphate;

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

Y+++ sol none 25°C 0.0 M 1997LBd (13383) 62
Kso(YPO4)=-25.02

Calculated from data for 0.10 M HClO4 solution.

Y+++ sol oth/un 25°C 0.0 C I 1993FKb (13384) 63
Kso(YPO4)=-25.60

In synthetic seawater, Ks(YPO4)=-22.92.

Y+++ sol none 25°C 0.0 C 1991FBa (13385) 64
Kso(YPO4)=-24.76

Y+++ ix R4N.X 25°C 0.20M U I 1966BEc (13386) 65
K(Y+H2L)=1.84

Medium: NH4ClO4. K=2.65 (I=0 corr)

P207---- 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

Y+++ gl KCl 25°C 0.50M U 1989APd (13672) 66
K(Y+H2L)=4.30

P3010---- 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

Y+++ gl KNO3 25°C 0.10M U T H B2=9.1 1974KRa (13920) 67
K(Y+2HL)=6.7

K(Y+2HL)=6.8 and B2=9.0 (35 C), K(Y+2HL)=6.5 and B2=8.9 (45 C)
DH(Y+2HL)=-19 kJ mol⁻¹; DH(B2)=-6

Y+++ gl NaClO4 ? 0.10M U B2=17.21 1962RKa (13921) 68
K(Y+HL)=4.97
K(Y+2HL)=8.87

P309--- H3L CAS 13566-25-1 (235)
Cyclotrimetaphosphate;

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

Y+++ cal oth/un 25°C 0.10M C H K1=3.19 1983GGb (13974) 69
Medium: 0.10 M HCl. DH(K1)=32.0 kJ mol⁻¹, DS(K1)=168 J K⁻¹ mol⁻¹.

P4012---- H4L CAS 13598-74-8 (234)
Cyclotetrametaphosphate;

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

Y+++ cal oth/un 25°C 0.10M C H K1=3.44 1983GGb (14024) 70
Medium: 0.10 M HCl. DH(K1)=17.8 kJ mol⁻¹, DS(K1)=125 J K⁻¹ mol⁻¹.

SCN- HL Thiocyanate CAS 463-56-9 (106)
Thiocyanate;

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

Y+++ cal non-aq 25°C 100% U H K1=1.6 B2=2.9 1992TIa (15340) 71
K3=0.5
Medium: DMF, 0.2 M R4NX. DH(K1)=8 kJ mol⁻¹, DH(B2)=4, DH(B3)=25

Y+++ sp NaClO4 20°C 0.60M U T K1=-0.07 1964KSe (15341) 72

S04-- H2L Sulfate CAS 7664-93-9 (15)
Sulfate;

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

Y+++ sol oth/un 25°C 0.66M C K1=1.83 2004SBb (16666) 73
Method: solubility of BaSO4 in 0.117 m YCl3 solution.
Calculated for I=0, K1=3.50.

Y+++ oth oth/un 15°C var U T H K1=3.51 1974QAa (16667) 74
Method:ultrasonic absorption. Medium:Y2(SO4)3. K1=3.58(25 C), 3.61(31.6 C)
DH(K1)=17.7 kJ mol⁻¹

Y+++ cal oth/un 25°C 0.0 U H 1969FPa (16668) 75
DH(K1)=13.7 kJ mol⁻¹

Y+++ cal oth/un 25°C 0.0 U H K1=3.34 B2=5.34 1969IEa (16669) 76
DH(K1)=15.1 kJ mol⁻¹, DH(K2)=3.05; DS(K1)=114.6 J K⁻¹ mol⁻¹, DS(K2)=48.5

Y+++ ISE NaClO4 25°C 2.0M U H K1=1.24 B2=1.68 1967CCd (16670) 77
By calorimetry: DH(K1)=16.9 kJ mol⁻¹, DS=80.3 J K⁻¹ mol⁻¹; DH(K2)=6.3, DS=30

Y+++ dis NaClO4 20°C 3.0M U K1=2.0 B2=3.4 1960PBa (16671) 78
B3=4.36

Y+++ oth oth/un 25°C 0.0 U K1=3.47 1954SJa (16672) 79

CH606P2 H4L Medronic acid CAS 1984-15-2 (2384)
Methanediposponic acid; CH2(P03H2)2

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

Y+++ gl KCl 25°C 0.50M U K(Y+H2L)=5.43 1989APd (18298) 80

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

Y+++ gl NaClO4 20°C 0.10M U K1=2.56 B2=4.41 1964PSd (18433) 81
K3=1.5

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

Y+++ ix R4N.X 25°C 0.05M C K1=5.74 B2=10.09 2001SBf (19156) 82
K(Y+HL)=2.08
Medium: 0.05 M NH4NO3. At I=0, K1=6.66, B2=11.27.

Y+++ gl KCl 25°C 1.0M U M K(Y(edta)+L)=2.90 1988KTa (19157) 83

Y+++ oth oth/un 25°C 0.10M U K1=5.46 B2=9.29 1971STe (19158) 84
Method: electrical migration or transference number

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

Y+++ oth oth/un ? ? U B2=3.74 1967MBa (20227) 85
Method: paper electrophoresis

Y+++ cal NaClO4 25°C 2.0M C H 1964GRa (20228) 86
DH(K1)=13.65 kJ mol⁻¹, DS(K1)=75.7 J K⁻¹ mol⁻¹; DH(B2)=22.55, DS(B2)=128;
DH(B3)=21.94, DS(B3)=139.

Y+++ gl NaClO4 20°C 0.10M U K1=1.97 B2=3.60 1962KPa (20229) 87

Y+++ EMF NaClO4 20°C 2.0M U K1=1.53 B2=2.66 1960SOb (20230) 88
B3=3.4
B4=3.3

Method: quinhydrone electrode

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
Y+++ gl oth/un 25°C .065M U TIH K1=5.28 B2=8.85 1975GSa (20384) 89
At 35 C: K1=5.22, K2=4.80; 45 C: 5.15, 5.00. At 35 C, I=0.15: K1=4.95,
K2=4.75

Y+++ gl NaClO4 20°C 0.10M U 1964PKa (20385) 90
K(Y+HL)=1.91
K(YHL+HL)=1.28

Y+++ gl NaClO4 25°C 2.0M U 1962BCa (20386) 91
K(Y+HL)=1.49
K(YHL+HL)=0.7

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
Y+++ cal NaClO4 25°C 2.0M C H 1964GRa (20657) 92
DH(K1)=-0.31 kJ mol⁻¹, DS(K1)=46.4 J K⁻¹ mol⁻¹; DH(B2)=-0.724, DS(B2)=82.0;
DH(B3)=-3.75, DS(B3)=96.2; DH(B4)=-3.9, DS(B4)=107.

Y+++ gl NaClO4 20°C 0.10M U K1=2.785 B2=4.88 1964PKb (20658) 93
B3=5.78

Y+++ EMF NaClO4 20°C 2.0M U K1=2.47 B2=4.40 1960SOa (20659) 94
B3=5.7
B4=6.3
B5=6.3

Method: quinhydrone electrode

Y+++ ix NaClO4 20°C 0.20M U K1=2.78 B2=4.70 1960SVa (20660) 95
B3=6.0

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

Y+++ gl NaClO4 30°C 0.2M U T K1=5.06 1977MSf (21759) 96

C2H6O2 L Ethyleneglycol CAS 107-21-1 (924)
1,2-Dihydroxyethane (Ethane-1,2-diol); HO.CH2.CH2.OH

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

Y+++ gl NaClO4 22°C 0.10M U 1972Mcd (22160) 97
K(YH-1L+H)=6.95

C2H6O6P2 H4L (5706)
Ethene-1,1-diphosphonic acid; H2C:C(P03H2)2

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

Y+++ gl KCl 25°C 0.15M U I 1989AMa (22178) 98
K(Y+H2L)=5.00

C2H8O7P2 H4L HEDPA CAS 2809-21-4 (436)
1-Hydroxyethane-1,1-diphosphonic acid; CH3.C(OH)(P03H2)2

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

Y+++ sp oth/un 25°C 0.70M U 1987APa (23405) 99
K(Y+H2L)=5.51

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

Y+++ gl KNO3 25°C 0.10M U K1=4.40 B2=7.04 1968PFa (24595) 100

C3H5NO2 HL (4234)
Isonitrosoacetone; CH3.CO.CH:N.OH, anti-Pyruvic aldehyde oxime

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

Y+++ gl diox/w 20°C 50% U K1=5.98 1971MAF (24652) 101
Medium: 50% dioxan, 0.1 M NaClO4

C3H6N2O2 L Methylglyoxime CAS 2140-03-6 (2981)
Methylglyoxime; CH3.C(:N.OH).CH:N.OH

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

Y+++ gl diox/w 20°C 50% U K1=6.43 B2=12.17 1971MAf (24814) 102
Medium: 50% dioxan, 0.1 M NaClO4

C3H602 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

Y+++ gl NaClO4 25°C 2.0M U K1=1.61 B2=2.81 1965CGa (25075) 103

Y+++ gl NaClO4 20°C 0.10M U K1=1.88 B2=3.06 1964PKa (25076) 104

C3H602S 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

Y+++ gl NaClO4 25°C 2.00M U 1968CMA (25179) 105
K(Y+HL)=1.70

Y+++ gl NaClO4 31°C 2.0M U 1963BCb (25180) 106
K(Y+HL)=1.38
K(YHL+HL)=0.7

C3H602S H2L CAS 107-96-0 (437)
3-Mercaptopropanoic acid; HS.CH2.CH2.COOH

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

Y+++ gl NaClO4 25°C 2.00M U 1968CMA (25233) 107
K(Y+HL)=1.51

C3H603 HL CAS 81598-26-7 (2521)
3-Hydroxypropanoic acid; HO.CH2.CH2.COOH

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

Y+++ gl NaClO4 25°C 2.00M U K1=1.43 1969JCc (25284) 108

C3H603 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

Y+++ gl NaClO4 25°C 0.20M U K1=2.80 B2=4.94 1964DVA (25572) 109
K3=1.22
K4=0.55

Y+++ gl NaClO4 20°C 0.10M U K1=3.017 B2=5.33 1964PKb (25573) 110
B3=6.95

Y+++ gl NaClO4 25°C 2.0M U K1=2.53 B2=4.70 1961CCa (25574) 111
K3=1.42

Y+++ ix NaClO4 20°C 0.20M U K1=2.83 B2=4.92 1960SVa (25575) 112
B3=6.8

Y+++ ix oth/un rt 0.20M U B2=4.96 1958PMa (25576) 113

C3H6O3 HL Methoxyacetic CAS 625-45-6 (29)
Methoxyethanoic acid; CH3.O.CH2.COOH

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

Y+++ gl NaClO4 20°C 0.10M U K1=2.00 B2=3.11 1964PKa (25610) 114

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

Y+++ gl NaCl 37°C 0.15M U M K1=3.92 B2=8.09 1991DWb (26298) 115
B(YH2L(Glu))=23.03

Y+++ gl KNO3 35°C 0.10M U K1=5.42 1990RSe (26299) 116

Y+++ gl KNO3 25°C 0.10M U K1=5.0 1967EMb (26300) 117

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

Y+++ gl KNO3 25°C 0.10M M M K1=5.53 1996AEa (27198) 118
Data for ternary complexes with dipicolinic acid.

Y+++ gl NaNO3 25°C 0.10M M I M K1=5.61 1995KDd (27199) 119
K(Y(egta)+L)=3.79
Data for 0.15 and 0.05 M NaNO3. At I=0, K1=5.86, K(Y(egta)+L)=4.08.

Y+++ gl NaClO4 20°C 0.10M M TIH 1991ELa (27200) 120
B(YHL)=3.50
Constant independent of I. DH(K1)=23.9 kJ mol⁻¹, DS=149 J K⁻¹ mol⁻¹

Y+++ EMF KCl 22°C 0.10M U K1=4.51 1968RPa (27201) 121

Y+++ gl oth/un 25°C 0.10M U K1=3.50 1965PGe (27202) 122

C3H8O2 L Propyleneglycol CAS 57-55-6 (2025)
Propan-1,2-diol; CH3.CH(OH).CH2(OH)

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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Y+++      gl  NaClO4 22°C 0.10M U                                1972MCd (27688) 123
                                                K(YH-1L+H)=6.95
*****
C3H8O3          L      Glycerol          CAS 56-81-5 (2707)
Propane-1,2,3-triol; HO.CH2.CH(OH).CH2.OH
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Y+++      gl  NaClO4 22°C 0.10M U                                1972MCd (27757) 124
                                                K(YH-1L+H)=6.85
-----
Y+++      gl  NaCl   25°C 0.10M U                                1970PKe (27758) 125
                                                K(YH-1L+H)=6.79
*****
C3H12N09P3     H6L     NTPA             CAS 6419-19-8 (2920)
Nitritotris(methylenephosphonic acid); N(CH2PO3H2)3
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Y+++      gl  KNO3   25°C 0.10M C                                1991SKb (28596) 126
                                                K(YL+H)=7.15
                                                K(YHL+H)=5.5
-----
Y+++      sol oth/un 25°C 0.03M U                                1988BKa (28597) 127
                                                K1=22.5
                                                B(YHL)=25.1
                                                B(YH2L)=28.1
                                                B(YH3L)=30.5
                                                B(YH4L)=33.5
B(MH5L) = 33.7
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Y+++      sol oth/un 25°C 0.03M U                                1979TKc (28598) 128
                                                K1=11.0
                                                K(Y+H+L)=19.4
*****
C4H2O4          H2L     Squaric acid     CAS 2892-51-5 (439)
3,4-Dihydroxy-3-cyclobutene-1,2-dione;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Y+++      cal NaClO4 25°C 0.10M U  H   K1=2.73  B2=4.25  19760Ca (28672) 129
DH(K1)=9.9 kJ mol-1, DS=85 J K-1 mol-1; DH(B2)=13.9, DS=128
-----
Y+++      gl  NaClO4 25°C 0.10M C  H   K1=2.727 B2= 4.25  19760Cb (28673) 130
By calorimetry: DH(K1)=9.92 kJ mol-1, DS(K1)=85.4 J K-1 mol-1;
DH(B2)=13.9, DS(B2)=128.
*****
C4H4O4          H2L     Maleic acid       CAS 110-16-7 (111)
cis-Butenedioic acid; HOOC.CH:CH.COOH
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Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo

Y+++ gl NaNO3 25°C 0.50M C K1=4.24 B2=6.32 1977KPa (29160) 131
B(YHL)=6.3
B(Y2H-2L2)=-2.0

Y+++ gl NaClO4 25°C 0.10M U K1=3.61 B2=5.55 1970RFa (29161) 132

C4H4O5 H2L Oxobutanedioic CAS 328-42-7 (1733)
2-Oxosuccinic acid, Oxalacetic acid; HOOC.CH2.CO.COOH

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

Y+++ gl oth/un 25°C ? U K1=5.6 B2=9.8 1956Gnc (29282) 133

C4H5NO5 H2L (7375)
Oxalohydroxamic acid; HOOC.CO.CH2.CO.NHOH

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

Y+++ gl KNO3 25°C 0.1M M K1=10.50 B2=20.20 1989LWa (29318) 134
K3=9.09

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

Y+++ gl NaClO4 25°C 0.20M U T K1=2.92 B2=5.21 1975Pmb (30379) 135
35 C: K1=2.95, K2=2.31; 45 C: K1=2.98, K2=2.34

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

Y+++ gl KNO3 20°C 0.10M U 1980SDa (30758) 136
B(YHL)=8.14

Y+++ gl KNO3 20°C 0.10M U K1=4.60 B2=7.56 1980Sdb (30759) 137
K(Y+HL)=1.85

Y+++ gl NaClO4 25°C 0.20M U T H K1=4.63 B2=7.74 1975Pmb (30760) 138
35 C: K1=4.65, K2=3.13; 45 C: K1=4.70, K2=3.15

Y+++ gl NaClO4 25°C 0.10M U K1=4.91 B2=8.19 1970RFa (30761) 139

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

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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Y+++      gl  KCl    25°C  1.0M U    M                    1988KTa (30948) 140
                                         K(Y(edta)+L)=1.26
-----

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Y+++      cal NaClO4 25°C  1.0M C    H                    1963GRd (30949) 141
DH(K1)=7.247 kJ mol-1, DS(K1)=126 J K-1 mol-1; DH(B2)=2.046,
DS(B2)=194; DH(B3)=-15.52, DS(B3)=198.
-----

