

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										

AsW11039----- 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

B04H4- 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+H2B03)=1.49										

Calculated from data for 0.02-0.16 M BaCl2. Data for 10-50 C.

DH(Ba+H2B03)=3.1 kJ mol-1, DS=39 J K-1 mol-1.

C03-- 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		1984MTb (3145)	7
							$K(\text{BaL(s)}=\text{Ba}+\text{L})=-6.87$		
							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			1973BSd (3146)	8
							Kso=-5.48		
Ba++	EMF	none	30°C	0.0	U			1969GSb (3147)	9
							Kso=ca.-8.1(resin membrane electrode)		
Ba++	gl	none	25°C	0.0	U			1969NRa (3148)	10
							$K(\text{Ba}+\text{HL})=1.52$		
Ba++	sol	oth/un	25°C	0.0	U			1968BBf (3149)	11
							Kso=-9.40		
Ba++	oth	none	25°C	0.0	U	T		1968KRa (3150)	12
							Kso=-8.25		
							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			1946NAa (3151)	13
							Kso(BaCO3(s))=-8.29		
							Method: H electrode. I=0 corr.		
Ba++	sol	oth/un	25°C	0.0	U	T		1939HJa (3152)	14
							Kso=-8.69		
							Medium: 0 corr. Kso=-8.56(40 C)		
Ba++	sol	none	25°C	0.0	U	T		1937TWa (3153)	15
							$K(\text{BaCO}_3(\text{s})=\text{Ba}+\text{CO}_3)=-9.26$		
							Extrapolated to zero ionic strength. T: 25-40C. At 40C, K=-9.53		
Ba++	sol	none	25°C	0.0	U			1935KAa (3154)	16
							Kso(BaCO3(s))=-8.31		
							+Kpso=-5.82		
							I=0 corr. +Kpso: $\text{BaCO}_3(\text{s})+\text{CO}_2(\text{g})+\text{H}_2\text{O}=\text{Ba}+2\text{HCO}_3$		
Ba++	oth	none	rt	0.0	U			1926HBa (3155)	17
							Kso(BaCO3(s))=-7.77		
							Method: tyndallometry. I=0 corr.		
Ba++	sol	none	16°C	0.0	U			1915JOa (3156)	18
							Kso(BaCO3(s))=-8.15		
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
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C6O3 L Benzenetrioxyde CAS 264911-91-3 (6002)

cis-Benzenetrioxyde;

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	KN03	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	NaN03	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	1990D0d (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 1963K0d (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 1951K0a (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 1923B0a (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 Kso(BaF2)=-5.98 1950TKa (6766) 59

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

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 Kso(BaL2(s))=-7.76 1974FRf (8493) 64

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), -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;

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Ba++      gl  R4N.X  25°C 5.00M U      K1=-0.15      1985MMa (9097) 74
*****
NO3-      HL      Nitrate      CAS 7697-37-2 (288)
Nitrate;
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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      1963VWa (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;
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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      1956BP a (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
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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		1923K0a (11022)	89
Medium: BaCl2 at various concentrations; method:colorimetry										

P04---			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	1995P0a (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			

PW11039-----			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		1984C0a (13400)	96

P207----			H4L	Pyrophosphate			CAS 2466-09-3	(198)		
Diphosphate; from (HO)2PO.O.PO(OH)2										

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

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

P3010-----			H5L				CAS 10380-08-2	(1001)		
Triphosphate; from (HO)2PO.O.PO(OH).O.PO(OH)2										

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ba++	oth	none	25°C	0	U			Kso(BaS)=-1.1 *Kso(BaS)=16.2	1988LIa (14323)	109
Derived from thermodynamic data and K(H+S=HS)=17.3. *****										
S04--		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 Kso(BaS04)=-10.02 (barite)	1998PKb (16001)	110
Solubility of BaS04 (labelled with 133Ba) in H2S04 (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										
Ba++	sol	none	RT	0.0	C I			K1=2.72 Kso(BaS04)=-10.05	1990FRa (16002)	111
Method: ICP spectroscopy. Calculated from data for 0.001-0.10 M Na2S04 BaS04 is barite.										
Ba++	sol	none	25°C	0.0	C			Kso(BaS04)=-10.008	1988MGb (16003)	112
Method: analysis of literature solubility data, using Pitzer parameters. SrS04 is barite.										
Ba++	oth	none	25°C	0.0	C TIH			Kso(BaS04)=-9.959	1988RAa (16004)	113
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.										
Ba++	sol	none	25°C	0.0	C TIH			Kso(BaS04)=-9.98 (1 bar)	1977BLa (16005)	114
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.										
Ba++	ISE	oth/un	30°C	0.0	U			Kso=-9.7 (resin membrane electrode)	1969GSb (16006)	115
Ba++	sol	oth/un	25°C	0.0	U T			Kso=-9.72	1969MUa (16007)	116
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										
Ba++	dis	NaCl04	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 1893KR a (16023) 132

