SC-Database
Software version = 5.81 Data version = 4.62
Experiment list contains 1225 experiments for
 (no ligands specified)
 Metal : Ba++
 (no references specified)
 (no experimental details specified)

****
e- HL Electron (442)
Electron;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ EMF none 25°C 0.00 U 1972KKb (361) 1
K(Ba+2e=Ba/Hg)=-56.15(-1.661V)

Ba++ oth none 25°C 0.0 U I 1962JTa (362) 2
K(Ba+2e)=-98.45(-2912 mV)
Method:combination of thermodynamic data. In MeOH: K=-99.50(-2943 mV)
****
AsO4--- H3L Arsenate CAS 7778-39-4 (1557)
Arsenate;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ oth none 25°C 0.0 M 1997SAb (1130) 3
Ks(Ba3(AsO4)2(s)+2H=3Ba+2HAsO4)=-26.50. Calc. from thermodynamic data
---
Ba++ sol oth/un 20°C var U 1956CHd (1131) 4
Kso(Ba3L2)=-50.11
****
AsW11O39------- H7L (2468)
alpha-Heteromonoarseno-polytungstate;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl NaNO3 25°C 1.00M U K1=3.53 1984COa (1176) 5
****
BO4H4- HL Borate CAS 10043-35-3 (991)
Borate; B(OH)4-

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl none 25°C 0.0 M TIH 1976REa (1304) 6
K(Ba+H2BO3)=1.49
Calculated from data for 0.02-0.16 M BaCl2. Data for 10-50 C.
DH(Ba+H2BO3)=3.1 kJ mol-1, DS=39 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
Ba++	sol	NaCl	25°C	1.0M	C	I	K(BaL(s)=Ba+L)=-6.87	1984MTb (3145)	7
I=0.1-6 M.Activity coeff. estimated from Pitzer's eq. At I=0 corr:K=-8.56									
Ba++	sol	none	25°C	0.0		U	Kso=-5.48	1973BSd (3146)	8
Ba++	EMF	none	30°C	0.0		U	Kso=ca.-8.1(resin membrane electrode)	1969GSb (3147)	9
Ba++	gl	none	25°C	0.0		U	K(Ba+HL)=1.52	1969NRa (3148)	10
Ba++	sol	oth/un	25°C	0.0		U	Kso=-9.40	1968BBf (3149)	11
Ba++	oth	none	25°C	0.0		U T	Kso=-8.25	1968KRa (3150)	12
Method: Estimated data. Temperature range 25-250 C Kso=-8.28(50 C); -8.63(100 C); -9.25(150 C); -10.04(200 C); -10.96(250 C)									
Ba++	EMF	none	25°C	0.0		U	Kso(BaCO3(s))=-8.29	1946NAa (3151)	13
Method: H electrode. I=0 corr.									
Ba++	sol	oth/un	25°C	0.0		U T	Kso=-8.69	1939HJa (3152)	14
Medium: 0 corr. Kso=-8.56(40 C)									
Ba++	sol	none	25°C	0.0		U T	K(BaCO3(s)=Ba+CO3)=-9.26	1937TWa (3153)	15
Extrapolated to zero ionic strength. T: 25-40C. At 40C, K=-9.53									
Ba++	sol	none	25°C	0.0		U	Kso(BaCO3(s))=-8.31 +Kpso=-5.82	1935KAa (3154)	16
I=0 corr. +Kpso: BaCO3(s)+CO2(g)+H2O=Ba+2HCO3									
Ba++	oth	none	rt	0.0		U	Kso(BaCO3(s))=-7.77	1926HBa (3155)	17
Method: tyndallometry. I=0 corr.									
Ba++	sol	none	16°C	0.0		U	Kso(BaCO3(s))=-8.15	1915JOa (3156)	18
Ba++	sol	none	16°C	0.0		U T		1914WEa (3157)	19

```
                                        Kso(BaCO3(s))=-8.71
Kso(BaCO3(s)/Kso(BaSO4(s))=0.61(16 C), 0.59(25 C), 0.61(38 C)
--------------------------------------------------------------------------------
Ba++       sol none   25°C  0.0  U                      1911MSa  (3158)  20
                                        Kso(BaCO3(s))=-8.09
                                        +Kso=-4.35
I=0 corr. +Kso: BaCO3(s)+H2CO3=Ba+2HCO3
--------------------------------------------------------------------------------
Ba++       sol none   16°C  0.0  U                      1900BOa  (3159)  21
                                        Kso(BaCO3(s))=-8.71
********************************************************************************
C6N6Fe----            H4L                        (2191)
Hexacyanoferrate (II); Fe(II)(CN)6----
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Ba++       ISE oth/un 25°C 0.00  U   H    K1=3.78        1975JLa  (3556)  22
DH=17.5 kJ mol-1
--------------------------------------------------------------------------------
Ba++       EMF oth/un 25°C  3.0M U        K1=1.16        1975LMd  (3557)  23
Background salt: LiClO4
--------------------------------------------------------------------------------
Ba++       sp  none   25°C  0.0  U        K1=3.80        1957CPa  (3558)  24
Also K1 for iso-PrOH/H2O mixtures
********************************************************************************
C6N6Fe---             H3L    Ferricyanide       (2491)
Hexacyanoferrate (III); Fe(III)(CN)6---
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Ba++       cal oth/un 25°C 0.10M U        K1=1.53        1982ARa  (3630)  25
--------------------------------------------------------------------------------
Ba++       EMF oth/un 25°C  3.0M U        K1=0.36        1975LMd  (3631)  26
Background salt: LiClO4
--------------------------------------------------------------------------------
Ba++       sol oth/un 25°C  3.0M U   H    K1=-0.60       1966MRb  (3632)  27
Medium: LiCl. By calorimetry: DH(K1)=-15.5 kJ mol-1, DS=-63 J K-1 mol-1
--------------------------------------------------------------------------------
Ba++       con none   25°C  0.0  U        K1=2.88        1952GMb  (3633)  28
********************************************************************************
C6O3                   L    Benzenetrioxide  CAS 264911-91-3  (6002)
cis-Benzenetrioxide;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Ba++       nmr alc/w  25°C 100%  U   H    K1=1.90        1987BBc  (3698)  29
In MeOH. DH=-7.9 kJ mol-1 by calorimetry
********************************************************************************
Cl-                    HL    Chloride         CAS 7647-01-0  (50)
Chloride;
```

```
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Ba++       con alc/w  25°C 100%  C T H    K1=2.67        1987DWa  (4511)  30
Medium: MeOH, DH(K1)=21.1 kJ mol-1, DS(K1)=122 J K-1 mol-1
--------------------------------------------------------------------------------
Ba++       ISE alc/w  25°C 100%  U        K1=2.48        1984DMa  (4512)  31
Medium: MeOH, 0.05 M NaClO4
--------------------------------------------------------------------------------
Ba++       gl  KNO3   25°C 3.00M U T H    K1=-0.48       1982MSb  (4513)  32
K1=-0.61(15 C), K1=-0.2(45 C), K1=-0.16(65 C), K1=-0.18(85 C)
DH=25.0 kJ mol-1, DS=75 J mol-1 K-1
--------------------------------------------------------------------------------
Ba++       con alc/w  25°C 100%  U        K1=2.63        1978LWb  (4514)  33
--------------------------------------------------------------------------------
Ba++       EMF NaNO3  25°C 0.10M C T H    K1=-0.44       1975SCd  (4515)  34
Method: Ag,AgCl electrode. Data for 15-60 C.
DH(K1)=-11.3 kJ mol-1, DS(K1)=-46.4 J K-1 mol-1.
--------------------------------------------------------------------------------
Ba++       EMF non-aq 25°C 100%  U        B2=3.45        1971DTb  (4516)  35
Medium: SeOCl2, 0.5 M Et4NClO4
--------------------------------------------------------------------------------
Ba++       ix  NaClO4   ?   1.0M U        K1=-0.7        1969PSa  (4517)  36
--------------------------------------------------------------------------------
Ba++       con non-aq 520°C 100%  U T      K1=3.0    B2=5.00   1968RFb  (4518)  37
Medium:BaCl2 var. K1=1.4(255 C), 1.7(298 C), 2.5(420 C);
K2=1.76(420 C); at p=1.0 g cm-3, also values at p=0.5-0.9
--------------------------------------------------------------------------------
Ba++       con none   18°C  0.0  U        K1=-0.13       1935MDa  (4519)  38
********************************************************************************
ClO3-                  HL    Chlorate         CAS 7790-93-4  (971)
Chlorate;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Ba++       sol none   25°C  0.0  U        K1=0.7         1935MDa  (6030)  39
********************************************************************************
ClO4-                  HL    Perchlorate      CAS 7001-90-3  (287)
Perchlorate;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Ba++       con mixed  25°C  20%  C        K1=1.22        2003SIa  (6148)  40
Medium: 20% w/w propylene carbonate/ethylene carbonate.
--------------------------------------------------------------------------------
Ba++       con non-aq 25°C 100%  C        K1=1.34        1992STa  (6149)  41
Medium: propylene carbonate.
--------------------------------------------------------------------------------
Ba++       con alc/w  30°C 100%  C TIH    K1=2.50        1990DOd  (6150)  42
Medium: MeOH. DH(K1)=16.1 kJ mol-1, DS=105 J K-1 mol-1. Also in ethylene
```

glycol/MeOH mixtures (0,20,40,60,80,100%)

Ba++ con alc/w 25°C 100% C T H K1=2.65 1987DWa (6151) 43
Medium: MeOH, DH(K1)=16.5 kJ mol-1, DS(K1)=106 J K-1 mol-1

****

CrO4-- H2L Chromate CAS 7738-94-5 (2382)
Chromate;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Ba++	sol	NaClO4	20°C	0.36M	U	TI		1972LLc	(6470)	44
							Kso=-8.693			

I=0.01, Kso-9.532; I=0.04, Kso=-9.252; I=0.16, Kso=-9.912, I=0, Kso=-9.87
Data also at 25 C, 1 M KCl: I=0(corr), Kso=-9.67

Ba++	oth	oth/un	20°C	0.50M	U			1963KOd	(6471)	45
							K=-2.76			

K: 2BaCrO4(s)+2H=2Ba+Cr2O7+H2O. Method:refractometry

Ba++	kin	oth/un	300°C	100%	U			1958DIb	(6472)	46
							Kso=-5.3(kinetic methods)			
							Kso=-5.4(solubility)			

Medium:(Na,K)NO3(liquid,eutectic);in m units

Ba++	sol	none	100°C	0.0	U			1951KOa	(6473)	47
							Kso=-7.82			

Ba++	sol	none	25°C	0.0	U			1943BRa	(6474)	48
							Kso=-9.93			

Ba++	oth	none	18°C	0.0	U	T		1923BOa	(6475)	49
							Kso=-9.80			

Kso=-9.62(28.1 C)

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Ba++	gl	alc/w	25°C	100%	C		K1=5.0	B2=9.4	1988TIa (6757)	50

Ba++	gl	KNO3	25°C	3.00M	U	T H	K1=-0.18		1982MSb	(6758) 51

K1=-0.24(15 C), K1=-0.03(45 C), K1=0.11(65 C), K1=0.19(85 C)
DH=12.9 kJ mol-1, DS=40.1 J mol-1 K-1

Ba++	ISE	alc/w	25°C	100%	C	I	K1=2.18		1978BBc	(6759) 52

Medium: MeOH, 0.05 M Et4NClO4. In H2O, 0.05 M Et4NClO4 K1=1.32

Ba++	sol	none	25°C	0.0	U	T		1972KEa	(6760)	53
							Kso(BaF2(s))=-5.879			

Kso=-5.872(10 C), -5.875(15 C), -5.875(20 C), -5.881(30 C), -5.888(35 C), -5.903(40 C), -5.912(45 C)

Ba++ sol none 25°C 0.0 U T 1972KEa (6761) 54
Kso(BaF2(s))=-5.983
Medium: D2O. Kso=-5.970(10 C); -5.970(15 C); -5.979(20 C); -5.988(30 C); -5.984(35 C); -5.998(40 C); -6.019(45 C)

Ba++ ISE NaClO4 25°C 1.0M U T K1=-0.15 1971BHc (6762) 55
K1=0.18(35 C)

Ba++ ISE NaNO3 25°C 1.0M U T H K1=-0.38 1971CVa (6763) 56
DH(K1)=17.2 kJ mol-1, DS=50.2 J K-1 mol-1. K1=-0.29(35 C)

Ba++ ISE NaClO4 25°C 1.0M U T H K1=-0.2 1968TWa (6764) 57
DH(K1)=0; K1=-0.3(2 C), -0.3(39 C)

Ba++ cal NaClO4 25°C 1.0M U H 1968TWa (6765) 58
DH(K1)=about 0

Ba++ sol none 25°C 0.0 U 1950TKa (6766) 59
Kso(BaF2)=-5.98

Ba++ con none 26°C 0.0 U T 1923BOa (6767) 60
Kso(BaF2)=-5.76
Kso=-5.80(9.5 C), -5.77(18 C)

****

I- HL Iodide CAS 10034-85-2 (20)
Iodide;

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

---

Ba++ dis oth/un var U 1968LKa (7893) 61
Kd(Ba+2I=BaI2(in TBP))=-0.08

****

IO3- HL Iodate CAS 7782-68-5 (1257)
Iodate;

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

---

Ba++ gl NaClO4 25°C 3.0M M I K1=0.97 1995POa (8491) 62
Kso=-7.13
At I=0: K=0.97

Ba++ sol NaClO4 25°C 1.00M U K1=2.06 B2=3.65 1985KSb (8492) 63
B3=4.75

Ba++ sol NaClO4 25°C 0.50M U I 1974FRf (8493) 64
Kso(BaL2(s))=-7.76
Medium: LiClO4. Kso=-7.60(I=1), -7.43(I=2), -7.35(I=3), -7.39(I=4),

-8.86(I=0 corr)

Ba++ sol none 25°C 0.0 U T 1969BMa (8494) 65
Kso(BaL2(H2O))=-8.80
Kso'(BaL2)=-8.34 (40 C)
Kso=-9.74(0 C), -9.41(8 C), -9.05(17 C), -8.61(30 C). Kso'=-8.11(50 C), -7.88(60 C), -7.65(70 C), -7.48(79 C), -7.33(86 C)

Ba++ sol none 25°C 0.0 U 1963LMb (8495) 66
Kso(BaL2)=-8.81

Ba++ sol none 25°C 0.0 U 1949DWa (8496) 67
Kso(BaL2)=-8.82

Ba++ sol none 25°C 0.0 U 1939NRa (8497) 68
Kso(BaL2)=-8.80

Ba++ con none 25°C 0.0 U K1=1.1 1935MDa (8498) 69
By solubility Kso(BaL2)=-8.82

Ba++ sol none 25°C 0.0 U T 1923BOa (8499) 70
Kso(BaL2)=-9.19
I=0 corr. Kso=-10.80(0 C), -10.08(10 C), -9.06(30 C), -8.72(40 C), -8.34 (50 C), -8.0(60 C), -7.74(70 C), -7.49(80 C), -7.24(90 C), -6.89(100 C)
****
MnO4- HL Permanganate CAS 13456-41-3 (5678)
Manganate(VII), Permanganate;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ sol oth/un 25°C dil U 1924SSa (8632) 71
Kso(BaMn(VI)O4)=-9.61
****
MoO4-- H2L Molybdate (443)
Molybdate;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ sol NaCl 25°C 0.10M U I 1972JOa (8715) 72
0.1<I<0.8, Kso(BaL)=-8+log[1.06+15.56I-5.68I**2]; 0.6<I<2.4, Kso=-8+log[2.65+10.95I-2.58I**2]; 3.6<I<5.2; Kso=-8+log[23.5-3.43*I]
****
NH3 L Ammonia CAS 7664-41-7 (414)
Ammonia

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ dis oth/un 25°C 0.5M C TI K1=-0.20 B2=-0.78 1990PSb (9096) 73
K3=-0.85
Medium: 0.5 M NH4ClO4;Also for I=1.5 K1=-0.36; K2=-0.74; K3=-1.0;

For I= 1.0 K1=-0.27; K2=-0.66; K3=-0.92;

Ba++ gl R4N.X 25°C 5.00M U K1=-0.15 1985MMa (9097) 74

****

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

Nitrate;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Ba++	sol	NaClO4	25°C	0.50M	U	I	K1=0.21	B2=0.11	1974FRf (9579)	75

Medium: LiClO4. K1=0.16, B2=-0.03(I=1). K1=0.14, B2=0.01(I=2). K1=0.20, B2=-0.15, B3=-1.5, B4=-1.1(I=3). K1=0.24, B2=0.03, B3=-0.6, B4=-1.4(I=4)

Ba++	ix	NaClO4	25°C	1.0M	U		K1=0.15		1969PSa (9580)	76

Ba++	oth	none	25°C	0.0	U		K1=1.1		1966MBb (9581)	77

Ba++	cal	KNO3	25°C	c	U	IH			1964VGb (9582)	78

DH1=-13.4 kJ mol-1, DS=-27.2 J K-1 mol-1. In LiNO3:DH(K1)=-7.9, DS=-8.8

Ba++	con	oth/un	25°C	0.0	U	T H	K1=0.94		1963VVa (9583)	79

Medium: 0 corr. K1=0.98(18 C). DH(K1)=-9.6 kJ mol-1, DS=-12 J K-1 mol-1

Ba++	con	oth/un	18°C	0.0	U		K1=0.92		1930RDa (9584)	80

****

OH- HL Hydroxide (57)

Hydroxide;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Ba++	cal	none	25°C	0.0	M	H			1965HWb (11014)	81

DH(Kso)=57.3 kJ mol-1 , DS=121 J K-1 mol-1, DH(K1)=4.6, DS=59

Ba++	EMF	NaClO4	25°C	3.0M	C		K1=0.00		1961COd (11015)	82

Method: H electrode

Ba++	EMF	oth/un	20°C	var	U		K1=2.2		1961KTa (11016)	83

K1(H+OH=H2O)=14.167 assumed. Method: H electrode

Ba++	kin	none	25°C	0.0	U		K1=0.85		1956BPa (11017)	84

Ba++	EMF	none	25°C	0.0	C		K1=0.68		1954GMb (11018)	85

Ba++	EMF	none	25°C	0.0	C	T H	K1=0.64		1954GMb (11019)	86

DH(K1)=7.3 kJ mol-1, DS=36.8; K1=0.62(5 C), 0.60(15 C), 0.69(35 C), 0.72(45 C). Method: H electrode

---

Ba++	kin	oth/un	25°C	0.10M	U	I	K1=0.37		1949BPb (11020)	87

Medium: 0.1 to 0.4 M. At I=0 corr K1=0.64

```
Ba++       EMF none   25°C  0.0  C        K1=0.64        1939DAa (11021)  88
--------------------------------------------------------------------------------
Ba++       oth oth/un 18°C  var  U        K1=0.72        1923KOa (11022)  89
Medium: BaCl2 at various concentrations; method:colorimetry
********************************************************************************
PO4---                H3L    Phosphate        CAS 7664-38-2  (176)
Phosphate;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Ba++       gl  NaNO3  25°C 0.10M M                         1996SSa (13109)  90
                                        K(Ba+HL)=1.36
--------------------------------------------------------------------------------
Ba++       gl  NaClO4 25°C    0  M  I     K1=0.78   B2=1.30   1995POa (13110)  91
In 3.0 M NaClO4: K1=-0.03, B2=0.0
--------------------------------------------------------------------------------
Ba++       sol oth/un 20°C  0.0  U                         1966SMb (13111)  92
                                        Ks(BaHL)=-7.42
--------------------------------------------------------------------------------
Ba++       sol oth/un 20°C  var  U                         1961CAb (13112)  93
                                        Kso(Ba3L2)=-22.47
                                        Ks(BaHL=Ba+HL)=-7.04
--------------------------------------------------------------------------------
Ba++       sol none   38°C  0.0  U                         1954HPa (13113)  94
                                        Ks(BaHL=Ba+HL)=-7.56
Also by quinhydrone electrode. At I=0.008 M Kso(Ba3L2)=-29.34?
--------------------------------------------------------------------------------
Ba++       sol oth/un 20°C  dil  U                         1929LAa (13114)  95
                                        Kso=-6.44
********************************************************************************
PW11O39-------        H7L                        (2467)
alpha-Heteromonophospho-polytungstate;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Ba++       gl  NaNO3  25°C 1.00M U        K1=2.47        1984COa (13400)  96
********************************************************************************
P2O7----              H4L    Pyrophosphate    CAS 2466-09-3  (198)
Diphosphate; from (HO)2PO.O.PO(OH)2
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Ba++       sp  oth/un 19?°C  var  U        K1=4.64        1957VAb (13562)  97
--------------------------------------------------------------------------------
Ba++       EMF oth/un 25°C  dil  U        K2=4.5         1950WCa (13563)  98
********************************************************************************
P3O10-----            H5L                        CAS 10380-08-2  (1001)
Tripolyphosphate; from (HO)2PO.O.PO(OH).O.PO(OH)2
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
```

Ba++ gl KNO3 45°C 0.10M U K1=3.95 1971TRa (13839) 99
K(Ba+HL)=2.65

Ba++ gl KCl 25°C 0.10M U K1=3.0 1964EMb (13840) 100
K(Ba+HL)=1.8?
K(BaL+H)=6.3?

Ba++ gl R4N.X 25°C 0.10M U K1=3.0 1962RKa (13841) 101
K(Ba+HL)=2.7
Medium: K,NH4Cl

Ba++ gl none 25°C 0.0 U T K1=6.3 1959WOa (13842) 102
Ks(NaBa2L(s)=Na+Ba+BaL)=-9.8
At 40 C: K1=6.1, Ks=-9.7

Ba++ EMF oth/un 25°C dil U B2=4.5 1950WCa (13843) 103

****

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

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

---

Ba++ sp R4N.X 25°C 0.10M U K1=0.08 1962RKa (13947) 104
Medium: NH4Cl

Ba++ oth none 25°C 0.0 U K1=3.35 1949JMa (13948) 105

****

P4O12---- H4L CAS 13598-74-8 (234)
Cyclotetrametaphosphate;

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

---

Ba++ sp R4N.X ? 0.10M U K1=1.00 1962RKa (13997) 106
Medium: NH4Cl

Ba++ con none 25°C 0.0 U K1=4.99 1950JMb (13998) 107

****

P4O13------ H6L Tetraphosphate (1102)
Tetraphosphate;

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

---

Ba++ sol oth/un 35°C var U T 1969BCc (14045) 108
Ligand:Polyphosphates with n>4; PnO3n+1 (n+2)-, Ks(BaL2(s)+L)=10.32,
Kso=-9.80,(BaL2(H2O)2;L=PO3-unit), Additional Temp.:Ks=10.07,Kso=-9.27(45C)

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	oth	none	25°C	0	U			1988LIa (14323)	109
							Kso(BaS)=-1.1		
							*Kso(BaS)=16.2		

Derived from thermodynamic data and K(H+S=HS)=17.3.

****

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

Sulfate;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	sol	none	25°C	0.0	M	T H	K1=2.49	1998PKb (16001)	110
							Kso(BaSO4)=-10.02 (barite)		

Solubility of BaSO4 (labelled with 133Ba) in H2SO4 (0-6.2 M). Data for 60 C. Pitzer equations. DH(Kso)=17.6 kJ mol-1. At 60 C, Kso=-9.68, K1=2.55

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	sol	none	RT	0.0	C	I	K1=2.72	1990FRa (16002)	111
							Kso(BaSO4)=-10.05		

Method: ICP spectroscopy. Calculated from data for 0.001-0.10 M Na2SO4 BaSO4 is barite.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	sol	none	25°C	0.0	C			1988MGb (16003)	112
							Kso(BaSO4)=-10.008		

Method: analysis of literature solubility data, using Pitzer parameters. SrSO4 is barite.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	oth	none	25°C	0.0	C	TIH		1988RAa (16004)	113
							Kso(BaSO4)=-9.959		

Critical evaluation of literature data for Kso and DH(Kso) as a function of T (25-300 C) and [NaCl]. DH(Kso)=28.61 kJ mol-1, DS=-102.5 J K-1 mol-1.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	sol	none	25°C	0.0	C	TIH		1977BLa (16005)	114
							Kso(BaSO4)=-9.98 (1 bar)		

Method: solubility in H2O (22-300 C) and in 0.20 m and 0.40 m NaCl (100-250 C), 1-500 bar. At 100 C, Kso=-9.59. DH(Kso)=26.6 kJ mol-1, DS=-102.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	ISE	oth/un	30°C	0.0	U			1969GSb (16006)	115

Kso=-9.7 (resin membrane electrode)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	sol	oth/un	25°C	0.0	U	T		1969MUa (16007)	116
							Kso=-9.72		

Kso=-9.49(50 C),-9.44(75 C),-9.45(100 C),-9.55(125 C),-9.7(150 C),-9.9(175C) ,-10.15(200 C),-10.45(225 C),-10.9(250 C),-11.45(275 C),-12.15(300 C);barite

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	dis	NaClO4	25°C	1.0M	U		K1=0.66 B2=1.42	1966SSd (16008)	117
Ba++	sol	oth/un	20°C	0.0	U		K1=2.3	1965LIb (16009)	118
Ba++	con	oth/un	25°C	0.0	U			1963NPb (16010)	119

```
                                        Kso(BaL)=-9.99
--------------------------------------------------------------------------------
Ba++       sol NaCl   25°C  5.0M U TI                    1960TEa (16011) 120
                                        Kso(BaL)=-7.50
Kso=-7.31(50 C), -7.02(80 C), -6.80(95 C); also Kso for lower conc NaCl.
At I=0 corr. Kso=-9.96(25 C), -9.71(50 C), -9.62(80 C), -9.59(95 C)
--------------------------------------------------------------------------------
Ba++       con oth/un 24°C  dil  U  I                   1958GBa (16012) 121
                                        Kso(BaL)=-10.00
Also Kso in EtOH/H2O, Me2CO/H2O mixtures
--------------------------------------------------------------------------------
Ba++       sol oth/un 25°C  0.0  U   H                  1955SIa (16013) 122
                                        Kso(BaL)=-9.87
DH(so)=25.0 kJ mol-1, DS=-104.9 J K-1 mol-1
--------------------------------------------------------------------------------
Ba++       vlt oth/un 25°C  0.0  U                       1953SKa (16014) 123
                                        Kso=-9.77
--------------------------------------------------------------------------------
Ba++       vlt oth/un 25°C  0.0  U                       1940CBa (16015) 124
                                        Kso(BaL)=-9.97
--------------------------------------------------------------------------------
Ba++       oth oth/un 25°C  0.0  U   H                  1933LHa (16016) 125
                                        Kso(BaL)=-10.06
From thermodynamic data. DH(so)=22.8 kJ mol-1, DS=-116 J K-1 mol-1
--------------------------------------------------------------------------------
Ba++       oth none   25°C  0.0  U                       1933NEa (16017) 126
                                        Kso(BaL)=-10.06
Method: tyndallometry
--------------------------------------------------------------------------------
Ba++       con oth/un 18°C  0.0  U T                     1923BOa (16018) 127
                                        Kso(BaL)=-10.03
Kso=-10.28(0.8 C), -9.90(27.8 C)
--------------------------------------------------------------------------------
Ba++       con oth/un 18°C  dil  U                       1919KVa (16019) 128
                                        Kso(BaL)=-10.01
--------------------------------------------------------------------------------
Ba++       con oth/un 25°C  0.0  U T                     1910MEa (16020) 129
                                        Kso(BaL)=-9.96
Kso=-10.06(18 C), -9.70(50 C), -9.58(100 C)
--------------------------------------------------------------------------------
Ba++       con oth/un 25°C  dil  U                       1901HUa (16021) 130
                                        Kso(BaL)=-10.02
--------------------------------------------------------------------------------
Ba++       con oth/un 18°C  dil  U T                     1893HOa (16022) 131
                                        Kso(BaL)=-10.00
Kso=-9.74(38 C)
--------------------------------------------------------------------------------
Ba++       con oth/un 18°C  dil  U                       1893KRa (16023) 132
                                        Kso(BaL)=-9.92
********************************************************************************
```

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	sol	none	25°C	0.0	U		K1=2.33 Kso(BaL)=-4.79	1951DMb (16806)	133
Also by conductivity									
Ba++	sol	none	25°C	0.0	U	T	K1=2.21	1949DWa (16807)	134
K1=2.28(35 C)									

SeO3-- H2L Selenite CAS 7783-00-8 (2391)
Selenite;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	con	oth/un	18°C	dil	U		Kso=-5.21	1968RVa (17040)	135
Ba++	sol	oth/un	25°C	0.0	U		Kso=-6.57	1965LSb (17041)	136
Medium:0 corr. In dilute solution: Kso=-6.37									

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	cal	oth/un	25°C	dil	U	H		1959SKa (17098)	137
DH(Kso(BaL))=21.9 kJ mol-1									
Ba++	sol	oth/un	25°C	dil	U	T	Kso(BaL)=-7.46	1958SSa (17099)	138
Kso=-7.53(15 C), -7.43(30 C), -7.64(40 C), -7.75(50 C), -7.86(75 C), -8.0(95 C)									
Ba++	vlt	oth/un	25°C	0.0	U		Kso=-7.30	1953SKa (17100)	139

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	sol	oth/un	20°C	var	U		K(Ba(OH)HL(s)=BaOH+HL)=-4.93	1961KTa (17207)	140

TeO4-- H2L Tellurate (5750)
Tellurate(VI); TeO4-- or TeO2(OH)4--

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ sol oth/un 20°C var U 1970KBd (17306) 141
Kso=-12.5
Kso(3Ba+TeO6)=-14.0
****
CH2O2 HL Formic acid CAS 64-18-6 (37)
Methanoic acid; H.COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ sol NaClO4 25°C 0.00 U I K1=0.88 B2=1.39 1977HFa (17593) 142

Ba++ gl oth/un 25°C 0.0 U T H K1=1.38 1956NAa (17594) 143
Medium: 0 corr. K1(35 C)=1.34, DH(K1)=-7.9 kJ mol-1, DS=-1.3 J K-1 mol-1

Ba++ sol none 25°C 0.0 U K1=0.60 1952CMf (17595) 144

Ba++ gl oth/un 25°C 0.0 U K1=1.38 1948SCa (17596) 145
****
CH3NO HL Formaldoxime CAS 62479-75-2 (4206)
Formaldoxime; CH2:N.OH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ oth oth/un 20°C 0.10M U K1=8.6 1971BJa (17668) 146
Paper electrophoresis, acetate-veronal buffer
****
CH3O5P H3L Phosphonoformic CAS 4428-95-9 (5654)
Phosphonoformic Acid; O:P(OH)2.COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl NaNO3 25°C 0.10M C K1=2.73 1994SCa (17700) 147
K(Ba+HL)=1.42
K(BaL+H)=6.26
****
CH4O3ClP H2L CAS 2565-58-4 (1973)
Chloromethylphosphonic acid; Cl.CH2.PO3H2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ EMF NaNO3 25°C 0.10M U K1=1.11 1970TNa (17928) 148
****
CH5O3P H2L CAS 13590-71-1 (1752)
Methylphosphonic acid; CH3.PO3H2

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

```
Ba++       gl  NaNO3  25°C 0.10M M        K1=1.29        1992SCa (18124) 149
**************************************************************************
CH5O4P                H2L                      CAS 86703-09-5  (1751)
Methylphosphoric acid;  CH3OP(O)(OH)2
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Ba++       gl  NaNO3  25°C 0.10M M        K1=1.23        1996SSa (18173) 150
**************************************************************************
CH6NO3P               H2L    AMPA              CAS 1066-51-3  (1981)
Aminomethylphosphonic acid; H2N.CH2.PO3H2
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Ba++       gl  NaNO3  25°C 0.10M C         K1=1.17        1994SCa (18226) 151
                                          K(Ba+HL)=0.67
                                          K(BaL+H)=9.58
**************************************************************************
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
--------------------------------------------------------------------------
Ba++       dis NaClO4 25°C  1.0M U        K1=0.58   B2=2.20?  1966SSd (18805) 152
--------------------------------------------------------------------------
Ba++       dis oth/un 20°C 0.10M U                          1963STc (18806) 153
                                          Kso=-6.0
Medium: KClO4
--------------------------------------------------------------------------
Ba++       con oth/un 18°C  0.0  U        K1=2.31        1932MDa (18807) 154
**************************************************************************
C2H3O2Br               HL    Bromoacetic acd  CAS 79-08-3  (1309)
Bromoethanoic acid; Br.CH2.COOH
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Ba++       sol oth/un 25°C  ->0  U        K1=0.24        1949DWa (19277) 155
**************************************************************************
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
--------------------------------------------------------------------------
Ba++       oth none   25°C    0  U T H    K1=1.75        1994SHd (19898) 156
Data also at 35, 45 55 C. DH(K1)=2.9 KJ mol-1, DS=43.4 J K-1 mol-1
--------------------------------------------------------------------------
Ba++       gl  alc/w  25°C 100%  M        K1=3.5    B2=5.5    1988PPa (19899) 157
Medium: MeOH
--------------------------------------------------------------------------
Ba++       gl  R4N.X  25°C 0.16M U  I     K1=0.48        1985RSa (19900) 158
```

K1=0.56 (I=0.04); 0.48 (0.25); 0.53 (0.49); 0.70 (1.00)

Ba++ sol NaClO4 25°C 0.00 U I K1=0.83 B2=1.25 1977HFa (19901) 159

Ba++ gl none 25°C 0.0 U K1=0.979 1964AMa (19902) 160

Ba++ gl non-aq 25°C 100% U K2=6.48 1964KLa (19903) 161
Medium: ethanoic acid

Ba++ sp non-aq 25°C 100% U B2=9.20 1961PSa (19904) 162
Medium: ethanoic acid

Ba++ gl oth/un 25°C 0.0 U T H K1=1.15 1956NAa (19905) 163
Medium: 0 corr. K1(35 C)=1.10; DH(K1)=-9.7 kJ mol-1, DS=-10.5 J K-1 mol-1

Ba++ sol oth/un 25°C 0.0 U K1=0.41 1952CMe (19906) 164

Ba++ EMF KCl 20°C 0.20M U K1=0.39 1938CKa (19907) 165
Method: H electrode

****

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

---

Ba++ EMF oth/un 25°C ->0 U K1=1.00 1954DMa (20494) 166
Method: H electrode

Ba++ sol oth/un 25°C ->0 U K1=1.04 1952CMf (20495) 167

Ba++ EMF KCl 20°C 0.20M U K1=0.66 1938CKa (20496) 168
Method: H electrode

****

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

---

Ba++ gl NaNO3 25°C 0.10M C M K1=3.45 2000KAb (21494) 169
K(BaA+L)=3.73
B(BaAL)=7.33
H2A=Dipicolinic acid.

Ba++ gl NaNO3 25°C 0.10M C K1=3.50 1989GAb (21495) 170

Ba++ sp NaClO4 25°C 1.0M C K1=-0.374 1989LWe (21496) 171

Ba++ sp oth/un 25°C 1.0M U K1=1.40 1987HAa (21497) 172

Ba++ sol oth/un 25°C ->0 U K1=0.77 1951MOa (21498) 173

****

C2H6OS L DMSO CAS 67-68-5 (329)
Dimethylsulfoxide; (CH3)2.SO

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Ba++	ISE	non-aq	25°C	100%	M		K1=1.63	B2= 1.99	1999NMa (22091)	174
							B3=2.31			
							B4=2.59			

Method: ISE based on benzo-12-crown-4 coupled to polyacrylamide.
Medium: propylenecarbonate, 0.01 M Et4NClO4.