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Y+++      EMF NaClO4 20°C 1.00M U          K1=5.24  B2=9.76  1963GTa (30950) 142
                                         B3=13.03
-----

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Method: quinhydrone electrode

```

C4H6O6          H2L    L-Tartaric acid  CAS 87-69-4 (92)
L-Tartaric acid, L-2,3-Dihydroxybutanedioic acid; HOOC.CH(OH).CH(OH).COOH
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Y+++      oth NaNO3 25°C  0.50M U    M    K1=2.68          1972PBd (31397) 143
                                         B(YLOH)=11.66
-----

```

Method: optical rotation

```

Y+++      ISE NaNO3 25°C  0.50M U    M                    1972RMa (31398) 144
                                         B(Cu2Y(OH)5L3)=54.40
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Y+++      gl  alc/w 25°C  50% U    I    K1=5.52          1972SSj (31399) 145
Medium: 0-50% EtOH, 0.05 M. K1(0%)=4.03; K1(25%)=4.68; K1(40%)=5.12
-----

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Y+++      oth oth/un 25°C  var  U          K1=4.07  B2=6.89  1966PBb (31400) 146
                                         K(2Y+L)=5.97
                                         K(Y+H-1L)=12.87
                                         K(Y+HL)=2.82
-----

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```

C4H7N04          H2L    Aspartic acid  CAS 56-84-8 (21)
Aminobutanedioic acid; H2N.CH(CH2.COOH).COOH
-----

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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Y+++      gl  KNO3  25°C  0.10M M    M    K1=8.42          1996AEa (31979) 147
Data for ternary complexes with dipicolinic acid.
-----

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Y+++      gl  NaClO4 30°C  0.10M U    I    K1=5.37          1984YLa (31980) 148
-----

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Y+++      gl  NaClO4 25°C  0.20M U T H    K1=4.75  B2=8.07  1975PMb (31981) 149
35 C: K1=4.77, K2=3.34; 45 C: K1=4.80, K2=3.36
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C4H7N04          H2L    IDA          CAS 142-73-4 (118)
Iminodiethanoic acid; HN(CH2.COOH)2
-----

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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Y+++	sp	oth/un	25°C	0.10M	U		K1=6.78	1997YSa (32400)	150
Y+++	gl	KCl	25°C	1.0M	U	M	K(Y(edta)+L)=3.54	1988KTa (32401)	151
Y+++	cal	KNO3	20°C	0.10M	U	HM	K(YA+L)=3.24 DH(YA+L)=-27.32 kJ mol ⁻¹ . DH(YAL)=-27.32, DS=307. H4A=EDTA	1971GKb (32402)	152
Y+++	gl	KNO3	25°C	0.10M	U	M	K1=6.78 B2=12.03	1962THa (32403)	153
Ternary complexes with N-(2-hydroxyethyl)diaminoethane-triethanoic acid ***** 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
Y+++	gl	diox/w	20°C	50%	U		K1=7.95 B2=14.97	1971MAF (32553)	154
Medium: 50% v/v dioxan, 0.1 M NaClO4 ***** 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
Y+++	gl	KNO3	25°C	0.10M	M	M	K1=5.46	1996AEa (32747)	155
Data for ternary complexes with dipicolinic acid.									
Y+++	gl	NaClO4	30°C	0.10M	U		K1=3.76 B2=6.58	1984YLa (32748)	156
Y+++	gl	NaClO4	30°C	0.2M	U		K1=4.43	1977MSf (32749)	157
Y+++	gl	NaClO4	25°C	0.10M	U		B2=8.05	1973TSe (32750)	158
***** C4H8N2O4 H2L CAS 39156-77-9 (3008) Hydrazine-N,N-diethanoic acid; H2N.N(CH2.COOH)2									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Y+++	EMF	KCl	25°C	0.10M	U		K1=4.1 B2=7.2 K3=0.1	1954VIa (33118)	159
***** 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
Y+++	gl	NaClO4	25°C	2.00M	U	H	K1=1.64 B2=2.79	1965CGa (33261)	160

By calorimetry: DH(K1)=22.6 kJ mol⁻¹, DS=107 J K⁻¹ mol⁻¹; DH(K2)=12.4, DS=67

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-----
Y+++      gl  NaClO4 25°C 0.50M U      K1=1.60  B2=2.71  1964SPa (33262) 161
*****

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C4H8O2S          HL          CAS 627-04-3 (3007)
S-Ethylthioethanoic acid; CH3.CH2.S.CH2.COOH
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values          Reference ExptNo
-----

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Y+++      gl  NaClO4 31°C 2.0M U      K1=1.42  B2=2.12  1963BCb (33415) 162
*****

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C4H8O3          HL          CAS 594-61-6 (81)
2-Hydroxy-2-methylpropanoic acid; (CH3)2C(OH).COOH
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values          Reference ExptNo
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```

Y+++      gl  NaClO4 25°C 0.20M U      K1=2.9    B2=5.60  1964DVa (33538) 163
                     K3=1.7
                     K4=1.4
-----

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```

Y+++      gl  NaClO4 25°C 2.0M U I    K1=3.11  B2=5.54  1964DVa (33539) 164
                     K3=1.74
                     K4=1.06
-----

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```

K1=3.22(I=0),3.12(I=0.1),3.05(I=0.5),3.08(I=1.0); K2=2.06(I=0),2.49(I=0.1),
2.45(I=0.5),2.44(I=1.0); K3=1.98(0),1.86(0.1),1.81(1.0); K4=1.37(0),1.22(0.1)
-----

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```

Y+++      gl  NaClO4 20°C 0.10M U      K1=3.204 B2=5.79  1964PKb (33540) 165
                     B3=7.51
-----

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Y+++      gl  NaClO4 25°C 0.50M U      K1=2.88  B2=5.32  1964SPa (33541) 166
                     B3=6.75
-----

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```

Y+++      gl  NaClO4 25°C 2.0M U      K1=2.86  B2=5.44  1961CCa (33542) 167
                     K3=1.86
-----

```

```

Y+++      ix  NaClO4 20°C 0.20M U      K1=3.11  B2=5.60  1960SVa (33543) 168
                     B3=7.3
-----

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*****
C4H8O4          HL          CAS 21620-60-0 (2326)
2,3-Dihydroxy-2-methylpropanoic acid; HO.CH2.C(OH)(CH3).COOH
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values          Reference ExptNo
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Y+++      gl  KNO3   25°C 0.10M C      K1=3.05  B2=5.49  1975PFb (33688) 169
                     K3=1.73
-----

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*****
C4H8O5          HL          CAS 56309-80-9 (2365)
2,3-Dihydroxy-2-hydroxymethylpropanoic acid; HO.CH2.C(CH2.OH)(OH).COOH
-----

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

```

Y+++ EMF KNO3 25°C 0.10M U K1=2.95 B2=5.33 1976PKb (33717) 170
K3=1.78

Y+++ gl NaClO4 25°C 0.50M U K1=2.65 B2=4.67 1964SPa (33718) 171
B3=5.26

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

Y+++ gl KNO3 25°C 0.10M U T K1=5.04 1978SSb (33928) 172

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

Y+++ gl KCl 20°C 0.10M U K1=3.7 1970RPa (34341) 173

C4H11NO3 L Tris buffer CAS 77-86-1 (550)
2-Amino-2-(hydroxymethyl)-propan-1,3-diol; (HO.CH2)3C.NH2

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

Y+++ gl NaClO4 25°C 0.10M C M K1=2.23 2001GYa (35066) 174
K(2Y+L+5OH)=40.04

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

Y+++ gl KCl 25°C 0.10M U K(Y+HL)=8.79 1965DKb (35895) 175

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

Y+++ cal NaClO4 25°C 0.10M U H K1=2.78 B2=4.46 1978COa (35952) 176
DH(K1)=11.3 kJ mol⁻¹, DS=91.1; DH(K2)=5.02, DS=48.9

C5H7NO3 HL (4313)
Isonitrosoacetylacetone; HO.N:CH.CO.CH2.CO.CH3

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

Y+++ gl diox/w 20°C 50% U K1=5.19 B2=8.87 1971MAf (37535) 177
Medium: 50% v/v dioxan, 0.1 M NaClO4

C5H7N04 HL (6083)

2-Acrylamidoglycolic acid; CH2:CH.CO.NH.CH(OH).COOH

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

Y+++ gl NaNO3 25°C 0.50M C K1=2.34 1977DPa (37543) 178
B(YH-1L)=-2.88
B(Y2H-3L3)=-9.40

C5H8N2O3 H2L (4317)

Methylacetyl glyoxime; CH3.C(:N.OH).C(:N.OH).CO.CH3

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

Y+++ gl diox/w 20°C 50% U K1=5.63 B2=10.51 1971MAf (37712) 179

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

Y+++ dis NaClO4 25°C 0.10M C K1=5.87 B2=10.64 1987SKc (38134) 180
K3=3.09
K4=1.74

Method: extraction of 88Y into heptane/acac phase.

K1 from literature.

Y+++ gl NaClO4 20°C 0.10M U M 1973TZa (38135) 181
K(Y(EDTA)+L)=3.60

Y+++ gl mixed 30°C 67% U K1=7.70 B2=13.62 1964DBb (38136) 182
K3=4.91

Medium: 67% acetone, 0.1 M NaClO4

Y+++ gl NaClO4 25°C 2.0M U K1=5.57 B2=10.16 1964YCa (38137) 183

Y+++ gl oth/un 30°C 0.10M U K1=5.87 B2=10.85 1960GFa (38138) 184
K3=3.25

Y+++ dis oth/un ? 0.10M U K1=6.4 B2=11.1 1960STb (38139) 185
B3=13.9

Y+++ gl mixed ? 75% U K1=7.73 B2=13.73 1956DBa (38140) 186
K3=4.77

Medium: acetone

Y+++ gl oth/un 30°C 0.0 U K1=6.4 B2=11.1 1955IFa (38141) 187

K3=2.8

C5H8O4 H2L CAS 498-21-5 (2234)
Methylsuccinic acid; HOOC.CH2.CH(CH3).COOH

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

Y+++ gl NaClO4 25°C 0.10M U K1=3.12 B2=4.91 1970RFa (38271) 188

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

Y+++ gl alc/w 25°C 25% U I K1=3.50 1973CSd (38369) 189
Medium: 0-40% (v/v) EtOH, 0.05 M. K1(0%)=3.25, K1(40%)=3.72

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

Y+++ EMF oth/un 25°C 0.10M U K1=3.94 1969PSc (38445) 190

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

Y+++ gl NaClO4 25°C 0.10M U B2=5.50 1981ZLa (38657) 191

Y+++ gl KCl 25°C 0.10M U T H K1=5.40 B2=10.21 1973SCf (38658) 192

Data for 35 C. DH(K1)=26 kJ mol⁻¹, DS(K1)=192 J K⁻¹ mol⁻¹;
DH(K2)=42, DS(K2)=234.

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

Y+++ gl NaClO4 25°C 0.10M U B2=5.10 1981ZLa (38760) 193

Y+++ gl KCl 25°C 0.10M U T H K1=4.52 B2= 8.92 1973SCf (38761) 194

Data for 35 C. DH(K1)=7 kJ mol⁻¹, DS(K1)=110 J K⁻¹ mol⁻¹;
DH(K2)=14, DS(K2)=131.

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

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-----
Y+++          gl NaCl  37°C 0.15M U            K1=4.82      1991DWb (39148) 195
                   B(YHL)=11.77
                   B(YH2L)=15.13
-----
Y+++          vlt NaClO4 25°C 0.5M C T H        K1=1.60      B2= 2.11  1978ZGb (39149) 196
Method: polarography. Medium: 0.50 M LiClO4, pH 6.3. Also data at 35 C.
DH(K1)=-8.02 kJ mol-1, DS(K1)=3.6 J K-1 mol-1. DH(B2)=-4.80, DS(B2)=24.
*****
C5H9NO4              H2L      MIDA                      CAS 4408-64-4 (190)
N-Methyliminodiethanoic acid; CH3.N(CH2.COOH)2
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Metal          Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
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Y+++          gl KCl   25°C 0.10M U            K1=6.77      B2=12.30  1980MGc (39295) 197
                   B3=14.64
                   B(Y+20H+L)=18.33
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*****
C5H10N2O3          HL      Glutamine                CAS 56-85-9 (18)
2-Aminopentanedioic acid 5-amide; H2N.CH(CH2.CH2.CO.NH2)COOH
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Metal          Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
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Y+++          gl NaClO4 30°C 0.2M U            K1=4.72                      1977MSf (39848) 198
-----

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Y+++          gl NaClO4 25°C 0.10M U            B2=8.05                      1973TSb (39849) 199
-----

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*****
C5H10N2O5          H2L                      (8080)
3-Hydroxy-2,4-diaminopentane-1,5-dioic acid;
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Metal          Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
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Y+++          gl KCl   20°C 0.1M U            K1=8.45                      1977ABf (40121) 200
-----

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*****
C5H10O3              HL                      CAS 4026-18-0 (422)
2-Hydroxy-3-methylbutanoic acid; CH3.CH2.C(OH)(CH3).COOH
-----

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

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Y+++          ix NaClO4 20°C 0.20M U            K1=2.60      B2=4.95  1960SVa (40272) 201
                   B3 > 6.0
-----

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*****
C5H10O3              HL                      CAS 617-31-2 (474)
2-Hydroxypentanoic acid; CH3.CH2.CH2.CH(OH).COOH
-----

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

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```

Y+++          gl NaClO4 25°C 1.0M U            K1=2.46                      1968GCa (40288) 202
-----

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*****
C5H10O4              HL                      CAS 4767-03-7 (4297)
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2,2-Bis(hydroxymethyl)propanoic acid; CH₃.C(CH₂OH)₂.COOH

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

Y+++ gl NaClO4 25°C 0.10M U K1=2.17 B2=3.73 1970RDa (40306) 203

C5H10O4 HL CAS 19860-56-1 (2327)
2,3-Dihydroxy-2-methylbutanoic acid; CH₃.CH(OH).C(OH)(CH₃).COOH

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

Y+++ gl KNO3 25°C 0.10M C K1=2.91 B2=5.15 1975PFb (40321) 204
K3=1.43

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

Y+++ gl KCl 25°C 0.10M U T H K1=4.79 B2= 9.06 1973SCf (40773) 205
Data for 35 C. DH(K1)=-35 kJ mol⁻¹, DS(K1)=-26 J K⁻¹ mol⁻¹;
DH(K2)=37, DS(K2)=206.

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

Y+++ gl NaNO3 25°C 0.10M M I M K1=5.72 1995KDd (41134) 206
K(Y(egta)+L)=3.84
Data for 0.15 and 0.05 M NaNO₃. At I=0, K1=5.91, K(Y(egta)+L)=4.08.

Y+++ gl KCl 20°C 0.10M U K1=4.6 1970RPa (41135) 207

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

Y+++ sp KCl 25°C 0.10M M I K1=6.21 1986PEa (42322) 208

C6H4O6 H4L CAS 5678-48-2 (871)
Tetrahydroxy-1,4-benzoquinone;

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

Y+++ EMF NaClO4 30°C 0.10M U K1=6.00 B2=8.30 1981HIa (42329) 209

C6H5NO2 HL Picolinic acid CAS 98-98-6 (391)
2-Pyridine-carboxylic acid; C₅H₄N.COOH

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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Y+++      gl  NaClO4 25°C 0.50M U          K1=3.68  B2=6.90  1977Ggb (42628) 210
                                         B3=9.19
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Y+++      gl  KNO3   25°C 0.10M U          K1=4.03  B2=7.36  1964THb (42629) 211
                                         B3=10.0
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*****
C6H5NO2          HL  Nicotinic acid  CAS 59-67-6 (419)
3-Pyridine-carboxylic acid; C5H4N.COOH
-----

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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Y+++      gl  NaClO4 25°C 0.20M U          K1=2.39          1973FDa (42691) 212
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*****
C6H5NO4          H2L  4-Nitrocatechol CAS 3316-09-4 (890)
1,2-Dihydroxy-4-nitrobenzene; O2N.C6H3(OH)2
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
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```

Y+++      gl  NaNO3  25°C 0.0 U      M  K1=9.75          1996KDb (42947) 213
                                         K(Y(egta)+L)=5.81
-----

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Extrapolated from data for I=0.05-0.15 M NaNO3.