Ba++	ISE	non-aq	25°C	100%	M		K1=1.61	B2=2.51	1988NHa (22092)	175

Medium: MeCN, 0.01 M Et4NClO4

****

C2H7NS HL CAS 60-23-1 (588)
2-Aminoethanethiol; H2N.CH2.CH2.SH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KNO3	25°C	0.10M	U		K1=1.37	1963TAa (22488)	176

****

C2H7O3P H2L CAS 71778-99-9 (1978)
Ethylphosphonic acid; CH3.CH2.PO3H2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	NaNO3	25°C	0.10M	M		K1=1.30	1992SCa (22567)	177

****

C2H8O7P2 H4L HEDPA CAS 2809-21-4 (436)
1-Hydroxyethane-1,1-diphosphonic acid; CH3.C(OH)(PO3H2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KNO3	25°C	0.10M	U		K1=3.35	1980ZRc (23359)	178
							K(Ba+HL)=2.72		

****

C3H4N2 L Imidazole CAS 288-32-4 (90)
1,3-Diazole, imidazole; C3H4N2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	NaNO3	25°C	0.50M	M		K1=-0.4	1998KSa (23860)	179

****

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
Ba++	sp	none	25°C	0.0	U	T	K1=2.28	1976KOa (24391)	180

Also data at 15,30,35 C. By competition with bromocresol purple

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	NaClO4	25°C	0.10M	U		K1=1.22	1968OVa (24392)	181
Ba++	gl	NaClO4	20°C	0.10M	U		K1=1.34 K(Ba+HL)=0.61	1963CAa (24393)	182
Ba++	con	oth/un	25°C	->0	U		K1=2.13	1951PJb (24394)	183
Ba++	EMF	oth/un	25°C	0.04M	U		K1=1.71	1949SDa (24395)	184
Ba++	EMF	KCl	25°C	0.20M	U		K1=1.23 K(Ba+HL)=0.44	1938CKa (24396)	185

****

C3H4O5 H2L Tartronic acid CAS 80-69-3 (839)
Hydroxypropanedioic acid; HO.CH(COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	NaClO4	20°C	0.10M	U		K1=1.80 K(Ba+HL)=0.87	1963CAa (24615)	186

****

C3H5NO4 H2L Aminomalonic ac CAS 1068-84-4 (2980)
2-Aminopropanedioic acid; HOOC.CH(NH2).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	EMF	oth/un	20°C	->0	U		K1=0	1945SKa (24669)	187

Method: H electrode

****

C3H6O2 HL Propionic acid CAS 79-09-4 (35)
Propanoic acid; CH3.CH2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	oth	none	25°C	0	U	T H	K1=2.46	1994SHd (24983)	188

Data also at 35, 45 55 C. DH(K1)=1.6 KJ mol-1, DS=52.4 J K-1 mol-1

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	sol	NaClO4	25°C	0.00	U	I	K1=0.67 B2=1.19	1977HFa (24984)	189
Ba++	sol	oth/un	25°C	->0	U		K1=0.15	1952CMf (24985)	190
Ba++	EMF	KCl	20°C	2.0M	U		K1=0.34	1938CKa (24986)	191

Method: H electrode

****

C3H6O3 HL L-Lactic acid CAS 79-33-4 (82)
L-2-Hydroxypropanoic acid; CH3.CH(OH).COOH

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

```
Ba++       gl  oth/un 25°C  1.0M U        K1=0.34   B2=0.42   1965VTa (25405) 192
--------------------------------------------------------------------------------
Ba++       EMF oth/un 25°C  ->0  U        K1=0.64        1954DMb (25406) 193
Method: H electrode
--------------------------------------------------------------------------------
Ba++       sol oth/un 25°C  ->0  U        K1=0.77        1952CMf (25407) 194
--------------------------------------------------------------------------------
Ba++       EMF KCl    20°C 0.20M U        K1=0.55        1938CKa (25408) 195
Method: H electrode
********************************************************************************
C3H6O4                 HL    Glyceric acid    CAS 473-81-4  (2520)
2,3-Dihydroxypropanoic acid; HO.CH2.CH(OH).COOH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Ba++       EMF KCl    20°C 0.20M U        K1=0.80        1938CKa (25630) 196
Method: H electrode
********************************************************************************
C3H7NO                  L    DMF              CAS 68-12-2  (598)
N,N-Dimethylformamide; HCO.N(CH3)2
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Ba++       ISE non-aq 25°C 100%  M        K1=0.76   B2= 1.90  1999NMa (25655) 197
                                         B3=2.25
Method: ISE based on benzo-12-crown-4 coupled to polyacrylamide.
Medium: propylenecarbonate, 0.01 M Et4NClO4.
--------------------------------------------------------------------------------
Ba++       ISE non-aq 25°C 100%  M        K1=1.28   B2=1.76   1988NHa (25656) 198
Medium: MeCN, 0.01 M Et4NClO4
********************************************************************************
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
--------------------------------------------------------------------------------
Ba++       sol oth/un 25°C  ->0  U      T K1=0.80        1951MOa (26141) 199
********************************************************************************
C3H7O6P               H2L                        (6830)
3-Hydroxy-2-oxopropylphosphoric acid; CH2(OH).CO.CH2.OPO3H2
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Ba++       gl  NaNO3  25°C 0.10M U        K1=1.14        1992LCb (27322) 200
********************************************************************************
C3H9O4P               H2L                        (6694)
(Phosphonylmethoxy)ethane; H2O3P.CH2.O.CH2.CH3
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
```

Ba++ gl NaNO3 25°C 0.10M M K1=1.33 1992SCa (28020) 201
****
C3H9O6P H2L CAS 57-03-4 (2984)
2,3-Dihydroxypropylphosphoric acid, Glycerol 1-phosphate; HO.CH2.CH(OH).CH2.OPO3H2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl NaNO3 25°C 0.10M U K1=1.18 1992LCb (28047) 202
****
C3H10NO3P H2L CAS 35869-68-2 (1989)
Dimethylaminomethylphosphonic acid; (CH3)2N.CH2.PO3H2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl KNO3 25°C 0.10M C K1=1.5 1993SKc (28100) 203
****
C3H10O6P2 H4L CAS 29712-42-3 (3554)
Propane-1,2-diphosphonic acid; CH3.CH(PO3H2).CH2(PO3H2)

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl KCl 20°C 0.10M U K1=2.20 1951SRa (28387) 204
K(Ba+HL)=1.3
****
C3H10O6P2 H4L CAS 4671-82-3 (3555)
Propane-1,3-diphosphonic acid; (H2O3P).CH2.CH2.CH2(PO3H2)

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl KCl 20°C 0.10M U K1=2.34 1951SRa (28394) 205
K(Ba+HL)=1.6
****
C3H11NO6P2 H4L (6735)
N-Methylimino-N,N-bis(methylenephosphonic acid); CH3.N(CH2PO3H2)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl KNO3 25°C 0.10M C K1=3.57 1993SKc (28445) 206
K(BaL+H)=10.62
K(BaHL+H)=5.4

Ba++ gl NaClO4 25°C 0.10M U K1=4.21 1988LDa (28446) 207
****
C3H12NO9P3 H6L NTPA CAS 6419-19-8 (2920)
Nitrilotris(methylenephosphonic acid); N(CH2PO3H2)3

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl KNO3 25°C 0.10M C H K1=6.34 1993SMa (28551) 208
K(BaL+H)=9.72

K(BaHL+H)=6.16
DH(K1)=-8.2, DH(BaHL)=-22.5, DH(BaH2L)=12.4 kJ mol-1.

Ba++ gl KNO3 25°C 0.10M C K1=6.34 1987SAa (28552) 209
K(BaL+H)=9.72
K(BaHL+H)=6.16
K(BaH2L+H)=5.1

****

C4H4O4 H2L Maleic acid CAS 110-16-7 (111)
cis-Butenedioic acid; HOOC.CH:CH.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	sp	none	25°C	0.0	U		K1=2.35	1976KOa (29047)	210
Ba++	con	oth/un	25°C	->0	U		K1=2.26	1940TDa (29048)	211

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	con	oth/un	25°C	->0	U		K1=1.59	1940TDa (29178)	212

****

C4H5N2Cl L CAS 872-49-1 (7589)
5-Chloro-1-methylimidazole;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	NaNO3	25°C	0.50M	M		K1=-0.10	1998KSa (29335)	213

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	NaNO3	25°C	0.50M	M		K1=-0.5	1998KSa (29575)	214

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	R4N.X	25°C	0.10M	C	TIH	K1=1.41	1984DDa (29935)	215
							B(BaHL)=5.95		

Medium: Et4NI. Data for 0.05-1.0 M and 15-45 C.DH(K1)=6.7 kJ mol-1, DS(K1)
=50 J K-1 mol-1; DH(BaHL)=5.9, DS=134. At I=0, K1=2.12, B(BaHL)=6.64.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	ix	oth/un	25°C	0.16M	U		K1=1.21	1954SCa (29936)	216

```
Ba++       con oth/un 25°C  ->0  U        K1=2.08        1951PJb (29937) 217
--------------------------------------------------------------------------
Ba++       EMF oth/un 25°C 0.15M U        K1=0.97        1946JOa (29938) 218
--------------------------------------------------------------------------
Ba++       con oth/un 25°C  ->0  U        K1=1.57        1940TDa (29939) 219
--------------------------------------------------------------------------
Ba++       EMF KCl    25°C 0.20M U        K1=1.03        1938CKa (29940) 220
                                          K(Ba+HL)=0.45
Method: H electrode
**************************************************************************
C4H6O4                H2L    Me-Malonic Acid  CAS 516-15-2  (816)
Methylpropanedioic acid; HOOC.CH(CH3).COOH
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Ba++       gl  NaClO4 25°C 0.10M U        K1=1.42        1968OVa (30115) 221
**************************************************************************
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
--------------------------------------------------------------------------
Ba++       cal NaNO3  25°C 1.00M U   H    K1=1.17        1980ARa (30587) 222
DH(K1)=1.63 kJ mol-1
--------------------------------------------------------------------------
Ba++       gl  NaClO4 20°C 0.10M U                       1963CAa (30588) 223
                                          K(Ba+H2L)=0.67
                                          K(Ba+HL)=1.38
--------------------------------------------------------------------------
Ba++       ix  oth/un 25°C 0.16M U        K1=1.36        1954SCa (30589) 224
At I=0.078 M K1=1.48
--------------------------------------------------------------------------
Ba++       kin oth/un 25°C  ->0  U        K1=1.32        1951BWa (30590) 225
                                          K(Ba+HL)=0.66
--------------------------------------------------------------------------
Ba++       con oth/un 25°C  ->0  U        K1=2.20        1940TDa (30591) 226
--------------------------------------------------------------------------
Ba++       EMF KCl    25°C 0.20M U        K1=1.30        1938CKa (30592) 227
                                          K(Ba+HL)=0.67
**************************************************************************
C4H6O5                H2L    Diglycolic acid  CAS 110-99-6  (243)
Di(carboxy)methyl ether, 2,2'-Oxydiethanoic acid; HOOC.CH2.O.CH2.COOH
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Ba++       gl  KNO3   25°C 0.10M U        K1=2.15        1974MSa (30853) 228
**************************************************************************
C4H6O6                H2L    DL-Tartaric acd  CAS 133-37-9  (94)
DL-Tartaric acid,DL-2,3-Dihydroxybutanedioic acid; HOOC.CH(OH).CH(OH).COOH
--------------------------------------------------------------------------
```

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	NaClO4	25°C	1.00M	M	M	K(Ba+H2L+(ascorbate))=3.91	1988MOa	(31011) 229
Ba++	oth	oth/un	25°C	dil	C		K1=2.686	1982HKa	(31012) 230

Method: isotachophoresis. Medium: 0.006-0.019 M tartrate buffer, pH 5.1.

****

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

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	NaClO4	37°C	0.20M	U		K1=2.19	1967TTb	(31201) 231
Ba++	dis	NaClO4	20°C	0.10M	U		K1=<2.0	1963STc	(31202) 232
Ba++	ix	oth/un	25°C	0.16M	U	I	K1=1.68	1954SCa	(31203) 233

I=0.078 M: K1=1.76

Ba++	oth	oth/un	25°C	0.15M	U		K1=1.95	1946JOa	(31204) 234

METHOD:E

Ba++	con	oth/un	25°C	->0	U		K1=2.54	1940TDa	(31205) 235
Ba++	EMF	KCl	25°C	0.20M	U		K1=1.62 K(Ba+HL)=0.88	1938CKa	(31206) 236

****

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

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	NaNO3	25°C	0.10M	C	M	K1=3.75 K(BaA+L)=3.93 B(BaAL)=7.53	2000KAb	(31817) 237

H2A=Dipicolinic acid.

Ba++	gl	KNO3	25°C	0.10M	M		K1=2.57	1981GVa	(31818) 238
Ba++	gl	KCl	25°C	0.10M	U		K1=1.14	1953LMa	(31819) 239

****

C4H7NO4 H2L IDA CAS 142-73-4 (118)

Iminodiethanoic acid; HN(CH2.COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KNO3	20°C	0.10M	U	H	K1=1.67	1964ANa	(32200) 240

By calorimetry: DH(K1)=0.4 kJ mol-1, DS=33.4 J K-1 mol-1

Ba++ EMF oth/un 20°C ->0 U K1=1.67 1945SKa (32201) 241
Method: H electrode
****
C4H8O2 HL CAS 107-92-6 (1118)
n-Butanoic acid; CH3.CH2.CH2.COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ oth none 25°C 0 U T H K1=2.47 1994SHd (33329) 242
Data also at 35, 45 55 C. DH(K1)=1.6 KJ mol-1, DS=52.6 J K-1 mol-1

Ba++ sol NaClO4 25°C 0.00 U I K1=0.61 B2=0.88 1977HFa (33330) 243

Ba++ sol none 25°C 0.0 U K1=0 1952CMf (33331) 244

Ba++ EMF KCl 25°C 0.20M U K1=0.31 1938CKa (33332) 245
Method: H electrode
****
C4H8O3 HL CAS 594-61-6 (81)
2-Hydroxy-2-methylpropanoic acid; (CH3)2C(OH).COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ EMF NaClO4 25°C 1.0M U K1=0.36 B2=0.51 1965VTa (33446) 246
Method: quinhydrone electrode.
****
C4H8O3 HL CAS 300-85-6 (30)
3-Hydroxybutanoic acid; CH3.CH(OH).CH2.COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ EMF KCl 25°C 0.20M U K1=0.43 1938CKa (33620) 247
Method: H electrode
****
C4H9NO L CAS 127-19-5 (477)
N,N-Dimethylacetamide; CH3.CO.N(CH3)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ ISE non-aq 25°C 100% C K1=0.92 B2=1.23 1990NKa (33761) 248
B3=1.69
B4=1.85
Medium: propylene carbonate, 0.01 M Et4NClO4.
****
C4H10O2S L CAS 111-48-8 (4275)
3-Thiapentan-1,5-diol; HO.CH2.CH2.S.CH2.CH2.OH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl NaClO4 25°C 1.0M C K1=-0.08 1979SRa (34683) 249

****

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
Ba++	gl	R4N.X	25°C	1.00M	C	I	K1=0.02	1982SSf (35054)	250

In 90 % (v/v) DMSO/water mixture: K1=0.41 (I=0.25 M)

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KNO3	25°C	0.10M	C		K1=5.93	2000SDa (35104)	251
							K(BaL+H)=8.42		
							K(BaHL+H)=5.57		
							K(BaH2L+H)=3.8		

****

C4H11O4P H2L (5867)
n-Butyl phosphoric acid; C4H9.O.PO(OH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	NaNO3	25°C	0.10M	C		K1=1.22	1988MSa (35286)	252

****

C4H12O6P2 H4L CAS 4071-77-6 (3592)
Butane-1,4-diphosphonic acid; H2O3P.CH2.CH2.CH2.CH2.PO3H2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KCl	20°C	0.10M	U		K1=2.28	1951SRa (35577)	253
							K(Ba+HL)=1.5		

****

C4H12O7P2 H3L CAS 52811-47-9 (7665)
N-Butyldiphosphoric acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	NaNO3	25°C	0.10M	M		K1=2.38	1999SSa (35585)	254

****

C5H2O2F6 HL HFA CAS 1522-22-1 (195)
1,1,1,5,5,5-Hexafluoropentane-2,4-dione; F3C.CO.CH2.CO.CF3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	diox/w	30°C	75%	U		B2=8.0	1953UFe (35921)	255

****

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
--------------------------------------------------------------------------------
Ba++       sol KCl    25°C 0.30M U        K1=1.55        1965CDa (35937) 256
                                          Kso=-8.28
********************************************************************************
C5H4NBr                 L                     CAS 1120-87-2  (8780)
4-Bromopyridine;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Ba++       gl  NaNO3  25°C 0.50M C        K1=-0.06       2002KSb (36003) 257
********************************************************************************
C5H4NCl                 L                     CAS 626-60-8  (322)
3-Chloropyridine; C5H4N.Cl
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Ba++       gl  NaNO3  25°C 0.50M C        K1=-0.18       2002KSb (36023) 258
********************************************************************************
C5H4N2O4              H2L    Orotic acid      CAS 65-86-1  (624)
1,2,3,6-Tetrahydro-2,6-dioxo-4-pyrimidinecarboxylic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Ba++       gl  NaClO4 25°C 0.50M U  I                     1983MDa (36109) 259
                                          K(Ba+H2L)=1.91 (2.36 in 0.1 M)
                                          K(Ba+2H2L)=3.47
                                          K(Ba+HL)=3.89
                                          K(Ba+2HL)=7.27
********************************************************************************
C5H4O2S                HL    2-Thenoic acid   CAS 527-72-0  (2312)
Thiophene-2-carboxylic acid; C4H3S.COOH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Ba++       gl  NaClO4 30°C 0.20M U T H    K1=2.06        1976SSd (36254) 260
********************************************************************************
C5H5N                   L    Pyridine         CAS 110-86-1  (31)
Pyridine, Azine;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Ba++       gl  NaNO3  25°C 0.50M C        K1=-0.20       2002KSb (36595) 261
********************************************************************************
C5H5N2Br                L                     CAS 1072-97-5  (2630)
5-Bromo-2-aminopyridine; C5H3N(Br)(NH2)
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
```

Ba++ gl NaNO3 25°C 0.50M C K1=-0.34 2002KSb (36859) 262
****
C5H5O2F3 HL CAS 367-57-7 (163)
1,1,1-Trifluoropentane-2,4-dione; CF3.CO.CH2.CO.CH3

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl diox/w 30°C 75% U B2=8.0 1953UFe (37049) 263
****
C5H6N2 L 2-Aminopyridine CAS 504-29-0 (1478)
2-Aminoazine, 2-Pyridylamine; C5H4N.NH2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl NaNO3 25°C 0.50M C K1=-0.29 2002KSb (37124) 264
****
C5H6N2O HL (3035)
2-Aminopyridine 1-oxide; C5H4N(-O)(NH2)

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ sp NaClO4 25°C 0.50M U 1963SBd (37203) 265
K(Ba+HL)=0.09
****
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
---
Ba++ gl diox/w 28°C 70% U K1=5.35 B2=10.05 1992ZHa (37913) 266

Ba++ gl NaNO3 25°C 0.10M C K1=1.70 1982HNa (37914) 267

Ba++ gl diox/w 24°C 50% U K1=2.5 1979ACa (37915) 268

Ba++ gl diox/w 20°C 17% C K1=4.86 B2=8.21 1976JWa (37916) 269

Ba++ gl diox/w 30°C 75% U B2=9.0 1953UFb (37917) 270
****
C5H8O4 H2L CAS 595-46-0 (1144)
Dimethylmalonic acid; HOOC.C(CH3)2.COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl NaClO4 25°C 0.10M U K1=1.35 1968OVa (38208) 271
****
C5H8O4 H2L CAS 601-75-2 (479)
Ethylpropanedioic acid; HOOC.CH(C2H5).COOH

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

```
--------------------------------------------------------------------------------
Ba++       sp  none   25°C  0.0  U T      K1=2.26        1976KOa (38236) 272
Also data at 15,30,35 C. Determined colourimetrically
--------------------------------------------------------------------------------
Ba++       gl  NaClO4 25°C 0.10M U        K1=1.39        1968OVa (38237) 273
********************************************************************************
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
--------------------------------------------------------------------------------
Ba++       gl  oth/un 25°C  ->0  U        K1=2.04        1951PJb (38309) 274
********************************************************************************
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
--------------------------------------------------------------------------------
Ba++       gl  NaNO3  25°C 0.10M C    M   K1=1.96        2000KAb (39066) 275
                                          K(BaA+L)=2.01
                                          B(BaAL)=5.61
H2A=Dipicolinic acid.
--------------------------------------------------------------------------------
Ba++       gl  KNO3   25°C 0.10M M        K1=2.30        1981GVa (39067) 276
--------------------------------------------------------------------------------
Ba++       gl  KCl    25°C 0.10M U        K1=1.28        1953LMa (39068) 277
********************************************************************************
C5H9NO4               H2L    MIDA             CAS 4408-64-4  (190)
N-Methyliminodiethanoic acid; CH3.N(CH2.COOH)2
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Ba++       gl  KCl    25°C 0.10M U   H    K1=2.61   B2=4.94   1968NPb (39239) 278
By calorimetry: DH(K1)=-4.4 kJ mol-1, DS=35.1 J K-1 mol-1
--------------------------------------------------------------------------------
Ba++       cal KNO3   20°C 0.10M U   H                  1965ANa (39240) 279
DH(K1)=-3.3 kJ mol-1, DS=38.5 J K-1 mol-1
--------------------------------------------------------------------------------
Ba++       gl  KCl    20°C 0.10M U        K1=2.59        1955SAa (39241) 280
--------------------------------------------------------------------------------
Ba++       EMF oth/un 20°C  ->0  U        K1=3.45        1945SKa (39242) 281
Method: H electrode
********************************************************************************
C5H10NO7P             H4L    PMIDA            CAS 5994-61-6  (2433)
N-(Phosphonomethyl)iminodiethanoic acid; H2O3P.CH2.N(CH2.COOH)2
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Ba++       gl  KNO3   25°C 0.10M C        K1=5.61        2000SDa (39667) 282
                                          K(BaL+H)=7.36
```

K(BaHL+H)=4.7

Ba++ gl KCl 30°C 0.10M U K1=5.1 1958OMb (39668) 283

Ba++ EMF KCl 20°C 0.10M U K1=5.35 1949SAa (39669) 284
K(Ba+HL)=1.69

Method: H electrode

****

C5H10O2 HL n-Valeric acid CAS 109-52-4 (3027)
Pentanoic acid; CH3(CH2)3.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	sol	oth/un	25°C	->0	U		K1=-0.20	1952CMf (40201)	285

****

C5H10O2 HL Pivalic acid CAS 75-98-9 (3026)
Trimethylethanoic acid, 2,2-Dimethylpropanoic acid; (CH3)3C.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	sol	oth/un	25°C	->0	U		K1=0.08	1952CMf (40215)	286

****

C5H10O5 L D-Ribose CAS 50-69-1 (512)
D-Ribose;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	cal	none	25°C	0.0	U	H	K1=0.18	1991MLa (40347)	287

DH(K1)=-15 kJ mol-1

****

C5H11NO2 HL Nor-Valine CAS 760-78-1 (689)
2-Aminopentanoic acid; CH3.CH2.CH2.CH(NH2).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	NaNO3	25°C	0.10M	C	M	K1=3.35	2000KAb (40835)	288
							K(BaA+L)=3.65		
							B(BaAL)=7.25		

H2A=Dipicolinic acid.

****

C5H11O8P H2L Ribose-5-phosph CAS 4300-28-1 (2756)
Ribose-5-phosphoric acid, Ribofuranoside 5 Phosphoric acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	NaNO3	25°C	0.10M	C		K1=1.17	1988MSa (41421)	289

****

C5H13NO7P2 H4L CAS 75006-88-1 (640)
1-Acetylaminopropylidene-1,1-diphosphoric acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Ba++	gl	KNO3	30°C	0.15M	U		K1=5.28	B2=7.74	1983LSa (41754)	290
							K(Ba+HL)=2.36			

****

C5H13NO7P2 H4L CAS 88216-82-4 (641)
1-Propanoylaminoethylidene-1,1-diphosphoric acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KNO3	30°C	0.15M	U		K1=4.72	1983LSa (41758)	291
							K(Ba+HL)=2.22		
							K(Ba+BaL)=1.97		

****

C5H14NO4P H2L (8071)
1-Amino-2-hydroxypentane-2-phosphonic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	NaClO4	25°C	0.1M	U		K1=3.92	1975SLa (41837)	292
							K(Ba+HL)=2.96		

****

C6H3N3O7 HL Picric acid CAS 88-89-1 (593)
2,4,6-Trinitrophenol; HO.C6H2(NO2)3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	con	none	30°C	0.0	U	I M	K2=1.67	1979PSa (42093)	293
Ba++	sp	oth/un	25°C	->0	U		K1=3.60	1960KAb (42094)	294

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	NaNO3	20°C	0.10M	U		K1=1.65	1960ANb (42499)	295
Ba++	gl	oth/un	25°C	0.0	U		K1=1.63	1957LUa (42500)	296
Ba++	gl	NaNO3	25°C	0.10M	U		K1=2.4	1957SYb (42501)	297

****

C6H5NO4 H2L 3-Nitrocatechol CAS 6665-98-1 (2685)
1,2-Dihydroxy-3-nitrobenzene; O2N.C6H3(OH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KCl	25°C	0.10M	M		K1=2.71	1986HAc (42858)	298

****

C6H5NO4 H2L 4-Nitrocatechol CAS 3316-09-4 (890)

1,2-Dihydroxy-4-nitrobenzene; O2N.C6H3(OH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KCl	25°C	0.10M	M		K1=2.6 B2=4.9	1985HAa (42918)	299

****

C6H6NBr L (8782)
5-Bromo-2-methylpyridine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	NaNO3	25°C	0.50M	C		K1=-0.24	2002KSb (43194)	300

****

C6H6NCl L CAS 10445-91-7 (8781)
4-(Chloromethyl)pyridine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	NaNO3	25°C	0.50M	C		K1=-0.12	2002KSb (43210)	301

****

C6H6NO6P H2L CAS 330-13-2 (5865)
4-Nitrophenylphosphoric acid; NO2.C6H4.O.PO.(OH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	NaNO3	25°C	0.10M	C		K1=1.06	1988MSa (43247)	302

****

C6H6O2 H2L Hydroquinone CAS 123-31-9 (3646)
1,4-Dihydroxybenzene; HO.C6H4.OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	nmr	oth/un	25°C	0.0	U		K1=0.4	1992AVa (43896)	303

Medium: pH 7.4 buffer

****

C6H6O3 L CAS 39078-11-0 (8605)
1,2:3,4:5,6-Trianhydro-cis-inositol;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	cal	non-aq	25°C	100%	C	H	K2=1.90	1992BCf (44006)	304

Medium: MeOH. DH(K2)=-9.6 kJ mol-1, DS(K2)=4.0 J K-1 mol-1.

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KCl	20°C	0.10M	U		K1=4.10	1964PCa (44409)	305
							K(Ba+HL)=2.0		

```
**************************************************************************
C6H7N                   L    Picoline         CAS 109-06-8  (320)
2-Methylpyridine; C5H4N.CH3
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Ba++       gl  NaNO3  25°C 0.50M C        K1=-0.19       2002KSb (44602) 306
**************************************************************************
C6H7N                   L    beta-Picoline    CAS 108-99-6  (324)
3-Methylpyridine; C5H4N.CH3
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Ba++       gl  NaNO3  25°C 0.50M C        K1=-0.16       2002KSb (44691) 307
**************************************************************************
C6H7O4P                 H2L                      CAS 701-64-4  (5866)
Phenyl phosphoric acid; C6H5O.PO(OH)2
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Ba++       gl  NaNO3  25°C 0.10M C        K1=1.19        1988MSa (45231) 308
**************************************************************************
C6H8N2O4                H2L                        (3100)
Cyanomethyliminodiethanoic acid; NC.CH2.N(CH2.COOH)2
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Ba++       gl  KCl    20°C 0.10M U        K1=1.98        1955SAa (45416) 309
**************************************************************************
C6H8O4                  H2L                      CAS 5445-51-2  (69)
Cyclobutane-1,1-dicarboxylic acid; C4H6(COOH)2
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Ba++       gl  NaClO4 25°C 0.10M U        K1=1.46        1966OCb (45505) 310
**************************************************************************
C6H8O6                  H3L    Tricarballylic   CAS 99-14-9  (1620)
1,2,3-Propanetricarboxylic acid; HOOC.CH2.CH(COOH).CH2.COOH
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Ba++       gl  NaClO4 20°C 0.10M U        K1=1.95        1964COb (45562) 311
                                         K(Ba+HL)=1.15
                                         K(Ba+H2L)=0.73
**************************************************************************
C6H8O6                  H2L    Ascorbic acid    CAS 50-81-7  (285)
Ascorbic acid (Vitamin C);
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
```

```
Ba++       gl  NaClO4 25°C 1.00M M    M                  1988MOa (45626) 312
                                        K(Ba+H2L+(tartrate))=3.91
--------------------------------------------------------------------------------
Ba++       gl  NaClO4 20°C 1.00M M                       1983MOa (45627) 313
                                        K(Ba+HL)=1.03
                                        K(Ba+2HL)=1.85
********************************************************************************
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
--------------------------------------------------------------------------------
Ba++       oth oth/un 25°C  dil  C        K1=4.150       1982HKa (46036) 314
                                        K(Ba+HL)=2.686
Method: isotachophoresis. Medium: 0.006-0.019 M citrate buffer, pH 5.1.
--------------------------------------------------------------------------------
Ba++       gl  oth/un 32°C 0.10M U        K1=3.6         1965PPb (46037) 315
--------------------------------------------------------------------------------
Ba++       gl  NaClO4 20°C 0.10M U        K1=2.89        1964COb (46038) 316
                                        K(Ba+HL)=1.75
                                        K(Ba+H2L)=0.79
--------------------------------------------------------------------------------
Ba++       sol oth/un 35°C    ?  U T H    K1=3.6         1959DMb (46039) 317
DH(K1)=-75.3 kJ mol-1, DS=-176. K1=3.2(45 C)
--------------------------------------------------------------------------------
Ba++       ix  oth/un 25°C .078M U  I     K1=2.84        1954SCa (46040) 318
I=0.16: K1=2.54
--------------------------------------------------------------------------------
Ba++       ix  R4N.X  25°C .165M U        K1=2.30        1948SRa (46041) 319
Medium: 0.165 M NH4Cl. At I=0.16 M K1=1.8
--------------------------------------------------------------------------------
Ba++       EMF oth/un 25°C 0.15M U        K1=2.98        1946JOa (46042) 320
********************************************************************************
C6H8O7P2              H3L                    CAS 101378-64-7  (7666)
Phenyldiphosphoric acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Ba++       gl  NaNO3  25°C 0.10M M        K1=2.31        1999SSa (46345) 321
********************************************************************************
C6H9NO6               H3L                    CAS 41035-84-1  (4367)
N-Carboxymethyl-L-aspartic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Ba++       gl  KNO3   25°C 0.10M U        K1=3.21        1975GNb (46375) 322
********************************************************************************
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
Ba++	gl	KNO3	20°C	0.10M	C	TIH R	K1=4.85	1982ANa (46703)	323

IUPAC evaluation

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KCl	20°C	0.10M	U	T	K1=4.83	1966IMb (46704)	324
Ba++	gl	KNO3	25°C	0.10M	U	T	K1=4.72	1960BMb (46705)	325

K1=4.87(0.5 C), 4.66(42.4 C). DH(K1)=-8.4 kJ mol-1, DS=63 J K-1 mol-1

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	EMF	oth/un	30°C	0.0	U	T H	K1=5.587	1956HMa (46706)	326

Method: H electrode. K1=5.968(0 C), 5.914(10 C), 5.875(20 C)
DH(K1)=-2.1 kJ mol-1, DS=105 J K-1 mol-1

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	EMF	oth/un	25°C	0.0	U			1956MAa (46707)	327

Method: H electrode. DG(K1)=-33.47 kJ mol-1, DH=-4.2, DS=100 J K-1 mol-1

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KCl	20°C	0.10M	U	T	K1=4.82	1955SAa (46708)	328
Ba++	EMF	oth/un	20°C	0.0	U		K1=6.41	1945SKb (46709)	329

Method: H electrode

****

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
Ba++	gl	KCl	20°C	0.10M	U		K1=2.88	1955SAa (47840)	330

****

C6H10O4 H2L CAS 595-84-6 (481)
(Methylethyl)propanedioic acid; HOOC.C(CH3)(C2H5).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	sp	none	25°C	0.0	U		K1=2.74	1976KOa (48024)	331

****

C6H10O4 H2L Adipic acid CAS 124-04-9 (401)
1,6-Hexanedioic acid; HOOC.(CH2)4.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	oth/un	25°C	->0	U		K1=1.92	1951PJa (48064)	332
Ba++	con	oth/un	25°C	->0	U		K1=1.85	1940TDa (48065)	333

****

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

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

Ba++ gl KNO3 25°C 0.10M U K1=2.29 1974MSa (48331) 334
****
C6H11NO4S H3L CAS 58033-48-5 (3124)
N-2-Mercaptoethyliminodiethanoic acid; HS.CH2.CH2.N(CH2.COOH)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl KCl 20°C 0.10M U K1=3.55 1955SAa (48610) 335
K(Ba+HL)=2.16
****
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
---
Ba++ gl KCl 20°C 0.10M U K1=3.42 1955SAa (48694) 336
****
C6H11NO7S H3L CAS 39716-94-4 (3125)
N-2-Sulfoethyliminodiethanoic acid (taurine-NN-diacetic acid)

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ EMF KCl 20°C 0.10M U K1=3.01 1949SAa (48846) 337
Method: H electrode
****
C6H12NO7P H4L CAS 55339-27-0 (3127)
N-2-Phosphoethyliminodiethanoic acid; H2O3P.CH2.CH2.N(CH2.COOH)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl KCl 20°C 0.10M U K1=3.64 1949SAa (49034) 338
K(Ba+HL)=1.72
Method: H electrode
****
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
---
Ba++ cal NaClO4 25°C 0.10M U H K1=1.2 1983EHa (49224) 339
DH1=6.8 kJ mol-1, DS1=46.3 J K-1 mol-1
****
C6H12N2O4 H2L N,N-EDDA CAS 5835-29-0 (2333)
1,2-Diaminoethane-N,N-diethanoic acid; H2N.CH2.CH2.N(CH2.COOH)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl KCl 20°C 0.10M U K1=3.19 1955SAa (49299) 340
****
C6H12O6 L CAS 488-58-4 (2283)

epi-Inositol;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ ISE none 25°C 0.0 C K1=0.26 1975AHa (49630) 341
****
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
---
Ba++ EMF KCl 20°C 0.20M U K1=0.95 1938CKa (49700) 342
Method: H electrode
****
C6H14O3 L Diglyme CAS 111-96-6 (6769)
bis-2-Methoxyethyl ether, 2,5,8-Trioxanonane; CH3.O.CH2CH2.O.CH2CH2.O.CH3

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ cal non-aq 25°C 100% C H 1992BSc (51048) 343
Medium: propylene carbonate. DH(K1)=-17.2 kJ mol-1.
****
C6H15NO3 Triethanolamine CAS 102-71-6 (447)
Tris-(2-hydroxyethyl)amine; L

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl R4N.X 25°C 1.00M C I K1=0.36 1982SSf (51283) 344
In 90 % (v/v) DMSO/water mixture: K1=0.58 (I=0.25 M)
****
C6H16NO4P H2L (8073)
1-Amino-2-hydroxy-4-methylpentane-2-phosphonic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl NaClO4 25°C 0.1M U K1=3.89 1975SLa (51562) 345
K(Ba+HL)=2.92
****
C6H16NO4P HL CAS 387383-55-3 (8776)
N,N,N-Trimethyl-2-(phosphonomethoxy)ethylamine;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl NaNO3 25°C 0.10M M K1=0.79 2002FGb (51573) 346
****
C6H17N2O3P H2L (7486)
N,N,N'-Trimethyldiaminoethane-N'-methylphosphonic acid;
(CH3)2N.CH2CH2.N(CH3)CH2PO3H2

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

---

Ba++	gl	KNO3	25°C	0.10M	C	K1=6.29		1999DOa (51825)	347
						K(BaL+H)=9.57			
						K(BaHL+H)=8.32			
						K(BaH2L+H)=6.47			
						K(BaH3L+H)=4.4			

****

C6H18N2O6P2 H4L (1363)
N,N'-Dimethyldiaminoethane-N,N'-dimethylphosphonic acid;
CH3N(CH2PO3H2).CH2.CH2.N(CH2.PO3H2)CH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KNO3	25°C	0.10M	C		K1=3.12	1999DOa (51949)	348
							K(BaL+H)=10.20		
							K(BaHL+H)=7.3		

****

C6H18N2O6P2 H4L (7487)
N,N-Dimethyldiaminoethane-N',N'-dimethyldiphosphonic acid;
(CH3)2N.CH2CH2.N(CH2PO3H2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KNO3	25°C	0.10M	C		K1=3.37	1999DOa (51969)	349
							K(BaL+H)=11.07		
							K(BaHL+H)=7.8		

****

C6H18N3OP L HMPA CAS 680-31-9 (603)
Hexamethylphosphoramide, Tris-(dimethylamino)phosphine oxide;((CH3)2N)3PO

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Ba++	ISE	non-aq	25°C	100%	M		K1=3.20	B2=4.49	1988NHa (51978)	350

Medium: MeCN, 0.01 M Et4NClO4

****

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
Ba++	gl	KNO3	25°C	0.10M	C	H	K1=7.10	1993SMa (52321)	351
							K(BaL+H)=10.26		
							K(BaHL+H)=8.54		
							K(BaH2L+H)=7.05		
							K(BaH3L+H)=5.78		

DH(K1)=-2.8, DH(BaHL)=-20.3, DH(BaH2L)=-8.6, DH(BaH3L)=-9.4, DH(BaH4L)=2.4 kJ mol-1.