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Y+++      gl  KNO3   25°C 0.10M U          K1=9.36  B2=16.16  1981BDa (42948) 214
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*****
C6H5O3Cl         HL          CAS 7599-81-1 (2689)
5-Hydroxy-2-(chloromethyl)-4H-pyran-4-one;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
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```

Y+++      sp  KCl    25°C 0.10M M  I  K1=5.85          1986PEa (43092) 215
-----

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```

*****
C6H5O3I         HL          CAS 16065-34-2 (2690)
5-Hydroxy-2-(iodomethyl)-4H-pyran-4-one;
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```

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

Y+++      sp  KCl    25°C 0.10M M  I  K1=5.97          1986PEa (43098) 216
-----

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*****
C6H5O4Br         L          CAS 40838-32-2 (1084)
6-Bromo-5-hydroxy-2-(hydroxymethyl)-4H-pyran-4-one;
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```

```

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

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```

Y+++      sp  KCl    25°C 0.10M M  I  K1=5.35          1986PEa (43118) 217
-----

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```

*****
C6H5O4Cl         HL  Chlorokojic aci (3086)
3-Chloro-5-hydroxy-2-hydroxymethyl-4-pyrone;
-----

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

Y+++ gl oth/un 30°C 0.10M U K1=6.00 B2=11.32 1972DSd (43139) 218

C6H5O4I L (1085)
6-Iodo-5-hydroxy-2-hydroxymethyl-4H-pyran-4-one;

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

Y+++ sp KCl 25°C 0.10M M I K1=5.43 1986PEa (43160) 219

C6H6O HL Phenol CAS 108-95-2 (457)
Hydroxybenzene, phenol; C6H5.OH

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

Y+++ sp NaClO4 25°C 0.10M U K1=2.40 1966PMa (43550) 220

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

Y+++ gl NaNO3 25°C 0.0 U M K1=9.88 1996KDb (43867) 221
K(Y(egta)+L)=5.87
Extrapolated from data for I=0.05-0.15 M NaNO3.

Y+++ gl KNO3 25°C 0.05M M I K1=10.37 B2=19.93 1981BDc (43868) 222
Also data for I=0.2 and 0.35 M. At I=0, K1=11.08, K2=9.56.

Y+++ gl NaClO4 30°C 0.20M U M K1=9.81 1979MSd (43869) 223
K(Y(hedta)+L)=7.35
hedta is N-(hydroxyethyl)diaminoethane-N,N',N'-triethanoic acid.

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

Y+++ gl NaClO4 30°C 0.20M U M K1=10.68 1979MSd (44001) 224
K(Y(hedta)+L)=6.71
hedta is N-(hydroxyethyl)diaminoethane-N,N',N'-triethanoic acid.

Y+++ gl NaClO4 30°C 0.20M U M K1=10.68 1978MSk (44002) 225
K(Y(nta)+L)=7.34

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
Y+++	gl	NaCl04	30°C	0.10M	U	M		K1=5.96 B2=11.10 B(YLA)=13.37 K(YA+L)=6.43 K(YB+L)=5.62 K(YC+L)=4.85	1989NOb (44111)	226
H2A=iminodiacetic acid, H2B=hydroxyethyliminodiethanoic acid, H3C=nitrilo-triethanoic acid										

Y+++	sp	KCl	25°C	0.10M	C			K1=6.47 B2=11.85 B3=16.07 K(Y+HL=YL+H)=-2.03 K(YL+HL=YL2+H)=-3.12 K(YL2+HL=YL3+H)=-4.28	1987PEa (44112)	227
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Y+++	sp	KCl	25°C	0.10M	M	I		K1=6.50	1986PEa (44113)	228
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Y+++	gl	NaCl04	30°C	0.10M	U			K1=6.70 B2=12.09 K3=3.88	1970DSc (44114)	229
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C6H6O3	HL	Allomaltol	CAS	644-46-2	(2688)
5-Hydroxy-2-methyl-4H-pyran-4-one;					

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Y+++	sp	KCl	25°C	0.10M	M	I		K1=6.32	1986PEa (44131)	230

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
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Y+++	gl	NaCl04	30°C	0.10M	U	M		K1=5.32 B2=10.33 B(YLA)=12.51 K(YA+L)=5.83 K(YB+L)=5.21 K(YC+L)=4.54	1989NOb (44258)	231
------	----	--------	------	-------	---	---	--	---	-----------------	-----

H2A=iminodiacetic acid, H2B=hydroxyethyliminodiethanoic acid, H3C=nitrilo-triethanoic acid

Y+++	sp	KCl	25°C	0.10M	M	I		K1=6.06	1986PEa (44259)	232
------	----	-----	------	-------	---	---	--	---------	-----------------	-----

Y+++	gl	oth/un	30°C	0.10M	U			K1=6.18 B2=11.37 K3=4.15	1972DSd (44260)	233
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Y+++	gl	NaCl04	25°C	2.0M	U			K1=5.43 B2=10.81	1964YCa (44261)	234

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
Y+++	gl	KNO3	25°C	0.10M	U			K1=14.16 B(Y2L3)=43.97	2005ATa (44518)	235
Y+++	gl	KNO3	25°C	0.10M	U	TIH		K1=14.54 B2=28.34	1980BDd (44519)	236
Data for I=0.05-0.2 M and for I=0.10 M (35 C). Also DH and DS values.										
Y+++	gl	NaClO4	30°C	0.20M	U	M		K1=14.19 K(Y(hedta)+L)=9.67	1979MSd (44520)	237
hedta is N-(hydroxyethyl)diaminoethane-N,N',N'-triethanoic acid.										
Y+++	gl	NaClO4	25°C	0.50M	C			K1=12.54 B2=21.71 B(YHL2)=29.32	1976LAF (44521)	238
Y+++	gl	NaClO4	25°C	0.10M	U			K1=13.72 K(Y+HL)=5.13	1970SSi (44522)	239
***** 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
Y+++	gl	NaNO3	25°C	0.50M	C			K1=6.8 B2=10.17 B(YHL)=9.3 B(YH-1L)=0.95 B(Y2H-3L3)=-1.9	1977KPa (46311)	240
Y+++	gl	KNO3	25°C	0.10M	U	M		B(Y(IDA)L)=9.6	1975TDa (46312)	241
Y+++	sp	NaNO3	25°C	0.50M	C	M		K1=6.79 B2=10.13 B(YH2L)=10.86 B(YHL)=9.04 B(YH-1L)=0.97 B(Y2H-3L2)=-3.69	1974RKc (46313)	242
B(YCu(H-3/2)L2)=6.40, (i.e. a binuclear complex). Glass electrode also used										
Y+++	oth	KNO3	32°C	0.10M	U			K(Y+H3L=YL+3H)=-6.86 K(YL=Y(OH)L+H)=-6.30 K(Y(OH)L=Y(OH)2L+H)=-8.91 K(Y+HL=YL+H)=-1.08	1973TPa (46314)	243
Y+++	gl	alc/w	25°C	25%	U	I		K1=8.62 Medium: EtOH/H2O, 0.05 M (NaCl,NaClO4). 0%, K1=7.87, 50%, K1=9.82	1972BKd (46315)	244
Y+++	oth	oth/un	25°C	0.10M	U			K1=7.75 B2=10.95 K(YL+HL)=2.50	1971STe (46316)	245

Constants obtained by survey of literature data

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Y+++	sol	NaClO4	25°C	0.10M	U			K1=7.81 Kso=-11.03	1966SSg (46317)	246
Y+++	ix	oth/un	25°C	0.14M	U			K(Y+H2L)=3.6	1947TMa (46318)	247

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
Y+++	ISE	NaClO4	25°C	0.10M	C	I		K1=11.30	1997LBb (47100)	248
Method: Cu ISE and competitive complexation by Cu. Data for 0.1-5.0 M. At I=0.0 M, K1=13.18.										
Y+++	gl	alc/w	30°C	50%	C			K1=10.78	1994S0a (47101)	249
Medium: 50% v/v MeOH/H2O, 0.10 M NaClO4.										
Y+++	ISE	KNO3	25°C	0.10M	C			K1=11.45	1980NSf (47102)	250
Competitive method using Cd ion-selective electrode.										
Y+++	gl	KNO3	20°C	1.0M	C			K2=8.02	1978GHb (47103)	251
Y+++	gl	diox/w	30°C	50%	U			K(YL+A)=5.43	1978SGf (47104)	252
HA=tropolone										
Y+++	gl	NaClO4	25°C	0.50M	U			K1=11.09	1977GGb (47105)	253
Y+++	cal	KNO3	20°C	0.10M	U	HM		K(YA+L)=3.73	1971GKb (47106)	254
H4A=EDTA. DH(YA+L)=-29.29 kJ mol-1, SD=-28.5 J K-1 mol-1. DH(YLA))=-31.8 kJ mol-1, DS=310 J K-1 mol-1										
Y+++	gl	oth/un	20°C	0.20M	U			B(YL(OH))=6.83	1970VMa (47107)	255
Y+++	gl	KCl	20°C	0.10M	U			K1=11.41 B2=20.43	1965ANb (47108)	256
Y+++	gl	KNO3	25°C	0.10M	U	T H T		K1=11.48 B2=20.43	1962MFb (47109)	257
15 C: K1=11.46, K2=9.09; 20 C: 11.46, 9.03; 30 C: 11.54, 8.94; 35 C: 11.56, 8.84; 40 C: 11.60, 8.83. DH(K1)=11.3 kJ mol-1, DS=258; DH(K2)=-17.5, DS=113										
Y+++	vlt	KNO3	20°C	0.10M	U			B(Y2L3)=36.8	1957NOa (47110)	258
Y+++	vlt	KNO3	20°C	0.10M	U			K1=11.41	1956SGa (47111)	259

C6H10N2O5 H2L ADA CAS 26239-55-4 (2747)
 N-(2-Acetamido)iminodiethanoic acid; H2N.CO.CH2.N(CH2.COOH)2

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

Y+++ gl KNO3 25°C 0.10M M M K1=7.05 1996AEa (47858) 260
 Data for ternary complexes with dipicolinic acid

 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

Y+++ gl mixed 30°C 67% U K1=7.14 B2=12.94 1964DBb (47934) 261
 K3=5.62

Medium: 67% acetone, 0.1 M NaClO4

 C6H10O2S HL (4370)
 Ethyl thioacetoacetate; CH3.CS.CH2.CO.OCH2.CH3

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

Y+++ gl mixed 30°C 75% U K1=7.02 B2=13.04 1970DRa (47968) 262
 K3=5.57

Medium: 75% acetone, 0.1 M

 C6H10O3 HL CAS 16841-19-3 (3649)
 1-Hydroxycyclopentanecarboxylic acid; HO.C5H8.COOH

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

Y+++ gl NaClO4 25°C 0.10M U K1=2.998 B2=5.43 1966PRb (47999) 263
 K3=1.84
 K4=1.69

 C6H10O3 HL CAS 141-97-9 (3068)
 Ethyl acetoacetate; CH3.CO.CH2.CO2.C2H5

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

Y+++ gl mixed 30°C 75% U K1=6.40 B2=11.93 1969DRa (48020) 264
 Medium: 75% acetone, 0.1 M NaClO4

 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

Y+++ gl NaClO4 25°C 0.10M U M K1=4.60 1997PPb (48491) 265
 K(Y(edta)+L)=4.19

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

Y+++ gl alc/w 30°C 50% C K1=9.06 1994SOa (48812) 266
Medium: 50% v/v MeOH/H2O, 0.10 M NaClO4.

Y+++ gl KNO3 20°C 1.00M U K1=8.12 B2=15.82 1974CMd (48813) 267
K(YL2(OH)+H)=10.15

Y+++ oth NaNO3 20°C 0.10M U M K1=8.6 B2=16.20 1966JMc (48814) 268
Method: paper electrophoresis. Ternary complexes with HEDTA

Y+++ gl KCl 25°C 0.10M U K1=8.38 B2=15.69 1965DTa (48815) 269

Y+++ ISE KNO3 25°C 0.10M U K1=9.22 B2=16.83 1963TLa (48816) 270

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

Y+++ gl KNO3 25°C 0.10M U K1=7.78 B2=14.12 1962THb (49285) 271

C6H12O4 HL CAS 1112-33-0 (1246)
2,3-Dihydroxy-2,3-dimethylbutanoic acid; (CH3)2.C(OH).C(OH)(CH3).COOH

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

Y+++ gl KNO3 25°C 0.10M U K1=3.18 B2=5.47 1979PPa (49502) 272
K3=1.71

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

Y+++ gl KCl 25°C 0.20M U K1=2.38 B2=4.52 1963K0c (49768) 273

C6H13NO2 HL Isoleucine CAS 73-32-5 (424)
2-Amino-3-methylpentanoic acid; CH3.CH2.CH(CH3).CH(NH2).COOH

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

Y+++ gl NaNO3 25°C 0.10M M M K1=6.11 1996KdD (49920) 274
*K(YL)=-8.29
*K(Y(OH)L)=-8.74
K(Y(egta)+L)=4.22

Data for 0.05-0.15 M NaNO3. At I=0, K1=6.29, K(Y(egta)+L)=4.40.

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

Y+++ gl NaNO3 25°C 0.10M M M K1=6.09 1996KdD (50123) 275
*K(YL)=-8.31
*K(Y(OH)L)=-8.76
K(Y(egta)+L)=4.20

Data for 0.05-0.15 M NaNO3. At I=0, K1=6.29, K(Y(egta)+L)=4.42.

Y+++ gl KCl 25°C 0.10M U T H K1=4.26 B2= 8.16 1973SCf (50124) 276

Data for 35 C. DH(K1)=33 kJ mol-1, DS(K1)=194 J K-1 mol-1;
DH(K2)=53, DS(K2)=252.

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

Y+++ gl NaNO3 25°C 0.10M M M K1=6.00 1996KdD (50198) 277
*K(YL)=-8.35
*K(Y(OH)L)=-8.79
K(Y(egta)+L)=4.16

Data for 0.05-0.15 M NaNO3. At I=0, K1=6.23, K(Y(egta)+L)=4.39.

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

Y+++ oth NaNO3 20°C 0.10M U K1=7.2 B2=12.80 1966JMc (50418) 278
Method: paper electrophoresis

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

Y+++ gl KCl 20°C 0.10M U K1=3.1 1970RPa (50840) 279

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

Y+++ gl KCl 20°C 0.10M U K1=3.2 1970RPa (51019) 280

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

Y+++ gl KCl 25°C 0.10M C 1998HGa (51455) 281
B(YH-6L2)=-16.4

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

Y+++ gl NaCl 25°C 0.15M C K1=11.106 1998DMa (52370) 282
B(YH-1L)=3.935
B(YHL)=17.001
B(YH2L)=22.808

Y+++ gl KNO3 25°C 0.10M C 1991SKb (52371) 283
K(YL+H)=7.17
K(YHL+H)=5.9

Y+++ dis R4N.X 20°C 0.10M U K1=15.06 1970TIa (52372) 284
Medium: NH4Cl, method: chromatography

C7H4N2O6 HL CAS 2460-59-5 (3139)
3,5-Dinitrosalicylaldehyde; HO.C6H2(NO2)2.CHO

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

Y+++ sp NaClO4 25°C 0.10M U K1=1.75 1966PMa (52397) 285

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

Y+++ gl NaNO3 25°C 0.10M U I M K1=5.89 1996KDC (52509) 286
*K(YL)=-6.22
K(Y(egta)+L)=5.24

Data for 0.05 and 0.15 M NaNO3. At I=0, K1=6.31, *K(YL)=-7.40,
K(Y(egta)+L)=5.57.

Y+++ gl oth/un 24°C 0.20M U K1=5.41 1972PSd (52510) 287
Medium: LiCl

C7H5N04 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

Y+++ gl KNO3 25°C 0.10M M M K1=5.56 1996AEa (52822) 288
Data for ternary complexes with aspartic acid, serine, asparagine and
N-(2-acetamido)iminodiacetic acid

Y+++ cal NaClO4 25°C 0.50M C H 1963GRd (52823) 289
DH(K1)=-6.02 kJ mol⁻¹, DS(K1)=141 J K⁻¹ mol⁻¹; DH(B2)=-22.22,
DS(B2)=226; DH(B3)=-51.20, DS(B3)=234.

Y+++ EMF oth/un 20°C 0.50M U K1=8.46 B2=15.73 1961GRa (52824) 290
K3=5.61

C7H5NO4 HL CAS 5274-70-4 (3148)
3-Nitrosalicylaldehyde; HO.C6H3(NO2).CHO

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

Y+++ sp NaClO4 25°C 0.10M U K1=3.27 1966PMa (52884) 291

C7H5NO4 HL CAS 97-51-8 (1887)
5-Nitrosalicylaldehyde; O2N.C6H3(OH).CHO

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

Y+++ sp NaClO4 25°C 0.10M U K1=3.17 1966PMa (52938) 292

C7H5O2Cl HL (3747)
2-Hydroxy-6-chlorobenzaldehyde (6-chlorosalicylaldehyde)

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

Y+++ sp NaClO4 25°C 0.10M U K1=4.87 1966PMa (53160) 293

C7H5O2Cl HL CAS 1927-94-2 (3143)
3-Chlorosalicylaldehyde; HO.C6H3(Cl).CHO

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

Y+++ sp NaClO4 25°C 0.10M U K1=3.77 1966PMa (53191) 294

C7H5O2Cl HL CAS 2420-26-0 (3144)
4-Chlorosalicylaldehyde; HO.C6H3(Cl).CHO

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

Y+++ sp NaClO4 25°C 0.10M U K1=4.09 1966PMa (53209) 295

C7H5O2Cl HL CAS 635-93-8 (3145)
5-Chlorosalicylaldehyde; HO.C6H3(Cl).CHO

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Y+++	sp	NaClO4	25°C	0.10M	U		K1=3.94	1966PMa (53225)	296

C7H6O5		HL					Thiotropolone	CAS 1073-38-7 (8477)	
2-Mercapto-2,4,6-cycloheptatrien-1-one;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Y+++	gl	diox/w	30°C	50%	M	I	K1=5.08 K3=3.37	B2= 9.70 1978SSi (53549)	297
Medium: 50% v/v dioxane/H2O, 0.10 M NaClO4. Data for 0.005 and 0.2 M NaClO4.									

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
Y+++	sp	NaClO4	25°C	0.10M	U		K1=4.34	1966PMa (53634)	298

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
Y+++	dis	non-aq	25°C	100%	C		K(YL3+TOPO)=4.99 K(YL3+2TOPO)=7.39	2001NCa (53699)	299
TOPO is trioctylphosphane oxide. Medium: toluene.									

Y+++	sp	NaClO4	25°C	0.10M	U		K1=7.46	1970HOa (53700)	300
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Y+++	gl	KN03	25°C	0.10M	U		K1=7.18 K3=5.01 K4=3.42	B2=13.26 1969CMB (53701)	301

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
Y+++	gl	NaNO3	25°C	0.10M	U	I M	K1=8.68 *K(YL)=-7.72 K(Y(egta)+L)=6.91	1996KDC (54340)	302
Data for 0.05 and 0.15 M NaNO3. At I=0, K1=9.03, *K(YL)=-8.81, K(Y(egta)+L)=6.21.									

Y+++	gl	alc/w	24°C	20%	C	M	K(Y(ada)+L)=3.22	1996MIa (54341)	303
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Medium: 20% w/w EtOH/H2O, 0.10 M KNO3.
 ada: N-(acetamido)-iminodiethanoic acid.

 Y+++ ix mixed 20°C 50% U 1976TRa (54342) 304
 K(Y+HL)=2.56
 K(Y+2HL)=4.60
 K(Y+3HL)=6.20

Medium: 50% v/v acetone/H2O, 0.25 M NaClO4

 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

 Y+++ gl NaClO4 30°C 0.20M U M K1=12.59 1979MSd (54774) 305
 K(Y(hedta)+L)=7.25
 hedta is N-(hydroxyethyl)diaminoethane-N,N',N'-triethanoic acid.

 Y+++ gl NaClO4 30°C 0.20M U M K1=12.59 1978MSk (54775) 306
 K(Y(nta)+L)=7.68

 C7H6O6S H3L CAS 5965-83-3 (399)
 5-Sulfosalicylic acid, 2-Hydroxy-5-sulfobenzoic; H03S.C6H3(OH).COOH

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

 Y+++ gl KNO3 20°C 0.10M U T K1=7.92 1982DBa (55080) 307

 Y+++ gl KNO3 25°C 0.20M U T K1=6.61 1975PMc (55081) 308
 35 C: K=6.61; 45 C: K=6.78

 C7H6O9S2 H3L CAS 56507-30-3 (2659)
 3,5-Disulfosalicylic acid; (H03S)2.C6H2(OH).COOH

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

 Y+++ gl NaClO4 25°C 0.50M C T K1=8.64 B2=14.38 1976LAF (55105) 309
 B(YHL)=12.7

 C7H7NOS HL (2034)
 N-Thioformyl-N-phenylhydroxylamine; H(C:S)N(C6H5)OH

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

 Y+++ gl diox/w 30°C 70% U K1=7.49 B2=13.10 1981MBb (55157) 310

 C7H7NO2 HL Anthranilic CAS 118-92-3 (1589)
 2-Aminobenzoic acid, Anthranilic acid; H2N.C6H4.COOH

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

Y+++ gl alc/w 24°C 20% C M K1=2.505 1996MIa (55271) 311
K(Y(ada)+L)=3.24

Medium: 20% w/w EtOH/H2O, 0.10 M KNO3.
ada: N-(acetamido)-iminodiethanoic acid.

Y+++ gl NaNO3 25°C 0.10M M I M K1=4.22 1995KDc (55272) 312
K(Y(egta)+L)=3.85

Data for 0.05 and 0.15 M NaNO3. At I=0, K1=4.59, K(Y(egta)+L)=4.34.

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

Y+++ gl KNO3 25°C 0.1M M K1=11.07 B2=21.27 1989LWa (55618) 313
K=9.45

Y+++ gl mixed 25°C 75% U 1970SEa (55619) 314

K(Y+HL)=7.24

K(YHL+HL)=6.50

Medium: 75% acetone, 0.1 M NaClO4

C7H7NO5S H2L CAS 3577-63-7 (3181)

5-Sulfoanthranilic acid; (5-sulfo-2-aminobenzoic acid)

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

Y+++ gl NaNO3 25°C 0.10M M I M K1=4.14 1995KDc (55681) 315
K(Y(egta)+L)=3.59

Data for 0.05 and 0.15 M NaNO3. At I=0, K1=4.46, K(Y(egta)+L)=3.86.

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

Y+++ gl NaNO3 25°C 0.0 U M K1=9.95 1996KDb (56084) 316
K(Y(egta)+L)=6.05

Extrapolated from data for I=0.05-0.15 M NaNO3.

C7H8O4 HL Methyl kojic CAS 1506-07-8 (2686)

3-Hydroxy-6-(hydroxymethyl)-2-methyl-4H-pyran-4-one;

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

Y+++ sp KCl 25°C 0.10M M I K1=6.48 1986PEa (56136) 317

C7H8O5 HL CAS 2029-29-4 (2687)

3-Hydroxy-2,6-bis(hydroxymethyl)-4H-pyran-4-one;

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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Y+++      sp  KCl    25°C 0.10M M I      K1=6.08      1986PEa (56155) 318
*****
C7H11N04      H2L                      CAS 499-82-1 (3163)
Piperidine-2,6-dicarboxylic acid; C5H9N(COOH)2
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Y+++      gl  KNO3   25°C 0.10M U          K1=6.00      B2=11.40     1963THb (56815) 319
*****
C7H11N06      H3L                      (2926)
2-Aminobutanoic-N-propane-1,3-dioic acid; HOOC.CH(C2H5)NH.CH(COOH)2
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Y+++      gl  KNO3   25°C 0.1M U          K1=8.50      1982KKc (56854) 320
*****
C7H12N2O3      HL   Gly-Pro          CAS 704-15-4 (257)
Glycyl-proline; H2N.CH2.CO.NC4H7.COOH
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Y+++      gl  KNO3   25°C 0.15M M T H      K1=3.80      1979SKd (57130) 321
Data for 35 and 45 C. At 35 C, K1=3.90, DH(K1)=21.9 kJ mol-1,
DS(K1)=145 J K-1 mol-1.
*****
C7H12O3      HL                      (4422)
3-Methyl ethylacetoacetate; CH3.CO.CH(CH3).CO.OCH2.CH3
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Y+++      gl  mixed  30°C 75% U          K1=8.20      1971DRb (57279) 322
Medium: 75% acetone, 0.1 M
*****
C7H12O4      H2L                      CAS 510-20-3 (482)
Diethylpropanedioic acid (Diethylmalonic acid); HOOC.C(C2H5)2.COOH
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Y+++      gl  KNO3   25°C 0.10M U          K1=4.60      B2=7.05     1968PFa (57375) 323
*****
C7H12O6      HL   Quinic acid      CAS 77-95-2 (2578)
1,3,4,5-Tetrahydroxycyclohexane-1-carboxylic acid;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Y+++      gl  NaCl   20°C 0.10M U          K1=2.89      1977SSc (57415) 324
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C7H13NO5 H2L (8081)
4-Hydroxy-2-aminopentane-1,5-dioic acid;

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

Y+++ gl KCl 20°C 0.1M U K1=7.02 1978KPe (57558) 325
Data for threo isomer. For erythro isomer: K1=6.32

C7H14O3 HL CAS 65311-45-1 (6266)
3-Hydroxy-3,4-dimethyl-pentanoic acid; CH3.CH2.C(OH)(CH3).CH(CH3).COOH

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

Y+++ gl NaClO4 25°C 0.10M C K1=2.78 B2=4.52 1976SPa (57882) 326

C8H5N5O6 H3L Murexide (453)
Purpuric acid (Murexide is ammonium salt);

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

Y+++ sp KNO3 12°C 0.10M U 1965GEa (58543) 327
K(Y+H2L)=3.36

C8H6O4 H2L Phthalic acid CAS 88-99-3 (113)
Benzene-1,2-dicarboxylic acid; C6H4(COOH)2

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

Y+++ gl alc/w 24°C 20% C M K1=3.81 1996MIa (59037) 328
K(Y(ada)+L)=4.99

Medium: 20% w/w EtOH/H2O, 0.10 M KNO3.
ada: N-(acetamido)-iminodiethanoic acid.

Y+++ gl NaNO3 25°C 0.10M M I M K1=4.85 1995KDb (59038) 329
K(Y(egta)+L)=4.33

Data for 0.05 and 0.15 M NaNO3. At I=0, K1=5.14, K(Y(egta)+L)=4.69.

Y+++ gl NaClO4 30°C 0.10M U K1=4.04 B2=7.12 1966KPb (59039) 330

C8H6O4 H2L Isophthalic aci CAS 212-91-5 (1619)
Benzene-1,3-dicarboxylic acid; C6H4(COOH)2

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

Y+++ cal NaClO4 25°C 0.10M U H K1=2.51 1982CBc (59063) 331
DH= 15.04 kJ mol⁻¹, DS= 99 J K⁻¹ mol⁻¹

C8H7NO2 HL CAS 532-54-7 (4363)
Isonitrosoacetophenone, Phenylglyoxal 2-oxime;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Y+++	gl	diox/w	20°C	50%	U		K1=6.32 B2=11.94	1971MAf (59110)	332
Medium: 50% v/v dioxan, 0.1 M NaClO4									

C8H7NO3		HL					(7376)		
benzoylhydroxamic acid; C6H5COCONHOH									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Y+++	gl	KNO3	25°C	0.1M	M		K1=9.66 B2=18.56 K3=7.62	1989LWa (59131)	333

C8H7O2Cl		HL					CAS 1450-74-4 (6325)		
2-Hydroxy-5-chloro-acetophenone; Cl(HO)C6H3.CO.CH3									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Y+++	gl	alc/w	25°C	20%	M	I	K1=6.29	1994KDa (59224)	334
Medium: 20% v/v EtOH/H2O, 0.10 M NaNO3. Also data for 0.05 and 0.15 M NaNO3. At I=0 (20% v/v), K1=6.58, *K(YL)=-8.76, *K(Y(OH)L)=-8.90.									

C8H8N2O		L					CAS 4856-97-7 (3820)		
2-(Hydroxymethyl)benzimidazole;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Y+++	gl	diox/w	30°C	50%	U	T H	B2=16.47	1988NOa (59314)	335
40 C: B2=16.38; 50 C: B2=16.30. DH=-16.3 kJ mol-1, DS=262 J K-1 mol-1									

C8H8N2O2		HL					Phenylglyoxime (3222)		
Phenylglyoxime; C6H5.C(:N.OH).CH:N.OH									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Y+++	gl	diox/w	20°C	50%	U		K1=6.82 B2=12.79	1971MAf (59345)	336
Medium: 50% dioxan, 0.1 M NaClO4									

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
Y+++	gl	alc/w	25°C	20%	M	I	K1=6.63	1994KDa (59472)	337
Medium: 20% v/v EtOH/H2O, 0.10 M NaNO3. Also data for 0.05 and 0.15 M NaNO3. At I=0 (20% v/v), K1=6.93, *K(YL)=-8.68, *K(Y(OH)L)=-9.23.									

C8H8O2		HL					CAS 583-80-2 (3191)		
beta-Methyltropolone;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Y+++	sp	alc/w	?	3%	U			K1=7.38	1967GDb (59606)	338
Medium: 3% EtOH, 0.2 M NaClO4										

C8H8O3		H2L						CAS 490-78-8	(6324)	
2,5-Dihydroxyacetophenone; (HO)2C6H3.CO.CH3										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Y+++	gl	alc/w	25°C	20%	M	I		K(Y+HL)=6.44	1994KDa (59685)	339
Medium: 20% v/v EtOH/H2O, 0.10 M NaNO3. Also data for 0.05 and 0.15 M NaNO3. At I=0 (20% v/v), K1=6.70, *K(YHL)=-8.59, *K(Y(OH)HL)=-9.02.										

C8H8O3		HL		o-Anisic acid				CAS 579-75-9	(2337)	
2-Methoxybenzoic acid; CH3O.C6H4.COOH										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Y+++	gl	NaClO4	25°C	0.10M	M	H		K1=1.66	1988CLb (59757)	340
DH=9.32 kJ mol ⁻¹ , DS=63 J K ⁻¹ mol ⁻¹										

C8H8O3		HL		m-Anisic acid				CAS 586-38-9	(2804)	
3-Methoxybenzoic acid; CH3O.C6H4.COOH										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Y+++	gl	NaClO4	25°C	0.10M	M	H		K1=1.87	1988CLb (59923)	341
DH=11.6 kJ mol ⁻¹ , DS=75 J K ⁻¹ mol ⁻¹										

C8H8O3		HL						CAS 148-52-8	(3193)	
3-Methoxysalicylaldehyde; CH3O.C6H3(OH).CHO										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Y+++	gl	NaNO3	25°C	0.10M	M	I	M	K1=4.853	1995KDd (59933)	342
K(Y(egta)+L)=3.645										
Data for 0.15 and 0.05 M NaNO3. At I=0, K1=5.076, K(Y(egta)+L)=3.938.										

C8H8O3		HL		p-Anisic acid				CAS 100-09-4	(1373)	
4-Methoxybenzoic acid; CH3O.C6H4.COOH										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Y+++	gl	NaClO4	25°C	0.10M	M	H		K1=2.01	1988CLb (59966)	343
DH=14.2 kJ mol ⁻¹ , DS=86 J K ⁻¹ mol ⁻¹										

C8H8O4		HL						CAS 520-45-6	(4478)	
3-Acetyl-2-hydroxy-6-methylpyran-4-one, Dehydroethanoic acid;										


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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Y+++      gl  diox/w 35°C 50% U          K1=4.80  B2=8.78  1971MAa (60101) 344
Medium: 50% dioxan, 0.1 M NaClO4
*****
C8H9NO2          HL                      CAS 4389-45-1 (3226)
3-Methyl-2-aminobenzoic acid; CH3.C6H3(NH2).COOH
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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Y+++      gl  NaNO3 25°C 0.10M M I M    K1=5.56          1995KDC (60237) 345
                                K(Y(egta)+L)=5.18
Data for 0.05 and 0.15 M NaNO3. At I=0, K1=5.78, K(Y(egta)+L)=5.30.
*****
C8H9NO4          H2L                      (4520)
Dehydroethanoic acid oxime;
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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Y+++      gl  diox/w 35°C 50% U          K(Y+HL)=4.16
                                K(Y+2HL)=7.38
Medium: 50% dioxan, 0.1 M NaClO4
*****
C8H10O4          L                      CAS 34241-51-5 (5701)
3-Acetyl-6-methylhydropyran-2,4-dione;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Y+++      gl  alc/w 22°C 20% U          K1=4.57  B2=8.24  1988ZTa (60857) 347