Ba++	gl	KCl	25°C	0.10M	U		K1=11.14	1980RZa (52322)	352
							K(BaL+H)=9.22		

K(BaH2L+H)=7.14
K(BaHL+H)=8.41
K(BaH3L+H)=6.25

Ba++ gl KNO3 25°C 0.10M U K1=7.88 1979RZa (52323) 353
K(Ba+HL)=6.95
K(Ba+H2L)=4.31
K(Ba+H3L)=3.53

****

C6O2Cl4 L Chloranil CAS 118-75-2 (4344)
2,3,5,6-Tetrachloro-1,4-benzoquinone;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	sp	alc/w	?	100%	U	M	K(BaI2+L)=1.15 K(Ba(SCN)2+L)=4.48	1969PPf (52376)	354

Medium: MeOH

****

C7H4NO4Cl H2L CAS 4722-94-5 (3780)
4-Chloropyridine-2,6-dicarboxylic acid; Cl.C5H2N(COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	NaClO4	22°C	0.10M	U		K1=3.19	1964BBe (52384)	355

****

C7H5NO4 H2L Quinolinic acid CAS 89-00-9 (567)
2,3-Pyridinedicarboxylic acid; C5H3N.(COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KNO3	25°C	0.10M	U		K1=2.1	1958YYa (52622)	356

****

C7H5NO4 H2L CAS 499-80-9 (566)
2,4-Pyridinedicarboxylic acid; C5H3N.(COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KNO3	25°C	0.10M	U		K1=2.1	1958YYa (52650)	357

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	NaNO3	25°C	0.10M	C		K1=3.60	2000KAb (52753)	358
Ba++	gl	oth/un	25°C	0.10M	U		K1=3.43	1966BSe (52754)	359

By ion exchange: K2=0.5

```
Ba++       gl  NaNO3  20°C 0.10M U        K1=3.46        1960ANb (52755) 360
--------------------------------------------------------------------------
Ba++       gl  KNO3   25°C 0.10M U        K1=3.4         1957SYb (52756) 361
**************************************************************************
C7H5NO5               H3L                    CAS 499-51-4  (3150)
4-Hydroxypyridine-2,6-dicarboxylic acid; HO.C5H2N(COOH)2
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Ba++       gl  NaClO4 22°C 0.10M U        K1=3.98        1964BBa (53073) 362
--------------------------------------------------------------------------
Ba++       gl  oth/un 20°C 0.10M U        K1=3.9         1963ANd (53074) 363
                                        K(BaL+H)=7.86
**************************************************************************
C7H6N2O4              H2L                    CAS 2683-49-0  (3753)
4-Aminopyridine-2,6-dicarboxylic acid  (4-aminodipicolinic acid)
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Ba++       gl  KNO3   20°C 0.10M U        K1=3.68        1965ABa (53505) 364
--------------------------------------------------------------------------
Ba++       gl  NaClO4 22°C 0.10M U        K1=3.76        1964BBa (53506) 365
**************************************************************************
C7H6O2                 HL    Benzoic Acid     CAS 65-85-0  (462)
Benzenecarboxylic acid; C6H5.COOH
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Ba++       gl  alc/w  25°C 100%  M        K1=3.7    B2=5.9    1988PPa (53823) 366
Medium: MeOH
**************************************************************************
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
--------------------------------------------------------------------------
Ba++       gl  alc/w  25°C 100%  M                        1988JTa (54154) 367
                                        K(Ba+HL)=3.5
                                        K(Ba+2HL)=5.8
Medium: MeOH
--------------------------------------------------------------------------
Ba++       cal alc/w  25°C 100%  U   H                    1988PPa (54155) 368
Medium: MeOH. DH(BaL)=24.3 kJ mol-1; DS=118. DH(BaL2)=3.7; DS=127
--------------------------------------------------------------------------
Ba++       kin oth/un 25°C  ->0  U                        1951BWa (54156) 369
                                        K(Ba+HL)=0.21
**************************************************************************
C7H6O6S               H3L                    CAS 5965-83-3  (399)
5-Sulfosalicylic acid, 2-Hydroxy-5-sulfobenzoic; HO3S.C6H3(OH).COOH
--------------------------------------------------------------------------
```

```
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Ba++       gl  NaNO3  25°C 0.10M C        K1=2.68        1982HNa (54940) 370
*************************************************************************
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
-------------------------------------------------------------------------
Ba++       gl  oth/un 25°C  ->0  U        K1=0.23        1958LUa (55209) 371
*************************************************************************
C7H7NO2               H2L    Salicylaldoxime  CAS 94-67-7  (1486)
2-Hydroxybenzaldehyde oxime; HO.C6H4.CH:N.OH
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Ba++       gl  oth/un 25°C  ->0  U                        1958LUa (55306) 372
                                       K(Ba+HL)=0.53
                                       K(Ba+2HL)=3.72
*************************************************************************
C7H7NO2                HL                     CAS 3222-47-7  (3154)
6-Methylpyridine-2-carboxylic acid; CH3.C5H3N.COOH
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Ba++       gl  NaNO3  20°C 0.10M U        K1=2.05        1960ANb (55427) 373
*************************************************************************
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
-------------------------------------------------------------------------
Ba++       gl  NaNO3  25°C 0.10M C        K1=3.20        2000KHa (55588) 374
*************************************************************************
C7H8N2O2                L                     CAS 15513-52-7  (5516)
3-Nitro-2,6-dimethylpyridine;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Ba++       gl  NaNO3  25°C 0.50M C        K1=<-1.30      1984ERa (55898) 375
*************************************************************************
C7H9N                  L    3,5-Lutidine       (323)
3,5-Dimethylpyridine; C5H3N.(CH3)2
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Ba++       gl  NaNO3  25°C 0.50M C        K1=-0.18       2002KSb (56285) 376
*************************************************************************
C7H9NO3S               HL                     CAS 87655-41-2  (5520)
2,6-Dimethylpyridine-3-sulfonic acid;
```

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	NaNO3	25°C	0.50M	C		K1=<-1.0	1984ERa (56450)	377

****

C7H9NO8 H4L (8068)

2-Aminopropane-1,3-dioic-N,N-bis(ethanoic acid);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KNO3	25°C	0.1M	U		K1=5.50	1976NGb (56467)	378

****

C7H9NO8 H4L CAS 4379-32-2 (5702)

2-Aminopropane-1,3-dioic-N-2-butane-1,4-dioic acid; (HOOC)2CH.NH.CH(COOH)CH2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KNO3	25°C	0.10M	U		K1=2.96	1988KMa (56472)	379

****

C7H11NO6 H3L (2926)

2-Aminobutanoic-N-propane-1,3-dioic acid; HOOC.CH(C2H5)NH.CH(COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KNO3	25°C	0.10M	U		K1=1.90	1982KKa (56839)	380

****

C7H11NO6 H3L CAS 40199-58-4 (3165)

N-(2'-Carboxyethyl)iminodiethanoic acid; HOOC.CH2.CH2.N(CH2.COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	EMF	KCl	20°C	0.10M	U		K1=3.40	1949SAa (56878)	381

Method: H electrode

****

C7H11NO6 H3L MNTA (1026)

Nitrilo(2-propanoic)-diethanoic acid; HOOC.CH(CH3).N(CH2.COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KNO3	20°C	0.10M	U		K1=4.79	1974RMf (56904)	382
Ba++	gl	KCl	20°C	0.10M	U		K1=4.86	1966IMa (56905)	383

****

C7H11NO6P2 H4L CAS 4712-06-5 (4470)

Amino(phenyl)methylenediphosphonic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KCl	25°C	0.10M	U		K1=5.16 K(Ba+HL)=4.36	1969DMd (56939)	384

****

C7H12N2O5 H2L Gly-Glu CAS 7412-78-4 (280)
Glycyl-glutamic acid; H2N.CH2.CO.NH.CH(CH2.CH2.COOH).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KNO3	20°C	0.10M	U		K1=2.90	1980BBc (57174)	385

****

C7H12N3O5P H2L PMEC CAS 117087-39-5 (8366)
1-[2-(Phosphonomethoxy)ethyl]cytosine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	NaNO3	25°C	0.10M	M		K1=1.38 K(Ba+HL)=0.0 K(BaL+H)=5.6	1999BHb (57200)	386

****

C7H12O4 HL CAS 96740-23-7 (2249)
1,5-Dimethoxy-pent-2,4-dione, CH3.O.CH2.CO.CH2.CO.CH2.O.CH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	diox/w	24°C	50%	U		K1=2.5	1979ACa (57289)	387

****

C7H12O4 H2L CAS 534-59-8 (480)
Butylpropanedioic acid (Butylmalonic acid); HOOC.CH(C4H9).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	sp	none	25°C	0.0	U	T	K1=2.24	1976KOa (57334)	388

Also data at 15,30,35 C. Determined colourimetrically

****

C7H12O4 H2L CAS 510-20-3 (482)
Diethylpropanedioic acid (Diethylmalonic acid); HOOC.C(C2H5)2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	sp	none	25°C	0.0	U	T	K1=2.41	1976KOa (57357)	389

Also data at 15,30,35 C. Determined colourimetrically

****

C7H13NO4S H2L (3184)
N-(2-Methylthioethyl)iminodiethanoic acid; CH3.S.CH2.CH2.N(CH2.COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KCl	20°C	0.10M	U		K1=2.62	1955SAa (57545)	390

****

C7H13NO5 H2L CAS 62117-07-1 (3171)
N-(2-Methoxyethyl)iminodiethanoic acid; CH3.O.CH2.CH2.N(CH2.COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KCl	20°C	0.10M	U		K1=3.56	1955SAa (57573)	391

****

C7H14N2O4 H2L TriMe-EDDA CAS 7597-26-4 (265)
1,3-Propanediamine-N,N'-diethanoic acid; HOOC.CH2.NH.(CH2)3.NH.CH2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	cal	NaClO4	25°C	0.10M	U	H	K1=1.3	1983EHa (57816)	392

DH1=2.5 kJ mol-1, DS1=33.6 J K-1 mol-1

****

C7H14N4O4P H2L CAS 550359-20-1 (9059)
[[2-(4-Amino-2-imino-1(2H)-pyrimidinyl)ethoxy]methyl]phosphonic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	NaNO3	25°C	0.10M	M		K1=0.82	2003FHa (57842)	393

****

C7H22N2O13P4 H8L DPPH CAS 54622-43-4 (2651)
2-Hydroxy-1,3-diaminopropane-N,N,N'N'-tetramethylphosphonic acid;
HO.CH(CH2.N(CH2.PO3H2)2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	ISE	KNO3	25°C	0.1M	U		K1=5.93	1985SNd (58385)	394
							B(BaHL)=16.51		
							B(BaH3L)=34.30		
							B(BaH2L)=26.30		
							B(BaH4L)=40.76		
							B(BaH5L)=45.74		
							B(Ba2L)=7.29		

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	sp	non-aq	25°C	100%	U	T H	K1=4.41	1994GSb (58488)	395

At 35 C: K1=4.37; 45 C: K1=4.30; 55 C: K1=4.24. DH(K1)=-11 kJ mol-1, DS=48
Medium: DMSO

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	sp	non-aq	20°C	100%	U		K1=4.46	1992PSa (58489)	396

Medium: DMF, 0.01 M Me4NI

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	sp	alc/w	25°C	100%	U	I	K1=5.40	1988KGa (58490)	397

Medium: MeOH. Also in DMF (K1=4.43) and DMSO (4.05).

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	sp	alc/w	25°C	100%	U	I	K1=5.40	1987GKb (58491)	398

Medium: MeOH. Also in DMF (K1=4.43) and DMSO (K1=4.05)

Ba++ sp non-aq 25°C 100% U K1=3.89 1983PSc (58492) 399
Medium: DMSO
****
C8H5O2F3S HL TTA CAS 326-91-0 (165)
4,4,4-Trifluoro-1-(2-thienyl)butane-1,3-dione; F3C.CO.CH2.CO.C4H3S

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl diox/w 20°C 17% C K1=5.94 B2=10.53 1976JWa (58601) 400

Ba++ gl diox/w 30°C 75% U B2=10.6 1953UFe (58602) 401
****
C8H5O3F3 HL CAS 15788-03-1 (3215)
1,1,1-Trifluoro-3-2'-furoylacetone; F3C.CO.CH2.CO.C4H3O

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl diox/w 30°C 75% U B2=10.2 1953UFe (58714) 402
****
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
---
Ba++ gl NaCl 25°C 0.10M U K1=2.28 1989SKa (58946) 403

Ba++ gl oth/un 25°C .493M U T H K1=2.58 1975PAc (58947) 404
10-15 C: K1=2.59; 20 C: 2.58

Ba++ EMF oth/un 25°C 0.15M U K1=0.92 1946JOa (58948) 405

Ba++ con oth/un 25°C 0.0 U K1=2.33 1940TDa (58949) 406
****
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
---
Ba++ con oth/un 25°C 0.0 U K1=1.55 1940TDa (59048) 407
****
C8H8N2O4 H2L (3823)
4-(Methylamino)pyridine-2,6-dicarboxylic acid; CH3.NH.C5H2N(COOH)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl NaClO4 22°C 0.10M U K1=3.81 1964BBa (59352) 408
****
C8H8O2S HL 2-Thenoylaceton CAS 3151-27-2 (3224)
2-Thenoylacetone, 1-(2'-Thienyl)butane-1,3-dione; C4H3S.CO.CH2.CO.CH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	diox/w	30°C	75%	U		B2=9.2	1953UFe (59636)	409

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
Ba++	gl	alc/w	25°C	100%	M			1988JTa (59722)	410
							K(Ba+HL)=3.7		
							K(Ba+2HL)=5.5		

C8H8O3 HL Mandelic Acid CAS 611-72-3 (80)
2-Phenyl-2-hydroxyethanoic acid; C6H5.CH(OH).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	kin	oth/un	25°C	0.0	U		K1=0.70	1951BWa (59811)	411
Ba++	con	oth/un	25°C	0.0	U		K1=0.77	1938BDa (59812)	412

C8H8O4 HL (6840)
3-Acetyl-4-Hydroxy-6-methyl-2-pyrone;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	mixed	24°C	50%	U		K1=2.24 B2=4.20	1993ZMa (60106)	413

Medium: 50% v/v acetone/H2O

C8H9N3O7 H2L Uramildiacetic CAS 13055-06-5 (185)
5-Amino-2,4,6-trioxo-1,3-perhydrodiazimino-N,N-diethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	cal	KNO3	25°C	0.1M	C	H		1981CSb (60620)	414

DH(K1)=-12.5 kJ mol-1, DS=67 K J mol-1

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KNO3	25°C	0.10M	U	T	K1=6.02	1977SVa (60621)	415
Ba++	cal	R4N.X	20°C	0.1M	C			1976ANb (60622)	416
							DH1= -11.3 kJ/mol		

in Me4NCl

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	R4N.X	25°C	0.10M	C		K1=6.16	1975JTa (60623)	417
Ba++	gl	KNO3	20°C	0.10M	U		K1=6.13 B2=9.83	1963IFb (60624)	418
Ba++	ISE	oth/un	20°C	0.0	U		K1=6.78	1946SKa (60625)	419

****
C8H9O3P H2L CAS 1707-08-0 (1969)
2-Styrylphosphonic acid; C6H5.CH:CH.PO3H2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl KNO3 25°C 0.12M U K1=2.50 1979RZb (60672) 420
****
C8H11NO L CAS 20819-02-5 (5524)
4-Methoxy-2,6-dimethylpyridine;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl NaNO3 25°C 0.50M C K1=<-0.7 1984ERa (61034) 421
****
C8H11NO2 H2L Dopamine CAS 579-59-9 (251)
2-(3',4'-Dihydroxyphenyl)ethylamine; (HO)2.C6H3.CH2.CH2.NH2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl KCl 25°C 0.10M U T H 1986CVb (61077) 422
K(Ba+HL)=3.02
K(Ba+2HL)=4.12
Data for 0-37 C. At 37 C, K(Ba+HL)=2.92, K(Ba+2HL)=3.92.
DH(Ba+HL)=-26.6 kJ mol-1, DS=31 J K-1 mol-1; DH(Ba+2HL)=-12.5, DS=20.6
****
C8H11NO3 H2L Noradrenaline CAS 138-65-8 (253)
Norepinephrine, 3,4-Dihydroxyphenylethanolamine; (HO)2C6H3.CH(CH2.NH2).OH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl KCl 25°C 0.10M U T H K1=3.97 B2= 4.49 1982CVa (61162) 423
Data for 0 and 37 C. DH(K1)=-24.3 kJ mol-1, DS(K1)=-15 J K-1 mol-1;
DH(K2)=-11.8, DS(K2)=-19.
****
C8H11NO8 H4L CAS 24868-49-3 (2572)
2-Amino(N,N-diethanoic)-1,4-butanedioic acid;HOOCCH(N(CH2COOH)2)CH2COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl KNO3 25°C 0.10M U K1=4.02 1975NGa (61185) 424
****
C8H11NO8 H4L CAS 7408-20-0 (2608)
Amino-di(butanedioic acid);HN(CH(COOH)CH2.COOH)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl KNO3 25°C 0.1M C K1=2.18 1999VZb (61201) 425

Ba++ gl KNO3 25°C 0.1M U K1=2.18 1978MNa (61202) 426

****

C8H12N2O8 H4L CAS 35039-85-1 (4537)
1,2-Diaminoethane-N,N'-dimalonic acid; (HOOC)2.CH.NH.CH2.CH2.NH.CH(COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KNO3	20°C	0.10M	U		K1=3.92 K(Ba+HL)=1.8	1973DSc	(61493) 427
Ba++	gl	KNO3	25°C	0.10M	U		K1=3.32 K(Ba+HL)=1.85 K(Ba+BaL)=1.94	1972GBd	(61494) 428

****

C8H12N5O4P H2L CAS 106941-25-7 (6693)
9-(2-(Phosphonylmethoxy)ethyl)adenine; H2O3P.CH2.O.CH2.CH2.adenine

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	NaNO3	25°C	0.10M	M		K1=1.30	1992SCa	(61651) 429

****

C8H13NO6 H3L (3835)
2-Amino-2-carboxypropane-N,N-diethanoic acid; HOOCC(CH3)2N(CH2COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KNO3	20°C	0.10M	U		K1=3.19	1974RMf	(61758) 430
Ba++	gl	KCl	20°C	0.10M	U		K1=5.61	1966IMa	(61759) 431

****

C8H13NO6 H3L (5681)
2-Aminobutanoic-N,N-diethanoic acid; CH3CH2CH(COOH)N(CH2COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KNO3	20°C	0.10M	U		K1=4.48	1974RMf	(61783) 432

****

C8H13NO6S H3L (5675)
2-Mercapto-1-aminoethane-N,N,S-triethanoic acid; HOOC.CH2.S.CH2.CH2.N(CH2COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	NaClO4	25°C	0.10M	U		K1=3.10	1975POa	(61818) 433

****

C8H13N6O4P H2L (7462)
9-[2-(Phosphonomethoxy)ethyl]-2,6-diaminopurine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	NaNO3	25°C	0.10M	M		K1=1.33 K(Ba+HL)=0.0	1999BSa	(61875) 434

****

C8H14N2O4 H2L CAS 124099-98-5 (5607)
1,4-Piperazine-N,N'-diethanoic acid; HOOC.CH2.C4H8N2.CH2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	cal	NaClO4	25°C	0.10M	U	H	K1=1.4	1985EHa	(61945) 435

DH(K1)=1.8 kJ mol-1, DS=33.3 J K-1 mol-1

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	EMF	KCl	20°C	0.10M	U		K1=1.6	1963IPb	(61946) 436

Method: H electrode

****

C8H14O7 H2L (241)
Di(carboxymethoxy)ethyl ether; (HOOC.CH2.O.CH2.CH2)2O

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KNO3	25°C	0.10M	U		K1=2.29	1974MSa	(62147) 437

****

C8H16N2O4 H2L (266)
N,N'-Dimethylethylenediamine-N,N'-diethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KNO3	25°C	0.10M	C		K1=2.66	1993WLa	(62527) 438
Ba++	cal	NaClO4	25°C	0.10M	U	H	K1=2.5	1983EHa	(62528) 439

DH1=-3.8 kJ mol-1, DS1=34.9 J K-1 mol-1

****

C8H16N2O6 H2L CAS 50730-95-5 (4548)
Ethylenediiminobis(3-hydroxy-2-propanoic acid);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	EMF	oth/un	20°C	0.10M	U		K1=2.3	1972DKa	(62584) 440
Ba++	gl	KNO3	20°C	0.10M	U		K1=2.3	1970DKa	(62585) 441

****

C8H16O4 L 12-Crown-4 CAS 294-93-9 (174)
1,4,7,10-Tetraoxacyclododecane; cyclo(-O.(CH2.CH2.O)3.CH2.CH2-)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	cal	non-aq	25°C	100%	C	H	K2=2.39	1992BCf	(62659) 442

Medium: MeOH. DH(K2)=-6.3 kJ mol-1, DS(K2)=25 J K-1 mol-1.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	cal	alc/w	25°C	100%	U	H T	K1=2.56	1987BUa	(62660) 443

Medium: MeOH. DH(K1)=-21.4 kJ mol-1; DS=-23 J K-1 mol-1; DH(B2)=-27.3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	cal	non-aq	25°C	100%	C	H	K2=<2	1986BUe	(62661) 444

DH(K1)=-21.4 kJ mol-1, DS(K1)=-23 J K-1 mol-1; DH(K2)=-5.6.
Medium: MeOH.

Ba++ EMF non-aq 25°C 100% U T K1=4.63 B2=7.9 1982MRb (62662) 445
Medium: anhydrous propylene carbonate, 0.1M Et4NClO4
****
C8H17NO3 L CAS 41775-76-2 (6751)
10-Aza-1,4,7-trioxacyclododecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ vlt non-aq 25°C 100% C K1=5.7 2000HHa (62760) 446
Medium: acetonitrile, 0.1 M Et4NClO4. Method: dc polarography.
****
C8H18N2O2 L CAS 294-92-8 (654)
1,7-Dioxo-4,10-diazacyclododecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ cal non-aq 25°C 100% C H K1=2.34 B2= 2.34 1986BUe (62843) 447
DH(K1)=-13.3 kJ mol-1, DS(K1)=-15 J K-1 mol-1; DH(K2)=>15.
Medium: MeOH.
****
C8H18N2O2 L CAS 122-96-3 (5902)
N,N-Bis(2-hydroxyethyl)piperazine;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl NaCl 25°C 0.10M C K1=2.04 1999HLb (62858) 448
B(BaHL)=9.76
****
C8H18O4 L Triglyme CAS 112-49-2 (2358)
1,2-Bis(methoxyethoxy)ethane; CH3O.C2H4O.CH2.CH2.OC2H4.OCH3

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ cal non-aq 25°C 100% C H 1992BSc (62982) 449
Medium: propylene carbonate. DH(K1)=-32.6 kJ mol-1.
****
C8H19NO5 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
---
Ba++ gl mixed 25°C 90% C I K1=1.14 1982SSf (63055) 450
Medium: 90% DMSO/H2O

Ba++ gl KNO3 25°C 1.0M C K1=0.85 1980SAb (63056) 451
****
C9H4N2F4 L CAS 124005-68-1 (7590)

N-(2,3,5,6-Tetrafluorophenyl)imidazole;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	NaNO3	25°C	0.50M	M		K1=-0.38	1998KSa (63505)	452

****

C9H6N2O6S H2L CAS 15851-63-3 (1433)
7-Nitro-8-hydroxyquinoline-5-sulfonic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	oth/un	25°C	0.0	U		K1=1.78 B2=3.10	1955NUa (63911)	453

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	oth/un	20°C	0.0	U		K1=2.07	1952NAa (64237)	454

****

C9H7N3O2S H2L TAR CAS 2246-46-0 (707)
4-(2'-Thiazolylazo)-resorcinol; C3H2NS.N:N.C6H3(OH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	alc/w	25°C	50%	U			1967NPb (64696)	455

K(Ba+HL) < 3
Medium: 50% MeOH, 0.1 M NaClO4

****

C9H8O4 HL Acetylsalicylic CAS 50-78-2 (1240)
2-Acetoxybenzoic acid, Acetylsalicylic acid; CH3.CO.O.C6H4.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	vlt	NaClO4	25°C	0.50M	C	T H	K1=4.80	1989GRb (64895)	456

Method: polarography. Medium: 0.50 M NH4ClO4, pH 4.8. Data for 25-45 C.
DH(K1)=-23.6 kJ mol-1, DS(K1)=12.7 J K-1 mol-1.

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	sp	NaClO4	?	0.20M	U		K1=2.43	1967GDb (64933)	457

****

C9H9NO2 HL CAS 34790-24-4 (3261)
Isonicotinoylacetone; C5H4N.CO.CH2.CO.CH3

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

Ba++ gl diox/w 30°C 75% U B2=8.8 1953UFe (65040) 458
****
C9H9NO2 HL CAS 40614-52-6 (3262)
Picolinoylacetone; C5H4N.CO.CH2.CO.CH3

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl diox/w 30°C 75% U B2=10.0 1953UFe (65043) 459
****
C9H9N3O4 HL CAS 89314-30-7 (8506)
2-[(4-Nitrophenyl)hydrazono]-propanoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl alc/w 30°C 40% M M K1=2.45 B2= 3.35 1995RRd (65149) 460
K(BaL+A)=2.94
K(BaL+en)=5.46
K(BaL+pro)=2.19
K(BaL+B)=2.83
Medium: 40% v/v EtOH/H2O, 0.10 M KNO3. K(BaL+ala)=2.24, K(BaL+gly)=0.80;
H2A is catechol, HB is hydroxyproline.

Ba++ gl alc/w 30°C 40% M M 1995RRd (65150) 461
K(Ba(phen)+L)=2.43
K(BaA+L)=1.26
Medium: 40% v/v EtOH/H2O, 0.10 M KNO3. H2A is salicylic acid.
****
C9H10N2O2 HL CAS 5330-70-1 (8505)
2-(Phenylhydrazono)-propanoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl alc/w 30°C 40% M M K1=2.62 B2= 4.14 1995RRd (65216) 462
K(BaL+A)=2.87
K(BaL+en)=5.40
K(BaL+pro)=2.15
K(BaL+B)=2.60
Medium: 40% v/v EtOH/H2O, 0.10 M KNO3. K(BaL+ala)=1.55, K(BaL+gly)=0.72;
H2A is catechol, HB is hydroxyproline.

Ba++ gl alc/w 30°C 40% M M 1995RRd (65217) 463
K(Ba(phen)+L)=2.60
K(BaA+L)=1.33
Medium: 40% v/v EtOH/H2O, 0.10 M KNO3. H2A is salicylic acid.
****
C9H10N2O4 H2L CAS 5648-29-1 (3871)
4-(N',N'-Dimethylamino)pyridine-2,6-dicarboxylic acid;

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

Ba++ gl NaClO4 22°C 0.10M U K1=3.86 1964BBa (65266) 464
****
C9H10N2O5 H3L (4645)
4,5,6,7-Tetrahydroindazol-3-one-5,5-dicarboxylic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl diox/w 25°C 50% U 1969ZSa (65276) 465
K(Ba+H2L)=2.30
K(Ba+HL)=4.52
****
C9H10O8 H4L CAS 3724-52-5 (1264)
cis-1,2,3,4-Cyclopentanetetracarboxylic acid; C5H6.(COOH)4

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl NaClO4 25°C 0.19M U K1=5.38 B2= 8.22 1986MSc (65638) 466
****
C9H11NO HL CAS 10229-63-7 (3872)
N-(Salicylidene)aminoethane; HO.C6H4.CH:N.CH2.CH3

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ sp non-aq 25°C 100% C K1=1.21 2002CCc (65668) 467
Medium: acetonitrile.
****
C9H11NO5 H2L CAS 57362-11-5 (3876)
N-(2'-Furfuryl)iminodiethanoic acid; C4H3O.CH2.N(CH2.COOH)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl KNO3 20°C 0.10M U K1=2.68 1963IFa (66450) 468
****
C9H11N3O7 H3L (3877)
N-(1-Methyl-2,4,6-trioxo-perhydropyrimidinyl)iminodiethanoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl KNO3 20°C 0.10M U K1=6.06 B2=9.91 1963IFb (66523) 469
****
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
---
Ba++ gl KNO3 25°C 0.1M U K1=6.90 1982KBe (66730) 470
****
C9H13NO3 H2L (-)Adrenaline CAS 51-43-4 (252)
4-(1-Hydroxy-2-(methylamino)ethyl)-1,2-dihydroxybenzene,

Epinephrine;CH3NHCH(OH)C6H3(OH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KCl	25°C	0.10M	U	T H	K1=4.02 B2= 5.91	1983CVa (66859)	471

Data for 0 and 37 C. DH(K1)=-37.4 kJ mol-1, DS(K1)=-58.0 J K-1 mol-1; DH(K2)=-12.5, DS(K2)=-13.9.

****

C9H13NO6 H3L (3881)

2,6-Dicarboxypiperidyl-N-ethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KNO3	25°C	0.10M	U		K1=3.40	1968KTd (66880)	472

****

C9H13NO8 H4L (7012)

1,3-Dicarboxypropane-1-iminodiethanoic acid; HOOC.CH(N(CH2COOH)2)CH2CH2COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KNO3	25°C	0.10M	U		K1=3.54	1977GNb (66906)	473
Ba++	gl	KNO3	25°C	0.1M	U		K1=3.54	1976NGb (66907)	474

****

C9H13N2O9P H3L UMP-5 CAS 58-97-9 (2948)

Uridine-5'-monophosphoric acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	R4N.X	25°C	0.10M	C	T	K(Ba+HL)=1.74	1991SMa (66970)	475

IUPAC evaluation

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	NaNO3	25°C	0.10M	C		K(Ba+HL)=1.13	1988MSa (66971)	476

****

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
Ba++	nmr	non-aq	32°C	100%	U		K(Ba(NO3)2+L)=0.34	1980MCa (67049)	477

Medium: DMSO-d6

****

C9H14N2O9 H4L CAS 56360-11-3 (2576)

2-Hydroxy-1,3-diaminopropane-N,N'-di(1,3-propanedioic acid)

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

```
Ba++       gl  KNO3   25°C 0.10M U        K1=2.00        1975KGa (67135) 478
                                          K(Sr+HL)=1.65
*******************************************************************************
C9H14N2O12P2          H4L    UDP              CAS 58-98-0  (3288)
Uridine-5'-diphosphoric acid;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Ba++       gl  NaNO3  25°C 0.10M M        K1=2.29        1999SSa (67160) 479
                                          K(Ba+H2L)=1.1
                                          K(BaHL+H)=5.2
*******************************************************************************
C9H14N3O8P            H2L    CMP-5            CAS 63-37-6  (1243)
Cytidine-5'-monophosphoric acid, Cytidilic acid;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Ba++       gl  R4N.X  25°C 0.10M C      T K1=1.72        1991SMa (67249) 480
IUPAC evaluation
-------------------------------------------------------------------------------
Ba++       gl  NaNO3  25°C 0.10M C        K1=1.11        1988MSa (67250) 481
*******************************************************************************
C9H14N5O3P            H2L                   CAS 121149-93-7  (2512)
9-(4-Phosphonobutyl)adenine;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Ba++       gl  NaNO3  25°C 0.10M M        K1=1.22        2000GKa (67357) 482
                                          K(Ba+HL)=0.0
                                          *K(BaHL)=-6.5
*******************************************************************************
C9H15NO6              H3L                     (7177)
2-Aminopentanoic-N,N-diethanoic acid; C3H7C(COOH)N(CH2COOH)2
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Ba++       gl  KNO3   20°C 0.10M U        K1=4.41        1974RMf (67403) 483
*******************************************************************************
C9H15N3O11P2          H3L    CDP              CAS 63-38-7  (2187)
Cytidine-5'-diphosphoric acid;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Ba++       gl  NaNO3  25°C 0.10M M        K1=2.27        1999SSa (67587) 484
                                          K(Ba+HL)=1.1
                                          K(BaL+H)=5.22
*******************************************************************************
C9H16N2O6             H2L                   CAS 24709-35-8  (3274)
N-(2-(2-Ethoxycarbonylamino)ethyl)iminodiethanoic acid;
-------------------------------------------------------------------------------
```

```
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Ba++       gl  KCl    20°C 0.10M U        K1=2.0         1955SAa (67627) 485
**************************************************************************
C9H16O4               H2L                      CAS 57218-62-9  (484)
Ethyl(2-methylpropyl)propanedioic acid; HOOC.C(C2H5)(CH2.CH(CH3)2).COOH
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Ba++       sp  none   25°C  0.0  U        K1=2.67        1976KOa (67785) 486
**************************************************************************
C9H18O2Si              HL                       CAS 17940-02-2  (3275)
6-Trimethylsilylhexane-2,4-dione; (CH3)3.Si.CH2.CH2.CO.CH2.CO.CH3
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Ba++       gl  diox/w 30°C  75%  U        B2=9.8         1953UFd (67965) 487
**************************************************************************
C9H19N2O4+             H2L                        (3277)
2-Di(carboxymethyl)aminoethyltrimethylammonium cation
           +
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Ba++       gl  KCl    20°C 0.10M U        K1=1.34        1955SAa (68001) 488
**************************************************************************
C9H24N3O9P3            H6L    NOTPH             CAS 83843-39-3  (224)
1,4,7-Triazacyclononane-N,N',N"-tris(methylenephosphonic acid);
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Ba++       gl  KCl    25°C  1.0M U        K1=4.37        1984KMa (68311) 489
                                          K(Ba+HL)=2.16
--------------------------------------------------------------------------
Ba++       gl  oth/un 25°C 1.00M U        K1=4.37        1982PSc (68312) 490
                                          K(Ba+HL)=2.16
**************************************************************************
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
--------------------------------------------------------------------------
Ba++       gl  none   25°C  0.0  C                       1990CDc (68508) 491
                                          Kso(BaH2L)=-16.8
                                          K(Ba2L)=-13.5
Additional technique: spectrophotometry.
**************************************************************************
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
-------------------------------------------------------------------------
Ba++       gl  oth/un 25°C  0.0  U        K1=1.20        1955LUa (68700) 492
*************************************************************************
C10H7NO2               HL                     CAS 86-59-9  (873)
Quinoline-8-carboxylic acid;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Ba++       gl  oth/un 25°C  0.0  U        K1=1.22   B2=3.70   1955LUa (68755) 493
*************************************************************************
C10H7O2F3              HL                     CAS 326-06-7  (196)
3-Benzoyl-1,1,1-trifluoroacetone; CF3.CO.CH2.CO.C6H5
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Ba++       gl  diox/w 30°C  75%  U        B2=15.4        1953UFe (69136) 494
*************************************************************************
C10H8N2                 L    2,2'-Bipyridyl   CAS 366-18-7  (25)
2,2'-Bipyridine; (C5H4N)2
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Ba++       cal KCl    25°C 0.25M U   H    K1=-0.25       1997MKb (69528) 495
DH(K1)=-14 kJ mol-1; DS=-42 J K-1 mol-1
-------------------------------------------------------------------------
Ba++       gl  oth/un 25°C 0.20M U TIH    K1=-0.33       1993DGa (69529) 496
DH(K1)=23 kJ mol-1, DS(K1)=72 J K-1 mol-1. Data for 5-45 C, 0.20-
0.75 M BaCl2
-------------------------------------------------------------------------
Ba++       gl  KCl    25°C 0.25M U T H    K1=-0.24       1985CRa (69530) 497
K1=-0.10(10 C);K1=-0.38(40 C). DH(K1)=-16.3 kJ mol-1, DS=-58 J K-1 mol-1
*************************************************************************
C10H9O2Br              HL                     CAS 4023-81-8  (1182)
4-Bromo-1-phenyl-1,3-butanedione; Br.C6H4.CO.CH2.CO.CH3
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Ba++       gl  diox/w 20°C  75%  M T      K1=6.59   B2=11.61  1980GMd (70434) 498
*************************************************************************
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
-------------------------------------------------------------------------
Ba++       gl  diox/w 20°C  17%  C        K1=5.78   B2=9.94   1976JWa (70708) 499
-------------------------------------------------------------------------
Ba++       gl  diox/w 30°C  75%  U        B2=9.4         1953UFe (70709) 500
*************************************************************************
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
Ba++	gl	NaClO4	25°C	0.10M	U		K1=2.0	1968SMb (70845)	501

****

C10H11NO4 H2L CAS 1137-73-1 (2567)
N-Phenyliminodiethanoic acid; C6H5.N(CH2.COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	EMF	KCl	20°C	0.10M	U		K1=1	1947SWa (71000)	502

****

C10H11NO5 H3L CAS 100844-86-8 (2108)
N-(2-Hydroxyphenyl)iminodiethanoic acid; HO.C6H4.N(CH2.COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KNO3	20°C	0.10M	U		K1=4.27	1963IFb (71038)	503
							K(Ba+HL)=2.50		

****

C10H11NO7S H3L (3335)
N-(2-Sulfophenyl)iminodiethanoic acid; HO3S.C6H4.N(CH2.COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	EMF	KCl	20°C	0.10M	C		K1=3.48	1947SWa (71066)	504

Method: H electrode

****

C10H12N2O2 HL CAS 89314-29-4 (8507)
2-[(4-Methylphenyl)hydrazono]-propanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	alc/w	30°C	40%	M	M	K1=3.00 B2= 4.78	1995RRe (71194)	505
							K(BaL+A)=2.73		
							K(BaL+en)=5.31		
							K(BaL+pro)=2.02		
							K(BaL+B)=2.51		

Medium: 40% v/v EtOH/H2O, 0.10 M KNO3. K(BaL+ala)=1.47, K(BaL+gly)=0.65.
H2A is catechol, HB is hydroxyproline.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	alc/w	30°C	40%	M	M		1995RRe (71195)	506
							K(Ba(phe)+L)=2.68		
							K(BaA+L)=1.50		

Medium: 40% v/v EtOH/H2O, 0.10 M KNO3. H2A is salicylic acid.

****

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
-------------------------------------------------------------------------
Ba++       gl  NaNO3  20°C 0.10M C   H    K1=3.40        1981ANb (71250) 507
DH1=-7.1 kJ mol-1   DS1=40.6 J K-1 mol-1
-------------------------------------------------------------------------
Ba++       gl  KNO3   20°C 0.10M U        K1=3.40        1963IFc (71251) 508
*************************************************************************
C10H12N4O6             HL                     CAS 40281-74-1  (3910)
Purin-6-one 9-riboside N(1)-oxide    (Inosine N(1)-oxide)
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Ba++       sp  NaClO4 25°C 0.10M U        K1=1.2         1965SIa (71509) 509
*************************************************************************
C10H12O2               HL                     CAS 1946-74-3  (202)
3-Isopropyltropolone;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Ba++       dis NaClO4 25°C 0.10M U        K1=1.87   B2=2.74   1962DYa (71571) 510
*************************************************************************
C10H13N2O11P          H3L    Orotidylic acid  CAS 68244-58-6  (6665)
Orotidine-5'-monophosphoric acid, uridine-5-carboxylic acid-5-monophosphoric acid;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Ba++       gl  NaNO3  25°C 0.10M M        K1=1.62        1991BSc (71792) 511
                                        K(BaH-1L+H)=8.78
*************************************************************************
C10H13N3O7             H3L                      (3912)
1,3-Dimethyluramil-N,N-diethanoic acid;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Ba++       gl  KNO3   20°C 0.10M U        K1=6.00   B2=9.88   1963IFb (71803) 512
*************************************************************************
C10H13N4O8P            H3L    IMP             CAS 131-99-7  (843)
Inosine-5'-monophosphoric acid;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Ba++       gl  NaNO3  25°C 0.10M M                        1994SMb (71857) 513
                                        K(Ba+HL)=1.28
                                        *K(BaHL)=-8.61
*************************************************************************
C10H13N4O9P            H3L                      (3930)
Inosine-5'-monophosphoric acid N(1)-oxide;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
```

```
Ba++       sp  NaClO4 25°C 0.10M U                        1965SIa (71884) 514
                                          K(Ba+HL)=1.6
********************************************************************************
C10H13N5O5             HL    Guanosine        CAS 118-00-3  (1402)
2-Aminopurin-6-one-9-riboside;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Ba++       nmr non-aq 21°C 100%  U                        1973SFa (72008) 515
                                          K(Ba+HL)=1.70
Medium: (CH3)2SO
********************************************************************************
C10H14N5O6PS           H2L    AMPS             CAS 19341-57-2  (8152)
Adenosine-5'-monothiophosphoric acid, 5-Thioadenylic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Ba++       gl  NaNO3  25°C 0.10M M        K1=0.99        1997SSg (72152) 516
********************************************************************************
C10H14N5O7P            H2L    AMP-2            CAS 81012-86-4  (2437)
Adenosine-2'-monophosphoric acid, 2-Adenylic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Ba++       gl  R4N.X  25°C 0.10M C      T K1=1.76        1991SMa (72184) 517
IUPAC evaluation
--------------------------------------------------------------------------------
Ba++       gl  NaNO3  25°C 0.10M U        K1=1.12        1989MSf (72185) 518
--------------------------------------------------------------------------------
Ba++       gl  KNO3   40°C 0.10M U T H    K1=1.64        1967TMf (72186) 519
K1=1.82(0.4 C),1.77(12 C),1.71(25 C). At 25 C: DH(K1)=-8.4 kJ mol-1, DS=5
********************************************************************************
C10H14N5O7P            H2L    AMP-3            CAS 84-21-9  (2438)
Adenosine-3'-monophosphoric acid, 3-Adenylic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Ba++       gl  R4N.X  25°C 0.10M C      T K1=1.74        1991SMa (72236) 520
IUPAC evaluation
--------------------------------------------------------------------------------
Ba++       gl  NaNO3  25°C 0.10M U        K1=1.08        1989MSf (72237) 521
--------------------------------------------------------------------------------
Ba++       gl  KNO3   40°C 0.10M U T H    K1=1.62        1967TMf (72238) 522
K1=1.81(0.4 C),1.75(12 C),1.69(25 C). At 25 C: DH(K1)=-7.9 kJ mol-1, DS=5 J
--------------------------------------------------------------------------------
Ba++       gl  KNO3   25°C 0.10M U        K1=1.69        1962TMa (72239) 523
********************************************************************************
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
Ba++	gl	NaNO3	25°C	0.10M	M		K1=1.18 K(BaL+H)=4.6 K(Ba+HL)=-0.4	2003BSa (72441)	524
Ba++	gl	NaNO3	25°C	0.10M	M		K1=1.18	1996SSd (72442)	525
Ba++	gl	R4N.X	25°C	0.10M	C	T	K1=1.78	1991SMa (72443)	526

IUPAC evaluation

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	NaNO3	25°C	0.10M	U		K1=1.17	1989MSf (72444)	527
Ba++	gl	NaNO3	25°C	0.10M	C		K1=1.17	1988SMb (72445)	528
Ba++	gl	KNO3	40°C	0.10M	U T H		K1=1.66	1967TMf (72446)	529

K1=1.85(0.4 C),1.80(12 C),1.73(25 C). At 25 C: DH(K1)=-8.4 kJ mol-1, DS=5 J

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	NaClO4	25°C	0.10M	U		K1=1.14	1964SBa (72447)	530
Ba++	gl	KNO3	25°C	0.10M	U		K1=1.73	1962TMa (72448)	531

****

C10H14N5O8P H2L CAS 4061-78-3 (3931)
Adenosine-5'-monophosphoric acid N(1)-oxide;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	NaClO4	25°C	0.10M	U		K(Ba+HL)=1.15 K(BaL+H) > 10.79	1964SBa (72522)	532

By spectrophotometry: K1 < 2.86

****

C10H14N5O8P H3L GMP-5 CAS 85-32-5 (2947)
Guanosine-5'-monophosphoric acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	NaNO3	25°C	0.10M	M		K(Ba+HL)=1.32 *K(BaHL)=-9.02	1994SMb (72586)	533

****

C10H15NO6 H3L (3915)
N-(1'-Carboxycyclopentyl)iminodiethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KCl	20°C	0.10M	U		K1=5.50	1966IMa (72669)	534

****

C10H15N2O8P H2L TMP-5 CAS 365-07-1 (2949)
Thymidine-5'-monophosphoric acid, Thymidylic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	R4N.X	25°C	0.10M	C	T	K(Ba+HL)=1.72	1991SMa (72699)	535

IUPAC evaluation

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	NaNO3	25°C	0.10M	C		K(Ba+HL)=1.11	1988MSa (72700)	536

****

C10H15N4O14P3 H5L ITP CAS 35908-31-7 (2148)

Inosine 5'-triphosphoric acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	NaNO3	25°C	0.10M	C		K(Ba+HL)=3.28 K(BaHL+H)=5.5 K(Ba+H2L)=2.3	2001SBc (72763)	537

For pyrimidine nucleoside 5'-triphosphoric acid, K1=3.18, K(Ba+HL)=2.1, K(BaL+H)=5.4

****

C10H15N5O10P2 H3L ADP CAS 20398-34-9 (2181)

Adenosine-5'-diphosphoric acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	NaNO3	25°C	0.10M	M		K1=2.37 K(BaL+H)=5.15 K(Ba+HL)=1.12	2003BSa (72978)	538
Ba++	gl	NaNO3	25°C	0.10M	C	M	K1=2.36 K(BaL+A)=3.26 B(BaLA)=5.62	2000KHa (72979)	539

H2A=salicylhydroxamic acid.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	R4N.X	25°C	0.10M	C	T	K1=2.58 K(Ba+HL)=1.51	1991SMa (72980)	540

IUPAC evaluation

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KNO3	40°C	0.10M	U	T H	K1=2.25 K(Ba+HL)=1.37	1967TMf (72981)	541

K1=2.53(0.4 C),2.45(12 C),2.36(25 C); K=1.55(0.4 C),1.50(12 C),1.44(25 C). At 25 C:DH(K1)=-12.1 kJ mol-1,DS=4.2 J K-1 mol-1; DH(Ba+HL)=-7.5,DS=4

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KNO3	25°C	0.10M	U		K1=2.36	1962TMa (72982)	542

****

C10H16N2O8 H4L EDDS CAS 52759-67-8 (1100)

1,2-Diaminoethane-N,N'-di-1,4-butanedioic acid; (CH2.NH.CH(COOH)CH2.COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KNO3	25°C	0.10M	U		K1=2.98 K(Ba+HL)=0.96	1989VZc (73112)	543
Ba++	gl	KNO3	25°C	0.10M	U		K1=2.12 K(Ba+HL)=1.46 K(Ba+BaL)=0.90	1971GBc (73113)	544
Ba++	dis	KNO3	20°C	0.10M	U		K1=3.8	1968MJa (73114)	545

Method: paper electrophoresis. By glass electrode, K1=3.10, K(Ba+HL)=1.30

****

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
Ba++	cal	NaClO4	25°C	0.50M	U	T H		1983VBa (73596)	546

DH(K1)=-24.60 kJ mol-1

Ba++	EMF	KCl	20°C	0.10M	C		K1=7.8	1981SFa (73597)	547

Method: Pt/H2 electrode.

Ba++	gl	KNO3	20°C	0.10M	C	I R	K1=7.73	1978ANa (73598)	548

IUPAC evaluation

Ba++	gl	KNO3	20°C	0.10M	U		K1=7.76	1978NLb (73599)	549
Ba++	oth	KNO3	20°C	0.10M	U		K1=8	1965JMb (73600)	550

Method: electrophoresis

Ba++	cal	KNO3	25°C	0.10M	U	H		1965WHa (73601)	551

DH(K1)=-22.1 kJ mol-1, DS=75.2 J K-1 mol-1

Ba++	cal	KNO3	20°C	0.10M	U	H		1963ANf (73602)	552

DH(K1)=-20.6 kJ mol-1, DS=79 J K-1 mol-1

Ba++	gl	KNO3	25°C	0.10M	U	T H T	K1=7.63	1960BMc (73603)	553

K1=8.07(0.5 C), 7.76(13.2 C), 7.36(42.4 C); DH(K1)=-25 kJ mol-1, DS=54

Ba++	ix	none	?	0.0	U		K1=9.92	1957KFa (73604)	554
Ba++	gl	oth/un	20°C	0.17M	U	H		1956CSb (73605)	555

DG(K1)=-43.5 kJ mol-1, DH=-20.2, DS=79.5 J K-1 mol-1

Ba++	EMF	oth/un	25°C	0.0	U	H		1956MAa (73606)	556

Method: H electrode. DG(K1)=-43.9 kJ mol-1, DH=-17, DS=92 J K-1 mol-1.

Ba++	EMF	NaClO4	25°C	0.10M	U		K1=7.9	1956SRb (73607)	557