                                K3=3.12
*****
C8H10O5          H2L                      CAS 145-73-7 (138)
7-Oxa-bicyclo[2.2.1]-heptan-2,3-dicarboxylic acid;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Y+++      gl  KCl 30°C 0.10M C          K1=5.77  B2=9.85  1996SZa (60878) 348
For the -5-en-2-exo isomer, K1=6.03, B2=10.84.
*****
C8H12N2O8        H4L                      CAS 35039-85-1 (4537)
1,2-Diaminoethane-N,N'-dimalonic acid; (HOOC)2.CH.NH.CH2.CH2.NH.CH(COOH)2
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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Y+++      vlt KNO3 25°C 0.10M U          K1=10.47          1972GBd (61532) 349
*****
C8H12O2          HL                      CAS 874-23-7 (3203)
2-Acetylcyclohexanone;
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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Y+++      gl  mixed  25°C  75%  U          K1=8.46  B2=16.05  1971DRa (61678) 350
Medium: 75% acetone, 0.1 M NaClO4
*****
C8H12O2          HL      Dimedone          CAS 126-81-8 (1137)
5,5-Dimethyl-1,3-cyclohexanedione;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Y+++      gl  oth/un 30°C 0.10M U          K1=2.78  B2=5.37  1975DSa (61692) 351
*****
C8H12O4          H2L          CAS 1076-97-9 (2224)
Cyclohexane-1,4-dicarboxylic acid; C6H10.(COOH)2
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Y+++      gl  NaClO4 25°C 0.10M M  H      K1=4.24          1986CDb (61718) 352
DH(K1)=17.2 kJ mol-1, DS=141 J K-1 mol-1
*****
C8H13NO6S        H3L          (5675)
2-Mercapto-1-aminoethane-N,N,S-triethanoic acid; HOOC.CH2.S.CH2.CH2.N(CH2COOH)2
-----

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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Y+++      gl  NaClO4 25°C 0.10M U          K1=8.36          1975POa (61834) 353
K(Y+HL)=2.63
*****
C8H14O3          HL          CAS 607-97-6 (4489)
3-Ethylethylacetoacetate; CH3.CO.CH(C2H5).CO.OC2H5
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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Y+++      gl  mixed  30°C  75%  U          K1=9.03          1971DRb (62083) 354
Medium: 75% acetone, 0.1 M
*****
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
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Y+++      gl  KCl     25°C  0.10M U          K(Y+HL)=17.7
K(Y+H2L)=9.2
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-----
Y+++      ix  oth/un 25°C 0.10M U          K1=24.04        1965TIc (62909) 356
*****
C8H18N2O10P2     H6L          CAS 2310-83-0 (5667)
-----

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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

Y+++ ix R4N.X 20°C 0.10M U K1=18.82 1970TIc (62922) 357
K(Y+HL)=13.80
K(Y+H2L)=11.92

C8H19N05 L Bis-tris CAS 6976-37-0 (2827)
Bis-(2-hydroxyethyl)imino-tris(hydroxymethyl)methane;

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

Y+++ gl NaCl 30°C 0.10M C K1=5.76 B2= 9.01 2002Nwa (63070) 358
B(Y2L)=6.01

Constants expressed on the molality scale.

C8H19O4P HL CAS 107-66-4 (2130)
Dibutylphosphoric acid; (C4H9O)2P(O)OH

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

Y+++ dis oth/un 20°C ? U K1=1.91 1961SSa (63196) 359

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

Y+++ gl KCl 25°C 0.10M U K1=12.87 1965DKb (63346) 360
K(Y+HL)=6.48

C8H24N2O12P4S H8L CAS 33424-58-7 (2648)
1,7-Diaza-4-thiaheptane-1,1,7,7-tetra(methylphosphonic acid);
S(CH2.CH2.N(CH2.PO3H2)2)2

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

Y+++ ix KCl 20°C 0.10M U K1=13.01 1971TIa (63488) 361
K(Y+HL)=10.14

C8H24N2O13P4 H8L CAS 25007-19-4 (2647)
1,7-Diaza-4-oxaheptane-1,1,7,7-tetra(methylphosphonic acid);
O(CH2.CH2.N(CH2.PO3H2)2)2

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

Y+++ dis oth/un 20°C 0.10M U K1=15.30 1969TIa (63496) 362
Method: chromatography

 C9H5N04 HL CAS 22308-86-7 (4607)
 3-Nitroso-4-hydroxycoumarin (oximidobenzotetronic acid);

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

 Y+++ sp diox/w 20°C 50% U K1=2.76 B2=4.65 1977MBb (63617) 363

C9H6N04BrS 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

 Y+++ gl NaClO4 25°C 0.10M U K1=5.50 B2=10.36 1973MAa (63707) 364
 K3=4.2

 C9H6N04IS 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

 Y+++ gl oth/un 20°C 0.10M U K1=6.23 1977SKd (63836) 365

 Y+++ gl KNO3 25°C 0.20M U T K1=5.23 1975PMc (63837) 366
 35 C: K=5.16; 45 C: K=4.92

 C9H6N2O5S H2L CAS 5263-74-1 (2738)
 7-Nitroso-8-hydroxyquinoline-5-sulfonic acid;

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

 Y+++ gl alc/w 27°C 50% C H K1=5.99 B2=11.0 1986EAa (63878) 367

C9H6O6 H3L Hemimellitic ac CAS 569-51-7 (1621)
 1,2,3-Benzenetricarboxylic acid; C6H3.(COOH)3

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

 Y+++ gl NaClO4 25°C 0.10M U H K1=4.76 1994CRa (63979) 368
 K(Y+HL)=2.81

DH(K1)=18.5 kJ mol⁻¹; DS=153 J K⁻¹ mol⁻¹

C9H7NO HL Oxine CAS 148-24-3 (504)
 8-Hydroxyquinoline (8-quinolinol);

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

 Y+++ sol none RT 0.0 U 1981FCa (64375) 369
 Kso(YL3)=-32.64

Method: spectrophotometry.

Y+++ gl diox/w 30°C 50% U K1=9.09 B2=17.24 1970GMb (64376) 370
Medium: 50% dioxan, 0.3 M NaClO4

C9H7NO2 HL CAS 1127-45-3 (4614)
8-Hydroxyquinoline-N-oxide;

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

Y+++ gl diox/w 30°C 50% U K1=7.21 1970GMb (64414) 371
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

Y+++ gl KNO3 30°C 0.20M U T K1=5.77 1975PMc (64590) 372
40 C: K=5.71; 50 C: K=5.62

Y+++ cal KNO3 20°C 0.10M U HM 1971GKb (64591) 373
K(YA+L)=4.31

DH(YA+L)=-21.11 kJ mol⁻¹, DS=10.45 J K⁻¹ mol⁻¹

DH(YAL): DH=-23.57, DS=347.8. H4A=EDTA

C9H8O4 H2L CAS 97652-17-0 (3855)
3-Carboxy-4-methyltropolone;

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

Y+++ sp NaClO4 ? 0.20M U K1=8.47 1967GDc (64958) 374
K(YHL)=10.61

Y+++ gl NaClO4 25°C 0.20M U K1=8.26 B2=14.88 1966GDa (64959) 375
K3=3.96

C9H8O4 H2L CAS 15872-28-3 (8407)
Bicyclo[2.2.1]hepta-2,5-diene-2,3-dicarboxylic acid;

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

Y+++ gl KCl 30°C 0.10M U K1=4.16 1996SZa (64984) 376

C9H10O4 H2L (7232)
Bicyclo[2.2.1]hept-5-en-2-endo,3-cis-dicarboxylic acid;

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

Y+++ gl KCl 30°C 0.10M C K1=4.03 B2=6.91 1996SZa (65580) 377
for the -2,5-dien-2-exo isomer, K1=4.16.

C9H10O5 H2L CAS 54384-22-4 (8406)
1-Methyl-(exo,exo)-7-oxabicyclo[2.2.1]hept-5-ene-2,3-dicarboxylic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Y+++	gl	KCl	30°C	0.10M	U			K1=5.13 B2= 8.00	1996SZa (65612)	378

C9H10O5 H2L (7233)
1-Methyl-7-oxa-bicyclo[2.2.1]hept-5-en-2-exo,3-cis-dicarboxylic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Y+++	gl	KCl	30°C	0.10M	C			K1=5.13 B2=8.00	1996SZa (65627)	379

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
Y+++	gl	NaCl	25°C	0.15M	U	H		K1=3.49	1992ZNa (65988)	380

By calorimetry: DH(K1)=6.38 kJ mol⁻¹, DS(K1)=88.22 J K⁻¹ mol⁻¹.

Y+++	gl	KNO3	35°C	0.10M	U			K1=5.27	1990RSe (65989)	381
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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
Y+++	gl	KNO3	25°C	0.10M	U				1977SAb (66244)	382

K(Y+HL)=4.43
K(Y+2HL)=8.48

At 35 C, I=0: K(Y+HL)=5.09, K(Y+2HL)=9.69

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
Y+++	gl	diox/w	30°C	75%	U			K1=6.96	1988MKd (66512)	383

C9H11N3O3 HL CAS 58336-41-7 (6169)
N-(2-Hydroxy-3-methoxybenzylidene)semicarbazide; CH3O(OH)C6H3.CH:N.CO.NH.NH2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Y+++	gl	diox/w	30°C	75%	U			K1=10.50	1988MKd (66519)	384

C9H12N2O6 HL Uridine CAS 58-96-8 (828)

Uracil-1-beta-D-ribofuranoside;

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

Y+++ gl KNO3 35°C 0.10M U M K1=5.20 1990RSc (66717) 385
K(YA+L)=4.89
K(YB+L)=4.72
K(YC+L)=4.47
H2A=Iminodiethanoic acid, H3B=NTA, H4C=EDTA

Y+++ gl KNO3 35°C 0.10M U M K1=4.49 1990RSc (66718) 386
K(YL+Ala)=9.59
K(YL+Phe)=9.41
K(YL+Trp)=9.60

C9H12N2O10 H5L CAS 80921-06-8 (2924)
2,3-Diaminopropanoic-N,N'-di-1,3-propanedioic acid;
(HOOC)2CH.NH.CH(COOH).CH2.NH.CH(COOH)2

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

Y+++ ISE KNO3 25°C 0.10M U K1=11.34 1983KBd (66749) 387
Hg-electrode.

C9H13NO6 H3L (3881)
2,6-Dicarboxypiperidyl-N-ethanoic acid;

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

Y+++ gl KNO3 25°C 0.10M U K1=10.83 B2=18.58 1968TKe (66897) 388

C9H13N3O5 L Cytidine CAS 65-46-3 (2152)
Cytidine, Cytosine-1-beta-D-ribofuranoside;

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

Y+++ gl KNO3 35°C 0.10M U M K1=3.30 1990RSc (67087) 389
K(Y+HA+L)=8.32
B(YBL)=15.69
B(YCL)=20.50
H2A=Iminodiethanoic acid, H3B=NTA, H4C=EDTA

Y+++ gl KNO3 35°C 0.10M U M K1=2.70 1990RSe (67088) 390
K(YL+Ala)=5.20
K(YL+Phe)=5.35
K(YL+Trp)=5.29

C9H16N2O6 H3L MEDTA CAS 40423-02-7 (5717)
N-Methyldiaminoethane-N,N',N'-triethanoic acid; HOOC.CH2.N(CH3)CH2.CH2.N(CH2.COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Y+++	cal	NaClO4	25°C	0.50M	M	IH		K1=12.89	1986RCa (67647)	391
DH=-10.1 kJ mol ⁻¹ , DS=213 J K ⁻¹ mol ⁻¹										

C9H16O4		H2L						CAS 1636-27-7	(485)	
Dipropylpropanedioic acid (Di-n-propylmalonic acid);										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Y+++	gl	KNO3	25°C	0.10M	U			K1=4.74 B2=7.36	1968PFa (67781)	392

C9H28N3O15P5		10L		DTPPH				CAS 15827-60-8	(2921)	
Diethylenetriamine-N,N,N',N'',N'''-penta(methylphosphonic acid);										
H2O3PCH2.N(CH2CH2.N(CH2PO3H2)2)2 H										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Y+++	dis	KCl	20°C	0.10M	U			K(Y+H4L)=9.48	1968TIa (68417)	393

C10H6O4		H2L						CAS 475-38-7	(6120)	
5,8-Dihydroxy-1,4-naphthoquinone;										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Y+++	sp	alc/w	25°C	50%	U			K(Y+HL)=6.904 K(Y+HL+L)=16.3 B(Y(OH)2L)=24.72	1993ISb (68489)	394
Medium: 50% v/v EtOH/H2O; 0.1 M NaClO4										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Y+++	sp	alc/w	25°C	50%	M			K(Y+HL)=6.904 B(YL(OH)2)=24.72 K(Y+H2L=YHL+H)=-1.47 K(Y+L+HL)=16.3	1993ISc (68490)	395
Medium: 50% v/v ethanol/H2O, 0.1 M NaClO4. K(YHL+H2L=YHL2+2H)=-10.2, K(YHL=YL(OH)2+3H)=-21.4, K(YHL2=YL(OH)2+H2L+H)=-11.22.										

C10H6O8		H4L		Pyromellitic Ac				CAS 89-05-4	(519)	
Benzene-1,2,4,5-tetracarboxylic acid; C6H2.(COOH)4										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Y+++	gl	NaClO4	25°C	0.10M	U	H		K1=4.57 K(Y+HL)=3.62	1994CRa (68532)	396
DH(K1)=20.2 kJ mol ⁻¹ , DS=155 J K ⁻¹ mol ⁻¹ ; DH(Y+HL)=15.3, DS=121										

C10H7NO2		HL						CAS 131-91-9	(2668)	

1-Nitroso-2-naphthol, alpha-Nitroso-beta-naphthol;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Y+++	sp	KCl	25°C	0.10M	M	I		K1=4.09	1976PEa (68598)	397
Y+++	gl	diox/w	30°C	75%	U			K1=9.02 B2=17.74 B3=25.04	1957CFa (68599)	398

 C10H7NO2 HL CAS 132-53-6 (2524)
 2-Nitroso-1-naphthol;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Y+++	gl	diox/w	30°C	75%	U			K1=8.3 B2=15.9 B3=23.3	1957CFa (68666)	399

 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
Y+++	gl	NaClO4	30°C	0.10M	U			K1=2.58 B2=5.04	1969DNc (68724)	400

 C10H7NO2 HL CAS 86-59-9 (873)
 Quinoline-8-carboxylic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Y+++	gl	NaClO4	30°C	0.10M	U			K1=2.60	1969DNc (68773)	401

 C10H7NO5S H2L CAS 14090-74-5 (2676)
 1-Nitroso-2-hydroxynaphthalene-7-sulfonic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Y+++	gl	KCl	25°C	0.10M	M			K1=4.28	1979LSb (68821)	402

 C10H7NO5S H2L (4766)
 1-Nitroso-2-hydroxynaphthalene-6-sulfonic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Y+++	sp	KCl	25°C	0.10M	C			K1=4.24	1973Pmb (68857)	403

 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
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Y+++ gl KCl 25°C 0.10M U I K1=2.87 1967MAi (68898) 404
K1=3.97(I=0)

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

Y+++ sp KCl 25°C 0.10M U K1=4.82 1978PPb (68955) 405

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

Y+++ gl KNO3 25°C 0.20M U T K1=3.44 1975PMc (69038) 406
35 C: K=3.43; 45 C: K=3.37

Y+++ gl KCl 25°C 0.10M U I K1=4.48 B2=7.83 1967MAi (69039) 407
B3=11.29

K1=6.24(I=0)

C10H8O2 H2L CAS 92-44-4 (1658)

2,3-Dihydroxynaphthalene;

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

Y+++ gl NaClO4 20°C 0.10M U M K(YA+L)=7.70, H4A=EDTA 1973PAC (69785) 408

C10H8O5S H3L DHNSA (877)

2,3-Dihydroxynaphthalene-6-sulfonic acid;

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

Y+++ gl NaClO4 30°C 0.20M U M K1=10.09 1979MSd (69869) 409
K(Y(hedta)+L)=8.06

hedta is N-(hydroxyethyl)diaminoethane-N,N',N'-triethanoic acid.

Y+++ gl NaClO4 30°C 0.20M U M K1=10.06 1978MSl (69870) 410
K(Y(edta)+L)=6.81

Y+++ gl NaClO4 25°C 0.50M C K1=10.14 B2=18.22 1976LAF (69871) 411
B3=24.0
B(YHL2)=24.8

Y+++ gl KNO3 30°C 0.20M U T K1=8.64 1975PMc (69872) 412
40 C: K=8.21; 50 C: K=7.89

C10H10O5 HL CAS 13522-48-0 (4722)

3-Mercapto-1-phenylbut-2-en-1-one; C6H5.CO.CH:CH.C(SH).CH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Y+++	gl	mixed	30°C	75%	U			K1=3.85 K2=7.27 K3=3.18	1969DNb (70641)	413

Medium: 75% acetone, 0.1 M NaClO4

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
Y+++	gl	alc/w	25°C	80%	U			K1=8.29 K2=14.64 K3=4.42	1967DZa (70784)	414

Medium: 80% MeOH, 0.1 M NaCl

Y+++	gl	alc/w	24°C	80%	U			K1=8.29 K2=14.64 K3 = 4.42	1967DZb (70785)	415
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Medium: 80% v/v MeOH/H2O, 0.1 M NaCl

Y+++	gl	mixed	30°C	67%	U			K1=8.21 K2=14.89 K3=5.68	1964DBb (70786)	416
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Medium: 67% acetone, 0.1 M NaClO4

Y+++	dis	oth/un	?	0.10M	U			K1=6.55 K2=11.4 K3=14.4	1960STb (70787)	417
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Y+++	gl	none	?	0.0	U			K1=8.24 K2=14.98 K3=5.59	1958DBa (70788)	418
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C10H10O6 H2L CAS 5411-14-3 (2394)
1,2-Phenylenedioxodiethanoic acid; C6H4(O.CH2.COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Y+++	gl	NaClO4	25°C	0.10M	M			K1=3.78	1977HCb (70864)	419

C10H11NO3 HL (1960)
N-Hydroxyacetoacetanilide; CH3.CO.CH2.CO.N(OH).C6H5

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Y+++	gl	diox/w	20°C	82%	U			K1=7.44 K2=13.73 K3=6.22	1979KSb (70946)	420

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
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Y+++ gl KNO3 25°C 0.10M U K1=8.63 B2=16.01 1964THa (71283) 421

C10H12O2 HL CAS 1946-74-3 (202)

3-Isopropyltropolone;

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

Y+++ gl diox/w 30°C 50% U M K1=7.85 B2=15.28 1980SGa (71612) 422
K3=5.95
K(Y(NTA)+L)=6.41

Y+++ gl alc/w 25°C 80% U K1=9.0 B2=16.50 1968DZb (71613) 423
K3=6.2
K4=4.8

Medium: 80% MeOH, 0.1 M NaCl

Y+++ sp alc/w ? 3% U K1=7.28 1967GDb (71614) 424

Medium: 3% EtOH, 0.2 M NaClO4

C10H14N5O7P H2L AMP-5 CAS 18422-05-4 (842)

Adenosine-5'-monophosphoric acid, 5-Adenylic acid;

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

Y+++ gl R4N.X 25°C 0.10M C T K1=4.48 1991SMa (72501) 425
K(Y+HL)=2.76

IUPAC evaluation

Y+++ ix NaCl 25°C 0.15M U K1=5.7 19600La (72502) 426

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

Y+++ sp R4N.X 25°C 0.10M C K1=18.5 1994KCa (74310) 427

Medium: Me4NCl

Y+++ cal NaClO4 25°C 0.10M C H 1987YJa (74311) 428

DH(K1)=-1.68 kJ mol⁻¹, DS(K1)=327 J K⁻¹ mol⁻¹.

Y+++ gl NaClO4 20°C 0.02M U M 1982MPd (74312) 429

K(YL+PO4)=3.40

Y+++ gl NaClO4 25°C 0.50M U K1=16.58 1977GGb (74313) 430

Y+++ gl KCl 25°C 1.00M U K2=2.24 1976BKa (74314) 431

K(YL+HL)=1.39

K(2YL+L)=4.81

Y+++ sp KCl 25°C 0.10M U K2=2.24 1975BKa (74315) 432
K(2YL+L)=4.81
K(YL+HL)=1.39

Y+++ gl KCl 25°C 1.0M C K2=2.24 1974BKe (74316) 433
K(YL+HL)=1.39
K(2YL+L=Y2L3)=4.81

Y+++ gl KNO3 25°C 0.10M U T M 1973TRb (74317) 434
K(YL+HA)=4.02
K(YL+H)=5.43
K(YL+HA)(2 C)=4.10, K(35 C)=3.86, K(45 C)=3.80; K(YL+H)(2 C)=5.86,
K(35 C)=5.24, K(45 C)=5.22, H5A=tripolyphosphoric acid

Y+++ gl KNO3 25°C 0.10M U T M 1973TRb (74318) 435
K(YL+A)=5.3
K(2 C)=5.4, K(35 C)=5.2, K(45 C)=5.0, H4A=adenosine triphosphate

Y+++ gl KNO3 25°C 0.10M U M 19700Za (74319) 436
K(YL+A)=7.63
K(YL+B)=7.05
K(YL+C)=7.32
K(YL+D)=3.15
H4A=tiron; H3B=2,3-dihydroxynaphthalene-6-sulphonic acid, H2C=catechol,
H2D=iminodiacetic acid, K(YL+E)=2.95, H2E=hydroxyethyl iminodiacetic acid

Y+++ gl NaClO4 25°C 0.10M U M 1969AIb (74320) 437
K(YL+A)=7.19, A4A=tiron

Y+++ nmr oth/un 40°C 0.10M U 1969MGc (74321) 438
K(Y(OH)L(H2O)n-1+H)=11.9
K(YL(H2O)n+H) < 2

Y+++ sp oth/un 19°C 0.10M U K1=16.9 1965VAa (74322) 439

Y+++ sol oth/un 20°C 0.15M U I K1=18.21 1963TTa (74323) 440
Kso=-25.13(I=0.1)

Y+++ ix R4N.X 22°C 0.50M U K1=17.70 1962TIa (74324) 441

Y+++ cal KNO3 20°C 0.10M U H 1958SRa (74325) 442
DH(K1)=1.33 kJ mol⁻¹, DS=350 J K⁻¹ mol⁻¹

Y+++ gl oth/un 20°C 0.01M U K1=17.98 1955WSa (74326) 443
Polarography also used

Y+++ gl KCl 20°C 0.10M U I T K1=17.38 1954SGa (74327) 444
By polarography K1=17.8. In 0.1 M KNO3 K1=18.08

Y+++ vlt KNO3 20°C 0.10M U T K1=17.56 1953WSa (74328) 445

Y+++ gl KCl 20°C 0.10M U K1=18.0 1952VIa (74329) 446

C10H16N5O13P3 H4L ATP CAS 56-65-5 (403)
Adenosine-5'-triphosphoric acid;

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

Y+++ gl R4N.X 25°C 0.10M C T K1=6.64 1991SMa (74840) 447
K(Y+HL)=3.64

IUPAC evaluation

Y+++ gl KNO3 35°C 0.10M U M 1972TRc (74841) 448
K(Y(EDTA)+L)=5.2

Y+++ ix NaCl 25°C 0.15M U K1=11.1 1960La (74842) 449

C10H16O2 HL CAS 100563-25-5 (4706)
2-Butanoylcyclohexanone; CH3.CH2.CH2.CO.C6H9O

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

Y+++ gl oth/un 30°C 0.10M U K1=9.13 B2=17.15 1972DSe (74926) 450

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

Y+++ gl NaClO4 25°C 0.50M U K1=14.32 1977Ggb (75535) 451

Y+++ gl KNO3 25°C 0.10M U M 19700Za (75536) 452

K(YL+A)=8.70
K(YL+B)=8.45
K(YL+C)=8.20
K(YL+D)=4.85

H4A=tiron; H3B=2,3-dihydroxynaphthalene-6-sulphonic acid; H2C=catechol,
H2D=iminodiacetic acid. K(YL+E)=4.48, H2E=hydroxyethyl iminodiacetic acid

Y+++ gl KNO3 25°C 0.10M U M 1963TLb (75537) 453

K(YL+A)=5.10
K(YL+B)=4.39

Id=iminodiacetic acid

Y+++ EMF oth/un 20°C 0.10M U K1=15.03 1962PMa (75538) 454

Y+++ gl KNO3 15°C 0.10M U T H K1=14.69 1961MFb (75539) 455

K1=14.67(20 C), 14.65(25 C), 14.62(30 C), 14.71(35 C), 14.65(40 C)

DH(K1)=-1.2 kJ mol⁻¹(25 C), DS1=277 J K⁻¹ mol⁻¹

Y+++ gl KNO3 25°C 0.10M U K1=14.49 1956SPa (75540) 456
By polarography K1=14.8

C10H19N3O4 HL Leu-Gly-Gly CAS 1187-50-4 (1230)
Leucyl-glycyl-glycine; H2N.CH(CH2.CH(CH3)2).CO.NH.CH2.CO.NH.CH2.COOH

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

Y+++ gl KNO3 25°C 0.10M U T H K1=3.30 1981SKg (75697) 457
Data for 35 and 45 C. DH(K1)=5.44 kJ mol⁻¹, DS(K1)=81.4 J K⁻¹ mol⁻¹.

C10H20N2O4 H2L (4753)
N,N'-Diethylethylenedinitrilo-N,N'-diethanoic acid;

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

Y+++ gl KNO3 25°C 0.10M U K1=6.8 1973PSb (75787) 458

C11H8O3 H2L CAS 86-48-6 (1129)
1-Hydroxy-2-naphthoic acid;

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

Y+++ gl KNO3 30°C 0.05M U I K1=8.76 B2=17.05 1976SSb (77022) 459

Y+++ gl diox/w 25°C 75% U K1=4.97 1975DJa (77023) 460

C11H8O3 H2L CAS 2083-08-1 (1131)
2-Hydroxy-1-naphthoic acid;

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

Y+++ gl diox/w 25°C 75% U K1=4.72 1975DJa (77067) 461

C11H8O3 HL CAS 483-35-6 (3347)
2-Hydroxy-3-methyl-1,4-naphthoquinone;

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

Y+++ gl diox/w 35°C 75% M K1=4.81 B2=8.37 1986SSc (77081) 462

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

Y+++ gl KNO3 20°C 0.10M U T H K1=8.70 B2=17.07 1977SKc (77135) 463
Further data at 30, 40 C. DH(B2)=-70.3 kJ mol⁻¹

Y+++ gl diox/w 25°C 75% U K1=5.28 1975DJa (77136) 464

 C11H8O4 HL CAS 7555-37-5 (4812)
 3-Acetyl-4-hydroxycoumarin

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

Y+++ gl diox/w 35°C 50% U K1=4.02 B2=7.10 1971MAa (77189) 465
 Medium: 50% dioxan, 0.01 M NaClO4

 C11H9NO2 H2L CAS 7470-09-9 (8481)
 2-Hydroxy-1-naphthaldoxime;

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

Y+++ gl diox/w 25°C 75% U K1=8.24 B2=15.59 1978MCd (77320) 466
 Medium: 75% v/v dioxane/H2O, 0.10 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

Y+++ gl diox/w 35°C 50% U 1971MAa (77432) 467
 K(Y+HL)=3.35
 K(Y+2HL)=5.91
 Medium: 50% dioxan, 0.01 M NaClO4

 C11H9N3O2 H2L PAR CAS 1141-59-9 (636)
 4-(2'-Pyridylazo)-1,3-dihydroxybenzene; C5H4N.N:N.C6H3(OH)2

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

Y+++ sp NaClO4 20°C 0.10M U K1=9.1 1967SNb (77604) 468
 K(Y+HL)=10.2

 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

Y+++ gl KNO3 35°C 0.10M U K1=5.48 1990RSe (78240) 469

 C11H12O3 HL CAS 94-02-0 (3351)
 Ethyl benzoylacetate; C6H5.CO.CH2.CO2.C2H5

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

Y+++ gl mixed 25°C 75% U K1=8.56 B2=15.74 1971DRa (78405) 470
 Medium: 75% acetone, 0.1 M NaClO4

C11H13NO3 H2L CAS 63467-38-9 (1961)
4-Methyl-N-hydroxyacetoacetanilide; CH3.CO.CH2.CO.N(OH).C6H4.CH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Y+++	gl	diox/w	20°C	82%	U			K1=7.16 B2=13.67 K3=6.09	1979KSb (78503)	471

C11H13NO4 L CAS 15658-60-3 (4587)
Diethyl 2,6-pyridinedicarboxylate; Dipicolinic acid diethyl ester;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Y+++	sp	non-aq	20°C	100%	C			K1=6.9 B2=13.50 B3=17.3	1997RPa (78540)	472

Medium: acetonitrile.

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
Y+++	gl	KNO3	25°C	0.10M	C			K1=13.63 K(Y+HL)=5.85 K(Y+2HL)=12.32	1989YSa (78645)	473

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
Y+++	sp	oth/un	25°C	?	U			K(Y+HL)=13.41	1974VKa (78683)	474

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
Y+++	gl	KNO3	25°C	0.10M	U			K1=6.84 B2=11.58	1964THa (78895)	475

C11H15NO5 HL CAS 1429-25-0 (2696)
3-Hydroxy-6-(hydroxymethyl)-2-(4-morpholinylmethyl)-4H-pyran-4-one;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Y+++	sp	KCl	25°C	0.10M	M	I		B(YHL)=11.57	1986POa (79054)	476

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

Y+++ vlt KNO3 20°C 0.10M U K1=18.78 1964ICb (79348) 477

C11H18N2O8 H4L CAS 38539-29-0 (2573)
1,3-Diaminopropane-N,N'-di(1,4-butanedioic acid)

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

Y+++ gl KNO3 25°C 0.10M U K1=10.18 1976GKd (79376) 478

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

Y+++ gl KNO3 20°C 0.10M U K1=14.40 1964LAa (79478) 479
Also K1=14.26

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

Y+++ gl KNO3 25°C 0.10M M K1=14.15 1986PLc (79580) 480

C11H18N2O9 H4L CAS 668-21-1 (2562)
2-Hydroxy-1,3-diaminopropane-N,N'-di(1,4-butanedioic) acid

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

Y+++ gl KNO3 25°C 0.10M U K1=11.05 1976GKd (79609) 481

C11H18O2 HL CAS 40072-58-3 (4820)
2-(3'-Methylbutanoyl)cyclohexanone (2-isovaleryl cyclohexanone);

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

Y+++ gl mixed 30°C 75% U K1=9.56 B2=18.16 1972DSd (79658) 482
Medium: 75% acetone

C11H18O2 HL CAS 5601-52-5 (4821)
2-Butanoyl-6-methylcyclohexanone (2-butyryl-6-methylcyclohexanone);

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

Y+++ gl mixed 30°C 75% U K1=10.58 B2=20.48 1972DSd (79669) 483

Medium: 75% acetone

C11H1809 H3L CAS 64020-00-4 (8225)

1,1,1-Tris(carboxymethoxymethyl)ethane;

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

Y+++ gl R4N.X 25°C 0.10M C K1=6.6 2001V5a (79678) 484

Medium: 0.10 M Me4NCl. Also data for N-ethyl-, N-phenyl-, N-NH2-,
N,N-dibenzyl- and N-CH2OCH2COOH- derivatives.

C11H2004 H2L CAS 2283-16-1 (2854)

2,2-Dibutylpropanedioic acid; HOOC.C(C4H9)2.COOH

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

Y+++ gl KNO3 25°C 0.10M U K1=4.67 B2=7.23 1968PFa (79774) 485

C11H26N206 L Bistris-propane CAS 64431-96-5 (7920)

1,3-Bis[tris(hydroxymethyl)methylamino]propane;

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

Y+++ gl NaClO4 25°C 0.10M C M K1=3.55 2001GYa (79959) 486

K(2Y+L+20H)=18.66

K(2Y+L+40H)=31.87

K(2Y+L+50H)=36.55

K(2Y+L+60H)=40.66

C12H10N6O4S H2L CAS 77327-19-6 (8343)

2-[4-Amino-3-(1,2,4-triazolylazo)]naphthol-4-sulphonic acid;

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

Y+++ gl NaClO4 30°C 0.10M U T H B2=13.13 1982GMb (80790) 487

B3=18.66

Data for 40 and 50 C. Also DH and DS values.

C12H11N3OS HL (6787)

2-Hydroxy-1-naphthaldehyde thiosemicarbazone;

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

Y+++ gl diox/w 20°C 75% U I K1=7.64 B2=14.77 1992SSc (80898) 488

Medium: 75% v/v dioxan/H2O; 0.1 M NaClO4

C12H11N3O2 HL CAS 50536-09-5 (6323)

2-Hydroxy-1-naphthaldehyde-semicarbazone; HO.C10H6.CH:N.NH.CO.NH2

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

Y+++ gl diox/w 20°C 75% U I K1=9.214 B2=16.715 1992SSc (80927) 489
Medium: 75% v/v dioxan/H2O; 0.1 M NaClO4