```
Ba++       cal oth/un 25°C 0.05M U   H                    1954CHa (73608) 558
Medium: BaCl2. DH(K1)=-21.3 kJ mol-1, DS=75.2 J K-1 mol-1
--------------------------------------------------------------------------------
Ba++       EMF oth/un 20°C  0.0  U   H    K1=7.78         1954CMb (73609) 559
Method: H electrode. DH(K1)=-17.2 kJ mol-1, DS=92 J K-1 mol-1
--------------------------------------------------------------------------------
Ba++       EMF KCl    20°C 0.10M U      T K1=7.76         1947SAa (73610) 560
                                          K(Ba+HL)=2.07
Method: H electrode
********************************************************************************
C10H16N2O8            H4L                    CAS 63501-20-2  (2583)
meso-2,3-Diaminobutane-N,N'-di(1,3-propanedioic acid)
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Ba++       gl  KNO3   25°C 0.10M U        K1=4.04         1978SGc (74360) 561
                                          K(Ba+HL)=1.56
                                          K(Ba+BaL)=1.48
********************************************************************************
C10H16N2O9            H4L                    CAS 616-90-0  (2615)
Bis-(2-aminoethylether)-N,N'di(1,3-propanedioic acid); ((HOOC)2CH.NH.CH2.CH2)2O
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Ba++       gl  KNO3   25°C 0.10M U        K1=4.28         1979KBd (74375) 562
                                          K(Ba+HL)=2.42
********************************************************************************
C10H16N2O11P2         H4L                    CAS 491-97-4  (7674)
Thymidine-5'-diphosphoric acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Ba++       gl  NaNO3  25°C 0.10M M                         1999SSa (74388) 563
                                          K(Ba+HL)=2.33
********************************************************************************
C10H16N5O13P3         H4L    ATP             CAS 56-65-5  (403)
Adenosine-5'-triphosphoric acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Ba++       gl  NaNO3  25°C 0.10M C    M   K1=3.70         2000KHa (74700) 564
                                          K(BaL+A)=3.30
                                          B(BaLA)=7.00
H2A=salicylhydroxamic acid.
--------------------------------------------------------------------------------
Ba++       gl  R4N.X  25°C 0.10M C      T K1=3.57         1991SMa (74701) 565
                                          K(Ba+HL)=1.88
IUPAC evaluation
--------------------------------------------------------------------------------
Ba++       nmr R4N.X  22°C 0.10M U                        1985PHb (74702) 566
```

```
                                        K(Ba+H3L)=2.26
--------------------------------------------------------------------------------
Ba++       gl  KNO3   40°C 0.10M U T H    K1=3.12        1966TMb (74703) 567
                                        K(Ba+HL)=1.75
K1=3.58(0.4 C),3.42(12 C),3.29(25 C); K=2.02(0.4 C),1.92(12 C),1.85(25 C).
At 25 C:DH(K1)=-16.3 kJ mol-1, DS=8.4 J K-1 mol-1; DH(Ba+HL)=-8.8,DS=8.4
--------------------------------------------------------------------------------
Ba++       gl  KNO3   25°C 0.10M U        K1=3.29        1962TMb (74704) 568
                                        K(Ba+HL)=1.85
--------------------------------------------------------------------------------
Ba++       gl  R4N.X  25°C 0.10M U        K1=3.73        1961NAa (74705) 569
Medium: Et4NBr
********************************************************************************
C10H16N5O14P3         H5L    GTP              CAS 86-01-1  (404)
Guanosine-5'-triphosphoric acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Ba++       gl  NaNO3  25°C 0.10M C                        2001SBc (74881) 570
                                        K(Ba+HL)=3.41
                                        K(BaHL+H)=5.75
                                        K(Ba+H2L)=2.65
********************************************************************************
C10H17NO4             H2L                   CAS 2848-06-8  (3916)
N-(Cyclohexyl)iminodiethanoic acid; C6H11.N(CH2.COOH)2
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Ba++       gl  KNO3   20°C 0.10M U        K1=2.37        1963IFb (74974) 571
********************************************************************************
C10H17NO5             H2L                   CAS 6243-06-7  (3326)
N-(2-Hydroxycyclohexyl)iminodiethanoic acid; HO.C6H10.N(CH2.COOH)2
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Ba++       gl  KNO3   20°C 0.10M U        K1=3.26        1963IFb (74986) 572
********************************************************************************
C10H17NO5             H2L                     (3917)
N-(Tetrahydropyran-2-ylmethyl)iminodiethanoic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Ba++       gl  KNO3   20°C 0.10M U        K1=3.61        1963IFa (75000) 573
********************************************************************************
C10H18N2O4S           H2L                     (6638)
1-Thia-4,7-diazacyclononane-N,N'-diethanoic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Ba++       gl  KNO3   25°C 0.10M C        K1=2.87        1993WLa (75215) 574
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C10H18N2O5 H2L (5608)
1-Oxa-4,7-diazacyclononane-N,N'-diethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KNO3	25°C	0.10M	U		K1=3.13	1990CCa (75232)	575
Ba++	cal	NaClO4	25°C	0.10M	U	H	K1=3.3	1985EHa (75233)	576

DH(K1)=-3.3 kJ mol-1, DS=53.0 J K-1 mol-1

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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
Ba++	gl	NaClO4	30°C	0.10M	U		K1=6.05	1981MMc (75335)	577
Ba++	cal	KNO3	25°C	0.10M	U	H		1965WHa (75336)	578

DH(K1)=-22.6 kJ mol-1, DS=41.8 J K-1 mol-1

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	EMF	KCl	30°C	0.10M	U		K1=6.2	1960HRa (75337)	579
Ba++	gl	KCl	20°C	0.10M	U		K1=5.54	1959KRa (75338)	580
							K(Ba+HL)=0.65		

****

C10H18O8 H2L CAS 32775-08-9 (240)
1,12-Dicarboxy-2,5,8,11-tetraoxadodecane; (HOOC.CH2.O.CH2.CH2.O.CH2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KNO3	25°C	0.10M	U		K1=2.29	1974MSa (75618)	581

****

C10H19NO4 H2L (3328)
N-(3,3-Dimethylbutyl)iminodiethanoic acid; (CH3)3C.CH2.CH2.N(CH2.COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KCl	20°C	0.10M	U		K1=2.41	1955SAa (75638)	582

****

C10H20N2O6 H2L (7208)
1,2-Diaminoethane-N,N'-bis(3-hydroxy-2-butanoic acid)); (CH2NHCH(COOH)CH(OH)CH3)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KNO3	20°C	0.10M	U		K1=2.2	1970DKa (75834)	583

****

C10H20N2O6 H2L CAS 96817-35-5 (4755)
1,2-Diaminoethane-N,N'-bis(4-hydroxy-2-butanoic acid);

```
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Ba++       sp  oth/un 20°C 0.10M U        K1=2.2         1972DKa (75845) 584
*************************************************************************
C10H20O2               HL    Capric acid      CAS 334-48-5  (2542)
Decanoic acid; CH3.(CH2)8.COOH
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Ba++       gl  oth/un 20°C  var  U                         1981HTc (75904) 585
                                          Kso=-8.23
*************************************************************************
C10H20O3S2              L                     CAS 40253-98-3  (8606)
1,4,10-Trioxa-7,13-dithiacyclopentadecane;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Ba++       cal non-aq 25°C 100%  C   H    K1=1.68        1988BUb (75911) 586
Medium: acetonitrile. DH(K1)=-1.9 kJ mol-1, DS(K1)=26 J K-1 mol-1.
*************************************************************************
C10H20O5                L    15-Crown-5       CAS 33100-27-5  (576)
1,4,7,10,13-Pentaoxacyclopentadecane; cyclo(-(O.CH2.CH2)5-)
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Ba++       ISE R4N.X  25°C  0.1M C  I   T K1=1.69        2003ADa (75972) 587
IUPAC Tentative. Medium: 0-0.1 M various.
-------------------------------------------------------------------------
Ba++       con mixed  25°C  20%  C        K1=3.81        2003SIa (75973) 588
Medium: 20% w/w propylene carbonate/ethylene carbonate.
-------------------------------------------------------------------------
Ba++       cal oth/un 25°C       C T    T K1=1.66        2000VGa (75974) 589
                                          DH1=-4.52 kJ/mol
Medium: 0.899 M BaCl2; for T=35 K1=1.64 DH1=-4.60 kJ/mol
for T=45 K1=1.62;
-------------------------------------------------------------------------
Ba++       con non-aq 25°C 100%  C   H    K1=1.26   B2= 1.41  1999WBa (75975) 590
Medium: N,N-dimethylformamide. By calorimetry: DH(K1)=-11.5 kJ mol-1,
DH(K2)=-3.8 kJ mol-1.
-------------------------------------------------------------------------
Ba++       cal non-aq 25°C 100%  C   H    K1=>5          1992BSc (75976) 591
Medium: propylene carbonate. DH(K1)=-39.2 kJ mol-1.
-------------------------------------------------------------------------
Ba++       cal non-aq 25°C 100%  C   H    K1=>5          1988BUb (75977) 592
Medium: acetonitrile. DH(K1)=-40.8 kJ mol-1.
-------------------------------------------------------------------------
Ba++       cal oth/un 25°C 0.10M U   H  T K1=1.71        1976ITb (75978) 593
DH=-4.77 kJ mol-1.
*************************************************************************
C10H21NO4               L                     CAS 66943-05-3  (5818)
```

1-Aza-4,7,10,13-tetraoxacyclopentadecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	sp	non-aq	25°C	100%	U		B2=>12.0	1998ACa (76182)	594

Medium: CH3CN

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C10H22N2O3 L Cryptand 2,1 CAS 31249-95-3 (835)
4,7,13-Trioxa-1,10-diazacyclopentadecane (Trioxa(2,1)cryptand);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	sp	non-aq	20°C	100%	U		K1=1.8	1992PSa (76307)	595

Medium: DMF, 0.01 M Me4NI

Ba++	ISE	alc/w	25°C	100%	U		K1=2.7	1988CFa (76308)	596

Medium: MeOH

Ba++	cal	alc/w	25°C	100%	U	H	K1=2.72 B2=5.14	1986BUa (76309)	597

Medium: MeOH. DH(B2)=-11.3 kJ mol-1; DS=8 J K-1 mol-1

Ba++	cal	non-aq	25°C	100%	U	H	K1=>6.5	1986BUb (76310)	598

In CH3CN. DH=-35.0 kJ mol-1

Ba++	cal	alc/w	25°C	100%	U	H	K1=2.72	1985BUc (76311)	599

Medium: MeOH, 0.05 M Et4NClO4. DH=+4.1 kJ mol-1

****

C10H22O5 L Tetraglyme CAS 143-24-8 (121)
2,5,8,11,14-Pentaoxapentadecane; (CH3.O.CH2.CH2.O.CH2.CH2.)2O

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	cal	non-aq	25°C	100%	U	H	K1=3.27	1993BDb (76438)	600

Medium: acetone. DH=-27.8 kJ mol-1; TDS=-9.2

Ba++	con	non-aq	25°C	100%	C	H	K1=4.30	1992BSc (76439)	601

Medium: propylene carbonate. By calorimetry, DH(K1)=-39.4 kJ mol-1,
DS(K1)=-50.3 J K-1 mol-1.

Ba++	cal	non-aq	25°C	100%	U	H	K1=1.74	1991TNa (76440)	602

Medium: MeOH. DH(K1)=-23.8 kJ mol-1; TDS=-14.1

****

C10H22O6 L Penta-Et-Glycol CAS 4792-15-8 (5466)
1,14-Dihydroxy-3,6,9,12,-Tetraoxatetradecane; HO.(CH2.CH2.O)4.CH2.CH2.OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	cal	alc/w	25°C	90%	U	IH	K1=3.45	1982HLa (76480)	603

Medium: 90% w/w MeOH/H2O. DH=-31.8 kJ mol-1, DS=-12.1 J K-1 mol-1

****

C10H26N2O12P4 H8L CAS 28698-30-8 (3342)
N,N,N',N'-Tetra(phosphomethyl)cyclohexane-1,2-diamine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Ba++	gl	oth/un	25°C	0.10M	U		K1=2.87		1959BYa (76757)	604

****

C11H8O2S2 HL CAS 1138-14-3 (3352)
Di-2-thenoylmethane; C4H3S.CO.CH2.CO.C4H3S

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Ba++	gl	diox/w	30°C	75%	U		B2=11.4		1953UFe (76985)	605

****

C11H9NO3 HL CAS 1137-48-0 (1449)
N-Phenyl-2-furylhydroxamic acid; C4H3O.CO.N(C6H5).OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Ba++	gl	diox/w	25°C	70%	U		K1=6.46	B2=11.72	1992DAc (77390)	606

For N-p-tolyl derivative, K1=7.12, K2=5.94, for N-m-Cl, K1=6.60,
K2=5.40; for N-p-Cl, K1=6.86, K2=5.66.

****

C11H10N2O L (7591)
4'-(Imidazol-1-yl)acetophenone;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Ba++	gl	NaNO3	25°C	0.50M	M		K1=-0.18		1998KSa (77668)	607

****

C11H11NO6 H3L CAS 1147-65-5 (425)
N-(2'-Carboxyphenyl)iminodiethanoic acid; HOOC.C6H4.N(CH2.COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Ba++	EMF	KCl	20°C	0.10M	U		K1=3.57		1947SWa (77823)	608

Method: H electrode

****

C11H11NO6 H3L (3357)
N-(3-Carboxyphenyl)iminodiethanoic acid; HOOC.C6H4.N(CH2.COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Ba++	EMF	KCl	20°C	0.10M	C		K1=1		1947SWa (77844)	609

Method: H electrode

****

C11H11NO6 H3L CAS 86363-45-6 (3358)
N-(4-Carboxyphenyl)iminodiethanoic acid; HOOC.C6H4.N(CH2.COOH)2

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

---
Ba++ EMF KCl 20°C 0.10M C K1=<1 1947SWa (77849) 610
Method: H electrode
****
C11H11O2F HL CAS 38440-21-0 (2906)
1-(4-Fluorophenyl)-1,3-pentanedione; F.C6H4.CO.CH2.CO.CH2.CH3

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl diox/w 20°C 75% M T K1=7.22 B2=12.00 1980GMd (77966) 611
****
C11H12N2O7 H3L CAS 76268-70-5 (3360)
N-(2-Hydroxy-5-nitrobenzyl)iminodiethanoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl KCl 20°C 0.10M U K1=4.81 1952SAb (78342) 612
K(Ba+HL)=1.75
****
C11H12O2 HL CAS 4023-79-4 (305)
1-(4-Methylphenyl)butane-1,3-dione; CH3.C6H4.CO.CH2.CO.CH3

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl diox/w 20°C 75% M T K1=7.06 B2=12.03 1980GMd (78372) 613
****
C11H13NO5 H2L CAS 4596-54-7 (3945)
N-(2'-Methoxyphenyl)iminodiethanoic acid; CH3O.C6H4.N(CH2.COOH)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl KNO3 20°C 0.10M U K1=2.08 1963IFb (78601) 614
****
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
---
Ba++ gl KCl 20°C 0.10M U K1=4.40 1952SAb (78615) 615
K(Ba+HL)=1.96
****
C11H13N3O3 H2L (3363)
Biacetyl oxime salicyloylhydrazone;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl alc/w 20°C 50% U B2=4.26 1961VLc (78726) 616
Medium: 50% EtOH, 0.1 M KCl
****
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
Ba++	gl	NaNO3	20°C	0.10M	C		K1=2.55	1981ANb (78877)	617

****

C11H14N4O4 L Tubercidin CAS 69-33-0 (6412)
7-Deazaadenosine, Tubercidin;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	NaNO3	25°C	0.50M	C		K1=-0.14	2002KSb (78958)	618

****

C11H15N4O7P H2L CAS 16719-46-3 (6026)
Tubercidin-5'-monophosphoric acid, 7-Deazaadenosine-5-monophosphoric acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	NaNO3	25°C	0.10M	C		K1=1.13	1988SMb (79069)	619
							K(Ba+HL)=0.1		

****

C11H17NO3 H2L Isoprenaline CAS 586-06-1 (3950)
3,4-Dihydroxy-1-(1'-hydroxy-2'-(propylamino)ethyl)benzene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KCl	25°C	0.10M	U T H		K1=3.42 B2= 4.52	1988CVa (79156)	620

Data for 0 and 37 C. DH(K1)=-17.4 kJ mol-1, DS(K1)=7.1 J K-1 mol-1;
DH(K2)=-12.6, DS(K2)=-20.6.

****

C11H17NO6 H3L (3951)
N-(2'-Carboxycyclohexyl)iminodiethanoic acid; HOOC.C6H10.N(CH2.COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KCl	20°C	0.10M	U		K1=5.07	1966IMa (79165)	621

****

C11H17NO8S H3L CAS 91649-51-3 (8438)
N,N,S-Tris(carboxymethyl)methionine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KCl	25°C	0.10M	C			1984RFd (79175)	622
							K(Ba+HL)=2.67		

****

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

Ba++ gl KNO3 25°C 0.10M U K1=7.90 1980KBb (79261) 623

Ba++ gl KNO3 20°C 0.10M U K1=8.40 1978NLb (79262) 624

Ba++ gl KCl 25°C 0.10M U K1=8.48 1970AIa (79263) 625
DL-isomer. For D-isomer, K1=8.45

Ba++ gl KCl 30°C 0.10M U K1=8.48 1963GHa (79264) 626

****

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
Ba++	gl	KNO3	20°C	0.10M	U		K1=3.95 K(Ba+HL)=2.21	1964LAa (79423)	627
Ba++	EMF	KCl	20°C	0.10M	C		K1=4.24 K(Ba+HL)=2.11	1948SAa (79424)	628

Method: H electrode

****

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
Ba++	gl	KNO3	25°C	0.10M	U		K1=4.91 K(BaL+H)=7.34	1966TKa (79541)	629
Ba++	oth	KNO3	20°C	0.10M	U		K1=5	1965JMb (79542)	630

Method: electrophoresis

Ba++ gl KCl 20°C 0.10M U K1=4.92 1964DSc (79543) 631
By polarography: K1=5.45

Ba++ gl KCl 30°C 0.10M U K1=4.65 1963GHa (79544) 632

Ba++ gl KCl 20°C 0.10M U K1=5.00 1959KRa (79545) 633
K(Ba+HL)=2.06

****

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
Ba++	gl	KNO3	25°C	0.10M	U		K1=1.95 K(Ba+HL)=1.14	1974KGa (79590)	634

****

C11H22O5 L 16-Crown-5 CAS 55477-28-8 (1592)
1,4,7,10,13-Pentaoxacyclohexadecane; cyclo(-(O.CH2.CH2)5.CH2.CH2-)

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ con none 25°C 0.0 C K1=1.84 1991TKa (79848) 635
Self medium (ca. 0.008M).

Ba++ dis none 25°C 0.0 C M 1989TKc (79849) 636
K(BaL+2A=BaA2L(org))=2.92
Method: extraction of metal picrate/L from H2O into benzene.
K(Ba+2HA(org)+L(org)=BaA2L(org)+2H)=0.07. HA is picric acid.
****
C12H5N7O12 L Dipicrylamine CAS 131-73-7 (1942)
Di(2,4,6-trinitrophenyl)amine; HN(C6H2(NO2)3)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ dis non-aq 25°C 100% U K1=2.1 1969PKb (80070) 637
Medium: nitrobenzene. K1=1.4(tracer amounts Ba++)
****
C12H8N2 L Phenanthroline CAS 66-71-7 (144)
1,10-Phenanthroline;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ cal KCl 25°C 0.25M U H K1=-3.4 1997MKb (80416) 638
DH(K1)=-10 kJ mol-1; DS=-22 J K-1 mol-1

Ba++ gl KCl 25°C 0.25M U T H K1=0.57 1985CRa (80417) 639
K1=0.66(10 C);K1=0.48(40 C).
DH=-10.0 kJ mol-1, DS=-21 J mol-1 K-1
****
C12H9NO2S HL CAS 74706-50-6 (3392)
Isonicotinoyl-2-thenoylmethane; C5H4N.CO.CH2.CO.C4H3S

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl diox/w 30°C 75% U B2=10.8 1953UFe (80571) 640
****
C12H9NO2S HL (3416)
Pyridine-2-carbonyl-(2-thenoyl)methane; C5H4N.CO.CH2.CO.C4H3S

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl diox/w 30°C 75% U B2=12.0 1953UFe (80573) 641
****
C12H11NO2S HL CAS 29556-14-7 (2049)
N-(4-Tolyl)-2-thenoylhydroxamic acid; C4H3SCON(OH)C6H4CH3

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

Ba++ gl diox/w 25°C 70% U K1=7.36 B2=13.54 1992DAc (80834) 642
****
C12H11NO9 H5L (3975)
N-(2',5'-Dicarboxy-4'-hydroxyphenyl)iminodiethanoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl KNO3 25°C 0.10M U 1967UKa (80853) 643
K(Ba+HL)=3.90
****
C12H12NO6Cl H3L (4004)
(alpha-Carboxy-4'-chlorobenzyl)iminodiethanoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl KCl 20°C 0.10M U K1=4.21 1966IMb (80983) 644
****
C12H12N2O3 HL Nalidixic acid CAS 389-08-2 (1401)
1-Ethyl-1,4-dihydro-7-methyl-4-oxo-1,8-naphthyridine-3-carboxylic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ sp KCl 25°C 0.10M U K1=1.0 1978TSb (81067) 645
****
C12H12N2O4Cl2 L CAS 53-85-0 (8151)
5,6-Dichloro-1-(beta-D-ribofuranosyl)benzimidazole;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl NaNO3 25°C 0.50M M K1=-0.16 1998KSd (81102) 646
****
C12H13NO6 H3L CAS 17335-88-5 (3981)
1-(Carboxybenzyl)iminodiethanoic acid; C6H5.CH(COOH).N(CH2.COOH)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl KCl 20°C 0.10M U K1=4.28 1966IMb (81243) 647
****
C12H15NO4 H2L CAS 36369-62-7 (4928)
(Phenethylimino)diethanoic acid; C6H5.CH2.CH2.N(CH2.COOH)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl KCl 20°C 0.10M U K1=2.40 1971KTl (81464) 648
K(Ba+HL)=1.24
****
C12H15NO5 H3L CAS 56042-30-9 (4929)
N-(4-Hydroxyphenethylimino)diethanoic acid; HO.C6H4.CH2.CH2.N(CH2.COOH)2

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

```
--------------------------------------------------------------------------------
Ba++       gl  KCl    25°C 0.10M U                        1971KTl (81509) 649
                                        K(Ba+HL)=2.52
                                        K(Ba+H2L)=1.32
********************************************************************************
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
--------------------------------------------------------------------------------
Ba++       gl  KCl    25°C 0.10M U        K1=2.59        1979TSa (81601) 650
                                        K(Ba+HL)=2.28
                                        K(Ba+BaL)=1.9
********************************************************************************
C12H16O4                L                       CAS 25887-95-6  (686)
2,3-Benzo-1,4,7,10-tetraoxacyclododeca-2-ene;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Ba++       oth alc/w  35°C 3.0%  C        K1=1.44        1999MTd (81672) 651
Method: capillary zone electrophoresis. Medium: 3% v/v EtOH/H20, 0.005 M
acetate buffer, pH 5.5.
********************************************************************************
C12H18N2O8            H2L                       CAS 93031-52-8  (5829)
1,4-Dioxa-7,10-diazayclododecane-5,12-dione-7,10-diethanoic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Ba++       gl  R4N.X  25°C 0.10M C        K1=3.66        2002DCb (81831) 652
                                        K(BaL+H)=5.06
Medium: 0.10 M Me4NNO3.
********************************************************************************
C12H18N2O8            H4L                       CAS 77441-50-0  (2930)
cis-1,4-Diaminocyclohexane-N,N'-di(propanedioic acid)
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Ba++       gl  KNO3   25°C 0.10M U        K1=2.54        1982SGb (81850) 653
********************************************************************************
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
--------------------------------------------------------------------------------
Ba++       gl  KCl    20°C 0.10M U        K1=2.86        1976TTb (81891) 654
                                        K(Ba+HL)=2.54
                                        K(BaL+Ba)=2.3
********************************************************************************
C12H18N2O8            H4L                       CAS 82481-42-3  (2931)
```

trans-1,4-Diaminocyclohexane-N,N'-di(propanedioic acid)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KNO3	25°C	0.10M	U		K1=2.23	1982SGb (81899)	655

****

C12H19NO6 H3L (3991)

N-(2'-Carboxycycloheptyl)iminodiethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KCl	20°C	0.10M	U		K1=5.54	1966IMa (81981)	656

****

C12H20N2O8 H4L CAS 1798-13-6 (4935)

1,2-Diaminobutane-N,N,N',N'-tetraethanoic acid;
(HOOC.CH2)2N.CH2.CH(C2H5).N(CH2.COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KNO3	20°C	0.10M	U		K1=8.50	1969NDa (82020)	657

****

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
Ba++	gl	KNO3	20°C	0.10M	U		K1=1.80	1973DSc (82057)	658
Ba++	gl	KNO3	25°C	0.10M	U		K1=2.47 K(Ba+HL)=1.66 K(Ba+BaL)=2.66	1972GBe (82058)	659

****

C12H20N2O8 H4L CAS 61368-60-3 (3389)

1,2-Diaminoethane-N,N'-diethanoic-N,N'-di-2-propanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KNO3	20°C	0.10M	U		K1=6.66	1966MKb (82126)	660
Ba++	gl	KCl	30°C	0.10M	U		K1=6.86	1963GHa (82127)	661

****

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
Ba++	gl	KNO3	20°C	0.10M	U		K1=3.77 K(Ba+HL)=2.58	1964LAa (82212)	662
Ba++	EMF	KCl	20°C	0.10M	U			1948SAa (82213)	663

K(Ba+HL)=2.40
Method: H electrode
****
C12H20N2O8 H4L BDTA CAS 868-43-9 (1742)
DL-2,3-Diaminobutane-N,N,N',N'-tetraethanoic acid;
(HOOC.CH2)2N.CH(CH3).CH(CH3).N(CH2.COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KCl	25°C	0.10M	U		K1=8.53(DL) K1=8.51(D)	1970AIa (82283)	664
Ba++	gl	KCl	20°C	0.10M	U		K1=8.49	1966IPa (82284)	665
Ba++	oth	KNO3	20°C	0.10M	U		K1=11	1965JMb (82285)	666

Method: electrophoresis

Ba++	gl	KCl	20°C	0.10M	U		K1=8.53	1963MDa (82286)	667

****
C12H20N2O8 H4L CAS 63818-08-6 (2584)
meso-2,3-Diaminobutane-N,N'-di(1,4-butanedioic acid);
(CH(CH3).NH.CH(COOH)(CH2.COOH))2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KNO3	25°C	0.10M	U		K1=3.31 K(Ba+HL)=1.23 K(Ba+BaL)=1.04	1978SGc (82351)	668

****
C12H20N2O8 H4L CAS 22968-57-6 (3992)
meso-2,3-Diaminobutane-N,N,N',N'-tetraethanoic acid;
(HOOC.CH2)2N.CH(CH3).CH(CH3).N(CH2.COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KCl	20°C	0.10M	U		K1=6.45	1966IPa (82384)	669
Ba++	oth	KNO3	20°C	0.10M	U		K1=7	1965JMb (82385)	670

Method: electrophoresis

Ba++	gl	KCl	20°C	0.10M	U		K1=6.53 K(Ba+HL)=1.83	1963MDa (82386)	671

****
C12H20N2O8S H4L TEDTA CAS 923-74-0 (3394)
2,2'-Thiobis(ethyliminodiethanoic acid); S(CH2.CH2.N(CH2.COOH)2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KCl	20°C	0.10M	U		K1=5.34	1964PCa (82448)	672

K(Ba+HL)=2.9

****

C12H20N2O8S2 H4L (3395)

2,2'-Dithiobisethyleneiminodiethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KNO3	25°C	0.10M	U		K1=3.81 K(BaL+H)=9.01 K(Ba+HL)=3.25 B(Ba2L)=6.80	1988PGb (82487)	673

****

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
Ba++	cal	KNO3	25°C	0.10M	U	H		1965WHa (82523)	674

DH(K1)=-27.2 kJ mol-1, DS=62.7 J K-1 mol-1

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KCl	20°C	0.10M	U		K1=8.15 K(Ba+HL)=3.85	1964PCa (82524)	675

****

C12H20N2O10 H4L CAS 10258-50-1 (3993)

(2,3-Dihydroxytetramethylenedinitrilo)tetraethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KNO3	20°C	0.10M	U		K1=3.61 K(Ba+HL)=2.94 K(BaL+Ba)=2.26	1967DSb (82584)	676

****

C12H20O8 L CAS 62796-84-3 (2141)

1,4,7,10,13,16-Hexaoxacyclooctadecane-2,6-dione;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	cal	alc/w	25°C	100%	U	H	K1=3.13	1980BMa (82648)	677

Medium: MeOH. DH=-1.70 kJ mol-1.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	cal	alc/w	25°C	100%	U	H	K1=3.1	1980LIb (82649)	678

Medium: MeOH. DH=-1.70 kJ mol-1.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	cal	alc/w	25°C	100%	U	H	K1=3.1	1977ILa (82650)	679

Medium: MeOH. DH(K1)=-1.90 kJ mol-1

****

C12H20O8N2 H4L (6908)

2-Methyl-1,2-diaminopropane-N,N,N'N'-tetraethanoic acid;
(HOOC.CH2)2N.CH2.C(CH3)2.N(CH2.COOH)2

```
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Ba++       gl  KNO3   20°C 0.10M C        K1=6.98        1978NLa (82669) 680
*************************************************************************
C12H21NO6             H3L                        (7209)
1-Carboxy-1-aminoheptane-N,N-diethanoic acid; HOOC.CH(C6H13)N(CH2.COOH)2
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Ba++       gl  KNO3   20°C 0.10M U        K1=4.4         1985LBc (82692) 681
*************************************************************************
C12H21N3O5              L                      CAS 106724-75-8  (8231)
3,6,9,12,15-Pentaoxa-18,19,20-triazabicyclo[15.2.1]eicosa-1(19),17-diene;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Ba++       cal none   25°C  0.0  C   H    K1=1.7         1986BNb (82713) 682
DH(K1)=-8.41 kJ mol-1.
*************************************************************************
C12H21N3O6            H3L    NOTA              (5589)
1,4,7-Triazacyclononane-N,N',N"-triethanoic acid;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Ba++       gl  NaNO3  25°C 0.10M C T H    K1=5.10        1987BGc (82729) 683
DH(K1)=-5.8 kJ mol-1
*************************************************************************
C12H22N2O6            H2L                        (6394)
1,7-Dioxa-4,10-diazacyclododecan-4,10-diethanoic acid;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Ba++       gl  R4N.X  25°C 0.10M C        K1=6.652       1992ADa (82791) 684
Medium: 0.1 M Me4NNO3
*************************************************************************
C12H22N2O6            H2L                        (6641)
7,10-Diaza-1,4-Dioxacyclododecane-7,10-diethanoic acid;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Ba++       gl  R4N.X  25°C 0.10M C        K1=6.68        1992ADa (82805) 685
Medium: 0.1 M Me4NNO3
*************************************************************************
C12H23NO5               L                          (6793)
10-Methoxycarbonylethyl-1,4,7-trioxa-10-azacyclododecane;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Ba++       cal alc/w  25°C 100%  U   H                    1990KMb (82944) 686
Medium: MeOH.  DH=-19.1 kJ mol-1
```

****
C12H23N3O5 H2L (6393)
1-Oxa-4,7,10-triazacyclododecan-4,10-diethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	R4N.X	25°C	0.10M	C		K1=5.25 B(BaHL)=13.07	1992ADa (82972)	687

Medium: 0.1 M Me4NNO3
****
C12H24O2 HL Lauric acid CAS 143-07-7 (2540)
Dodecanoic acid, CH3.(CH2)10.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	oth	oth/un	20°C	var	U		Kso=-11.16	1981HTc (83110)	688

****
C12H24O4S2 L CAS 296-39-9 (4938)
1,4,10,13-Tetraoxa-7,16-dithiacyclooctadecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	cal	non-aq	25°C	100%	C	H	K1=3.07	1992BSc (83132)	689

Medium: propylene carbonate. DH(K1)=-22.3 kJ mol-1, DS(K1)=-16 J K-1 mol-1.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	cal	non-aq	25°C	100%	C	H	K1=3.73	1988BUb (83133)	690

Medium: acetonitrile. DH(K1)=-24.6 kJ mol-1, DS(K1)=-117 J K-1 mol-1.
****
C12H24O5S L Thia-18-crown-6 CAS 52559-79-2 (2263)
1-Thia-4,7,10,13,16-pentaoxacyclooctadecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	cal	alc/w	25°C	100%	U	H	K1=3.4	1980LIa (83154)	691

Medium: MeOH. DH=-26.0 kJ mol-1.
****
C12H24O6 L 18-Crown-6 CAS 17455-13-9 (577)
1,4,7,10,13,16-Hexaoxacyclooctadecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	EMF	alc/w	25°C	100%	C		K1=4.87	2004ZTa (83267)	692

Medium: 100% methanol, 0.05 M Bu4NClO4. Method: Ag electrode, competition with Ag+ ion.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	ISE	alc/w	25°C	100%	C	IH T	K1=7.2	2003ADa (83268)	693

IUPAC Tentative. Medium: 0-0.1 M various. DH(K1)=-47 kJ mol-1
In H2O: K1=3.79, DH(K1)=-31.7

Ba++ con mixed 25°C 20% C K1=3.51 2003SIa (83269) 694
Medium: 20% w/w propylene carbonate/ethylene carbonate.