C12H12N03Cl HL (1055)
2-Chloro-4-dimethylamino-benzylidenepyruvic acid; (CH3)2N.C6H3Cl.CH:CH.CO.COOH

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

Y+++ sp NaClO4 25°C 0.50M U K1=1.942 1987MSa (80977) 490

C12H13N03 HL (1054)
4-Dimethylamino-benzylidenepyruvic acid; (CH3)2N.C6H4.CH:CH.CO.COOH

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

Y+++ sp NaClO4 25°C 0.50M U K1=2.062 1987MSa (81207) 491

C12H16N2O8 H4L (6460)
1,4-Diaminobut-2-yne-N,N,N',N'-tetraethanoic acid;
(HOOC.CH2)2N.CH2.CC.CH2.N(CH2.COOH)2

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

Y+++ gl KCl 25°C 0.10M U K1=8.12 1979TSa (81605) 492
K(Y+HL)=6.05
K(Y+YL)=5.5

C12H17N04 HL (2695)
3-Hydroxy-6-(hydroxymethyl)-2-(1-piperidinylmethyl)-4H-pyran-4-one;

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

Y+++ sp KCl 25°C 0.10M M I B(YHL)=14.16 1986POa (81719) 493

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

Y+++ gl KNO3 25°C 0.10M C K1=5.52 B2=10.06 1988YSa (81822) 494

C12H18N2O8 H4L CAS 76079-31-7 (2587)
trans-1,2-Diaminocyclohexane-N,N'-di(propanedioic acid)

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

Y+++ EMF KNO3 25°C 0.10M U K1=13.85 1985SGa (81883) 495

Y+++ EMF KNO3 25°C 0.10M U K1=15.02 B2=19.22 1980SGb (81884) 496

C12H18N2O8 H4L (8011)

trans-1,4-Diaminobuten-2-N,N,N',N'-tetraethanoic acid

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

Y+++ gl KCl 20°C 0.10M U K1=9.10 1976TTb (81895) 497

K(Y+HL)=6.34

K(YL+Y)=4.9

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

Y+++ gl KNO3 25°C 0.10M U K1=8.50 1973GBd (82109) 498

C12H20N2O8 H4L CAS 40623-42-5 (3388)

1,2-Diaminoethane-N,N'-diethanoic-N,N'-dipropanoic acid;

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

Y+++ gl NaClO4 25°C 0.10M U IH K1=13.52 1988RNa (82182) 499

B(Y+HL)=6.29

DH(K1)=6.81 kJ mol⁻¹, DH(Y+HL)=30.6, DS(K1)=282 J K⁻¹ mol⁻¹

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

Y+++ gl NaClO4 25°C 0.50M M H K1=10.11 1985CBa (82241) 500

K(YL+H)=6.63

K(YHL+H)=5.48

DH(K1)=23.9 kJ mol⁻¹, DS=274 J K⁻¹ mol⁻¹ (by calorimetry)

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

Y+++ EMF KNO3 20°C 0.10M U K1=17.54 1962MMc (82573) 501

Y+++ ix R4N.X 20°C 0.10M U I K1=17.92 1962STc (82574) 502

At pH 3.0. At pH 3.5, K1=17.77. At I=0.5 M, pH 2.6: K=17.66

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
Y+++	gl	alc/w	25°C	100%	C		K1=8.66	1983ANb (83916)	503
The equilibration took 7-12 days. Medium: MeOH, 0.05 M Et4NClO4									

C12H30N6		L					CAS 296-35-5	(143)	
1,4,7,10,13,16-Hexaazacyclooctadecane; cyclo(-(NH.CH2.CH2)6-)									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Y+++	gl	NaNO3	25°C	0.20M	C		K1=8.52	1991KKa (84362)	504

C13H11NOS		H2L					(7306)		
2-(Salicylideneamino)thiophenol, Salicylaldehyde-2-mercaptoanil; HO.C6H4.CH:N.C6H4.SH									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Y+++	gl	alc/w	25°C	70%	U		K1=14.17 B2=25.59	1995IFa (85050)	505
Medium: 70% v/v EtOH/H2O, 0.10 M NaCl.									

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
Y+++	gl	diox/w	25°C	50%	U		K1=7.73 B2=14.73 B3=20.81	1972GDb (85185)	506
Medium: 50% dioxan, 0.25 M NaClO4									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Y+++	gl	mixed	25°C	75%	U		K1=8.0 B2=14.32	1969DSb (85186)	507
Medium: 75% dioxan, 0.1 M NaClO4									

C13H11NO5S		H2L					CAS 23117-22-8	(6287)	
N-Benzoyl-4-hydroxylaminobenzene sulfonic acid; C6H5.CO.N(OH).C6H4HSO3									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Y+++	gl	NaNO3	30°C	0.50M	U		K1=5.58 B2=10.47 B3=14.05	1976GMc (85223)	508

C13H11NS		HL					CAS 42152-36-3	(8401)	
2-[(Phenylmethylene)amino]benzenethiol;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Y+++	gl	alc/w	25°C	70%	U		K1=11.31 B2=20.94	1995IFa (85234)	509
Medium: 70% v/v EtOH/H2O, 0.10 M NaCl. Also data for p-Cl, p-NMe2, p-OH, p-OCH3, p-CH3, p-NO2 substituted benzaldehyde Schiff bases.									

C13H15N06 H3L (660)
2-(Carboxymethyl)benzylamine-N,N-diethanoic acid;

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

Y+++ gl KNO3 30°C 0.10M U K1=9.55 1985ZXa (85725) 510

C13H15N06 H3L (4999)
2-Benzylnitriilotriethanoic acid;

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

Y+++ oth oth/un 25°C 0.10M U K2=8.94 1962HKa (85746) 511

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

Y+++ gl KNO3 25°C 0.10M C K1=10.36 1982PPd (86211) 512
K(Y+HL)=6.82

C13H22N2O9 H4L DETAP CAS 36829-96-6 (5602)
Bis(2-aminoethyl)ether-N,N,N'-triethanoic acid-N'-(3-propanoic acid);

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

Y+++ gl KNO3 25°C 0.10M C K1=14.28 1985PLa (86313) 513
K(Y+HL)=8.77

C14H8O4 H2L Alizarin CAS 72-48-0 (1058)
1,2-Dihydroxyanthraquinone;

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

Y+++ gl oth/un 25°C 0.10M U K1=12.55 1981EIa (86653) 514

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

Y+++ gl alc/w 25°C 20% U M K1=5.78 B2=10.43 1988SIa (86816) 515
Medium: 20% EtOH/H2O (v/v), 0.1 NaClO4. Ternary complexes with salicylic
acid, sulfosalicylic acid, nitrosalicylic acid, phen and bpy

C14H11N5O8S2 H5L CAS 1105-53-9 (5084)
1,5-Bis(2-hydroxy-5-sulfophenyl)-3-cyanoformazan;

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

 Y+++ gl NaNO3 20°C 0.10M U K1=14.57 1971SEa (87022) 516

 C14H14N2O2 HL (6168)
 N-(2-Hydroxy-3-methoxybenzylidene)phenylhydrazine; C6H5.NH.N:CH.C6H3(OH)OCH3

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

Y+++ gl diox/w 30°C 75% U K1=9.03 B2=17.65 1988MKd (87660) 517

 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

Y+++ ISE R4N.X 25°C 0.10M C K1=2.38 1986XJa (88386) 518

 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

Y+++ gl NaClO4 25°C 0.50M U K1=18.83 1977GGb (88818) 519

Y+++ EMF KNO3 25°C 0.10M U T H K1=19.14 1962MHa (88819) 520
 DH(K1)=17.6 kJ mol⁻¹, DS=431 J K⁻¹ mol⁻¹. At 20 C: K(YL+H)=2.18

Y+++ vlt KNO3 20°C 0.10M U K1=19.15 1954SGa (88820) 521

 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

Y+++ sp R4N.X 25°C 0.10M C K1=22.5 1994KCa (89433) 522
 Medium: Me4NCl

Y+++ cal NaClO4 25°C 0.10M C H 1987YJa (89434) 523
 DH(K1)=-14.2 kJ mol⁻¹, DS(K1)=374 J K⁻¹ mol⁻¹.

Y+++ cal NaClO4 25°C 0.50M U H 1977CGc (89435) 524
 DH(K1)=-36.3 kJ mol⁻¹

Y+++ gl NaClO4 25°C 0.50M U K1=20.39 1977GGb (89436) 525

Y+++ sp oth/un 20°C dil U K1=21.95 1969Kaf (89437) 526

Y+++ EMF KNO3 25°C 0.10M U H K1=22.05 1962MTc (89438) 527
 DH(K1)=-21.8 kJ mol⁻¹, DS=349 J K⁻¹ mol⁻¹

Y+++ ix R4N.X 20°C 0.10M U K1=22.28 1962STc (89439) 528

Y+++ gl oth/un 25°C 0.10M U K1=22.40 1959HCa (89440) 529

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

Y+++ gl KCl 25°C 1.00M U M 1976BKa (89616) 530

K(YEDTA+L)=2.8
K(YEDTA+HL)=2.6
K(2YEDTA+L)=5.6

Y+++ gl KCl 25°C 0.10M U 1974KPd (89617) 531

K(Y+HL)=6,87

C14H24N2O10 EGTA CAS 67-42-5 (349)
Ethyleneglycol-0,0'-bis(2-aminoethyl ether)-N,N,N',N'-tetraethanoic acid; H4L

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

Y+++ gl NaNO3 25°C 0.0 U K1=17.10 1996KDb (89963) 532

Extrapolated from data for I=0.05-0.15 M NaNO3.

Y+++ gl NaNO3 25°C 0.10M U I K1=17.01 1996KDC (89964) 533

Data for 0.05 and 0.15 M NaNO3. At I=0, K1=17.18.

Y+++ gl NaNO3 25°C 0.10M M K1=16.95 1996KDD (89965) 534

Data for 0.05-0.15 M NaNO3. At I=0, K1=17.10.

Y+++ gl NaNO3 25°C 0.10M M I K1=16.95 1995KDB (89966) 535

Data for 0.05 and 0.15 M NaNO3. At I=0, K1=17.10.

Y+++ gl NaNO3 25°C 0.10M M I K1=16.95 1995KDC (89967) 536

Data for 0.05 and 0.15 M NaNO3. At I=0, K1=17.10.

Y+++ gl NaNO3 25°C 0.10M M I K1=16.951 1995KDD (89968) 537

Data for 0.15 and 0.05 M NaNO3. At I=0, K1=17.183.

Y+++ EMF KNO3 20°C 0.10M U K1=16.82 1962MMc (89969) 538

C14H24O9 H3L CAS 64020-01-5 (8224)

1,1,1-Tris[(2-carboxyethoxy)methyl]ethane;

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

Y+++ gl R4N.X 25°C 0.10M C K1=3.65 2001VSA (90055) 539

K(YL+H)=4.30

Medium: 0.10 M Me4NCl. Also data for N-ethyl-, N-CH2OH-, N-CH2O(CH2)2COOH-

derivatives.

C14H25N3O8 H4L DEATA CAS 97315-55-4 (5601)
N,N-Bis(2-aminoethyl)ethylamine-N',N',N'',N''-tetraethanoic acid;

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

Y+++ gl KNO3 25°C 0.10M C K1=17.13 1985TPa (90109) 540

C14H25N3O9 H4L CAS 4454-15-3 (5078)
(N-(2-Hydroxyethyl)-2,2'-iminodiethylene)dinitrilo)tetraethanoic acid;

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

Y+++ vlt KCl ? 0.10M U K1=13.21 1968VLa (90120) 541

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

Y+++ gl R4N.X 25°C 0.10M M K1=10.85 1986COB (90212) 542

C14H26N4O6 H3L DOTRA (6701)
1,4,7,10-Tetraazacyclododecane-1,4,7-triethanoic acid;

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

Y+++ sp R4N.X 25°C 0.10M C K1=21.1 1994KCa (90256) 543

Medium: Me4NCl

C15H12OS HL (1261)
mono-Thiodibenzoylmethane; C6H5.CO.CH2.CS.C6H5

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

Y+++ gl NaClO4 30°C 0.05M U K1=7.34 B2=14.04 1979VMa (91507) 544

K3=6.34

C15H13N3O HL CAS 104992-04-3 (6852)
2-((1H-Benzimidazo-2-yl-methyl)-iminomethyl)phenol;

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

Y+++ gl alc/w 30°C 60% U M K1=6.57 B2=12.70 1990DOb (91667) 545

K(YA+L)=5.27

K(YB+L)=5.07

K(YC+L)=4.66

H2A=iminodiethanoic acid, H3B=hydroxyethyliminodiethanoic acid, H3C=NTA.

Data also for 3-chloro and 3-methoxysalicylidene analogues

 C15H14NOCl HL CAS 268214-29-5 (8398)
 4-Chloro-3,5-dimethyl-2-[(phenylimino)methyl]phenol;

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

 Y+++ gl diox/w 30°C 75% M K1=7.42 2000ANa (91697) 546
 Medium: 75% v/v dioxan/H2O, 0.10 M NaClO4. Data for an extensive series of
 4'-substituted phenylimino derivatives.

 C15H20N2O6 H3L BEDTA CAS 65311-06-0 (2944)
 N-Benzylidiaminoethane-N,N',N'-triethanoic acid;

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

 Y+++ gl KNO3 25°C 0.10M C K1=12.69 1978MPb (92160) 547

C15H23N3O2 L CAS 36763-33-4 (5176)
 N,N,N',N'-Tetraethyl-2,6-pyridinedicarboxamide;

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

 Y+++ sp non-aq 25°C 100% M K1=7.6 B2=14.60 1997RPb (92292) 548
 B3=22.4

Medium: acetonitrile.

C15H25N3O10 H5L (5127)
 Diethylenetriamine-N,N,N'',N''-tetraethanoic acid-N'-propanoic acid;

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

 Y+++ EMF KCl ? 0.10M U K1=16.52 1966VLa (92386) 549

C15H36N3O9P3 H3L (6749)
 1,4,7-Triazacyclononane-N,N',N''-tris(methylenephosphonate monoethyl ester)

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

 Y+++ gl R4N.X 25°C 0.10M C K1=10.4 1992LRa (92614) 550

C16H11N3O10S2 H4L Chromotrope 2B CAS 548-80-1 (896)
 2-((4-Nitrophenyl)azo)chromotropic acid;

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

 Y+++ sp oth/un 25°C ? U 1964MDc (92871) 551
 K1eff=4.7 (pH 6.0)

 C16H12N3O4ClS H2L CAS 133131-00-7 (8468)
 7-Amino-8-[(4-chlorophenyl)azo]-4-hydroxy-2-naphthalenesulfonic acid;

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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Y+++      gl  NaCl   25°C 0.10M U          K1=6.53  B2=12.56  1997IHa (93122) 552
                                     B3=18.21

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Also data for the 4'-fluoro-, 4'-nitro-, 4'-methoxy-, 4'-dimethylamino-,
4'-hydroxy-, 4'-carboxy-, 4'-AsO(OH)2-, 2'-hydroxy- analogue

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C16H13N2O10AsS2      H5L      Thorin I          CAS 3688-92-4 (2609)
1-((2-Arsonophenyl)azo)-2-hydroxy-3,6-naphthalylidylsulfonic acid;

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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Y+++      gl  NaClO4 30°C 0.10M U          K(Y+H2L=YH2L)=5.66
                                     K(YHL+H)=7.21
                                     K(YL+H)=9.57
                                     K(YL+OH)=2.81

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C16H13N2O11AsS2 H6L Arsenazo I CAS 520-10-5 (277)
2-(2'-Arsonophenylazo)chromotropic acid;

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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Y+++      sp  oth/un 20°C 0.10M U          K(Y+H2L)=9.60

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C16H14O4 HL BHMMA (5929)
omega-Benzoyl-2-hydroxy-4-methoxy-3-methylacetophenone;

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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Y+++      gl  alc/w  30°C 25% M          K1=6.70  B2=12.82  1987DGb (93587) 555