Ba++ cal none 25°C 0.0 C H K1=3.72 2001DKa (83270) 695
DH(K1)=-31.7 kJ mol-1.

Ba++ nmr non-aq 27°C 100% C I K1=5.47 2001KZa (83271) 696
Method: 7Li nmr; competitive binding study. Medium: nitromethane.
In acetonitrile, K1=3.94

Ba++ nmr non-aq 27°C 100% U I K1=4.24 2000SMd (83272) 697
Competitive method by 7Li nmr. Medium: acetonitrile (AN). Also data for
50% w/w AN/nitrobenzene (K1=4.58) and 50% w/w AN/nitromethane (K1=5.39).

Ba++ cal R4N.X 25°C 0.0 C K1=3.50 1999BSb (83273) 698
DH(K1)=-31.5 kJ mol-1. Data for 0-0.10 M Et4NMClO4.
For I=0.10 M, K1=3.46, DH(K1)=-33.2

Ba++ con alc/w 25°C 90% C TIH T K1=6.55 1999SSc (83274) 699
Medium: 90% w/w MeOH/H2O. Data for 5-40C. DH(K1)=-42.96 kJ mol-1, DS(K1)
=-18.82 J K-1 mol-1. Data for 0-90% w/w MeOH/H2O. For 0%, K1=3.91.

Ba++ cal non-aq 25°C 100% C H K1=3.75 1999WBa (83275) 700
Medium: N,N-dimethylformamide. DH(K1)=-43.3 kJ mol-1.

Ba++ cal mixed 25°C 50% C IH K1=4.13 1998BJb (83276) 701
Medium: 50% (v/v) HCOOH/H2O. DH(K1)=-18.1 kJ mol-1
For 25% (v/v) HCOOH/H2O, K1=3.57, DH(K1)=-22.2 kJ mol-1

Ba++ cal none 25°C 0.0 C K1=3.72 1997DZa (83277) 702
DH(K1)=-31.71 kJ mol-1.

Ba++ cal R4N.X 25°C 0.10M C H T K1=3.50 1996BCh (83278) 703
Medium: 0.10 M Et4NClO4. DH(K1)=30.7 kJ mol-1.

Ba++ cal non-aq 25°C 100% U H T K1=4.10 1995OKa (83279) 704
Medium:DMF, 0.1 M NEt4ClO4. DH=-44.4 kJ mol-1, DS=-70.5 J K-1 mol-1.

Ba++ cal R4N.X 25°C 0.10M U H T K1=3.75 1995OKa (83280) 705
Medium: 0.1 M NEt4Cl. DH=-33.1 kJ mol-1, DS=-39.4 J K-1 mol-1.

Ba++ cal none 50°C 0.00 C T H K1=3.46 1995WIa (83281) 706
Method: isothermal flow calorimetry. Measurements at 1.52 MPa. Data for
15-125 C. DH(K1)=-29.4 kJ mol-1, DS(K1)=-25 J K-1 mol-1.

Ba++ cal non-aq 25°C 100% U H T K1=7.35 1993BDb (83282) 707
Medium: acetone. DH=-61.0 kJ mol-1; TDS=-19.2 Calorimetric titration

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Ba++ cal non-aq 25°C 100% C H K1=11.56 1992BSc (83283) 708

Medium: propylene carbonate. K1 detd by competitive calorimetric titration with diketopyridino-18-crown-6. DH(K1)=-64.3 kJ mol-1, DS(K1)=4.7.

Ba++ cal oth/un 25°C 0.05M M K1=7.31 1992BUb (83284) 709

Ba++ con non-aq 25°C 100% C K1=3.17 1992STa (83285) 710
Medium: propylene carbonate.

Ba++ nmr non-aq 30°C 100% U I K1=>6 1991ASc (83286) 711
Medium: nitromethane. In MeCN, K1>5; in DMF, K1=3.81.

Ba++ ix none 25°C 0.0 U K1=3.6 1991BMb (83287) 712

Ba++ vlt non-aq 25°C 100% C K1=>5 1991SSb (83288) 713
Method: competitive complexation with Tl+; use of Tl(Hg)/Tl couple.
Medium: acetonitrile, 0.05 M Et4NClO4.

Ba++ sp alc/w 25°C 100% U I K1=7.15 1989KSc (83289) 714
In MeOH. In DMF K1=5.29; in DMSO K1=4.68

Ba++ cal non-aq 25°C 100% C H K1=>5 1988BUb (83290) 715
Medium: acetonitrile. DH(K1)=-19.8 kJ mol-1, DS(K1)=103 J K-1 mol-1.

Ba++ cal alc/w 25°C 100% U H K1=7.38 1986BUa (83291) 716
Medium: MeOH. DH(K1)=-48.5 kJ mol-1; DS=-22 J K-1 mol-1

Ba++ cal non-aq 25°C 100% C H 1986BUe (83292) 717
Medium: MeOH. DH(K1)=-48.5 kJ mol-1, DS(K1)=-23.5 J K-1 mol-1.

Ba++ nmr non-aq 25°C 100% U K1=4.21 1985BPa (83293) 718
Medium: DMF

Ba++ cal alc/w 25°C 100% U H T K1=7.38 1985BUc (83294) 719
Medium: MeOH, 0.05 M Et4NClO4. DH=-48.5 kJ mol-1
K from a calorimetric competition reaction.

Ba++ vlt R4N.X 25°C 0.10M C K1=3.67 1985SKd (83295) 720
Method: polarography. Medium: 0.10 M Me4NI.

Ba++ cal alc/w 25°C 100% U H K1=3.87 1983SLb (83296) 721

Ba++ cal alc/w 25°C 90% U IH K1=6.56 1982HLa (83297) 722
Medium: 90% MeOH. DH=-43.25 kJ mol-1, DS=-5.78 J K-1 mol-1

Ba++ cal alc/w 25°C 100% U H K1=7.04 1980BMa (83298) 723
Medium: MeOH. DH=-43.6 kJ mol-1.

Ba++ cal alc/w 25°C 100% U H T K1=7.04 1980LIa (83299) 724
Medium: MeOH. DH=-44.6 kJ mol-1.

```
Ba++       cal alc/w  25°C 100%  U   H    K1=7.0         1977ILa (83300) 725
Medium: MeOH. DH(K1)=-42.8 kJ mol-1
--------------------------------------------------------------------------------
Ba++       cal alc/w  25°C  70%  U   H    K1=6.0         1976ITa (83301) 726
Medium: 70% w/w MeOH/H2O. DH(K1)=-44.6 kJ mol-1.
--------------------------------------------------------------------------------
Ba++       cal oth/un 25°C 0.10M U   H  T K1=3.87        1976ITb (83302) 727
DH=-31.7 kJ mol-1.
********************************************************************************
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
--------------------------------------------------------------------------------
Ba++       sp  non-aq 25°C 100%  U T H    K1=2.68        1994GSb (83814) 728
At 35 C: K1=2.64; 45 C: K1=2.56; 55 C: K1=2.38. DH(K1)=-18 kJ mol-1, DS=-10
Medium: DMSO
--------------------------------------------------------------------------------
Ba++       sp  non-aq 20°C 100%  U        K1=5.55        1992PSa (83815) 729
Medium: DMF, 0.01 M Me4NI
--------------------------------------------------------------------------------
Ba++       sp  alc/w  25°C 100%  U  I     K1=5.98        1989KSc (83816) 730
In MeOH. In DMF K1=4.25; in DMSO K1=3.45
--------------------------------------------------------------------------------
Ba++       cal alc/w  25°C 100%  U   H    K1=6.12        1986BUa (83817) 731
Medium: MeOH. DH(K1)=-10.0 kJ mol-1; DS=83 J K-1 mol-1
--------------------------------------------------------------------------------
Ba++       ISE non-aq 25°C 100%  U   H    K1=>8          1986BUb (83818) 732
In CH3CN. DH=-54.7 kJ mol-1
--------------------------------------------------------------------------------
Ba++       cal non-aq 25°C 100%  C   H                   1986BUe (83819) 733
Medium: MeOH. DH(K1)=-10 kJ mol-1, DS(K1)=83.2 J K-1 mol-1.
--------------------------------------------------------------------------------
Ba++       cal alc/w  25°C 100%  U   H    K1=6.12        1985BUc (83820) 734
Medium: MeOH, 0.05 M Et4NClO4. DH=-10.0 kJ mol-1
--------------------------------------------------------------------------------
Ba++       ISE alc/w  25°C 100%  U   H    K1=5.9         1983CFb (83821) 735
Medium: MeOH, 0.05 M Et4NClO4
********************************************************************************
C12H26O4S              HL    SDS              CAS 151-21-3  (2522)
Dodecyl sulfate; CH3(CH2)11.OSO3H
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Ba++       sol oth/un 21°C    ?  U        B2=6.4         1979KBb (83980) 736
                                         B(Ba2L4)=8.7
                                         B(Ba3L6)=9.5
********************************************************************************
C12H26O6                L    Pentaglyme       CAS 1191-87-3  (2498)
2,5,8,11,14,17-Hexaoxaoctadecane; (CH3.O.CH2.CH2.O.CH2.CH2.O.CH2.)2
```

```
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Ba++       cal non-aq 25°C 100%  U   H    K1=3.97        1993BDb (83991) 737
Medium: acetone. DH=-39.9 kJ mol-1; TDS=-17.3
--------------------------------------------------------------------------------
Ba++       con non-aq 25°C 100%  C   H    K1=>5.5        1992BSc (83992) 738
Medium: propylene carbonate. By calorimetry, DH(K1)=-51.5 kJ mol-1.
--------------------------------------------------------------------------------
Ba++       con oth/un 25°C 0.05M M        K1=2.31        1992BUb (83993) 739
K1=2.59 (by calorimetry)
--------------------------------------------------------------------------------
Ba++       cal alc/w  25°C  90%  U  IH    K1=2.33        1982HLa (83994) 740
Medium: 90% MeOH. DH=-29.7 kJ mol-1, DS=-16.4 J K-1 mol-1
********************************************************************************
C12H28N2O9P2          H4L                        (7242)
1,4,10-Trioxa-7,13-diazacyclopentadecane-7,13-diyldimethylenediphosphonic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Ba++       gl  R4N.X  25°C 0.10M U        K1=8.22        1996BJa (84151) 741
                                         K(Ba+HL)=4.81
                                         K(Ba+H2L)=2.31
Medium: 0.1 M Me4NCl
********************************************************************************
C12H28N4O2              L                      CAS 296-36-6  (2472)
1,10-Dioxa-4,7,13,16-tetraazacyclooctadecane;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Ba++       gl  NaNO3  25°C 0.10M U        K1=<2          1990WHa (84231) 742
--------------------------------------------------------------------------------
Ba++       gl  NaNO3  25°C 0.10M C        K1=<2          1989HBa (84232) 743
********************************************************************************
C12H32N4O12P4         H8L    DOTPH            CAS 91987-74-5  (229)
1,4,7,10-Tetraazacyclododecane-N,N',N",N"'-tetramethylenephosphonic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Ba++       gl  R4N.X  25°C 0.10M M        K1=10.65       1990DSa (84405) 744
                                         B(BaH3L)=38.13
                                         B(Ba2L)=17.12
                                         B(Ba2HL)= 25.78
Medium: Me4NNO3
--------------------------------------------------------------------------------
Ba++       gl  KNO3   25°C  1.0M U        K1=8.8         1984KMb (84406) 745
                                         K(Ba+HL)=6.1
                                         K(Ba+H2L)=1.9
********************************************************************************
C13H10N2O4            H2L                      CAS 62437-12-1  (4013)
```

4-(Phenylamino)pyridine-2,6-dicarboxylic acid; C6H5.NH.C5H2N(COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	NaClO4	22°C	0.10M	U		K1=3.75	1964BBa (84876)	746

C13H10N2O4 HL CAS 2029-61-0 (178)
N-Phenyl-2-nitrobenzohydroxamic acid; O2N.C6H4.CO.N(C6H5).OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	diox/w	25°C	50%	U	T	K1=3.51 B2=5.97	1977VKa (84896)	747

At 35 C: K1=3.44, K2=2.40

C13H10N2O4 HL CAS 17120-18-2 (220)
N-Phenyl-3-nitrobenzohydroxamic acid; O2N.C6H4.CO.N(C6H5).OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	diox/w	25°C	50%	U	T	K1=3.62 B2=6.13	1977VKa (84908)	748

At 35 C: K1=3.57, K2=2.47

C13H10O2S HL CAS 10471-74-6 (3405)
Benzoyl-2-thenoylmethane; C6H5.CO.CH2.CO.C4H3S

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	diox/w	30°C	75%	U		B2=11.8	1953UFa (84985)	749

C13H10O3 HL CAS 5910-23-6 (3399)
Benzoyl-2-furoylmethane; C6H5.CO.CH2.CO.C4H3O

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	diox/w	30°C	75%	U		B2=11.4	1953UFe (85000)	750

C13H11NO5 HL Oxolinic acid CAS 14698-29-4 (2755)
1-Ethyl-6,7-dioxymethylene-quinoline-4-one-3-carboxylic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	sp	KCl	25°C	0.10M	U		K1=1.1	1978TSb (85218)	751

C13H15NO6 H3L (4999)
2-Benzylnitrilotriethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	oth	oth/un	25°C	0.10M	U		K1=4.40	1962HKa (85734)	752

C13H15NO6 H3L (4026)
N-(1'-Carboxy-1'-phenylethyl)iminodiethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KCl	20°C	0.10M	U		K1=4.93	1966IMa (85751)	753

****
C13H15NO6 H3L (4025)
N-(alpha-Carboxy-4'-methylbenzyl)iminodiethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KCl	20°C	0.10M	U		K1=4.31	1966IMb (85757)	754

****
C13H15NO7 H3L CAS 50444-50-3 (4027)
N-(alpha-Carboxy-4'-methoxybenzyl)iminodiethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KCl	20°C	0.10M	U		K1=4.32	1966IMb (85766)	755

****
C13H17NO5 H2L (5001)
N-(4-Methoxyphenethylimino)diethanoic acid; CH3O.C6H4.CH2CH2N(CH2COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KCl	20°C	0.10M	U		K1=2.47	1971KTl (85980)	756
							K(Ba+HL)=1.38		

****
C13H20N2O8 H4L CAS 22991-70-4 (3413)
trans-1,2-Cyclopentane-iminodiethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	oth/un	20°C	0.10M	U		K1=7.75	1960KGa (86111)	757
Ba++	gl	KCl	20°C	0.10M	U		K1=7.75	1959KRa (86112)	758
							K(Ba+HL)=3.91		

****
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
Ba++	EMF	KCl	20°C	0.10M	C			1948SAa (86189)	759
							K(Ba+HL)=2.38		

Method: H electrode

****
C13H22N2O8 H4L CAS 1198-14-7 (5004)
1,2-Diaminopentane-N,N,N',N'-tetraethanoic acid; (HOOCCH2)2NCH2CH(C3H7)N(CH2COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KNO3	20°C	0.10M	U		K1=8.50	1969NDa (86222)	760

C13H22N2O8 H4L (7164)
2,4-Diaminopentane-N,N,N',N'-tetraethanoic acid;
(HOOCCH2)2NCH(CH3)CH2CH(CH3)N(CH2COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KNO3	20°C	0.10M	U		K1=3.81 K(BaL+H)=2.06	1981NSc (86249)	761

C13H22N2O8 H4L (5003)
3-Methyl-1,2-diaminobutane-N,N,N',N'-tetraethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KNO3	20°C	0.10M	U		K1=8.60	1969NDa (86277)	762

C13H22O8 L CAS 58484-46-1 (2140)
1,5,8,11,14,17-Hexaoxacyclononadecane-2,4-dione;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	cal	alc/w	25°C	100%	U	H	K1=1.41	1980LIb (86375)	763

Medium: MeOH. DH=-20.4 kJ mol-1.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	cal	alc/w	25°C	100%	U	H	K1=1.41	1977ILa (86376)	764

Medium: MeOH. DH(K1)=-20.4 kJ mol-1

C13H23N3O8 H4L (3414)
N-Methyl-2,2'-iminobis(ethyliminodiethanoic acid);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	EMF	KCl	20°C	0.10M	C		K1=7.21 K(Ba+HL)=2.61	1957SSa (86395)	765

Method: H electrode

C13H24N2O6 H2L (5610)
1,11-Dioxa-4,8-diazacyclotridecane-N,N'-diethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	R4N.X	25°C	0.10M	C		K1=3.37 *K(BaL)=-11.24	1998CCd (86410)	766

Medium: 0.10 M Me4NNO3.

Ba++ cal NaClO4 25°C 0.10M U H K1=2.5 1985EHa (86411) 767
DH(K1)=-1.4 kJ mol-1, DS=43.3 J K-1 mol-1
****
C13H26O5 L (6410)
15,15-Dimethyl-1,4,7,10,13-pentaoxacyclohexadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ con none 25°C 0.0 C K1=0.9 2001KMb (86467) 768
****
C13H26O6 L 19-Crown-6 CAS 55471-27-7 (8943)
1,4,7,10,13,16-Hexaoxacyclononadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ con oth/un 25°C dil C K1=1.95 1999TMa (86493) 769
Self medium (Ba(NO3)2).
****
C13H28O2Si2 L CAS 64277-56-1 (6291)
2,2,10,10-Tetramethyl-2,10-disilahendecan-5,7-dione;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl diox/w 30°C 75% U B2=7.8 1953UFe (86540) 770
****
C13H34N4O12P4 H8L (6686)
1,4,7,11-Tetraazacyclotridecane-N,N',N",N"'-tetramethylenephosphonic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl R4N.X 25°C 0.10M M 1990DSa (86585) 771
B(BaHL)=19.24
B(BaH2L)=28.94
B(Ba2L)=12.61
Medium: Me4NNO3
****
C14H9O2F3 HL (3429)
1,1,1-Trifluoro-1'-naphthoylacetone;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl diox/w 30°C 75% U B2=10.0 1953UFe (86870) 772
****
C14H12N2O4 HL (179)
N-3-Tolyl-3-nitrobenzohydroxamic acid; O2N.C6H4.CO.N(C6H4.CH3).OH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl diox/w 25°C 50% U T K1=3.61 B2=6.10 1977VKa (87258) 773
At 35 C: K1=3.53, K2=2.42

****

C14H12N2O4 HL CAS 85407-74-5 (180)
N-4-Tolyl-2-nitrobenzohydroxamic acid; O2N.C6H4.CO.N(C6H4.CH3).OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Ba++	gl	diox/w	25°C	50%	U	T	K1=3.59	B2=6.08	1977VKa (87271)	774

At 35 C: K1=3.50, K2=2.41

****

C14H12N2O4 HL (221)
N-4-Tolyl-3-nitrobenzohydroxamic acid; O2N.C6H4.CO.N(C6H4.CH3).OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Ba++	gl	diox/w	25°C	50%	U	T	K1=3.71	B2=6.21	1977VKa (87284)	775

At 35 C: K1=3.60, K2=2.41

****

C14H14N2O10 H5L CAS 41379-95-7 (5070)
2-Carboxymethylamino-5-(bis(carboxymethyl)amino)-1,4-dibenzoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KNO3	25°C	0.10M	U		K1=4.20	1973UWb (87671)	776

****

C14H15N2O8Cl H4L (1903)
4-Chloro-1,2-diaminobenzene-N,N,N',N'-tetraethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KCl	25°C	0.10M	U		K1=4.21	1990MDa (87746)	777
							B(BaHL)=8.29		

****

C14H16N2O8 H4L CAS 40774-59-2 (1901)
1,2-Diaminobenzene-N,N,N',N'-tetraethanoic acid; C6H4(N(CH2.COOH)2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	NaClO4	25°C	1.00M	C	H	K1=3.99	1992NSa (87942)	778

By calorimetry: DH(K1)=2.5 kJ mol-1, DS=86 J K-1 mol-1

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KCl	30°C	0.10M	U		K1=4.8	1963GHa (87943)	779
							K(Ba+HL)=2.3		
							K(Ba+H2L)=1.6		

****

C14H16N2O8 H4L (6108)
1,3-Phenylenediamine-N,N'-disuccinic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	NaCl	25°C	0.50M	C		K1=1.399	1989FRa (87991)	780

B(BaHL)=6.599
B(BaH2L)=10.819
****
C14H16N2O8 H4L CAS 91856-15-4 (8449)
1,4-Phenylenediamine-N,N'-disuccinic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl NaCl 25°C 0.50M C K1=0.77 1984RFe (88012) 781
****
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
---
Ba++ con mixed 25°C 20% C K1=3.35 2003SIa (88241) 782
Medium: 20% w/w propylene carbonate/ethylene carbonate.

Ba++ oth alc/w 35°C 3.0% C K1=0.96 1999MTd (88242) 783
Method: capillary zone electrophoresis. Medium: 3% v/v EtOH/H20, 0.005 M acetate buffer, pH 5.5.

Ba++ cal non-aq 25°C 100% C H 1999WBa (88243) 784
Medium: N,N-dimethylformamide. DH(K1)=-4.5 kJ mol-1.

Ba++ cal non-aq 25°C 100% C H K1=>5 1988BUb (88244) 785
Medium: acetonitrile. DH(K1)=-25.9 kJ mol-1.
****
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
---
Ba++ cal KNO3 25°C 0.10M U H 1965WHa (88587) 786
DH(K1)=-9.2 kJ mol-1, DS=122 J K-1 mol-1

Ba++ cal KNO3 20°C 0.10M U T H 1963ANb (88588) 787
DH(K1)=1.4 kJ mol-1, DS=171.0 J K-1 mol-1

Ba++ cal KNO3 20°C 0.10M U H K1=8.64 1963ANf (88589) 788
DH(K1)=1.4 kJ mol-1, DS=171 J K-1 mol-1

Ba++ EMF KCl 20°C 0.10M C K1=7.99 1954SGa (88590) 789
K(Ba+HL)=3.15
Method: H electrode
****
C14H22O5 H2L CAS 85785-29-1 (2250)
Di(hepta-4,6-dione)ether, (CH3.CO.CH2.CO.(CH2)3)2O

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

---
Ba++ gl diox/w 24°C 50% U K1=5.2 1979ACa (88992) 790
****
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
---
Ba++ cal oth/un 27°C 0.10M U H 1968CLd (89159) 791
DH(K1)=-28.8 kJ mol-1, DS=67 J K-1 mol-1

Ba++ cal KNO3 25°C 0.10M U H 1965WHa (89160) 792
DH(K1)=-30.5 kJ mol-1, DS=58.5 J K-1 mol-1

Ba++ gl KNO3 25°C 0.10M C K1=8.8 1960WAa (89161) 793
K(BaL+H)=5.3

Ba++ gl oth/un 20°C 0.10M U K1=8.63 1958DRa (89162) 794

Ba++ gl oth/un 25°C 0.10M U K1=8.62 1955WAa (89163) 795
****
C14H24N2O7 H3L (3440)
N-(2-Hydroxycyclohexyl)ethylenediamine-N,N',N'-triethanoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl KCl 20°C 0.10M U K1=4.00 1959KRa (89492) 796
K(Ba+HL)=2.06
****
C14H24N2O8 H4L (5075)
1,2-Diaminoethane-N,N'-diethanoic-N,N'-di-2-butyric acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl KNO3 20°C 0.10M U K1=5.81 1969NDc (89504) 797
****
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
---
Ba++ gl KNO3 25°C 0.10M U K1=2.80 1969GKb (89565) 798
K(Ba+HL)=2.11
B(Ba2L)=1.28
****
C14H24N2O8 H4L CAS 1633-00-7 (5076)
4-Methyl-1,2-diaminopentane-N,N,N',N'-tetraethanoic acid;
(HOOCCH2)2NCH2CH(N(CH2COOH)2CH2CH(CH3)2

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

---
Ba++ gl KNO3 20°C 0.10M U K1=8.75 1969NDa (89628) 799
****
C14H24N2O9 H4L CAS 87720-52-3 (1593)
2,2'-Oxybis(propyliminodiethanoic acid)

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl KCl 20°C 0.10M U K1=3.77 1961ISa (89709) 800
K(Ba+HL)=2.69

Ba++ gl KCl 20°C 0.10M U K1=5.88 1961KGa (89710) 801
K(Ba+HL)=3.40
****
C14H24N2O9 H4L BPETA CAS 87720-52-3 (5077)
Bis-(3-di(carboxymethyl)aminopropyl)ether;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl KCl 20°C 0.10M U K1=3.77 1961ISa (89724) 802
K(Ba+HL)=2.69
****
C14H24N2O10 EGTA CAS 67-42-5 (349)
Ethyleneglycol-O,O'-bis(2-aminoethyl ether)-N,N,N',N'-tetraethanoic acid; H4L

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl KNO3 25°C 0.10M U K1=8.80 1982JGa (89838) 803
K(BaL+H)=6.2
K(BaL+2H)=5.5

Ba++ cal KCl 25°C 0.10M U H 1965BBe (89839) 804
DH(K1)=-37.6 kJ mol-1, DS=32.6 J K-1 mol-1

Ba++ cal KNO3 25°C 0.10M U H 1965WHa (89840) 805
DH(K1)=-36.8 kJ mol-1, DS=29.7 J K-1 mol-1

Ba++ EMF KCl 20°C 0.10M C K1=8.41 1964PCa (89841) 806
K(Ba+HL)=4.26
Method: H electrode

Ba++ gl oth/un 25°C 0.10M U K1=8.0 1957SRa (89842) 807
****
C14H24N2O10 H4L (2655)
N,N'-Bis(2-hydroxyethane)-N,N'-ethanediaminedibutanedioic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl KNO3 25°C 0.1M U K1=3.53 1985MGb (89976) 808
****

C14H24O9 L CAS 63689-61-2 (2273)
1,4,7,10,13,16,19-Heptaoxacycloheneicosa-17,21-dione;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	cal	alc/w	25°C	100%	U	H	K1=1.73	1980LIb (90056)	809

****
C14H24O10 HL 18-6A2 CAS 76871-57-3 (5407)
1,2-Bis-carboxy-18-crown-6;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	alc/w	25°C	90%	U		K1=9.2 B(BaHL)=13.4	1984FWa (90060)	810

Medium: 90% v/v MeOH/H2O, 0.05 M R4NX
****
C14H25N3O7 H3L (5397)
1-Oxa-4,7,10-triazacyclododecane-4,7,10-triethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	R4N.X	25°C	0.10M	U		K1=9.92 K(Ba+HL)=4.34	1988ADa (90080)	811

****
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
Ba++	cal	R4N.X	25°C	0.10M	U	H		1989DSa (90176)	812

DH(BaL)=-24.7 kJ mol-1; DS=58.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	R4N.X	25°C	0.10M	C		K1=7.412	1987DDb (90177)	813
Ba++	gl	R4N.X	25°C	0.10M	M		K1=7.31	1986COb (90178)	814

****
C14H26N2O8 H2L (6658)
1,4,10,13-Tetraoxa-7,16-diaza-2,3-dicarboxycyclooctadecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	R4N.X	25°C	0.10M	U		K1=4.3 B(BaHL)=12.6 B(Ba(OH)L)=7.8	1990AFa (90220)	815

****
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

Ba++ gl R4N.X 25°C 0.10M M K1=7.39 1996CHc (90244) 816
Medium: 0.1 M Me4NCl.
****
C14H28N2O4 L Cryptand 2,1,1 CAS 31250-06-3 (836)
1,10-Diaza-4,7,13,18-tetraoxabicyclo[8,5,5]eicosane (2,1,1);

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl R4N.X 25°C 0.05M C H K1=2.6 1996BCh (90346) 817
Medium: 0.05 M Et4NClO4. By calorimetry: K1=2.6, DH(K1)=-11.6 kJ mol-1.

Ba++ sp non-aq 25°C 100% U T H K1=2.57 1994GSb (90347) 818
At 35 C: K1=2.54; 45 C: K1=2.51; 55 C: K1=2.47. DH(K1)=-6 kJ mol-1, DS=29
Medium: DMSO

Ba++ sp non-aq 20°C 100% U K1=1.6 1992PSa (90348) 819
Medium: DMF, 0.01 M Me4NI

Ba++ cal alc/w 25°C 100% U H K1=2.53 1986BUa (90349) 820
Medium: MeOH. DH(K1)=-5.5 kJ mol-1; DS=30

Ba++ ISE non-aq 25°C 100% U H K1=6.32 1986BUb (90350) 821
In CH3CN. DH=-32.4 kJ mol-1

Ba++ cal alc/w 25°C 100% U H K1=2.53 1985BUc (90351) 822
Medium: MeOH, 0.05 M Et4NClO4. DH=-5.5 kJ mol-1

Ba++ gl R4N.X 25°C 0.05M C I K1=<2.0 1975LSc (90352) 823
In 95% MeOH, 0.05 M Me4NBr: K1 < 2
****
C14H28O2 HL Myristic acid CAS 544-63-8 (2543)
Tetradecanoic acid; CH3(CH2)12.COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ oth oth/un 20°C var U 1981HTc (90508) 824
Kso=-14.17
****
C14H28O7 L 21-Crown-7 CAS 33089-36-0 (2264)
1,4,7,10,13,16,19-Heptaoxacycloheneicosane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ cal alc/w 25°C 100% U H K1=5.44 1980LIa (90515) 825
Medium: MeOH. DH=-28.5 kJ mol-1.
****
C14H30N2O4 L CAS 31255-13-7 (2448)
N,N'-Dimethyl-cyclo-1,10-diaza-4,7,13,16-tetraoxaoctadecane;

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

---
Ba++ gl alc/w 25°C 95% C K1=6.67 2004KVa (90572) 826
Medium: 95% MeOH/H2O, 0.01 M Et4NClO4.

Ba++ gl oth/un 25°C ? C K1=3.54 1991DMa (90573) 827

Ba++ ISE alc/w 25°C 100% U H K1=6.9 1983CFb (90574) 828
Medium: MeOH, 0.05 M Et4NClO4

Ba++ gl alc/w 25°C 93% U K1=5.95 1978WVa (90575) 829
Medium: 93% MeOH/H2O
****
C14H30N2O5 L CAS 23978-10-1 (2955)
1,10-Diaza-4,7,13,16,19-pentaoxacycloheneicosane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ ISE alc/w 25°C 100% U K1=5.1 1988CFa (90609) 830
Medium: MeOH

Ba++ ISE alc/w 25°C 100% U H K1=5.39 1986BUa (90610) 831
Medium: MeOH. DH(K1)=-8.5 kJ mol-1; DS=74 J K-1 mol-1

Ba++ ISE alc/w 25°C 100% U H K1=5.39 1985BUc (90611) 832
Medium: MeOH, 0.05 M Et4NClO4. DH=-8.5 kJ mol-1
****
C14H30N2O5 L (6722)
7,13-Bis(2-hydroxyethyl)-1,4,10-trioxa-7,13-diazacyclopentadecane
---
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl R4N.X 25°C 0.10M C K1=3.99 1995LLa (90626) 833
Medium: Et4NClO4
****
C14H30N4O2 L (6364)
1,7,10,16-Tetraaza-4,13-dioxabicyclo[14.2.2]eicosane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl NaNO3 25°C 0.10M U K1=<2 1990WHa (90658) 834
****
C14H30O7 L CAS 1072-40-8 (2499)
2,5,8,11,14,17,20-Heptaoxaheneicosane; CH3.O.(CH2.CH2.O)6.CH3

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ cal non-aq 25°C 100% U H K1=4.28 1993BDb (90685) 835
Medium: acetone. DH=-40.1 kJ mol-1; TDS=-15.8

Ba++ con non-aq 25°C 100% C H K1=5.01 1992BSc (90686) 836

Medium: propylene carbonate. By calorimetry, DH(K1)=-56.6 kJ mol-1,
DS(K1)=-94.3 J K-1 mol-1.

****

C14H32N2O10P2 H4L CAS 81963-60-2 (7240)
1,4,10,13-Tetraoxa-7,16-diazacyclooctadecane-7,16-diyldimethylenediphosphonic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Ba++	gl	R4N.X	25°C	0.10M	U		K1=8.56		1996BJa (90759)	837
							K(Ba+HL)=4.95			
							K(Ba+H2L)=1.74			

Medium: 0.1 M Me4NCl

****

C14H36N4O12P4 H8L CAS 107446-90-2 (2015)
1,4,7,11-Tetraazacyclotetradecane-N,N',N",N"'-tetramethylphosphonic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Ba++	gl	R4N.X	25°C	0.10M	M				1990DSa (90870)	838
							B(BaHL)=18.75			
							B(BaH2L)=29.64			
							B(BaH3L)=37.90			
							B(BaH4L)=45.43			

Medium: Me4NNO3

****

C15H12O2 HL Diphenylacac CAS 120-46-7 (362)
1,3-Diphenylpropane-1,3-dione, Dibenzoylmethane; C6H5.CO.CH2.CO.C6H5

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Ba++	gl	diox/w	20°C	17%	C		K1=5.81	B2=10.25	1976JWa (91537)	839
Ba++	gl	diox/w	30°C	75%	U		K1=6.10	B2=11.50	1953UFe (91538)	840

****

C15H14N2O5 H3L (5113)
2-Phenyl-4,5,6,7-tetrahydroindazol-3-one-5,5-dicarboxylic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Ba++	gl	diox/w	25°C	50%	U				1964STa (91725)	841
							K(Ba+HL)=4.32			
							K(Ba+H2L)=2.30			

****

C15H19NO7 L CAS 64397-58-4 (2170)
3,6,9,12,15-Pentaoxa-21-azabicyclo[15.3.1]heneicosa-1(21),17,19-triene-2,16-dione;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Ba++	cal	alc/w	25°C	100%	U	H	K1=4.34		1980BMa (92114)	842

Medium: MeOH. DH=-25.2 kJ mol-1.

Ba++ cal alc/w 25°C 100% U H K1=4.34 1980LIb (92115) 843
Medium: MeOH. DH=-25.2 kJ mol-1.

Ba++ sp alc/w 25°C 100% U H K1=4.34 1977ILc (92116) 844
Medium: Methanol. DH(K1)= -25.2 kJ mol-1

****

C15H19N3O8 H4L CAS 53793-56-9 (8631)
N,N'-[2,6-Pyridinediylbis(methylene)]bis[N-(carboxymethyl)]glycine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KCl	25°C	0.10M	U		K1=8.1	1984VOb (92131)	845

For the 4-methoxy derivative: K1=6.7; for the 4-dimethylamino derivative, K1=6.0.

****

C15H23NO5 L CAS 53914-89-9 (2262)
3,6,9,12,15-Pentaoxa-21-azabicyclo[15.3.1]heneicosa-1(21),17,19-triene;

Ba++ cal alc/w 25°C 100% U H K1=>5.5 1980BMa (92265) 846
Medium: MeOH. DH=-32.3 kJ mol-1.

Ba++ cal alc/w 25°C 100% U H K1=>5.5 1980LIa (92266) 847
Medium: MeOH. DH=-32.3 kJ mol-1.

Ba++ sp alc/w 25°C 100% U H K1=>6.0 1977ILc (92267) 848
Medium: Methanol. DH= -32.3 kJ mol-1

****

C15H23N3O12 H6L CAS 21979-64-6 (4069)
1,2,3-Tris(N,N-bis(carboxymethyl)amino)propane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KNO3	25°C	0.10M	U		K1=7.41	1968MMb (92319)	849
							K(Ba+HL)=5.42		
							K(Ba+H2L)=1.4		
							B(Ba2L)=1.6		

****

C15H24O6 HL CAS 57722-03-9 (2353)
1-Hydroxy-2-(1,4,7,10,13-pentaoxatridecyl)benzene; HO.C6H4.O(CH2CH2O)4CH3

Ba++ sp alc/w 25°C 100% U K1=6.43 1981EMb (92341) 850
Medium: MeOH

****

C15H27N3O7 H3L (7396)
4,7,11-Tris(carboxymethyl)-1-oxa-4,7,11-triazacyclotridecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl R4N.X 25°C 0.10M C K1=6.90 1997CCa (92478) 851
Medium: Me4NNO3
****
C16H9N2OBr3 HL CAS 84317-74-8 (5169)
1-(2,4,6-Tribromophenylazo)-2-hydroxynaphthalene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl mixed 25°C 75% U K1=5.08 1972MCb (92647) 852
Medium: 75% acetone, 0.1 M KNO3
****
C16H11N2OBr HL CAS 7150-24-5 (5172)
1-(4-Bromophenylazo)-2-hydroxynaphthalene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl mixed 25°C 75% U K1=5.94 1972MCb (92697) 853
Medium: 75% acetone, 0.1 M KNO3
****
C16H11N2OCl HL CAS 24390-65-6 (5170)
1-(2-Chlorophenylazo)-2-hydroxynaphthalene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl mixed 25°C 75% U K1=5.53 1972MCb (92712) 854
Medium: 75% acetone, 0.1 M KNO3
****
C16H11N2OCl HL CAS 10149-93-6 (5171)
1-(4-Chlorophenylazo)-2-hydroxynaphthalene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl mixed 25°C 75% U K1=5.92 1972MCb (92727) 855
Medium: 75% acetone, 0.1 M KNO3
****
C16H11N2OI HL CAS 25023-35-2 (5173)
1-(4-Iodophenylazo)-2-hydroxynaphthalene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl mixed 25°C 75% U K1=5.95 1972MCb (92742) 856
Medium: 75% acetone, 0.1 M KNO3
****
C16H11N2O2Cl H2L CAS 3566-94-7 (3474)
1-(5-Chloro-2-hydroxyphenylazo)-2-hydroxynaphthalene;

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

---
Ba++ gl diox/w 30°C 75% U K1=5.10 1957SFb (92759) 857
K(Ba+H2L=BaL+2H)=-17.6
****
C16H11N3O3 HL CAS 6410-09-9 (5151)
1-(2-Nitrophenylazo)-2-hydroxynaphthalene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl mixed 25°C 75% U K1=2.65 1972MCb (92796) 858
Medium: 75% acetone, 0.1 M KNO3
****
C16H11N3O3 HL CAS 6410-46-1 (5152)
1-(4-Nitrophenylazo)-2-hydroxynaphthalene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl mixed 25°C 75% U K1=3.38 1972MCb (92811) 859
Medium: 75% acetone, 0.1 M KNO3
****
C16H12N2O HL CAS 842-07-9 (5156)
1-Phenylazo-2-hydroxynaphthalene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl mixed 25°C 75% U K1=6.44 1972MCb (92917) 860
Medium: 75% acetone, 0.1 M KNO3
****
C16H12N2O2 H2L CAS 9486-98-2 (3462)
1-(2-Hydroxyphenylazo)-2-hydroxynaphthalene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl mixed 25°C 75% U 1972MCb (92950) 861
K(Ba+HL)=6.37
Medium: 75% acetone, 0.1 M KNO3

Ba++ gl diox/w 30°C 75% U K1=5.74 1957SFb (92951) 862
K(Ba+H2L=BaL+2H)=-18.5
****
C16H12N2O2 H2L CAS 14934-27-1 (5157)
1-(4-Hydroxyphenylazo)-2-hydroxynaphthalene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl mixed 25°C 75% U 1972MCb (92969) 863
K(Ba+HL)=6.26
Medium: 75% acetone, 0.1 M KNO3
****
C16H12N2O4S H2L CAS 13964-82-4 (3475)

1-(4-Sulfophenylazo)-2-hydroxynaphthalene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	mixed	25°C	75%	U		K1=3.0	1972MCb (92996)	864

Medium: 75% acetone, 0.1 M KNO3

****

C16H12N2O8S2 H4L Chromotrope 2R CAS 4197-07-3 (2604)
2-(Benzeneazo)-chromotropic acid, Acid Red 29

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KNO3	25°C	0.10M	U			1971KMb (93061)	865
							K(Ba+HL)=1.84		
Ba++	gl	KNO3	25°C	0.10M	U			1968NMb (93062)	866
							K(Ba+HL)=1.06		

****

C16H12N2O9S2 H5L CAS 26197-92-2 (4094)
2-(2'-Hydroxyphenylazo)chromotropic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KNO3	25°C	0.10M	U			1968NMb (93075)	867
							K(Ba+HL)=2.73		

****

C16H12N2O11S3 H5L (4095)
2-(2'-Sulphophenylazo)chromotropic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KNO3	25°C	0.10M	U			1968NMb (93082)	868
							K(Ba+HL)=2.66		

****

C16H12N2O11S3 H5L CAS 35310-44-2 (5179)
2-(3'-Sulfophenylazo)chromotropic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KNO3	25°C	0.10M	U			1968NMb (93086)	869
							K(Ba+HL)=1.44		

****

C16H12N2O11S3 H5L CAS 548-81-2 (5180)
2-(4'-Sulfophenylazo)chromotropic acid,
2-(4-sulfophenylazo)-1,8-dihydroxyaphthalene-3,6-diHSO3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KNO3	25°C	0.10M	U			1968NMb (93092)	870
							K(Ba+HL)=1.58		

****

C16H13N2O10AsS2 H5L Thorin I CAS 3688-92-4 (2609)
1-((2-Arsonophenyl)azo)-2-hydroxy-3,6-naphthalyldisulfonic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	oth/un	30°C	?	U		K1=3.4	1964PCa (93185)	871

****

C16H13N2O10AsS2 H5L (5204)
2-(2-Arsonophenylazo)-1-hydroxynaphthalene-3,6-disulfonic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KNO3	25°C	0.10M	U		K1=1.8	1971KTc (93225)	872

****

C16H13N2O11AsS2 H6L Arsenazo I CAS 520-10-5 (277)
2-(2'-Arsonophenylazo)chromotropic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KNO3	25°C	0.10M	U		K1=4.22	1971KTc (93248)	873
Ba++	gl	KNO3	25°C	0.10M	U			1968NMb (93249)	874
							K(Ba+HL)=4.15		

****

C16H14N4O2 H2L (3467)
5-Hydroxy-4-(2-hydroxyphenylazo)-3-methyl-1-phenylpyrazole;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	diox/w	30°C	75%	U		K1=6.12	1952SNa (93472)	875

****

C16H14N4O4S HL (5184)
5-Methyl-1-phenyl-4-(2-sulfophenylazo)-3-pyrazolone;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	diox/w	30°C	75%	U		K1=3.69	1969SSc (93506)	876

****

C16H20N2O8 H4L CAS 6411-02-5 (1919)
1-Phenyl-ethylenediamine-N,N,N',N'-tetraethanoic acid (DL)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KNO3	20°C	0.10M	U		K1=8.39	1989SLa (94031)	877
Ba++	gl	KNO3	20°C	0.10M	U		K1=8.39	1969NDb (94032)	878
Ba++	gl	KCl	25°C	0.10M	U		K1=8.06	1967OTb (94033)	879

****

C16H20N2O10 H6L (704)
1,2-Dihydroxy-3,6-di-(methyleneiminodiethanoic acid)-benzene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KNO3	25°C	0.10M	C		K1=4.36 K(Ba+H2L)=3.53 K(Ba+HL)=4.35 K(BaHL+H)=10.43 K(BaL+H)=11.86 B(Ba2L)=9.14	1988ZHa (94064)	880

****
C16H24N2O8 H4L CAS 38557-30-1 (1256)
Ethylene-bis(N,N'-(2,6-dicarboxy)piperidine); ((HOOC)2.C5H8N.CH2.)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	NaNO3	25°C	0.10M	U		K1=4.14	1979PBa (94318)	881

****
C16H24O6 L Benzo18-crown-6 CAS 14098-24-9 (513)
2,3-Benzo-1,4,7,10,13,16-hexaoxacyclooctadeca-2-ene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	oth	alc/w	35°C	3.0%	C		K1=2.88	1999MTd (94379)	882

Method: capillary zone electrophoresis. Medium: 3% v/v EtOH/H20, 0.005 M acetate buffer, pH 5.5.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	cal	non-aq	25°C	100%	C	H	K1=2.68	1999WBa (94380)	883

Medium: N,N-dimethylformamide. DH(K1)=-23.4 kJ mol-1.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	cal	non-aq	25°C	100%	U	H	K1=5.80	1993BDb (94381)	884

Medium: acetone. DH=-49.3 kJ mol-1; TDS=-16.4 Calorimetric titration

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	con	none	25°C	0.0	U		K1=2.90	1989TKa (94382)	885
Ba++	cal	non-aq	25°C	100%	C	H	K1=5.48	1986ICa (94383)	886

Medium: MeOH. DH(K1)=-37.2 kJ mol-1, DS(K1)=-19.9 J K-1 mol-1.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	sp	alc/w	25°C	100%	U		K1=5.35	1981EMb (94384)	887

Medium: MeOH

****
C16H24O14 H4L CAS 61696-54-6 (6104)
1,4,7,10,13,16-Hexaoxacyclooctadeca-2,3,11,12-tetracarboxylic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	R4N.X	25°C	0.10M	M		K1=6.2 B(BaHL)=10.4	1991FGb (94491)	888

Medium: 0.10 M Et4NNO3.

****
C16H25NO4 L (7444)
1-Aza-4,7,10,13-tetraoxa-1-phenyl-cyclopentadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ sp non-aq RT 100% C K1=3.70 2001AVa (94512) 889
Method: spectrophotometric titration. Medium: acetonitrile.

Ba++ sp non-aq 25°C 100% U K1=4.30 1998ACa (94513) 890
Medium: CH3CN
****
C16H26N2O4 L (5849)
2,3-Benzo-1,4,10,13-tetraoxa-7,16-diazacyclooctadeca-2-ene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ ISE alc/w 25°C 100% U K1=4.5 1988CFa (94555) 891
Medium: MeOH
****
C16H26N2O10 H2L CAS 93031-54-0 (5831)
1,4,7,10-Tetraoxa-13,16-diazacyclooctadecane-11,18-dione-13,16-diethanoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl R4N.X 25°C 0.10M C K1=4.68 2002DCb (94564) 892
K(BaL+H)=4.35
Medium: 0.10 M Me4NNO3.
****
C16H26N2O12 H4L (6659)
1,4,10,13-Tetraoxa-7,16-diaza-2,3,11,12-tetracarboxycyclooctadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl R4N.X 25°C 0.10M U K1=6.6 1990AFa (94586) 893
B(BaHL)=15.7
****
C16H26N2O12 H4L CAS 130190-52-2 (6660)
1,4,10,13-Tetraoxa-7,16-diaza-2,3,7,16-tetracarboxycyclooctadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl R4N.X 25°C 0.10M U K1=10.2 1990AFa (94600) 894
B(BaHL)=17.3
****
C16H28N2O8 H4L (5167)
1,2-Diaminoethane-N,N'-diethanoic-N,N'-di-2-(3-methyl)butanoic acid;

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

```
Ba++       gl  KNO3   20°C 0.10M U        K1=3.30        1969NDc (94706) 895
**************************************************************************
C16H28N2O8            H4L                        (5168)
1,2-Diaminoethane-N,N'-diethanoic-N,N'-di-2-pentanoic acid;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Ba++       gl  KNO3   20°C 0.10M U        K1=5.97        1969NDc (94732) 896
**************************************************************************
C16H28N2O8            H4L                        (5138)
1,2-Diaminooctane-N,N,N',N'-tetraethanoic acid;
(HOOCCH2)2N.CH2.CH(C6H13)N(CH2COOH)2
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Ba++       gl  KNO3   20°C 0.10M U        K1=8.65        1979MBd (94758) 897
**************************************************************************
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
--------------------------------------------------------------------------
Ba++       gl  R4N.X  25°C 0.10M M        K1=12.31       1996CHc (94877) 898
Medium: 0.1 M Me4NCl.
--------------------------------------------------------------------------
Ba++       gl  KCl    25°C 0.10M C        K1=11.75       1991CMb (94878) 899
--------------------------------------------------------------------------
Ba++       cal R4N.X  25°C 0.10M C   H                   1984DFa (94879) 900
Medium: 0.10 M Me4NNO3. DH(K1)=-35.6 kJ mol-1, DS(K1)=125 J K-1 mol-1.
--------------------------------------------------------------------------
Ba++       gl  R4N.X  25°C 0.10M C        K1=12.873      1982DSa (94880) 901
                                         K(Ba+HL)=6.415
--------------------------------------------------------------------------
Ba++       EMF KCl    20°C 0.10M C        K1=11.3        1981SFa (94881) 902
Method: Pt/H2 electrode.
**************************************************************************
C16H29N3O8            H3L                    CAS 259211-79-5  (7775)
1,4-Dioxa-7,10,13-triazacyclopentadecane-7,10,13-triethanoic acid;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Ba++       gl  R4N.X  25°C 0.10M C        K1=7.25        2000CDd (94962) 903
Medium: 0.10 M (Me4N)NO3.
**************************************************************************
C16H30N2O8            H2L                    CAS 72912-01-7  (1568)
1,4,10,13-Tetraoxa-7,16-diazacyclooctadecane-N,N'-diethanoic acid;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Ba++       cal R4N.X  25°C 0.10M C   H                   1989DSa (95027) 904
```

DH(BaL)=-43.1 kJ mol-1; DS=5.

Ba++ gl NaNO3 25°C 0.10M U K1=8.46 1988HSb (95028) 905

Ba++ gl R4N.X 25°C 0.10M U K1=7.63 1983CRb (95029) 906

****

C16H30N4O8 H4L (3473)

N,N'-Dimethyl-2,2'-ethylenedi-iminobis(ethylenediethanoic acid);

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

---

Ba++ gl KCl 20°C 0.10M U K1=6.24 1964PCa (95082) 907

K(Ba+HL)=2.84

****

C16H32N2O4 L Cryptand 1,2,1H CAS 119017-36-6 (6587)

4,7,14,20-Tetraoxa-1,10-diazabicyclo[8.7.5]docosane;

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

---

Ba++ gl alc/w 25°C 95% M K1=3.34 1990LNa (95116) 908

Medium: 95% MeOH, 0.05 M Bu4NBr. For the 9,13-dihydroxy- analogue: K1 < 2

****

C16H32N2O5 L Cryptand 2,2,1 CAS 31364-42-8 (837)

1,10-Diaza-4,7,13,16,21-pentaoxabicyclo[8,8,5]tricosane (2,2,1);

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

---

Ba++ ISE non-aq 25°C 100% C H K1=6.60 1999WBa (95176) 909

Medium: N,N-dimethylformamide. Method: competitive titration against Ag+, using Ag+ ISE. By calorimetry: DH(K1)=-40.3 kJ mol-1.

Ba++ gl R4N.X 25°C 0.05M C H K1=5.8 1996BCh (95177) 910

Medium: 0.05 M Et4NClO4. By calorimetry: DH(K1)=-31.0 kJ mol-1.

Ba++ EMF non-aq 25°C 100% C H K1=5.04 1995CDb (95178) 911

Medium: DMSO, 0.1 M Et4NClO4. DH=-39.6 kJ mol-1, DS=-36.3 J K-1 mol-1.

Ba++ sp non-aq 25°C 100% U T H K1=4.12 1994GSb (95179) 912

At 35 C: K1=4.06; 45 C: K1=3.94; 55 C: K1=3.82. DH(K1)=-19 kJ mol-1, DS=16

Medium: DMSO

Ba++ sp non-aq 20°C 100% U K1=6.9 1992PSa (95180) 913

Medium: DMF, 0.01 M Me4NI

Ba++ cal alc/w 25°C 100% U H 1986BUa (95181) 914

B(Ba2L2)=10.4

Medium: MeOH. DH=-38.2 kJ mol-1; DS=70

Ba++ ISE non-aq 25°C 100% U H K1=>11 1986BUb (95182) 915

In CH3CN. DH=-78.3 kJ mol-1

Ba++ ISE alc/w 25°C 100% U H K1=10.4 1985BUc (95183) 916
Medium: MeOH, 0.05 M Et4NClO4. DH=-38.2 kJ mol-1

Ba++ ISE non-aq 25°C 100% C I K1=5.44 1985CKa (95184) 917
Medium: DMSO. In PC: K1=13.54; in DMF:K1=6.60; in MeOH:K1=10.43

Ba++ sp non-aq 25°C 100% U K1=2.99 1983PSc (95185) 918
Medium: DMSO

Ba++ cal R4N.X 25°C 0.06M C H 1976KLc (95186) 919
Medium: 0.057 M Me4NBr. Method: flow microcalorimetry.
DH(K1)=-26.4 kJ mol-1, DS(K1)=32 J K-1 mol-1.

Ba++ gl R4N.X 25°C 0.05M C I K1=6.30 1975LSc (95187) 920
In 95% MeOH: K1=9.70
****
C16H32N4O4 L (6794)
4,10-Bis(N,N-dimethylethanamido)-1,7-dioxa-4,10-diazacyclododecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ cal alc/w 25°C 100% U H K1=4.94 1990KMb (95318) 921
Medium: MeOH. DH=-33.0 kJ mol-1
****
C16H32N8O4 L CAS 157599-02-5 (8676)
1,4,7,10-Tetraazacyclododecane-1,4,7,10-tetraacetamide;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl NaNO3 25°C 0.10M C K1=5.35 1995MHa (95374) 922
****
C16H34N2O5 L (6953)
7,13-Bis(2-methoxyethyl)-1,4,10-trioxa-7,13-diazacyclopentadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl R4N.X 25°C 0.10M C K1=3.45 1995LLa (95412) 923
Medium: Et4NClO4
****
C16H34N2O5 L DHPK-21 CAS 106288-71-5 (8327)
N,N'-Bis(2-hydroxypropyl)-1,4,10-trioxa-7,13-diazacylopentadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl NaNO3 25°C 0.10M C K1=3.19 1986HBe (95427) 924
****
C16H34N2O6 L CAS 69930-74-1 (1321)
N,N'-Bis(2-hydroxyethyl)-1,7,10,16-tetraoxa-4,13-diazacyclooctadecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	R4N.X	25°C	0.10M	C		K1=5.33	1995LLa (95446)	925

Medium: Et4NClO4

****

C16H36N4O4 L (6703)

1,4,7,10-Tetrakis(2-hydroxyethyl)-1,4,7,10-tetraazacyclododecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	R4N.X	25°C	0.10M	C		K1=4.84	2000DFb (95569)	926

Medium: 0.10 M Et4NClO4.

****

C17H12N2O10S2 H5L CAS 3440-76-4 (4119)

2-(2'-Carboxyphenylazo)chromotropic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KNO3	25°C	0.10M	U			1971KMb (95719)	927
							K(Ba+HL)=2.81		
Ba++	gl	KNO3	25°C	0.10M	U			1968NMb (95720)	928
							K(Ba+HL)=2.81		

****

C17H14N2O HL CAS 2046-17-5 (5214)

1-(2-Methylphenylazo)-2-hydroxynaphthalene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	mixed	25°C	75%	U		K1=6.42	1972MCb (95794)	929

Medium: 75% acetone, 0.1 M KNO3

****

C17H14N2O HL CAS 6756-41-8 (5215)

1-(4-Methylphenylazo)-2-hydroxynaphthalene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	mixed	25°C	75%	U		K1=6.97	1972MCb (95809)	930

Medium: 75% acetone, 0.1 M KNO3

****

C17H14N2O2 HL CAS 1229-55-6 (5216)

1-(2-Methoxyphenylazo)-2-hydroxynaphthalene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	mixed	25°C	75%	U		K1=6.97	1972MCb (95828)	931

Medium: 75% acetone, 0.1 M KNO3

****

C17H14N2O2 HL CAS 13441-91-1 (5217)

1-(4-Methoxyphenylazo)-2-hydroxynaphthalene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl mixed 25°C 75% U K1=6.79 1972MCb (95843) 932
Medium: 75% acetone, 0.1 M KNO3
****
C17H14N2O9S2 H4L (5228)
2-(2-Methoxyphenylazo)chromotropic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl KNO3 25°C 0.10M U K1=2.08 1971KMb (95944) 933
K(Ba+HL)=2.08
****
C17H24N4O6 H3L (7349)
3,6,9,15-Tetraazabicyclo[9.3.1]pentadeca-1(15),11,13-triene-3,6,9-triethanoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl R4N.X 25°C 0.10M C K1=9.131 1997DQa (96453) 934
K(BaL+H)=4.87
Medium:Me4NNO3
****
C17H30N4O8 H4L TRITA CAS 60239-20-5 (1018)
1,4,7,10-Tetraazacyclotridecane-1,4,7,10-tetraethanoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl KCl 25°C 0.10M C K1=8.56 1991CMb (96641) 935
K(BaL+H)=8.13

Ba++ cal KNO3 25°C 0.10M C H 1984DFa (96642) 936
DH(K1)=-13.0 kJ mol-1, DS(K1)=117 J K-1 mol-1.

Ba++ gl KNO3 25°C 0.10M C K1=8.342 1982DSa (96643) 937
K(Ba+HL)=3.641

Ba++ EMF KCl 20°C 0.10M C K1=7.2 1981SFa (96644) 938
Method: Pt/H2 electrode.

Ba++ gl KCl 20°C 0.10M U K1=7.24 1976SFb (96645) 939
****
C17H31N3O8 H3L CAS 282717-18-4 (7776)
1,4-Dioxa-7,10,14-triazacyclohexadecane-7,10,14-triethanoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl R4N.X 25°C 0.10M C K1=4.06 2000CDd (96681) 940
*K(BaL)=-9.41
Medium: 0.10 M (Me4N)NO3.

****
C17H32N4O6 H3L (7253)
1,4,7,10-Tetraazacyclododecane-1-propyl-4,7,10-triethanoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl R4N.X 25°C 0.10M M K1=7.71 1996CHc (96694) 941
Medium: 0.1 M Me4NCl.
****
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
---
Ba++ gl R4N.X 25°C 0.10M M K1=10.03 1996CHc (96711) 942
Medium: 0.1 M Me4NCl.
****
C17H32N4O8 H3L (7255)
1,4,7,10-Tetraazacyclododecane-1-(2,3-dihydroxypropyl)-4,7,10-triethanoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl R4N.X 25°C 0.10M M K1=10.03 1996CHc (96725) 943
Medium: 0.1 M Me4NCl
****
C17H34N4O4S L CAS 503465-04-1 (9247)
4,7,13,16-Tetraoxa-1,10,21,23-tetraazabicyclo[8.8.7]pentacosane-22-thione;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl alc/w 25°C 95% C K1=2.35 2004KVa (96756) 944
Medium: 95% MeOH/H2O, 0.01 M Et4NClO4.
****
C17H37N3O4 L CAS 119167-07-6 (6042)
4,7,10-Tri-(2-hydroxypropyl)-1-oxa-4,7,10-triazacyclododecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl NaNO3 25°C 0.10M U K1=3.30 1988HSb (96785) 945
****
C18H12N2O11S2 H5L (5251)
2-(2'-Oxalophenylazo)chromotropic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl KNO3 25°C 0.10M U 1971KMb (96868) 946
K(Ba+HL)=2.73
****
C18H14N2O10S2 H5L (5253)
2-(2-Phenylethanoic acidazo)chromotropic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KNO3	25°C	0.10M	U			1971KMb (96939)	947
							K(Ba+HL)=2.43		

****

C18H14N2O11S2 H5L (4132)
2-(2'-(Carboxyhydroxymethyl)phenylazo)chromotropic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KNO3	25°C	0.10M	U			1971KMb (96945)	948
							K(Ba+HL)=3.12		

****

C18H14N2O11S2 H5L (4133)
2-(2'-(Carboxymethoxy)phenylazo)chromotropic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KNO3	25°C	0.10M	U			1971KMb (96952)	949
							K(Ba+HL)=3.00		

****

C18H16N4O4 H2L (3500)
2-(4,5-Dihydro-3-methyl-5-oxo-1-phenyl-1H-pyrazol-4-ylazo)phenoxyethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	diox/w	30°C	75%	U		K1=3.1	1962SCc (97210)	950

****

C18H18O8 H2L (5631)
1,4-bis(2-Carboxymethoxyphenyl)-1,4-dioxabutane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	alc/w	25°C	90%	M		K1=4.95	1998KLa (97303)	951

Medium: 90% v/v MeOH/H2O, 0.1 M Me4NCl

****

C18H22O4 H2L B(CH2AcAcH)2 (2252)
1,3-Di(hexa-3,5-dione)-benzene; C6H4((CH2)2.CO.CH2.CO.CH3)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	diox/w	24°C	50%	U		K1=4.3	1979ACa (97560)	952

****

C18H26N6 L (6628)
3,6,14,17,23,24-Hexaazatricyclo[17.3.1.1]tetracosa-1(23),8,10,12(24),19,21-hexaene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KCl	25°C	0.10M	M		K1=<2	1996MBb (97712)	953

****
C18H27N2O3F L CAS 173417-90-8 (6571)
23-Fluoro-4,7,20-trioxa-1,10-diazatricyclo[8.7.5.1,12,16]tricosa-12,14,16(23)triene
;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ EMF non-aq 25°C 100% C H K1=2.55 1999BHa (97746) 954
Medium: MeOH, 0.05 M Et4NClO4. By calorimetry DH(K1)=-1.0 kJ mol-1.
Method: by competition with Ag+, using Ag/Ag+ electrode.
****
C18H28O5 L CAS 15196-73-3 (2359)
2,3-(4'-Dimethylethylbenzo)-1,4,7,10,13-pentaoxacyclopentadeca-2-ene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ EMF non-aq 25°C 100% U K1=5.35 B2=10.4 1982MRb (97801) 955
Medium: anhydrous propylene carbonate, 0.1M Et4NClO4
****
C18H28O6 H2L O(EAcAcE)2O CAS 73199-63-0 (2251)
1,11-Dioxacycloeicosane-5,7,15,17-tetraone;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl diox/w 24°C 50% U K1=5.4 1979ACa (97830) 956
****
C18H28O6 L CAS 85556-93-0 (642)
2,3-Benzo-8,15-dimethyl-1,4,7,10,13,16-hexaoxacycloocotadeca-2-ene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ cal alc/w 25°C 100% U H K1=2.50 1983SLb (97839) 957
Medium: MeOH
****
C18H28O10 H2L (OEOAcAcOE)2 CAS 62950-36-1 (2254)
1,4,10,13,16,22-Hexaoxacyclotetracosa-6,8,18,20-tetraone;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl diox/w 24°C 50% U K1=6.4 1979ACa (97868) 958
****
C18H30N2O11 H2L CAS 93049-99-1 (5832)
1,4,7,10,13-Pentaoxa-16,19-diazacycloeicosane-14,21-dione-16,19-diethanoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl R4N.X 25°C 0.10M C K1=4.69 2002DCb (97904) 959
Medium: 0.10 M Me4NNO3.
****
C18H30N2O12 H4L (7125)

1,4,10,13-Tetraoxa-7,16-diazacyclooctadecane-7,16-bis(malonic acid);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	NaCl	25°C	0.15M	U		K1=9.76	1995BGa (97926)	960

****

C18H30N4O12 H6L TTHA CAS 869-52-3 (694)
Triethylenetetraaminehexaethanoic acid;((HOOC.CH2)2N.CH2.CH2.N(CH2.COOH).CH2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KCl	30°C	0.10M	U		K1=8.22 K(Ba+H2L)=1.7 K(Ba+HL)=5.55 K(BaL+Ba)=3.41	1963GHa (98012)	961

****

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
Ba++	gl	KCl	25°C	0.10M	C		K1=4.37	1991CMb (98189)	962
Ba++	cal	KNO3	25°C	0.10M	C	H		1984DFa (98190)	963

DH(K1)=10.5 kJ mol-1, DS(K1)=109 J K-1 mol-1.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KNO3	25°C	0.10M	C		K1=3.854 K(Ba+HL)=2.519	1982DSa (98191)	964
Ba++	EMF	KCl	20°C	0.10M	C		K1=4.3	1981SFa (98192)	965

Method: Pt/H2 electrode.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KCl	20°C	0.10M	U		K1=4.32	1976SFb (98193)	966

****

C18H32N4O8 H4L (8192)
3-Methyl-1,5,8,11-tetraazacyclotridecane-1,5,8,11-tetraethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	EMF	KCl	20°C	0.10M	C		K1=8.0	1981SFa (98245)	967

Method: Pt/H2 electrode. For the 3-ethyl- derivative, K1=5.9;
for the 3,3-dimethyl- derivative, K1=3.3

****

C18H32N4O9 H4L CAS 189282-31-3 (8974)
4,7,10,13-Tetrakis-(carboxymethyl)-1-oxa-4,7,10,13-tetraazacyclopentadecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	R4N.X	25°C	0.10M	C		K1=8.74 K(BaL+Ba)=3.01	1999CDb (98255)	968

Medium: 0.10 M NMe4NO3.
****
C18H32O8 L CAS 473704-12-0 (8708)
4-[(2-Propenyloxy)methyl]-2,5,8,11,14,17,20-heptaoxabicyclo[7.6.6]heneicosane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ cal none 25°C 0.0 C H K1=1.93 2001ZKd (98272) 969
Self-medium, ca. 0.005 M. DH(K1)=-17.3 kJ mol-1, DS(K1)=-21 J K-1 mol-1.
****
C18H33NO9 HL 4NH18-C6A CAS 83572-66-1 (5404)
2-Carboxy-3-N-butylformamide-1,4,7,10,13,16-hexaoxacyclooctadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl alc/w 25°C 90% U K1=5.5 B2=11.4 1984FWa (98286) 970
Medium: 90% v/v MeOH/H2O, 0.05 M R4NX
****
C18H34N4O8 H3L (7256)
1,4,7,10-Tetraazacyclododecane-1-(2-hydroxy-3-methoxypropyl)-4,7,10-triethanoic
acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl R4N.X 25°C 0.10M M K1=9.90 1996CHc (98368) 971
Medium: 0.1 M Me4NCl
****
C18H34N4O9 H3L DO3A-B (7301)
10-[2,3-Dihydroxy-(1-hydroxymethyl)-propyl]-1,4,7,10-tetraazacyclododecane-1,4,7-tr
iethanoic ac.;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl KCl 25°C 0.10M C K1=9.05 1996TKa (98374) 972
****
C18H36N2O5 L Cryptand 1,2,2H (6605)
1,10-Diaza-4,7,14,20,23-Pentaoxabicyclo[8.8.7]pentacosane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl alc/w 25°C 95% M K1=5.05 1990LNa (98404) 973
Medium: 95% MeOH, 0.05 M Bu4NBr. For the 12,16-dihydroxy- analogue: K1=3.63
****
C18H36N2O5 L Cryptand 2,2,1H CAS 119017-37-7 (6588)
5,8,15,18,23-Pentaoxa-1,12-diazabicyclo[10.8.5]pentacosane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl alc/w 25°C 95% M K1=4.92 1990LNa (98413) 974
Medium: 95% MeOH, 0.05 M Bu4NBr. For the 9,16-dihydroxy- analogue: K1=5.51

****

C18H36N2O6 L Cryptand 3,2,1 (7303)
1,10-Diaza-4,7,13,16,19,24-hexaoxabicyclo[8,11,5]hexacosane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	cal	KCl	25°C	0.10M	U	IH	K1=7.21	1997ZIa (98418)	975

DH(K1)=-45.8 kJ mol-1, DS=-15.4 J K-1 mol-1. In 95% v/v MeOH/H2O: K1=11.0; DH(K1)=-63.1, DS=-1.0

****

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
Ba++	ISE	non-aq	25°C	100%	C	H	K1=8.01	1999WBa (98514)	976

Medium: N,N-dimethylformamide. Method: competitive titration against Ag+, using Ag+ ISE. By calorimetry: DH(K1)=-54.8 kJ mol-1.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	EMF	non-aq	25°C	100%	C	I	K1=17.90	1997DKb (98515)	977

Method: Ag electrode. Medium: acetonitrile, 0.05 M Bu4NClO4. DH(K1)=-108.8 kJ mol-1, DS=-22.3. In DMF, DH(K1)=-50.6; in Me2SO, -47.8; in PC, -103.4.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	R4N.X	25°C	0.05M	C	H	K1=9.5	1996BCh (98516)	978

Medium: 0.05 M Et4NClO4. By calorimetry: DH(K1)=-62.8 kJ mol-1.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	EMF	non-aq	25°C	100%	C	H	K1=6.21	1995CDb (98517)	979

Medium: DMSO, 0.1 M Et4NClO4. DH=-48.1 kJ mol-1, DS=-42.5 J K-1 mol-1.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	sp	non-aq	25°C	100%	U	T H	K1=5.02	1994GSb (98518)	980

At 35 C: K1=4.93; 45 C: K1=4.86; 55 C: K1=4.74. DH(K1)=-17 kJ mol-1, DS=41
Medium: DMSO

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	cal	non-aq	25°C	100%	C	H		1992BSc (98519)	981

Medium: propylene carbonate. DH(K1)=-105.1 kJ mol-1, DS(K1)=-27 J K-1 mol-1.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	cal	alc/w	25°C	100%	U	H		1986BUa (98520)	982
							B(Ba2L2) >12		

Medium: MeOH. DH=-68.9 kJ mol-1; DS=15

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	ISE	non-aq	25°C	100%	U	H	K1=>9	1986BUb (98521)	983

In CH3CN. DH=-108.8 kJ mol-1

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	con	none	25°C	0.0	C		K1=ca. 9	1986KHe (98522)	984

Method: conductance stopped-flow. Medium pH 11.3.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	ISE	alc/w	25°C	100%	U	H	K1=12.2	1985BUc (98523)	985

Medium: MeOH, 0.05 M Et4NClO4. DH=-68.9 kJ mol-1

Ba++ ISE non-aq 25°C 100% C I K1=6.22 1985CKa (98524) 986
Medium: DMSO. In DMF K1=7.70; in propylenecarbonate K1=17.1; in MeOH K1=12.9

Ba++ sp non-aq 25°C 100% U K1=5.13 1983PSc (98525) 987
Medium: DMSO

Ba++ cal R4N.X 25°C 0.06M C IH 1976KLc (98526) 988
Medium: 0.057 M Me4NBr. Method: flow microcalorimetry. DH(K1)=-59.0 kJ mol-1, DS(K1)=-17 J K-1 mol-1. In 95% (v/v) MeOH/H2O, DH(K1)=-84.1,DS=-53.