Medium: 25% v/v EtOH/H2O

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C16H23NO8 L CAS 53408-96-1 (1765)
2,3-(4'-Nitrobenzo)-1,4,7,10,13,16-hexaoxacyclooctadeca-2-ene;
4'-Nitrobenzo-18-crown-6

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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Y+++      ISE R4N.X 25°C 0.10M C          K1=3.26          1986XJa (94275) 556

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C16H27N3O9 H4L (5673)
N'-(Allyloxyethyl)diethylenetriamine-N,N,N",N"-tetraethanoic acid;

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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Y+++      gl  KCl    20°C 0.10M U          K1=18.81          1982TIa (94653) 557

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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

Y+++ gl R4N.X 25°C 0.10M U K1=24.9 1991BCc (94936) 558
Medium: 0.1 M Me4NNO3

Y+++ gl R4N.X 25°C 0.10M U K1=24.9 1989CJa (94937) 559
Medium: 0.10 M Me4NNO3.

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

Y+++ dis NaClO4 21°C 0.10M C I K1=5.7 B2=10.70 1978NMb (95907) 560
B3=14.9

Method: distribution of 90Y between 0.10 M NaClO4 solution and benzene.
Data for 1.0 M NaClO4 and for distribution into CHCl3 and toluene.

C17H14N2O5S H3L Calmagite CAS 3147-14-6 (2875)
1-(1-Hydroxy-4-methyl-2-phenylazo)-2-naphthol-4-sulfonic acid;

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

Y+++ gl NaClO4 25°C 0.10M M K1=15.70 B2=23.55 1978MPd (95932) 561
K3=5.90

C17H16O4 H2L CAS 58134-82-0 (6193)
Benzoyl-2-hydroxy-4-methoxy-3-methylacetophenone;
C6H5.CO.CH2.CO.C6H2(OH)(OCH3)(CH3)

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

Y+++ gl alc/w 30°C 75% U M B2=14.00 1991GDd (96165) 562
Medium: 75% v/v EtOH/H2O, 0.1 M NaClO4. K(Y(Acetylacetone)+L)=12.00

Y+++ gl alc/w 30°C 75% U T H K1=7.75 B2=14.70 1987DGd (96166) 563
20 C:K1=7.64, K2=7.14; 40 C:K1=8.02, K2=7.12; 50 C:K1=8.40, K2=8.06
DH(K1)=-31 kJ mol⁻¹, DS=50 J K⁻¹ mol⁻¹

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

Y+++ gl R4N.X 25°C 0.10M U K1=19.6 1991BCc (96663) 564
Medium: 0.1 M Me4NNO3

Y+++ gl R4N.X 25°C 0.10M U K1=19.6 1989CJa (96664) 565
Medium: 0.10 M Me4NNO3.

C17H32N4O6 H3L (6696)
1,4,7,10-Tetraazacyclododecane-1,4,7-tri(2-methyl)ethanoic acid;
C8H17N4(CH(CH3)COOH)3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Y+++ sp R4N.X 25°C 0.10M U K1=25.2 1993KRb (96690) 566

C17H32N4O7 H3L CAS 120041-08-9 (6702)
10-Hydroxypropyl-1,4,7,10-tetraazacyclododecane-1,4,7-triethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Y+++ sp R4N.X 25°C 0.10M C K1=22.2 1994KCa (96721) 567
Medium: Me4NCl

C18H14N2O2 HL CAS 15017-21-7 (6859)
2-Hydroxynaphthalidene benzoyl hydrazone; C6H5.CO.NH.N:CH.C10H6.OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Y+++ gl diox/w 20°C 75% U T HM K1=8.99 B2=17.64 1994Mca (96912) 568
B3=24.48
K(Y(edta)+L)=3.36
K(Y(Hedta)+L)=3.44
K(Y(nta)+L)=3.58

Medium: 75% v/v dioxane/H2O, 0.10 M NaClO4. Data for 30 and 40 C.
DH and DS values.

C18H14N2O3 H2L CAS 54009-54-0 (6860)
2-Hydroxynaphthalidene salicylic hydrazone; HO.C6H4.CO.NH.N:CH.C10H6.OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Y+++ gl diox/w 20°C 75% U T HM 1994Mca (96922) 569

K(Y+HL)=7.64
K(Y+2HL)=14.92
K(Y+3HL)=20.83
K(Y(nta)+L)=3.54

Medium: 75% v/v dioxane/H2O, 0.10 M NaClO4. Data for 30 and 40 C.
K(Y(edta)+L)=3.02, K(Y(Hedta)+L)=3.23. DH and DS values.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Y+++ gl diox/w 20°C 75% U T HM 1994Mca (96923) 570
K(Zr+HL)=6.94
K(Zr+2HL)=13.53
K(Zr+3HL)=18.74
K(Zr(nta)+L)=4.08

Medium: 75% v/v dioxane/H₂O, 0.10 M NaClO₄. Data for 30 and 40 C.

K(Zr(edta)+L)=3.33, K(Zr(Hedta)+L)=3.68. DH and DS values.

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

Y+++ EMF KNO₃ 25°C 0.10M C T H K1=19.48 1985HWb (97443) 571
K(YL+H)=7.25

Method: Hg (and glass) electrode, using Hg(II) as competitive indicator ion. Data for 10-35 C. DH(K₁)=-48.7 kJ mol⁻¹, DS(K₁)=210 J K⁻¹ mol⁻¹.

C18H₂₆N₆ L (6628)
3,6,14,17,23,24-Hexaazatricyclo[17.3.1.1]tetracos-1(23),8,10,12(24),19,21-hexaene;

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

Y+++ gl KCl 25°C 0.10M M K1=7.1 1996MBb (97725) 572

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

Y+++ gl R4N.X 25°C 0.10M U K1=16.1 1991BCc (98233) 573
Medium: 0.1 M Me₄NNO₃

Y+++ gl NaNO₃ 25°C 0.20M C K1=14.77 1991KKa (98234) 574

Y+++ gl R4N.X 25°C 0.10M U K1=16.3 1989CJa (98235) 575
Medium: 0.10 M Me₄NNO₃.

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

Y+++ cal non-aq 25°C 100% C H K1=11.16 2003DCa (98764) 576
Method: competitive titration calorimetry of AgL+. Medium: acetonitrile.
DH(K₁)=-198.3 kJ mol⁻¹, DS(K₁)=-451 J K⁻¹ mol⁻¹.

Y+++ gl alc/w 25°C 100% C K1=10.34 1983ANb (98765) 577
The equilibration took 7-12 days. Medium: MeOH, 0.05 M Et₄NC₁₀

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

Y+++ gl NaClO4 30°C 0.20M U M K1=9.81 1978MSk (99118) 578
K(Y(nta)+L)=7.74

C19H15N08 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

Y+++ con oth/un 25°C 0.10M U K1=4.13 B2=8.30 1981Eic (99142) 579

Y+++ sp KNO3 22°C 0.1M U 1975PTf (99143) 580
K(Y+H+L)=28.0
K(Y+HL)=16.84
K((Y+2H+L)=31.31
K(YHL+H)=3.28

C19H16N40 L LAMI (5930)
2-(2'-Lepidylazo)-N-methylisatin

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

Y+++ gl diox/w 30°C 75% M I K1=9.87 B2=19.19 1987DGc (99170) 581
Medium: 75% v/v dioxan/H2O, 0.15 M NaClO4

C19H19N07 H2L (7003)
3-Methoxy-5-(N,N-dicarboxymethyl)aminomethyl-4-hydroxybenzophenone;

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

Y+++ gl KCl 20°C 0.10M U K1=12.5 1981SYa (99259) 582
K(Y+HL)=6.5

C20H13N3O7S H3L Eriochrome Bl T CAS 1787-61-7 (997)
1-(1-Hydroxy-2-naphthylazo)-6-nitro-2-naphthol-4-sulfonic acid;

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

Y+++ gl NaClO4 25°C 0.10M M K1=10.70 B2=19.87 1978MPd (99578) 583
K3=5.35

C20H14N2O5S H3L Solochrome 6B CAS 3564-14-5 (3507)
1-(1-Hydroxy-2-naphthylazo)-2-naphthol-4-sulfonic acid, Mordant Black3, Eriochrome
blue-black B;

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

Y+++ gl alc/w 30°C 50% C M K1=11.99 B2=22.25 1994S0a (99668) 584
K(YA+L)=10.40
K(Y(nta)+L)=9.63

Medium: 50% v/v MeOH/H2O, 0.10 M NaClO4.
H2A is hydroxyethyliminodiethanoic acid.

Y+++ gl NaClO4 30°C 0.10M U T H K1=13.55 1991NNb (99669) 585
Also data for 40 and 50 C. DH and DS values.

Y+++ gl NaClO4 25°C 0.10M M K1=11.15 B2=21.15 1978MPd (99670) 586
K3=6.85

C20H35N5O10 H5L (6545)
1,4,7,10,13-Pentaazacyclopentadecane-N,N',N'',N''',N''''-pentaethanoic acid;

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

Y+++ gl NaNO3 25°C 0.20M C K1=16.07 1991KKa (100549) 587

C21H14O3 HL CAS 26073-81-4 (5306)
6,7-Dihydroxy-2,4-diphenylbenzopyranol,
6-hydroxy-2,4-diphenyl-7H-1-Benzopyran-7-one;

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

Y+++ sp oth/un ? ? U K(YOH+L)=9.36 1969PSf (101038) 588

C22H14O9 H5L CAS 4431-00-9 (3513)
Aurintricarboxylic acid;

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

Y+++ sp oth/un 25°C ? U K(Y+HL)=4.5(?) 1966MSc (101515) 589

C22H17AsN4O14S3 H6L Arsenazo M CAS 3563-69-7 (623)
2-(2-Arsonophenylazo)-7-(3-sulfophenylazo)-1,8-dihydroxynaphthalene-3,6-disulfonic
acid;

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

Y+++ sp NaClO4 25°C 0.1M U K(Y+H4L)=10.19 1975MBa (101557) 590

Room temperature

Y+++ sp oth/un ? ? U K1=15.59 1971SSi (101558) 591

C22H18N4O14As2S2 H8L Arsenazo III CAS 1668-00-4 (1148)
2,7-Bis(2'-arsonophenylazo)chromotropic acid;

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

Y+++ sp NaClO4 25°C 0.10M U 1975NMa (101659) 592
K(Y+H5L)=7.36

Y+++ dis KCl ? 0.30M U 1973AGb (101660) 593
K(2Y+2H4L)=22.56

Y+++ sp oth/un 20°C ? U 1972SSi (101661) 594
K(Y+H4L)=16.07

C22H19N3O4S HL CAS 84819-63-6 (8347)
N-(3,4-DiMe-5-isoxazolyl)-4-[[(2-hydroxy-1-naphthalenyl)methylene]amino]benzenesulfonamide;

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

Y+++ gl NaClO4 25°C 0.10M U K1=4.91 B2= 9.52 1982MBa (101690) 595

C22H20O13 H5L Carminic acid CAS 1260-17-9 (714)
Carminic acid;

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

Y+++ sp oth/un ? 0.10M U 1970PLc (101708) 596
K(YOH+2H3L)=17.76

C23H16O9Cl2S H4L Chrome azuro1 S CAS 1667-99-8 (711)
Chromazuro1 S;

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

Y+++ sp oth/un ? ? U M 1973GAb (102579) 597
K(YOH+phen+2H3L)=12.50

Y+++ sp oth/un 25°C ? U 1967SSi (102580) 598
K1eff=4.3 (pH 6.0)

C24H18N4O18As2S2 10L CAS 2604-69-5 (4164)
2,7-Bis(2'-arsono-5'-carboxyphenylazo)chromotropic acid;
H

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

Y+++ sp KNO3 20°C 0.20M U 1965BMD (102877) 599
B(YH12L2)=96.4

C24H42N6O12 H6L (6546)
1,4,7,10,13,16-Hexaazacyclooctadecane-N,N',N'',N''',N''',N''''-hexaethanoic acid;

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

Y+++ gl NaNO3 25°C 0.20M C K1=24.04 1991KKa (103390) 600
K(Y+H2L)=15.93

C25H28N2O13 H6L CAS 42281-29-8 (5335)
(Carbonylbis((6-hydroxy-5-methoxy-3-phenylene)methylenenitrilo))tetraethanoic acid;

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

Y+++ gl KCl 20°C 0.10M U K1=22.1 1973VIb (103667) 601
K(Y+HL)=16.1
K(Y+H2L)=10.2
K(Y+H3L)=6.4
K(YOH+L)=4.4

C26H34N6O8 H4L CAS 132709-65-0 (8941)
3,6,14,17,23,24-Hexaazatricyclo[2.3.1.1.0.0.0]dotriaconta-1,8,10,12,19,21-hexaene-3,6,14,17-tetraene
tic acid;

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

Y+++ gl KCl 25°C 0.10M M K1=ca. 20 1996MBb (104102) 602
K(YL+H)=4.2
K(YHL+H)=2.4

C26H38N6 L CAS 180684-75-7 (7295)
1,8,14,17,24,31-Hexaazatricyclo[25.3.1.1.0.0]dotriaconta-10,12,14,26,28,

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

Y+++ gl KNO3 25°C 0.20M C K1=5.0 1996FJa (104210) 603

C28H24N2O2 H2L Solvent Green 3 CAS 128-80-3 (1021)
1,4-Bis(4'-methylanilino)anthraquinone;

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

Y+++ sp mixed 20°C 40% U 1984IHa (104669) 604
K(Y+H3L=YHL+2H)=-7.03
Medium: 40% DMF, 0.1 M NaClO4

C31H32N2O13S H6L Xylenol orange CAS 63721-85-5 (432)
5,5'-Bis-N,N-bis(carboxymethyl)aminomethyl-4'-hydroxy-3,3'-dimethylfuchson-2''-sulf
onic acid;

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

Y+++ sp NaClO4 20°C 0.20M U 1966KSd (105511) 605
K(Y+HL)=12.81

Y+++ sp oth/un 25°C ? U 1962TOa (105512) 606

K(?)=5.5

Acetate buffer

C36H48O6 L CAS 76543-12-9 (7372)

p-tert-Butyloxacalix[3]arene;

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

Y+++ nmr non-aq 25°C 100% U 1997HDa (106392) 607

Keff(YA3+H3L=YL+3H+3A)=-23.2

Medium: DMSO; 0.2 M 1,4-Diazabicyclo[2.2.2]octane, pH 8.5. A=triflate.

For p-chlorooxacalix[3]arene, Keff(YA3+H3L=YL+3H+3A)=-17.57

C37H44N2O13S H6L MeThymo1 Blue (428)

3,3'-Bis(N,N-di(carboxymethyl)aminomethyl)thymolsulfonephthalein;

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

Y+++ gl NaCl04 30°C 0.10M U 1980NAb (106625) 608

K(Y+H3L)=4.39

K(Y+H2L)=6.92

K(YH2L+H)=4.61

Also data for YHnL(OH) species

Y+++ sp NaNO3 ? 0.20M U 1965TRa (106626) 609

B(Y2H2L2)=50.4

K(Y2HL2+H)=8.0

K(Y2L2+H)=9.5

C37H54N6O14S L CAS 357165-79-8 (8003)

1-[5-Dimethylaminonaphthalene-1-sulfonyl-aminoethyl]-4,7,10-tris[3'-carboxyl-1'-carboxypropyl]cyc

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

Y+++ sp NaCl 22°C 0.10M C 2001LPc (106638) 610

K(YL+H)=6.21

K(YHL+H)=3.73

C45H66N10O6 L CAS 362613-35-2 (7912)

Tris[3-(6-diethylcarbamoilpyridine-2-carboxamide)propyl]amine;

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

Y+++ sp non-aq 25°C 100% C I K1=7.1 2001RDa (107234) 611

K(Y+HL)=6.5

Medium: CH3CN. In 95% v/v CH3CN/H2O, K1=4.9, K(Y+HL)=5.1.

C62H94N2O4S2 L (8109)

5,11,17,23-Tetrakis(1,1-dimethylethyl)-25-27-bis[2-methylthio)ethoxy]...calix(4)are

ne;

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

Y+++ cal non-aq 25°C 100% U H K1=4.42 2001NJa (107710) 612
Method: microcalorimetry. Medium: MeCN.. DH(K1)=-94 kJ mol⁻¹

Y+++ cal non-aq 25°C 100% U H K1=4.57 2001NJa (107711) 613
Method: microcalorimetry. Medium: MeCN.. DH(K1)=-188 kJ mol⁻¹

C76H116N4O8 L (8156)
p-tert-Butylcalix(4)arene tetradiisopropylethanoamide;

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

Y+++ cal non-aq 25°C 100% U H K1=4.96 2001NJa (107887) 614
Method: microcalorimetry. Medium: MeCN.. DH(K1)=-70.8 kJ mol⁻¹

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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

END