Ba++ gl R4N.X 25°C 0.10M C H K1=9.7 1975ANa (98527) 989
Medium: Me4NCl. DH(K1)=-59.8 kJ mol-1, DS=-15.5

Ba++ gl R4N.X 25°C 0.05M C I K1=9.5 1975LSc (98528) 990
In 95% MeOH: K1=12
****
C18H36N4O4 L (6795)
4,10-Bis(N,N-dimethylpropanamido)-1,7-dioxa-4,10-diazacyclododecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ cal alc/w 25°C 100% U H K1=3.30 1990KMb (98780) 991
Medium: MeOH. DH=-44.5 kJ mol-1
****
C18H38N2O6 L CAS 72911-99-0 (649)
4,13-Bis(2-methoxyethyl)-1,7,10,16-tetraoxo-4,13-diazacyclooctadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl R4N.X 25°C 0.10M C K1=4.36 1995LLa (98837) 992
Medium: Et4NClO4

Ba++ gl NaNO3 25°C 0.10M C K1=3.72 1991DHa (98838) 993
****
C18H38N2O6 L (5802)
7,16-Di(2-hydroxypropyl)-1,4,10,13-tetraoxa-7,16-diazacyclooctadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl NaNO3 25°C 0.10M U K1=4.65 1986HBc (98851) 994
****
C18H40N2O10P2 H2L (7241)
1,4,10,13-Tetraoxa-7,16-diazacyclooctadecane-7,16-diyldimethylenediphosphonic acid bis(Et-ester);

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl R4N.X 25°C 0.10M U K1=5.74 1996BJa (98887) 995
Medium: 0.1 M Me4NCl
****

C19H18N4O4 H2L (4142)
4-(2'-(2''-Carboxyethoxy)phenylazo)-3-methyl-1-Phe-pyrazol-5(2H)-one;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	diox/w	30°C	75%	U		K1=4.07	1965SMh (99249)	996

****
C19H34N4O8 H4L cPenta CAS 98515-24-3 (8328)
1,4,8,12-Tetrazacyclopentadecane-N,N',N'',N'''-tetraethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	R4N.X	25°C	0.10M	C		K1=1.75	1988DDa (99464)	997

Medium: 0.10 M Me4NNO3.
****
C19H39N3O5 L CAS 60598-00-7 (1537)
4-Methyl-1,4,10-triaza-7,13,16,21,24-pentaoxa-bicyclo[8,8,8]hexacosane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	R4N.X	25°C	0.10M	U		K1=9.0	1978LMa (99489)	998
							K(Ba+HL)=2.9		

****
C20H14N2O HL (5291)
1-(1-Naphthylazo)-2-hydroxynaphthalene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	mixed	25°C	75%	U		K1=5.50	1972MCb (99598)	999

Medium: 75% acetone, 0.1 M KNO3
****
C20H14N2O HL CAS 2653-64-7 (5292)
1-(2-Naphthylazo)-2-hydroxynaphthalene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	mixed	25°C	75%	U		K1=6.02	1972MCb (99613)	1000

Medium: 75% acetone, 0.1 M KNO3
****
C20H14N2O11S3 H2L Hydroxynaphthol CAS 63451-35-4 (2835)
Hydroxynaphthol blue, 1-(2-Hydroxy-4-sulfo-1-naphthylazo)-2-naphthol-3,

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	sp	none	25°C	0.0	U			1978BRb (99725)	1001
							K1eff=1.75		

Keff at pH 10
****
C20H16N4O5S H2L EriochromeRed B CAS 14954-75-7 (3510)
4-(4,5-Dihydro-3-Me-5-oxo-1-Phe-1H-pyrazol-4-ylazo)-3-naphthol-1-sulfonic acid;

```
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Ba++       gl  diox/w 30°C  75%  U                        1957SFb (99795)1002
                                          K(Ba+H2L=BaL+2H)=-17.6
*******************************************************************************
C20H22O9              H2L                        (5624)
1,7-bis(2-Carboxymethoxyphenyl)-1,4,7-trioxaheptane;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Ba++       gl  alc/w  25°C  90%  M        K1=5.52         1998KLa (99937)1003
Medium: 90% v/v MeOH/H2O, 0.1 M Me4NCl
*******************************************************************************
C20H24O6                L    DiBz-18-Crown-6  CAS 14187-32-7  (604)
2,3:11,12-Dibenzo-1,4,7,10,13,16-hexaoxacyclooctadeca-2,11-diene
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Ba++       EMF alc/w  25°C 100%  C        K1=4.43         2004ZTa (100084)1004
Medium: 100% methanol, 0.05 M Bu4NClO4. Method: Ag electrode,
competition with Ag+ ion.
-------------------------------------------------------------------------------
Ba++       con mixed  25°C  20%  C        K1=3.48         2003SIa (100085)1005
Medium: 20% w/w propylene carbonate/ethylene carbonate.
-------------------------------------------------------------------------------
Ba++       oth alc/w  35°C 3.0%  C        K1=1.96         1999MTd (100086)1006
Method: capillary zone electrophoresis. Medium: 3% v/v EtOH/H20, 0.005 M
acetate buffer, pH 5.5.
-------------------------------------------------------------------------------
Ba++       vlt non-aq 25°C 100%  C        K1=4.32         1991SSb (100087)1007
Method: competitive complexation with Tl+; use of Tl(Hg)/Tl couple.
Medium: acetonitrile, 0.05 M Et4NClO4.
-------------------------------------------------------------------------------
Ba++       cal non-aq 25°C 100%  C   H    K1=>5           1988BUb (100088)1008
Medium: acetonitrile. DH(K1)=-24.4 kJ mol-1.
-------------------------------------------------------------------------------
Ba++       sol none   25°C  0.0  U  I     K1=1.95         1975SNa (100089)1009
K(BaCl+L=BaClL) = 2.15
*******************************************************************************
C20H27N2O5Cl           HL                       CAS 199472-61-2  (8623)
5-Chloro-7-(1,4,7,10-tetraoxa-13-azacyclopentadec-13-ylmethyl)-8-quinolinol;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Ba++       cal non-aq 25°C 100%  C   H                    1997ZBb (100355)1010
                                          K(Ba+HL)=4.28
Medium: MeOH. DH(K)=-20.6 kJ mol-1, DS(K)=12.8 J K-1 mol-1.
*******************************************************************************
C20H30O5S8             e L                      CAS 334475-13-7  (6048)
```

3,6-Bis(methylsulfanyl)-2,7-(4,7,10,13,16-pentaoxa-1,19-dithianodecan-1,19-diyl)tet
rathiafulvalen

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ nmr mixed 25°C 50% C K1=4.2 2001DMa (100435)1011
Medium: 50% v/v CDCl3/CD3CN. Method: 1H NMR
****
C20H31N2O4F L CAS 173417-87-3 (6461)
26-Fluoro-4,7,13,16-tetraoxa-1,10-diazatricyclo[8.8.7.1,20,24]hexacosa-20,22,24(26)
-triene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ EMF non-aq 25°C 100% C H K1=7.63 1999BHa (100438)1012
Medium: MeOH, 0.05 M Et4NClO4. By calorimetry DH(K1)=-25.3 kJ mol-1.
Method: by competition with Ag+, using Ag/Ag+ electrode.
****
C20H32N2O4 L CAS 61696-66-0 (6497)
4,7,13,16-Tetraoxa-1,10-diazatricyclo[8.8.7.1,20,24]hexacosa-20,22,24(26)-triene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ EMF non-aq 25°C 100% C H K1=5.94 1999BHa (100455)1013
Medium: MeOH, 0.05 M Et4NClO4. By calorimetry DH(K1)=-28.6 kJ mol-1.
Method: by competition with Ag+, using Ag/Ag+ electrode.
****
C20H36N4O8 H4L (8193)
3,3-Dimethyl-1,5,8,12-tetraazacyclotetradecane-1,5,8,12-tetraethanoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ EMF KCl 20°C 0.10M C K1=2.4 1981SFa (100575)1014
Method: Pt/H2 electrode.
****
C20H36O6 L DiCy-18-crown-6 CAS 16069-36-6 (1653)
2,3:11,12-Dicyclohexyl-1,4,7,10,13,16-hexaoxacyclooctadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ EMF alc/w 25°C 100% C K1=4.98 2004ZTa (100625)1015
Medium: 100% methanol, 0.05 M Bu4NClO4. Method: Ag electrode,
competition with Ag+ ion.

Ba++ con mixed 25°C 20% C K1=3.17 2003SIa (100626)1016
Medium: 20% w/w propylene carbonate/ethylene carbonate.

Ba++ nmr non-aq 27°C 100% C I K1=6.65 2001KZa (100627)1017
Method: 7Li nmr; competitive binding study. Medium: nitromethane.
In acetonitrile, K1=5.05

Ba++ vlt non-aq 25°C 100% C K1=>5 1991SSb (100628)1018
Method: competitive complexation with Tl+; use of Tl(Hg)/Tl couple.
Medium: acetonitrile, 0.05 M Et4NClO4.

Ba++ cal non-aq 25°C 100% C H K1=>5 1988BUb (100629)1019
Medium: acetonitrile. DH(K1)=-48.1 kJ mol-1.

Ba++ cal oth/un 40°C 0.0 U T K1=3.12 1971INa (100630)1020
Isomer B. K1(10 C)=3.44, K1(25 C)=3.27. For isomer A: K1=3.84(10 C), 3.57(25 C), 3.47(40 C)
****
C20H40N2O6 L Cryptand 2,2,2H (6606)
1,10-Diaza-4,7,14,17,23,26-Hexaoxabicyclo[10.8.8]octacosane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl alc/w 25°C 95% M K1=7.53 1990LNa (100783)1021
Medium: 95% MeOH, 0.05 M Bu4NBr. For the 12,19-dihydroxy- analogue: K1=8.62
****
C20H40N2O6 L Cryptand 3,2,1H (6589)
1,7-Diaza-4,11,14,17,23,26-hexaoxabicyclo[13.8.5]octacosane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl alc/w 25°C 95% M K1=5.21 1990LNa (100792)1022
Medium: 95% MeOH, 0.05 M Bu4NBr. For the 9,19-dihydroxy- analogue: K1=7.08
****
C20H40N2O7 L Cryptand 3,2,2 CAS 31255-22-8 (1763)
Cryptand 3,2,2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl alc/w 25°C 90% M K1=10.40 1977LSc (100807)1023
Medium: 90% (w/w) MeOH/H2O, 0.1 M Et4NBr.

Ba++ gl R4N.X 25°C 0.05M C I K1=6.0 1975LSc (100808)1024
In 95% MeOH: K1=10.40
****
C20H42N2O6 L (6402)
7,16-Bis(1,1-dimethyl-2-hydroxyethyl)-1,4,10,13-tetraoxa-7,16-diazacyclooctadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl NaNO3 25°C 0.10M C K1=2.73 1991DHa (100861)1025
****
C20H42N2O8 L CAS 106113-01-3 (5879)
7,16-Bis(((2-hydroxyethyl)oxy)ethyl)-1,4,10,13-Tetraoxa-7,16-Diazacyclooctadecane;

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

---
Ba++ gl NaNO3 25°C 0.10M C K1=4.91 1989HBa (100866)1026
****
C20H42N4O4 L CAS 39678-14-3 (1543)
4,7-Dimethyl-1,4,7,10-tetraaza-13,16,21,24-tetraoxa-bicyclohexacosane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl R4N.X 25°C 0.10M U K1=6.7 1978LMa (100885)1027
K(Ba+HL)=2.7
****
C20H44N4O4 L CAS 102202-74-4 (6041)
1,4,7,10-Tetra-(2-hydroxypropyl)-1,4,7,10-tetraazacyclododecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl NaNO3 25°C 0.10M U K1=3.74 1988HSb (100924)1028
****
C20H44N4O4 L (6730)
1,4,7,10-Tetra-(2-methoxyethyl)-1,4,7,10-tetrazacyclododecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl R4N.X 25°C 0.10M C K1=4.72 1993SFb (100937)1029
Medium: 0.1 M Et4NClO4.
****
C20H44N4O6 L CAS 118018-01-2 (5878)
4,7,13,16-Tetrakis(2-hydroxyethyl)-1,10-dioxa-4,7,13,16-tetraazacyclooctadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl NaNO3 25°C 0.10M C K1=4.30 1989HBa (100959)1030
****
C21H21N2O8Cl H2L Demeclocycline CAS 64-73-3 (5759)
7-Chloro-6-demethyltetracycline;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl KNO3 25°C 0.10M C K1=3.11 1979DDd (101183)1031
Also data for other tetracycline analogues.
****
C21H22O7 L (7458)
1,8-[(3,6,9-Trioxaundecane-1,11-diyl)dioxy]xanthone;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ sp alc/w 25°C 100% U K1=3.16 1996BCf (101207)1032
Medium: MeOH. K(L+H)=-1.85. Data also for the 3,6,9,12-tetraoxa and
3,6,9,12,15-pentaoxa analogues
****

C21H24O8 L CAS 78708-41-5 (799)
2,3:9,10-Dibenzo-1,4,8,11,14-pentaoxacyclohexadeca-2,9-diene-6-oxyethanoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl alc/w 25°C 80% M IH K1=5.73 1985AEb (101263)1033
Medium: 80% w/w MeOH/H2O, pH=9. Calorimetry:DH(K1)=-20.2 kJ mol-1, DS=42.0
J K-1 mol-1. At pH=3, K(Ba+HL)=2.71, DH(Ba+HL)=-17.7, DS(Ba+HL)=-7.6.
****
C21H27O8P L CAS 71817-08-8 (6905)
1,2:10,11-Dibenzo-16-methylphosphonyl)-3,6,9,12,15,17,20-heptaoxacycloeicosane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ nmr non-aq 20°C 100% U K1=3.0 1982BGe (101299)1034
Medium: Acetone-D6 ; Method - NMR H1.
****
C21H31N5O8 H3L (7254)
1,4,7,10-Tetraazacyclododecane-1-(4-nitrobenzyl)-4,7,10-triethanoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl R4N.X 25°C 0.10M M K1=8.01 1996CHc (101407)1035
Medium: 0.1 M Me4NCl.
****
C21H42N4O6S L CAS 503465-05-2 (9248)
4,12,18,21,26,29-Hexaoxa-1,7,9,15-tetraazabicyclo[13.8.8]hentriacontane-8-thione;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl alc/w 25°C 95% C K1=5.63 2004KVa (101461)1036
Medium: 95% MeOH/H2O, 0.01 M Et4NClO4.
****
C22H16N4O14S4 H6L Sulfonazo III CAS 1738-02-9 (4155)
2,7-Bis(2'-sulfophenylazo)chromotropic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ sp alc/w 25°C 60% U I 1969PMb (101535)1037
K(?)=5.66
pH 1.7-2.55, 60% ethanol. K(pH 2.0)=6.26, K(2.3)=7.06, K(2.55)=8.23
In 0.008 HCl, 40-75% ethanol: K(?)=5.76(40%), 7.06(60%), 8.23(75%)

Ba++ sp KNO3 20°C 0.20M U 1965BVa (101536)1038
B(BaH2L)=25.9
****
C22H17N4O14ClP2S2 H8L ClPhosphonazo 3 CAS 1914-99-4 (2577)
2,7-Bis((4-chloro-2-phosphophenyl)azo)chromotropic acid;

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

```
--------------------------------------------------------------------------------
Ba++       sp  KNO3   25°C 0.20M U                      1967BMc (101577)1039
                                          B(BaH6L2)=82.5
********************************************************************************
C22H20N2O4              L                      CAS 207461-96-9  (8955)
(5Z)-12,13,20,21-Tetrahydrotribenzo[b,f,l][1,8,11,14,4,5]tetraoxadiazacyclohexadeci
ne;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Ba++       sp  non-aq  RT  100%  C  I     K1=2.45        2000GDa (101694)1040
Medium: acetonitrile. In MeOH, K1=1.55.
********************************************************************************
C22H24N2O8            H2L    Tetracycline     CAS 60-54-8  (2201)
Tetracycline;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Ba++       gl  NaNO3  25°C 0.10M C    M   K1=4.00        1989GAb (101809)1041
                                          K(BaL+Gly)=3.80
********************************************************************************
C22H24N2O8            H4L                      CAS 91044-24-5  (1920)
meso-1,2-Diphenyl-1,2-diaminoethane-N,N,N',N'-tetraethanoic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Ba++       gl  KNO3   20°C 0.10M U        K1=3.20        1989SLa (101839)1042
********************************************************************************
C22H24N2O8            H4L                      CAS 91044-25-6  (1921)
rac-1,2-Diphenyl-1,2-diaminoethane-N,N,N',N'-tetraethanoic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Ba++       gl  KNO3   20°C 0.10M U        K1=8.36        1989SLa (101855)1043
--------------------------------------------------------------------------------
Ba++       gl  KCl    25°C 0.10M U        K1=9.11        1967OTb (101856)1044
********************************************************************************
C22H26N4O10           H4L    BAPTA              (7230)
1,2-Bis(o-aminophenoxy)ethane-N,N,N',N'-tetraethanoic acid;
((HOOCCH2)2NCH(OC6H4NH2)2
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Ba++       gl  R4N.X  25°C 0.10M C        K1=5.75        1993YTa (101972)1045
********************************************************************************
C22H26O10             H2L                      (5628)
1,10-bis(2-Carboxymethoxy-phenyl)-1,4,7,10-tetraoxadecane;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
```

Ba++ gl alc/w 25°C 90% M K1=5.94 1998KLa (102007)1046
Medium: 90% v/v MeOH/H2O, 0.1 M Me4NCl
****
C22H28N2O6 L CAS 449740-17-4 (8937)
N-(2-Pyridylmethylene)-4-aminobenzo-18-crown-6;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ sp non-aq 25°C 100% C I M 2002YPc (102015)1047
K(ZnA2L+Ba)=4.69
Medium: MeCN, 0.10 M n-Bu4NPF6. By 1H nmr in CDCl3, K(ZnA2L+Ba)=4.30.
A is p-thiocresol.
****
C22H28O7 L Dibenzo-21-Cr-7 CAS 14098-41-0 (2876)
2,3:11,12-Dibenzo-1,4,7,10,13,16,19-heptaoxacycloheneicosane-2,11-diene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ oth alc/w 35°C 3.0% C K1=2.07 1999MTd (102037)1048
Method: capillary zone electrophoresis. Medium: 3% v/v EtOH/H20, 0.005 M
acetate buffer, pH 5.5.

Ba++ cal non-aq 25°C 100% C H K1=4.21 1986ICa (102038)1049
Medium: MeOH. DH(K1)=-21.1 kJ mol-1, DS(K1)=9.7 J K-1 mol-1.
****
C22H31N2O6Cl HL CAS 184647-21-0 (8621)
5-Chloro-2-(1,4,7,10,13-pentaoxa-16-azacyclooctadec-16-ylmethyl)-8-quinolinol;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ cal non-aq 25°C 100% C H 1997ZBb (102138)1050
K(Ba+HL)=6.20
Medium: MeOH. DH(K)=-40.6 kJ mol-1, DS(K)=-17.5 J K-1 mol-1.
Method: competitive calorimetric titration.
****
C22H31N2O6Cl HL CAS 184647-19-6 (8620)
5-Chloro-7-(1,4,7,10,13-pentaoxa-16-azacylooctadec-16-ylmethyl)-8-quinolinol;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ cal non-aq 25°C 100% C H 1997ZBb (102142)1051
K(Ba+HL)=4.08
Medium: MeOH. DH(K)=-39.3 kJ mol-1, DS(K)=-55.4 J K-1 mol-1.
****
C22H36N2O6 L Bz-Cryptand 222 CAS 31250-18-7 (2269)
5,6-Benzo-4,7,13,16,21,24-hexaoxa-1,10-diazabicylo[8:8:8]hexacosa-5-ene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl R4N.X 25°C 0.05M U H K1=7.6 1998DBa (102266)1052

Medium: 0.05 M Et4NClO4. By calorimetry: DH(K1)=-50.5 kJ mol-1,

---

Ba++ EMF alc/w 25°C 100% U H K1=10.99 1987BUb (102267)1053
In MeOH, 0.05M Et4NClO4. DH=-53.9 kJ mol-1

****

C22H42N2O6 L (6401)
7,16-Bis(tetrahydrofurfuryl)-1,4,10,13-tetraoxa-7,16-diazacyclooctadecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	NaNO3	25°C	0.10M	C		K1=4.50	1991DHa	(102402)1054

****

C22H44N2O7 L Cryptand 3,2,2H (6607)
1,10-Diaza-4,7,14,17,20,26,29-Heptaoxabicyclo[13.8.8]hentriacontane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	alc/w	25°C	95%	M		K1=6.64	1990LNa	(102413)1055

Medium: 95% MeOH, 0.05 M Bu4NBr. For the 12,22-dihydroxy- analogue: K1=8.43

****

C22H44N2O8 L Cryptand 4,2,2 (7304)
1,10-Diaza-4,7,13,16,21,24,27,30-octaoxabicyclo[8,8,14]dotricontane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	cal	alc/w	25°C	95%	U	H	K1=5.37	1997ZIa	(102419)1056

Medium: 95% v/v MeOH/H2O, 0.1 M. DH(K1)=-38.4 kJ mol-1, DS=-25.8 J K-1 mol-1

****

C22H44N2O8 L Cryptand 3,3,2 CAS 132162-57-3 (1762)
Cryptand 3,3,2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	R4N.X	25°C	0.05M	C		K1=3.65	1975LSc	(102426)1057

****

C22H44N6O5S2 L CAS 503465-08-5 (9241)
9,20,23,28,31-Pentaoxa-1,4,6,12,14,17-hexaazabicyclo[15.8.8]tritriacontane-5,13-dithione;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	alc/w	25°C	95%	C		K1=3.87	2004KVa	(102436)1058

Medium: 95% MeOH/H2O, 0.01 M Et4NClO4.

****

C22H46N2O4 L CAS 69703-24-8 (2449)
N,N'-Bis(2-dimethylpropane)-cyclo-1,10-diaza-4,7,13,16-tetraoxaoctadecane)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	alc/w	25°C	93%	U		K1=2.4	1978WVa	(102450)1059

Medium: 93% MeOH/H2O
****
C22H48N6O2 L CAS 39678-22-3 (1542)
4,7,13,16-Tetramethyl-1,4,7,10,13,16-hexaaza-21,24-dioxabicyclohexacosane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Ba++	gl	R4N.X	25°C	0.10M	U		K1=3.7		1978LMa (102484)	1060
							K(Ba+HL)=1.2			

****
C23H16N4O13S3 H6L CAS 4568-04-1 (5327)
2-(2'-Carboxyphenylazo)-7-(2'-sulfophenylazo)chromotropic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Ba++	sp	alc/w	25°C	75%	U	I			1969PMb (102517)	1061
							K(?)=4.94			

pH=1.7-2.9,75% ethanol. K(pH=2)5.60, K(2.3)=6.28, K(2.55)=6.79, K(2.9)=7.26
In 0.002HCl,40-75% ethanol: K(?)=4.48(40%), 5.81(60%), 7.26(75%)
****
C23H18N4O14S4 H6L Me-sulfonazoIII CAS 92408-49-6 (2780)
Methyl-2,7-bis(2-sulfonphenylazo)chromotropic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Ba++	sp	NaClO4	25°C	0.10M	U				1975BUb (102610)	1062
							K1eff=5.70 at pH 6.99			
							B2eff=11.48 at pH 6.99			
							B(2,2)eff=17.53 at pH 6.99			

****
C23H23NO5 L CAS 218619-58-0 (7808)
Dibenzo-pyridino-18-crown-6;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Ba++	EMF	alc/w	25°C	100%	C		K1=2.70		2004ZTa (102655)	1063

Medium: 100% methanol, 0.05 M Bu4NClO4. Method: Ag electrode,
competition with Ag+ ion.
****
C23H25NO5S L CAS 464185-98-6 (9292)
4'-[(2-Benzothiazole)ethenyl]-2:3-benzo-15-crown-5;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Ba++	sp	non-aq	20°C	100%	C		K1=4.7	B2=10.80	2003FFa (102690)	1064

Medium: CH3CN.
****
C23H30N2O4 L CAS 361454-16-2 (8960)
N-(Phenylmethylene)-4-(1,4,7,10-tetraoxa-13-azacyclopentadec-13-yl)benzamine;

```
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Ba++       sp  non-aq  RT  100%  C        K1=3.86        2001AVa (102748)1065
Method: spectrophotometric titration. Medium: acetonitrile.
*************************************************************************
C23H33N2O6Cl            L                     CAS 184647-23-2  (8622)
5-Chloro-8-methoxy-2-(1,4,7,10,13-pentaoxa-16-azacyclooctadec-16-ylmethyl)-quinolin
e;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Ba++       cal non-aq 25°C 100%  C   H    K1=5.02        1997ZBb (102794)1066
Medium: MeOH. DH(K)=-30.6 kJ mol-1, DS(K)=-6.54 J K-1 mol-1.
*************************************************************************
C24H16O12N4S2         H6L    Carboxyazo III   CAS 7451-57-2  (1807)
2,7-Bis(2'-carboxyphenylazo)chromotropic acid;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Ba++       sp  alc/w  25°C  75%  U  I                     1969PMb (102863)1067
                                          K(?)=4.26
pH=2.0-2.9,75% ethanol. K(pH=2.3)=5.08, K(2.55)=5.74, K(2.9)=6.12.
In 0.004 HCl,40-75% ethanol: K(?)=3.33(40%), 4.20(60%), 5.74(75%)
*************************************************************************
C24H20B-               HL                     CAS 4358-26-3  (2489)
Tetraphenylborate;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Ba++       dis non-aq 25°C 100%  U  I     K1=1.70        1969PKb (102884)1068
Medium: 0.01-0.10 nitrobenzene. K1(0.01,0.05)=1.30, (tracer amounts Ba++)
*************************************************************************
C24H20N4O14Cl2P2S2    H8L                      (4165)
2,7-Bis(4'-chloro-5'-methyl-2'-phosphonophenylazo)chromotropic acid;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Ba++       sp  KNO3   25°C 0.20M U                       1967BMc (102915)1069
                                        B(BaH6L)=109.4
*************************************************************************
C24H20N4O14S4         H6L                     CAS 14979-11-4  (4163)
2,7-Bis(4'-methyl-2'-sulfophenylazo)chromotropic acid;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Ba++       sp  KNO3   25°C 0.20M U        K1=4.24        1967BVa (102920)1070
*************************************************************************
C24H24N2O8            H4L                     CAS 89593-26-0  (8632)
N,N'-[1,2-Ethynediylbis(2,1-phenylenemethylene)]bis[N-(carboxymethyl)]glycine;
-------------------------------------------------------------------------
```

```
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Ba++       gl  KCl    20°C 0.10M U        K1=4.4         1984VSc (102949)1071
*************************************************************************
C24H26N2O8            H4L                    CAS 89561-09-1  (8633)
N,N'-[1,2-Ethenediylbis(2,1-phenylenemethylene)]bis[N-(carboxymethyl)]glycine;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Ba++       gl  KCl    20°C 0.10M U        K1=4.6         1984VSc (102974)1072
*************************************************************************
C24H26N2O8            H4L                    CAS 89561-11-5  (8635)
N,N'-[1,2-Ethenediylbis(4,1-phenylenemethylene)bis[N-(carboxymethyl)]glycine;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Ba++       gl  KCl    20°C 0.10M U        K1=2.0         1984VSc (102979)1073
*************************************************************************
C24H28N2O8            H4L                    CAS 89561-10-4  (8634)
N,N'-[1,2-Ethanediylbis(2,1-phenylenemethylene)]bis[N-(carboxymethyl)]glycine;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Ba++       gl  KCl    20°C 0.10M U        K1=3.0         1984VSc (103007)1074
*************************************************************************
C24H32O8               L    DiBz-24-Crown-8  CAS 14174-09-5  (580)
2,3:14,15-Dibenzo-1,4,7,10,13,16,19,22-octaoxacyclotetracosa-2,14-diene;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Ba++       con mixed  25°C  20%  C        K1=3.73        2003SIa (103109)1075
Medium: 20% w/w propylene carbonate/ethylene carbonate.
-------------------------------------------------------------------------
Ba++       oth alc/w  35°C 3.0%  C        K1=1.20        1999MTd (103110)1076
Method: capillary zone electrophoresis. Medium: 3% v/v EtOH/H20, 0.005 M
acetate buffer, pH 5.5.
-------------------------------------------------------------------------
Ba++       cal non-aq 25°C 100%  C   H    K1=4.04        1986ICa (103111)1077
Medium: MeOH. DH(K1)=-24.6 kJ mol-1, DS(K1)=-5.0 J K-1 mol-1.
*************************************************************************
C24H35NO9              L                      CAS 330462-64-1  (8032)
6,7-Dimethoxy-4-(1,4,7,10,13-pentaoxa-16-azacyclooctadec-16-ylmethyl)-2H-1-benzopyr
an-2-one;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Ba++       sp  mixed  25°C  10%  C        K1=6.51        2001LWa (103241)1078
Method: fluorimetry. Medium: 10%v/v acetonitrile/H2O.
*************************************************************************
C24H36N4O4             L    Py-2-18-aneN2O4  CAS 103837-13-4  (8062)
```

7,16-Bis(2-pyridinylmethyl)-1,4,10,13-tetraoxa-7,16-diazacyclooctadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl KNO3 25°C 0.10M C K1=4.99 1986DSa (103264)1079
****
C24H36O21 H6L CAS 71735-94-9 (7414)
1,4,7,10,13,16,19,22,25-Nonaoxacycloheptacosane-2,3,11,12,20,21-hexacarboxylic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl R4N.X 25°C 0.10M M K1=6.5 1991FGb (103307)1080
B(BaHL)=10.7
Medium: 0.10 M Et4NNO3.
****
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
---
Ba++ EMF KCl 20°C 0.10M C K1=9.1 1981SFa (103371)1081
Method: Pt/H2 electrode.
****
C24H44O8 L Dicy-24-crown-8 CAS 17455-23-1 (2401)
2,3,14,15-Dicyclohexyl-1,4,7,10,13,16,19,22-octaoxacyclotetracosane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ con mixed 25°C 20% C K1=3.50 2003SIa (103426)1082
Medium: 20% w/w propylene carbonate/ethylene carbonate.
****
C24H46N2O6 L (6567)
7,16-Bis(trans-2-hydroxycyclohexyl)-1,4,10,13-tetraoxa-7,16-diazocyclooctadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl NaNO3 25°C 0.10M C K1=4.59 1991DCa (103453)1083
****
C24H48N4O6 L CAS 56698-26-1 (1536)
4,10,16,22,27,32-Hexaoxa-1,7,13,19-tetraazatricyclo-tetratriacontane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl R4N.X 25°C 0.10M U K1=8.2 1981GLa (103480)1084
****
C24H48N6O6S2 L CAS 503465-10-9 (9242)
9,12,23,26,31,34-Hexaoxa-1,4,6,15,17,20-hexaazabicyclo[18.8.8]hexatricontane-5,16-dithione;

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

---

Ba++ gl alc/w 25°C 95% C K1=4.18 2004KVa (103503)1085

Medium: 95% MeOH/H2O, 0.01 M Et4NClO4.

****

C24H52N4O6 L CAS 118018-00-1 (5877)

4,7,13,16-Tetrakis(2-hydroxypropyl)-1,10-Dioxa-4,7,13,16-tetraazacyclooctadecane;

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

---

Ba++ gl NaNO3 25°C 0.10M C K1=4.14 1989HBa (103554)1086

****

C25H30N3O5Cl HL CAS 172033-66-8 (8619)

5-Chloro-2-(3,6,12,15-tetraoxa-9,21-diazabicycloheneicosa-1,17,19-trien-9-ylmethyl-8-quinolinol;

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

---

Ba++ cal non-aq 25°C 100% C H 1997ZBb (103685)1087

K(Ba+HL)=5.49

Medium: MeOH. DH(K)=-37.1 kJ mol-1, DS(K)=-19.3 J K-1 mol-1.

****

C25H30N3O5Cl HL CAS 172033-54-4 (8618)

5-Chloro-7(3,6,12,15-tetraoxa-9,21-diazabicycloheneicosa-1,17,19-trien-9-ylmethyl)-8-quinolinol;

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

---

Ba++ cal non-aq 25°C 100% C H 1997ZBb (103689)1088

K(Ba+HL)=4.12

Medium: MeOH. DH(K)=-32.7 kJ mol-1, DS(K)=-30.8 J K-1 mol-1.

****

C25H50N4O5 L CAS 61136-92-3 (1535)

Pentaoxa-4,10,16,22,27-tetraaza-1,7,13,19-tricyclo-tetratriacontane;

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

---

Ba++ gl R4N.X 25°C 0.10M U K1=5.3 1981GLa (103833)1089

****

C25H50N4O8S L CAS 503465-06-3 (9249)

4,7,15,18,24,27,32,35-Octaoxa-1,10,12,21-tetraazabicyclo[19.8.8]heptatriacontane-11-thione;

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

---

Ba++ gl alc/w 25°C 95% C K1=7.51 2004KVa (103842)1090

Medium: 95% MeOH/H2O, 0.01 M Et4NClO4.

****

C26H25NO9S H4L Semi-Xylenol O (426)

3-(N,N-Di(carboxymethyl)aminomethyl)-2-cresolsulfonephthalein;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ sp KNO3 25°C 0.10M U K1=4.75 1974YOa (103943)1091
B(BaHL)=12.72
****
C26H27N3O10 H4L (7231)
2-((2-Amino-5-methylphenoxy)-methyl)-6-methoxy-8-aminoquinoline-N,N,N',N'-tetraetha
noic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl R4N.X 25°C 0.10M C K1=5.29 1993YTa (103958)1092
****
C26H28O4 H2L B(CH2AcAcCH2)2B (2253)
3,5,16,18-Tetraoxo[7.7]metacyclophane ;Cyclo-(-C6H4.(CH2)2.CO.CH2.CO.(CH2)2-)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl diox/w 24°C 50% U K1=6.4 1979ACa (104020)1093
****
C26H31NO8S2 L CAS 136195-71-6 (6832)
Crown Ether Styryl Dye;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ sp non-aq 25°C 100% U K1=5.85 B2=11.15 1992BFa (104034)1094
Medium: CH3CN
****
C26H32N2O2 L CAS 588691-41-2 (9066)
4-{2-[10-(2-Morpholinoethyl)-9-anthryl]ethyl}morpholine;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ sp diox/w 25°C 40% C K1=5.26 2003GHb (104038)1095
K(BaL+Ba)=2.37
Method: fluorescence spectroscopy. Medium: 40% w/w dioxane/H2O, 0.05 M
Et4NClO4.
****
C26H32N2S2 L CAS 677034-81-0 (9064)
4-(2-{10-[2-(1,4-Thiazinan-4-yl)ethyl]-9-anthryl}ethyl)thiomorpholine;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ sp non-aq 25°C 100% C K1=3.46 2003GHa (104044)1096
K(BaL+Ba)=2.72
Method: fluorescence spectroscopy. Medium: acetonitrile, 0.05 M Et4NClO4.
****
C26H34N4 L CAS 677034-80-9 (9063)
1-(2-{10-[2-Piperazinoethyl]-9-anthryl}ethyl)piperazine;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ sp non-aq 25°C 100% C K1=5.69 2003GHa (104073)1097
K(BaL+Ba)=3.44
Method: fluorescence spectroscopy. Medium: acetonitrile, 0.05 M Et4NClO4.
****
C26H34N6O8 H4L CAS 132709-65-0 (8941)
3,6,14,17,23,24-Hexaazatricyclotetracosa-1,8,10,12,19,21-hexaene-3,6,14,17-tetraace
tic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl KCl 25°C 0.10M M K1=11.0 1996MBb (104092)1098
****
C26H34O8 H2L (3082)
1,4-Bis(2-carboxybutoxyphenyl)-1,4-dioxabutane; (HOOCCH(C4H9)O(C6H4)OCH2)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl alc/w 25°C 90% M K1=5.35 1998KLa (104106)1099
Medium: 90% v/v MeOH/H2O, 0.1 M Me4NCl
****
C26H35N3O5 HL CAS 254900-33-9 (8919)
7-(10-Hydroxybenzoquinoline-9-ylmethyl)-1,4,10,13-tetraoxa-7,16-diazacyclooctadecan
e;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ cal alc/w 25°C 100% C H 1999SBg (104115)1100
K(Ba+HL)=4.22
Medium: MeOH. DH(K)=-19.2 kJ mol-1, DS(K)=16 J K-1 mol-1.
****
C26H36N2O6 L DiBzCryptand222 (746)
5,6,14,15-Dibenzo-4,7,13,16,21,24-hexaoxa-1,10-diazabicyclo[8.8.8]hexacosan-5,14-di
ene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl R4N.X 25°C 0.05M U H 1998DBa (104126)1101
Medium: 0.05 M Et4NClO4. By calorimetry: DH(K1)=-30.6 kJ mol-1,
---
Ba++ ISE alc/w 25°C 100% C I K1=8.87 1985CKa (104127)1102
Medium: MeOH. In propylenecarbonate K1=13.5; in DMF K1=4.32; in DMSO K1=3.48

Ba++ ISE NaClO4 25°C 0.10M U K1=5.65 1984CTc (104128)1103
****
C26H36N2O6Cl2 H2L (7215)
7,16-Bis((5-chloro-2-hydroxybenzyl)-1,4,10,13-tetraoxa-7,16-diazacyclooctadecane;

```
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Ba++       cal non-aq 25°C 100%  C   H                  1995ZBa (104155)1104
                                          K(Ba+H2L)=3.52
Medium: methanol. DH(K)=-32.2 kJ mol-1, DS(K)=-40.9 J K-1 mol-1.
*************************************************************************
C26H38N2O4              L                     CAS 80757-23-9  (2450)
N,N'-Bis(benzyl)-1,10-diaza-4,7,13,16-tetraoxacyclooctadecane;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Ba++       con alc/w  25°C 100%  M   H    K1=4.76        2000BSe (104182)1105
Medium: MeOH. By calorimetry: DH(K1)=-29.9 kJ mol-1, DS(K1)=-9.7
J K-1 mol-1.
-------------------------------------------------------------------------
Ba++       gl  alc/w  25°C  93%  U        K1=4.5         1978WVa (104183)1106
Medium: 93% MeOH/H2O
*************************************************************************
C26H45NO6S             HL                     CAS 1180-95-6  (7099)
Taurodeoxycholic acid, N-(Deoxycholyl)taurine;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Ba++       vlt R4N.X  25°C 0.10M U  I                   1994BFa (104274)1107
                                         Kso(BaL2)=-7.92
Medium Me4NCl.  Data also for I=0.2-0.75 M
*************************************************************************
C26H48N2O6              L                       (6003)
5,6,14,15-Dicyclohexyl-4,7,13,16,21,24-hexaoxa-1,10-diazabicyclo[8.8.8]hexacosane;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Ba++       EMF alc/w  25°C 100%  U   H    K1=9.75        1987BUb (104293)1108
In MeOH. DH=-35.5 kJ mol-1
*************************************************************************
C26H52N4O5              L                     CAS 78648-22-3  (1534)
4,10,16,22,33-Pentaoxa-1,7,13,19-tetraazatricyclo[11,11,6,5(7.19)pentatriacontane;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Ba++       gl  R4N.X  25°C 0.10M U        K1=3.7         1981GLa (104326)1109
*************************************************************************
C26H52N6O7S2            L                     CAS 503465-16-5  (9245)
4,12,20,26,29,34,37-Heptaoxa-1,7,9,15,17,23-hexaazabicyclo[21.8.8]nonatriacontane-8
,16-dithione;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Ba++       gl  alc/w  25°C  95%  C        K1=5.46        2004KVa (104337)1110
Medium: 95% MeOH/H2O, 0.01 M Et4NClO4.
```

****
C26H52N6O7S2 L CAS 503465-12-1 (9243)
9,12,15,26,29,34,37-Heptaoxa-1,4,6,18,20,23-hexaazabicyclo[21.8.8]nonatricontane-5,19-dithione;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl alc/w 25°C 95% C K1=4.04 2004KVa (104347)1111
Medium: 95% MeOH/H2O, 0.01 M Et4NClO4.
****
C27H32NO5S+ L CAS 423763-94-4 (8997)
3-Ethyl-2-[4-(2,3,5,6,8,9,11,12-octahydro-1,4,7,10,13-benzopentaoxacyclopentadecin-15-yl)butadien
---
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ sp non-aq 25°C 100% C K1=4.69 2002GVc (104515)1112
Medium: acetonitrile, 0.01 M Et4NClO4.
****
C27H47N3O6 L (8029)
Tripodal ionophore 3;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ sp non-aq 25°C 100% C 2001LFa (104623)1113
K(BaP+L=LiPL)=5.16
Method: Analyses by spectrophotometry. Medium: chloroform. P is picrate.
****
C28H35N3O6 L CAS 114880-42-1 (7377)
3-(p-13-Aza-1,4,7,10-tetroxacyclopentadecan-13ylstyryl)-7-dimethylamino-1,4-benzoxazin-2-one;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ sp non-aq RT 100% C K1=3.89 1998ABc (104761)1114
Medium: acetonitrile. Method: fluorescence spectroscopy.
****
C28H36N2O2 L CAS 588691-42-3 (9067)
4-{3-[10-(3-Morpholinopropyl)-9-anthryl]propyl}morpholine;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ sp diox/w 25°C 40% C K1=4.86 2003GHb (104776)1115
K(BaL+Ba)=2.47
Method: fluorescence spectroscopy. Medium: 40% w/w dioxane/H2O, 0.05 M Et4NClO4.
****
C28H36N2O7S2 HL CAS 150196-54-6 (7735)
3-(3-Sulfopropyl)-2-[4-[N-(1,4,7,10,13-pentaoxa-16-azacyclooctadeca)]]styryl-benzothiazolium;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ sp non-aq 18°C 100% C K1=1.9 1997LHa (104782)1116
Medium: acetonitrile.
****
C28H38O9 H2L (3355)
1,7-Bis(2-carboxybutoxyphenyl)-1,4,7-trioxaheptane; (HOOCCH(C4H9)O(C6H4)OCH2CH2)2O

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl alc/w 25°C 90% M K1=5.54 1998KLa (104809)1117
Medium: 90% v/v MeOH/H2O, 0.1 M Me4NCl
****
C28H38O10 H2L CAS 100113-54-0 (3391)
1,10-Bis(2-carboxybutoxyphenyl)-1,4,7,10-tetraoxadecane;
(HOOC(C4H9)O(C6H4)OCH2CH2OCH2)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl alc/w 25°C 90% M K1=5.85 1998KLa (104813)1118
Medium: 90% v/v MeOH/H2O, 0.1 M Me4NCl
****
C28H40N2O6 L (2443)
Bicyclo-NcN'-1,10-diaza-4,7,13,16-tetraoxaoctadecane;(c=(CH2.C6H4.O.CH2)2)

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl alc/w 25°C 93% U K1=2.25 1978WVa (104816)1119
Medium: 93% MeOH/H2O
****
C28H40O6 L CAS 29471-17-8 (1262)
2,3:11,12-Bis(4'-tert-butylbenzo)-1,4,7,10,13,16-hexaoxacyclooctadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ EMF non-aq 25°C 100% U K1=7.66 1982MRb (104834)1120
Medium: anhydrous propylene carbonate, 0.1M Et4NClO4
****
C28H40O10 L DiBz-30-crown10 CAS 104946-67-0 (1776)
2,3:17,18-Dibenzo-1,4,7,10,13,16,19,22,25,28-decaoxacyclotriaconta-2,17-diene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ vlt non-aq 25°C 100% C K1=>5 1991SSb (104871)1121
Method: competitive complexation with Tl+; use of Tl(Hg)/Tl couple.
Medium: acetonitrile, 0.05 M Et4NClO4.

Ba++ sp alc/w 25°C 100% U I K1=4.37 1987GKb (104872)1122
Medium: MeOH. In DMF K1=3.51, in DMSO K1=3.40

Ba++ EMF non-aq 25°C 100% U K1=9.33 1982MRb (104873)1123
Medium: anhydrous propylene carbonate, 0.1M Et4NClO4
****
C28H42N2O6 L (2451)
N,N'-Bis(4-methoxybenzyl)-1,10-diaza-4,7,13,16-tetraoxacyclooctadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl alc/w 25°C 93% U K1=4.5 1978WVa (104926)1124
Medium: 93% MeOH/H2O
****
C28H56N6O8S2 L CAS 503465-18-7 (9246)
4,12,15,23,29,32,37,40-Octaoxa-1,7,9,18,20,26-hexaazabicyclo[24.8.8]dotetracontane-8,19-dithione;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl alc/w 25°C 95% C K1=5.99 2004KVa (105038)1125
Medium: 95% MeOH/H2O, 0.01 M Et4NClO4.
****
C28H56N6O8S2 L CAS 503465-14-3 (9244)
9,12,15,18,29,32,37,40-Octaoxa-1,4,6,21,23,26-hexaazabicyclo[24.8.8]dotetratriconta
ne-5,22-dithio

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl alc/w 25°C 95% C K1=4.31 2004KVa (105048)1126
Medium: 95% MeOH/H2O, 0.01 M Et4NClO4.
****
C29H35NO5 L CAS 201154-06-5 (7825)
N-(1-Pyrenylmethyl)-1,4,7,10,13-pentaoxa-16-azacyclooctadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ sp mixed 25°C 90% C 1997KKa (105098)1127
K(Ba(SCN)2+L)=4.35
Method: fluorescence emission. Medium: MeOH/CHCl3 (9:1 v/v).
****
C29H40N2O6Cl2 L CAS 181706-77-4 (8627)
3,18-Dichlorooctahydro-5H,16H-6,15-(ethanoxyethanoxyethano)-dibenzotetraoxaazacyclo
heneicosine;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ cal non-aq 25°C 100% C H K1=3.58 1998ZBc (105135)1128
Medium: MeOH. DH(K1)=-12.0 kJ mol-1, DS(K1)=28.3 J K-1 mol-1.
****
C29H42N2O6 L (2444)
Bicyclo-NcN'-1,10-diaza-4,7,13,16-tetraoxaoctadecane;(c=(CH2.C6H4.O.CH2)2.CH2)

```
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Ba++       gl  alc/w  25°C  93%  U        K1=2.1         1978WVa (105146)1129
Medium: 93% MeOH/H2O
******************************************************************************
C30H30N20O10            L                     CAS 259886-49-2  (8959)
Cucurbit[5]uril;
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Ba++       sol none   25°C  dil  C        K1=1.32        2001BCf (105214)1130
Method: dissolution of ligand in a 0.002-0.02 M BaX2 solution; spectro
photometric measurement. For decamethylcucurbit[5]uril, K1=1.32.
******************************************************************************
C30H36N8O3                   Furan-cryptand   CAS 121954-37-8  (7451)
39,40,41-Trioxa-1,4,11,14,17,24,29,36-octaazapentacyclo[12.12.12.1.1.1]henLetetraco
ntadodecane;
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Ba++       sp  non-aq 25°C 100%  U   H    K1=5.8         1996AAb (105251)1131
Medium: MeCN
tacyclo[12.12.12.1(6,9).1(19,22).1(31,34]hentetetraconta-4,6,8.....dodecaene
******************************************************************************
C30H44N2O6              L                        (2445)
Bicyclo-NcN'-1,10-diaza-4,7,13,16-tetraoxaoctadecane;(c=(CH2.C6H4.O.(C2H4)2)
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Ba++       gl  alc/w  25°C  93%  U        K1=2.55        1978WVa (105309)1132
Medium: 93% MeOH/H2O
******************************************************************************
C30H57NO8              HL    18NH15-C5A       CAS 79145-86-1  (5405)
2-Carboxy-3-N-octadecanylformamide-1,4,7,10,13-pentaoxycyclopentadecane;
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Ba++       gl  alc/w  25°C  90%  U        K1=4.4    B2=8.2    1984FWa (105381)1133
Medium: 90% v/v MeOH/H2O, 0.05 M R4NX
******************************************************************************
C30H62N2O3              L                        (2956)
1,10-Di(decylaza)-4,7,13-trioxacyclopentadecane;
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Ba++       cal alc/w  25°C 100%  U   H    K1=5.84        1986BUa (105387)1134
Medium: MeOH. DH(K1)=-32.9 kJ mol-1; DS=1 J K-1 mol-1
******************************************************************************
C31H32N2O13S          H6L    Xylenol orange   CAS 63721-85-5  (432)
```

5,5'-Bis-N,N-bis(carboxymethyl)aminomethyl-4'-hydroxy-3,3'-dimethylfuchsone-2"-sulf
onic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KNO3	25°C	0.10M	C	M	K1=5.51	1998GBa	(105453)1135
							K(BaL+H)=10.86		
							K(BaL+Ba)=3.45		
							K(Ba2L+H)=9.30		
Ba++	sp	KNO3	25°C	0.10M	U		K1=6.67	1974YOa	(105454)1136
							K(Ba+HL)=5.04		
							K(Ba+H2L)=2.02		
							K(Ba+BaL)=4.57		
							K(Ba+BaHL)=2.0		

****

C31H46N2O6 L (2446)
Bicyclo-NcN'-1,10-Diaza-4,7,13,16-tetraoxaoctadecane;(c=(CH2.C6H4.O.C2H4)2.CH2)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	alc/w	25°C	93%	U		K1=2.45	1978WVa	(105551)1137

Medium: 93% MeOH/H2O

****

C32H30N2O8 H4L CAS 81374-97-2 (8216)
N,N'-[1,8-Naphthalenediylbis(3,1-phenylenemethylene)]bis[N-(carboxymethyl)]-glycine
;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KCl	25°C	0.10M	U		K1=2.7	1982LVa	(105588)1138

****

C32H30N2O8 H4L CAS 81374-96-1 (8215)
N,N'-[1,8-Naphthalenediylbis(4,1-phenylenemethylene)]bis[N-(carboxymethyl)]-glycine
;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KCl	25°C	0.10M	U		K1=3.4	1982LVa	(105593)1139

****

C32H32N2O12 H6L Cresolphthalexo CAS 2411-89-4 (1997)
o-Cresolphthalein-3,3'-bis(methyliminodiethanoic acid)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	oth/un	25°C	0.10M	U		K1=8.0	1981GMd	(105609)1140
							B(BaHL)=18.17		
							B(Ba2L)=11.65		
Ba++	gl	KCl	20°C	0.1M	U		K1=6.2	1954AGb	(105610)1141

K(Ba+HL)=4.8
K(Ba+H2L)=2.3
K(Ba+H3L)=1.3
K(Ba+BaL)=5.2
K(Ba+BaHL)=1
****
C32H37NO9S H4L SemiMeThymolBlu (427)
3-(N,N-Di(carboxymethyl)-aminomethyl)thymolsulfonephthalein;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ sp KNO3 25°C 0.10M U K1=4.54 1974YOa (105664)1142
B(BaHL)=13.41
****
C32H38N4O6Cl2 HL CAS 172033-56-6 (8675)
2,2'-[1,4,10,13-Tetraoxa-7,16-diazacyclooctadecane-7,16-diylbis(methylene)]bis[5-Cl
-8-quinolinol]

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ cal non-aq 25°C 100% C H K1=12.2 1995ZBa (105677)1143
K(Ba+HL)=12.2
Medium: methanol. DH(K)=-76.1 kJ mol-1, DS(K)=-22 J K-1 mol-1.
****
C32H38N4O6Cl2 H2L (7214)
7,16-Bis((5-chloro-8-hydroxy-7-quinolinyl)methyl)-1,4,10,13-tetraoxa-7,16-diazacycl
ooctadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ cal alc/w 25°C 100% U H 1996BBf (105689)1144
K(Ba+H2L)=3.60
Medium: MeOH; 0.1 M Me4NCl. DH(K)=-11.6 kJ mol-1. Data also for similar
lariat ligands with substituted oxine side chains
****
C32H40N4O4 L CAS 340963-90-8 (8926)
8,8'-[1,4,10,13-Tetraoxa-7,16-diazacyclooctadecane-7,16-diylbis(methylene)bisquinol
ine;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ cal alc/w 25°C 100% C H K1=6.73 2001DXa (105713)1145
Medium: MeOH. Method: competitive calorimetric titration.
DS(K1)=-63.8 J K-1 mol-1, DS(K1)=63.8 J K-1 mol-1.
****
C32H40N4O6 H2L CAS 254900-38-4 (8920)
7,16-Bis(8-hydroxyquinoline-2-ylmethyl)-1,4,10,13-tetraoxa-7,16-diazacyclooctadecan
e;

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

---
Ba++ cal alc/w 25°C 100% C H 1999SBg (105718)1146
K(Ba+H2L)=11.6
Medium: MeOH. DH(K)=-73.0 kJ mol-1, DS(K)=-23 J K-1 mol-1.
K and DH(K) determined by competitive calorimetric titration.
****
C32H40N4O8 H4L CAS 254900-32-8 (8918)
7,16-Bis(2,8-quinolinediol-7-ylmethyl)-1,4,10,13-tetraoxa-7,16-diazacyclooctadecane
;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ cal alc/w 25°C 100% C H 1999SBg (105725)1147
K(Ba+H4L)=3.57
Medium: MeOH. DH(K)=-29.4 kJ mol-1, DS(K)=-30 J K-1 mol-1.
****
C32H40N6O6Cl2 H2L CAS 254900-39-5 (8921)
7,16-Bis(3-(5-chloro-2-hydroxyphenyl)pyrazol-1-ylmethyl)-1,4,10,13-tetraoxa-7,16-di
azacyclooctad;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ cal alc/w 25°C 100% C H 1999SBg (105728)1148
K(Ba+H2L)=4.87
Medium: MeOH. DH(K)=-26.4 kJ mol-1, DS(K)=4.7 J K-1 mol-1.
****
C32H43N2O7S HL CAS 189057-31-6 (7756)
3-(4-Carboxybutyl)-2-[4-[N-(1,4,7,10,13-pentaoxa-16-azacyclooctadeca)]]styryl-benzo
thiazolium;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ sp non-aq 18°C 100% C K1=4.4 1997LHa (105755)1149
Medium: acetonitrile.
****
C32H46N2O8Cl2 L CAS 181706-75-2 (8626)
3,18-Dichlorododecahydro-5H,16H-6,15-(ethanoxyethanoxyethano)dibenzohexaoxadiazacyc
lohexacosine;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ cal non-aq 25°C 100% C H K1=4.01 1998ZBc (105785)1150
Medium: MeOH. DH(K1)=-19.0 kJ mol-1, DS(K1)=13.1 J K-1 mol-1.
****
C32H48N2O6 L (2447)
Bicyclo-NcN'-1,10-diaza-4,7,13,16-tetraoxaoctadecane;(c=(CH2.C6H4.O.C3H6)2)

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl alc/w 25°C 93% U K1=3.0 1978WVa (105801)1151

Medium: 93% MeOH/H2O
****
C32H58N2O12 H2L CAS 88454-81-3 (5409)
2,11-Bis(carboxy)-3,12-bis(octanylformamide)-18-crown-6 (anti);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	alc/w	25°C	90%	U		K1=9.5	1984FWa	(105836)1152

Medium: 90% v/v MeOH/H2O, 0.05 M R4NX
****
C32H58N2O12 H2L CAS 88454-82-4 (5408)
3,11-Bis-carboxy-2,12-bis(octanylformamide)-18-crown-6 (syn);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	alc/w	25°C	90%	U		K1=8.0 B(BaHL)=12.1	1984FWa	(105842)1153

Medium: 90% v/v MeOH/H2O, 0.05 M R4NX
****
C32H64N4O10 L CAS 42133-16-4 (8579)
4,10,13,19,25,28,33,36,41,44-Decaoxa-1,7,16,22-tetraazatricyclo[20.8.8.87,16]hexate
tracontane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	alc/w	25°C	90%	M		K1=6.7 K(BaL+Ba)=6.3	1977LSc	(105848)1154

Medium: 90% (w/w) MeOH/H2O, 0.1 M Et4NBr.
****
C32H66N2O4 L 22DD Kryptofix CAS 79495-97-9 (6655)
1,10-Didecyl-1,10-diaza-4,7,13,16-tetraoxacyclooctadecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	cal	alc/w	25°C	100%	U	H	K1=5.84	1985BUc	(105860)1155

Medium: MeOH, 0.05 M Et4NClO4. DH=-32.9 kJ mol-1
****
C33H39N11 L Pyr-cryptand CAS 141258-00-6 (7452)
1,4,12,15,18,26,31,39,42,43,44-Undecaazapentacyclo[13.13.13.1.1.1]tetratetetraconta
pentadecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	sp	non-aq	25°C	100%	U	H	K1=6.22	1996AAb	(105916)1156

Medium: CH3CN
.13.1(6,10).1(20,24).1(33,37)]tetratetraconta-4-6-8-10(44),11...pentadecaene
****
C33H41N3O6 L (8027)
Tripodal ionophore ;

```
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Ba++       sp  non-aq 25°C 100%  C                        2001LFa (105922)1157
                                        K(BaP+L=LiPL)=6.15
Method: Analyses by spectrophotometry. Medium: chloroform. P is picrate.
*************************************************************************
C34H42N2O4              L                    CAS 205743-21-1  (8942)
N,N'-Bis(1-naphthylmethyl)-1,4,10,13-tetraoxa-7,16-diazacyclooctadecane;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Ba++       con alc/w  25°C 100%  M   H    K1=2.45          2000BSe (106055)1158
Medium: MeOH. By calorimetry: DH(K1)=-21.8 kJ mol-1, DS(K1)=-26.5
J K-1 mol-1.
*************************************************************************
C34H42N2O6Cl2           L                    CAS 181706-79-6  (8629)
3,18-Dichlorooctahydro-5H,16H-6,15-(ethanoxyethanoxyethano)tribenzotetraoxadiazacyc
lodocosine;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Ba++       cal non-aq 25°C 100%  C   H    K1=4.03          1998ZBc (106056)1159
Medium: MeOH. DH(K1)=-4.80 kJ mol-1, DS(K1)=61.1 J K-1 mol-1.
*************************************************************************
C34H53O8Br            H2L                    CAS 38784-08-6  (2336)
5-Bromolasalocid;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Ba++       gl  alc/w  25°C 100%  M                        1988JTa (106096)1160
                                        K(Ba+HL)=6.62
                                        K(Ba+2HL)=5.8
Medium: MeOH
*************************************************************************
C34H54O8              H2L    Lasalocid      CAS 25999-20-6  (2335)
Lasalocid acid;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Ba++       nmr non-aq 20°C 100%  C                        1998MLa (106123)1161
                                        K(Ba+HL)=1.8
Medium: CD3OD. Method: 13C nmr.
-------------------------------------------------------------------------
Ba++       dis non-aq 25°C 100%  U                        1993LPa (106124)1162
                                        K(Ba+2HL=BaL2+2H)=-9.7
Method: extraction into CHCl3.  K is for Ba(aq)+2HL(org)=BaL2(org)+2H(aq).
-------------------------------------------------------------------------
Ba++       gl  alc/w  25°C 100%  M                        1988JTa (106125)1163
                                        K(Ba+HL)=6.74
                                        K(Ba+2HL)=8.8
```

Ba++ cal alc/w 25°C 100% U H 1988PPa (106126)1164
Medium: MeOH. DH(BaL)=5.9 kJ mol-1; DS=148. DH(BaL2)=13.3; DS=229

Ba++ gl alc/w 25°C 100% U 1982BDc (106127)1165
K(Ba+4HL)=6.58
Medium: MeOH
****
C34H64O10 H2L D218-6A2 CAS 88454-79-9 (5406)
11,12-Bis(dodecanyl)-1,2-bis(carboxy)-1,4,7,10,13,16-hexaoxacyclooctadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl alc/w 25°C 90% U K1=9.8 1984FWa (106177)1166
B(BaHL)=14.1
Medium: 90% v/v MeOH/H2O, 0.05 M R4NX
****
C35H45N9 L CAS 312304-65-7 (7962)
29,32,35-TriMe-1,14,29,32,35,38,39,40,41-Nonaazahexacyclohentetraconta-3,5,7,8,10,12,16,18,20,21,
---
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl R4N.X 25°C 0.10M U K1=6.56 2001BBa (106201)1167
K(BaL+H)=7.9
K(BaHL+H)=8.60
K(BaH2L+H)=6.00
Medium: 0.10 M NMe4NO3.
****
C36H36N24O12 L Cucurbituril CAS 283175-97-3 (6744)
Cucurbit[6]uril;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ cal mixed 25°C 50% C H K1=3.08 2000ZKb (106253)1168
Medium: 50% v/v formic acid/H2O. DH(K1)=-13.2 kJ mol-1, DS(K1)=15 J K-1 mol-1.

Ba++ cal mixed 25°C 50% C IH K1=2.83 1998BJb (106254)1169
Medium: 50% (v/v) HCOOH/H2O. DH(K1)=-17.4 kJ mol -1.
Also data for 0-40% (v/v). In H2O, K1=5.23, DH(K1)=-10.6 kJ mol-1.
****
C36H44O7P2 L (5725)
1,17-Di(diphenylphosphinyl))-3,6,9,12,15-pentaoxaseptadecane;
Ph2PO.C2H4(O.C2H4)4OC2H4POPh2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ cal non-aq 25°C 100% U K1=5.0 B2=7.0 1991SGa (106332)1170
Medium: CH3CN; Ba as Ba(NCS)2

****
C36H47N3O6 L (8028)
Tripodal ionophore 2;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ sp non-aq 25°C 100% C 2001LFa (106373)1171
K(BaP+L=LiPL)=5.77
Method: Analyses by spectrophotometry. Medium: chloroform. P is picrate.
****
C36H58N10O10S4 H5L CAS 136685-24-0 (6875)
(1-Cys-,1'-Cys,4-Cys-,4'-Cys)-dithiobis(Ac-1-Cys-Pro-D-Val-4-Cys-NH2);

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl non-aq 20°C 100% U K1=9.09 B2=16.21 1993EAa (106441)1172
Method: circular dichroism. Medium: MeCN, ClO4-
****
C36H62O11 HL Monensin CAS 17090-79-8 (737)
Monensin, 1,6-dioxaspiro[4,5]decane derivative;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ ISE alc/w 25°C 100% M K1=7.14 1984CTa (106490)1173
Medium: MeOH. In EtOH K1=9.9

Ba++ ISE non-aq 25°C 100% M K1=7.03 1984CTa (106491)1174
Medium: N,N-dimethylformamide. In DMSO K1=5.14
****
C37H44N2O13S H6L MeThymol Blue (428)
3,3'-Bis(N,N-di(carboxymethyl)aminomethyl)thymolsulfonephthalein;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ sp KNO3 25°C 0.10M U K1=6.93 1974YOa (106586)1175
B(BaHL)=18.03
B(BaH2L)=26.19
K(Ba+BaL=Ba2L)=4.65
K(Ba+BaHL=Ba2HL)=1.9
****
C40H36O4P2 HL CAS 126763-08-4 (7791)
1,2-Bis[2-(diphenylphophinylmethyl)phenoxy]-ethane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ EMF non-aq 25°C 100% C K1=8.57 1997PKc (106730)1176
Medium: nitrobenzene
****
C40H36O5P2 L CAS 86341-96-0 (5724)
1,7-Di(2-diphenylphosphinyl)phenyl-1,4,7-trioxaheptane;Ph2PO.C6H4.O.C2H4.O.C2H4.O.C

6H4.POPh2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	EMF	non-aq	25°C	100%	C		K1=11.36	1997PKc (106742)	1177

Medium: nitrobenzene

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	EMF	non-aq	25°C	100%	C		K1=8.91 B2=13.42	1997PKc (106743)	1178

Medium: nitrobenzene

****

C40H50N20O10 L CAS 143902-45-8 (8935)

Decamethylcucurbit[5]uril;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	cal	mixed	25°C	50%	C	IH	K1=3.02	2000ZKb (106804)	1179

Medium: 50% v/v formic acid/H2O. DH(K1)=-37.4 kJ mol-1, DS(K1)=-67.8 J K-1 mol-1. By potentiometry in aqueous 0.05 M Et4NCl, K1=<2.

****

C40H64O12 L Nonactin CAS 6833-84-7 (4179)

Nonactin

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	oth	alc/w	30°C	100%	U		K1=1.61	1973ZFa (106837)	1180

Method: vapour pressure osmometry. Medium:MeOH. In EtOH, K1=2.30

****

C41H66O12 L Monactin CAS 7182-54-9 (4180)

Monactin

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	oth	alc/w	30°C	100%	U		K1=2.18	1973ZFa (106884)	1181

Method: vapour pressure osmometry. Medium:MeOH. In EtOH, K1=2.32

****

C42H40O5P2 L CAS 163172-12-6 (2080)

Bis((2-diphenylphosphinylmethyl)phenyl)diethyleneglycol ether;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	EMF	non-aq	25°C	100%	C		K1=7.07	1997PKc (106922)	1182

Medium: nitrobenzene

****

C42H52N4O6 L CAS 405917-44-4 (9250)

Tetraoxadiazacyclooctadecane-7,16-diylbis(methylene)bis-methyl-4-pyridinylidenecyclohexadienone;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	sp	R4N.X	25°C	0.10M	C			2004COa (106961)	1183

K(Ba+H2L=BaL+2H)=>15.30
Medium: buffered 0.1 M Et4NCl, pH 8.5.
****
C42H68N2O4 L CAS 188593-77-3 (8954)
2,17-Didodecyl-6,7,9,10,12,13-hexahydro-dibenzo[b,f][1,8,11,14,4,5]tetraoxadiazacyclohexadecine
---
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ sp non-aq RT 100% C I K1=5.3 2000GDa (106972)1184
Medium: acetonitrile. In MeOH, K1=1.95.
****
C42H68O12 L CAS 20261-85-2 (5373)
Dinactin;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ oth alc/w 30°C 100% U K1=2.08 1973ZFa (106977)1185
Method: vapour pressure osmometry. Medium: MeOH
****
C44H44O6P2 L CAS 126763-09-5 (7790)
1,8-Bis[2-(diphenylphosphinylmethyl)phenoxy]-3,6-dioxaoctane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ EMF non-aq 25°C 100% C K1=8.00 1997PKc (107126)1186
Medium: nitrobenzene
****
C44H48O10 L CAS 155500-94-0 (7357)
5,17-Di-tert-butyl-26,28-bis(carboethoxymethoxy)calix[4]diquinone;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ sp non-aq 23°C 100% U K1=5.7 1997BGa (107131)1187
Medium: 4/1 v/v CH2Cl2/CH3CN; 0.1 M Bu4NBF4
Data also for other related calix[4]diquinones
****
C44H50N2O10 H2L CAS 329183-28-0 (8807)
25,27-Bis(carboxymethoxy)-26,28-bis[(N,N-diethylaminocarbonyl)methoxy]calix[4]arene
;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl non-aq 25°C 100% C K1=8.95 B2=14.12 2000ABb (107141)1188
B(BaHL2)=23.63
B(Ba2HL2)=28.61
Medium: MeOH, 0.05 M Et4NClO4.
****
C44H52N4O8 L CAS 246035-33-6 (2925)
25,27-Bis(N,N-diethylaminocarbonylmethoxy)-26,28-bis(aminocarbonylmethoxy)calix[4]a

rene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ sp non-aq 25°C 100% C K1=2.5 1999USa (107156)1189
Medium: MeOH, 0.10 M Et4NCl
****
C44H72N4O8 L CAS 61894-23-3 (8580)
7,16:25,34-Bis(ethanoxyethanoxyethano)dibenzo[1,4,17,20,7,14,23,30]tetraoxatetraaza
cyclodotriac..

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl alc/w 25°C 90% M K1=5.9 1977LSc (107192)1190
K(BaL+Ba)=6
Medium: 90% (w/w) MeOH/H2O, 0.1 M Et4NBr. In H2O, K1=4.4.
****
C46H46N2O4 L CAS 185118-12-1 (7824)
N,N'-Bis(1-pyrenylmethyl)-1,4,10,13-tetraoxa-7,16-diazacyclooctadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ sp mixed 25°C 90% C 1997KKa (107247)1191
K(Ba(SCN)2+L)=2.15
Method: fluorescence emission. Medium: MeOH/CHCl3 (9:1 v/v).
****
C46H48O8P2 L CAS 119494-80-3 (7785)
1,14-Bis[2-(diphenylphosphinyl)phenoxy]-3,6,9,12-tetraoxatetradecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ EMF non-aq 25°C 100% C K1=8.57 1997PKc (107276)1192
Medium: nitrobenzene
****
C46H58O6 HL (6716)
Calix[4]arene-O(1)-ethanoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl alc/w 25°C 100% C K1=7.0 1993ABb (107295)1193
B(BaHL)=19.6
B(BaH2L)=31.8
B(BaH3L)=41.4
Medium: MeOH, 0.01 M Et4NClO4. Data also for tert-butyl and ethyl esters
****
C48H52O8P2 L CAS 126763-11-9 (7786)
1,14-Bis[2-(diphenylphosphinylmethyl)phenoxy]-3,6,9,12-tetraoxatetradecane;

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

Ba++ EMF non-aq 25°C 100% C K1=12.50 1997PKc (107370)1194
Medium: nitrobenzene
****
C48H52O9P2 L CAS 198490-22-1 (7788)
1,17-Bis[2-(diphenylphosphinyl)phenoxy]-3,6,9,12,15-pentaoxaheptadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ EMF non-aq 25°C 100% C K1=15.29 1997PKc (107374)1195
Medium: nitrobenzene
****
C48H60O8 H2L R-Bu-Calixarene CAS 147513-53-9 (6705)
4-tert-Butylcalix[4]arenedicarboxylic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl alc/w 25°C 100% C K1=8.3 1993ABb (107399)1196
B(Ba2L)=11.58
Medium: MeOH, 0.01 M Et4NClO4. Data also for di-tert-butyl ester
****
C48H64O4 L CAS 105880-81-7 (8677)
tert-Butylcalix-4-arene tetramethyl ether;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ sp non-aq 25°C 100% C K1=3.28 2004BCb (107420)1197
Medium: acetonitrile, 0.01 M Et4NClO4.
****
C50H56O9P2 L CAS 198490-23-2 (7787)
1,17-Bis[2-(diphenylphosphinylmethyl)phenoxy]-3,6,9,12,15-pentaoxaheptadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ EMF non-aq 25°C 100% C K1=13.93 1997PKc (107454)1198
Medium: nitrobenzene
****
C52H64O12 H4L R-Bu-Calixarene CAS 113215-72-8 (6704)
5,11,17,23-Tetra-(t-butyl)-25,26,27,28-tetrakis[(hydroxycarbonyl)methoxy]calix[4]ar
ene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl alc/w 25°C 100% C K1=17.96 1993ABb (107487)1199
B(BaHL)=26.26
B(BaH2L)=33.53
In methanol; 0.01 M (CH3CH2)4NClO4
****
C52H68N4O8 CAS 150588-24-2 (3074)
25,26,27,28-Tetrakis-(N,N-diethylaminocarbonylmethoxy)calix[4]arene; L

```
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Ba++       EMF non-aq 25°C 100%  C   H    K1=6.53        1999USa (107497)1200
Medium: MeOH, 0.10 M Et4NCl.  Method: by competition with Ag+.
DH(K1)=-8.2 kJ mol-1
*************************************************************************
C52H68N4O8              L                        (4823)
25,27-Bis(N,N-diethylaminocarbonylmethoxy)-26,28-bis(N-butylaminocarbonylmethoxy)ca
lix[4]arene;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Ba++       sp  non-aq 25°C 100%  C        K1=<1          1999USa (107505)1201
Medium: MeOH, 0.10 M Et4NCl
*************************************************************************
C52H69N3O6            H2L                     CAS 136158-03-7  (9132)
Tetra-t-butyl-calix[4]azacrown dione;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Ba++       sp  non-aq 20°C 100%  C        K1=3.03        2003OAa (107522)1202
Medium: 100% acetonitrile, 0.01 M Et4NClO4.
*************************************************************************
C54H90N6O18             L    Valinomycin      CAS 2001-95-8  (2142)
Valinomycin, Potassium Ionophore
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Ba++       cal alc/w  25°C 100%  U        K1=3.34        1977ILa (107546)1203
Medium: MeOH
*************************************************************************
C56H80O8                L                        (9259)
5,11,17,23-Tetra(t-butyl)-25,26,27,28-tetramethoxyethoxycalix[4]arene;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Ba++       sp  non-aq 25°C 100%  C        K1=5.09        2004BCb (107612)1204
Medium: acetonitrile, 0.01 M Et4NClO4.
*************************************************************************
C58H78O11              HL                     CAS 465527-74-6  (9287)
7,13,19,25-Tetra-t-butyl-28-methoxy-27,29,30-triethylacetate-2,3-dihomo-3-oxacalix[
4]arene;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Ba++       sp  alc/w  25°C 100%  C        K1=3.2         2001MAa (107620)1205
Medium: MeOH, 0.01 M Et4NCl.
*************************************************************************
C58H80O10               L                        (9264)
5,11,17,23-Tetra-t-butyl-25,27-di(2-methoxyethoxy)-26,28-di(ethylacetate)calix[4]ar
```

ene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ sp non-aq 25°C 100% C B2=4.94 2004BCb (107629)1206
Medium: acetonitrile, 0.01 M Et4NClO4.
****
C60H82N2O10 L CAS 155377-20-1 (8806)
5,11,17,23-Tetra-butyl-25,27-bis(carboxymethoxy)-bis[(N,N-diethylaminocarbonyl)meth
oxy]calix[4]ar

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl non-aq 25°C 100% C K1=9.6 B2=16.38 2000ABb (107664)1207
B(BaHL2)=25.23
Medium: MeOH, 0.05 M Et4NClO4.
****
C60H84N4O8 L (8174)
25,26,27,28-Tetrakis-(N-ethylaminocarbonylmethoxy)calix[4]arene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ sp alc/w 25°C 100% U H K1=3.2 2000ABa (107672)1208
Medium: 100% MeOH, DH(K1)=-10.1 kJ mol-1 by colorimetry
****
C60H84N4O8 L CAS 246035-32-5 (2735)
25,27-Bis(N,N-diethylaminocarbonylmethoxy)-26,28-bis(aminocarbonylmethoxy)-t-butylc
alix[4]arene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ sp non-aq 25°C 100% C K1=3.3 1999USa (107677)1209
Medium: MeOH, 0.10 M Et4NCl
****
C62H84O14 L CAS 135581-11-2 (8630)
9,23-Dioxpentacyclo[23.3.1.13,7.111.15.117.21]dotriacontane, ethanoic acid
derivative;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ sp non-aq 25°C 100% C K1=>6 1991ACc (107691)1210
Medium: acetonitrile, 0.01 M Et4NClO4.
****
C64H80O6 L (9262)
5,11,17,23-Tetra-t-butyl-25,27-di(phenylmethoxy)-26,28-di(2-methoxyethoxy)-calix[4]
arene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ sp non-aq 25°C 100% C K1=3.11 2004BCb (107760)1211

Medium: acetonitrile, 0.01 M Et4NClO4.
****
C66H80O8 L (9261)
5,11,17,23-Tetra(t-butyl)-25,27-diethoxycarbonylmethoxy-26,28-diphenylmethoxycalix[4]arene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ sp non-aq 25°C 100% C K1=2.74 2004BCb (107775)1212
Medium: acetonitrile, 0.01 M Et4NClO4.
****
C68H100N4O8 L CAS 246035-35-8 (3034)
25,27-Bis(N,N-diethylaminocarbonylmethoxy)-26,28-bis(N-butylaminocarbonylmethoxy)-t-butylcalix[4]

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ sp non-aq 25°C 100% C K1=3.7 1999USa (107802)1213
Medium: MeOH, 0.10 M Et4NCl
****
C68H100N4O8 L CAS 114155-16-7 (7183)
4-tert-Butylcalix[4]arene tetradiethylacetamide;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ cal alc/w 25°C 100% U H 1995ABc (107810)1214
Medium: 100% Methanol. DH(K1)=2.5 kJ mol-1, DS(K1)=144 J K-1 mol-1.
****
C69H102N4O9 L CAS 116352-85-3 (9286)
para-t-Butyldihomooxacalix[4]arene tetra(diethyl)amide;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ sp alc/w 25°C 100% C K1=4.4 2004MFa (107831)1215
Medium: MeOH, 0.01 M Et4NCl.
****
C77H82O9 L CAS 253317-20-3 (9288)
p-Tert-butyldihomooxacalix[4]arene tetraphenyketone;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ sp alc/w 25°C 100% C K1=4.9 1999MAb (107891)1216
Medium: MeOH, 0.01 M Et4NCl.
****
C96H144O24 L CAS 169888-22-6 (7534)
C-Undecylcalix[4]resorcinarene octa-alpha-(methyl ethanoate);

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ dis non-aq 25°C 100% U 1995FDa (107962)1217

K=5.13
Medium: CDCl3. Method: by H2O/CDCl3 extraction of picrate salt.
K: MA(org)+L(org)=MLA(org) where A=picrate.
****
C102H174N6O73 L CAS 571203-64-0 (9253)
4,13-Bis(2-(6-deoxy-b-cyclodextrin-6-yl)aminoethylamidomethyl)-4,13-diazatrioxacycl
opentadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl R4N.X 25°C 0.10M C K1=4.47 2003WWa (107972)1218
K(Ba+HL)=3.81
K(Ba+H2L)=3.04
Medium: 0.10 M Et4NClO4.
****
C114H198N6O73 L CAS 571203-66-2 (9254)
4,13-Bis(8-(6-deoxy-beta-cyclodextrin-6-yl)aminooctylamidomethyl)-4,13-diazatrioxac
yclopentadecan

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ gl R4N.X 25°C 0.10M C K1=4.82 2003WWa (107999)1219
K(Ba+HL)=4.54
K(Ba+H2L)=4.10
Medium: 0.10 M Et4NClO4.
****
C120H192O24 L CAS 175349-58-3 (7495)
C-Undecylcalix[4]resorcinarene octa-alpha-(tert-butyl ethanoate);

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ dis non-aq 25°C 100% U 1995FDa (108005)1220
K=5.34
Medium: CDCl3. Method: by H2O/CDCl3 extraction of picrate salt.
K: MA(org)+L(org)=MLA(org) where A=picrate.
****
C120H200N8O16 L CAS 169888-21-5 (7490)
C-Undecylcalix[4]resorcinarene octa-alpha-(N,N-diethyl acetamide);

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Ba++ dis non-aq 25°C 100% U 1995FDa (108016)1221
K=8.75
Medium: CDCl3. Method: by H2O/CDCl3 extraction of picrate salt.
K: MA(org)+L(org)=MLA(org) where A=picrate.
****
Polymer H2L X-14885A (4547)
Antibiotic X14885A, calcium ionophore

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

```
--------------------------------------------------------------------------------
Ba++       gl  alc/w  25°C 100%  U        K1=5.8         1989ABb (108074)1222
Medium: MeOH
********************************************************************************
Polymer                                              (5379)
Dextran derivative of N-propyliminodiethanoic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Ba++       gl  oth/un 20°C 0.10M U        K1=1.40        1968VGa (108162)1223
********************************************************************************
Polymer                                              (4199)
Polystyrene (54 mole %) and maleic anhydride copolymer
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Ba++       gl  KNO3   25°C  1.0M U                        1954MKa (108378)1224
                                          K'=1.36
See reference for definitions. Also data for Ca, Mg, Sr
********************************************************************************
Polymer                                              (4201)
Polyvinylethylether (62% mole %) and maleic anhydride copolymer
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Ba++       gl  KNO3   25°C  1.0M U                        1954MKa (108383)1225
                                          K'=2.00
See reference for definitions. Data also for Ca, Mg, Sr
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EXPLANATORY NOTES

DATA Flags are :-

T Data at other TEMPERATURES
I Data with various BACKGROUNDS
H Data for THERMOCHEMICAL quantities
M Data for TERNARY Complexes

EVALUATION Flags are :-

T or IUP=T signifies EVALUATION RATING = Tentative by IUPAC
R or IUP=R signifies EVALUATION RATING = Recommended by IUPAC

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