Kso(BaL)=-9.92

S203-- 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
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K1=2.28(35 C)

Se03-- 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			1968RVa (17040)	135

Kso=-5.21

Ba++	sol	oth/un	25°C	0.0	U			1965LSb (17041)	136
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Kso=-6.57

Medium:0 corr. In dilute solution: Kso=-6.37

Se04-- 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			1958SSa (17099)	138
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Kso(BaL)=-7.46
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			1953SKa (17100)	139
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Kso=-7.30

Si03-- H2L Silicate CAS 7699-41-4 (747)
Silicate; Si02(OH)2--

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

K(Ba(OH)HL(s)=BaOH+HL)=-4.93

Te04-- H2L Tellurate (5750)
Tellurate(VI); Te04-- or Te02(OH)4--

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	sol	oth/un	20°C	var	U		Kso=-12.5 Kso(3Ba+TeO6)=-14.0	1970KBd (17306)	141

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 K(Ba+HL)=1.42 K(BaL+H)=6.26	1994SCa (17700)	147

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 acid 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 NaCl04 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 NaCl04 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)₂SO

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

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
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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	KN03	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	NaN03	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	KN03	25°C	0.10M	U		K1=3.35 K(Ba+HL)=2.72	1980ZRC (23359)	178

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	NaN03	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	1976K0a (24391)	180

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

Ba++	gl	NaCl04	25°C	0.10M	U	K1=1.22	19680Va (24392)	181
Ba++	gl	NaCl04	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	NaCl04	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; HOOCH(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

Ba++	sol	NaCl04	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
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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)
						K(BaL+H)=9.72	208	

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; H00C.CH:CH.COOH			

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
<hr/>									
Ba++	sp	none	25°C	0.0	U		K1=2.35	1976K0a (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; H00C.CH:CH.COOH							

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
<hr/>									
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
<hr/>									
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
<hr/>									
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; H00C.CH2.CH2.COOH			

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
<hr/>									
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.

Ba++	ix	oth/un	25°C	0.16M	U	K1=1.21	1954SCa (29936)	216
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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; HOOCH(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	19680Va (30115)	221

C4H6O5 H2L Malic acid CAS 617-48-1 (393)

2-Hydroxybutane-1,4-dioic acid, Hydroxy-succinic acid; HOOCH2CH(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
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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; HOOCH2OCH2COOH

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 acid CAS 133-37-9 (94)

DL-Tartaric acid,DL-2,3-Dihydroxybutanedioic acid; HOOCH(OH).CH(OH).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	NaCl04	25°C	1.00M	M		K(Ba+H2L+(ascorbate))=3.91	1988M0a (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									
Ba++	gl	NaCl04	37°C	0.20M	U		K1=2.19	1967TTb (31201)	231
Ba++	dis	NaCl04	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	1946J0a (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	1938CKa (31206)	236
K(Ba+HL)=0.88									

C4H7NO4		H2L		Aspartic acid		CAS 56-84-8	(21)		
Aminobutanedioic acid; H2N.CH(CH2.COOH).COOH									
Ba++	gl	NaNO3	25°C	0.10M	C	M	K1=3.75	2000KAb (31817)	237
K(BaA+L)=3.93									
B(BaAL)=7.53									
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									
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	NaCl04	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	NaCl04	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 B3=1.69 B4=1.85	1990NKa (33761)	248

Medium: propylene carbonate, 0.01 M Et₄NC104.

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	NaCl04	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				

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)

C4H11N08P2 H5L CAS 2439-99-8 (2129)
N-Carboxymethyl-N,N-bis(methylenephosphonic acid); $\text{HOOC.CH}_2.\text{N}(\text{CH}_2.\text{PO}_3\text{H}_2)_2$

Ba++	gl	KN03	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; C4H9.0.PO(OH)2

Ba++	gl	NaNO3	25°C	0.10M	C	K1=1.22	1988MSa	(35286)	252
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C4H12O6P2 H4L CAS 4071-77-6 (3592)
Butane-1,4-diphosphonic acid; H2O3P.CH2.CH2.CH2.CH2.PO3H2

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;

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				

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 Kso=-8.28	1965CDa (35937)	256

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					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					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					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; H00C.C(CH3)2.C00H

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

Ba++ gl NaClO4 25°C 0.10M U K1=1.35 19680Va (38208) 271

 C5H8O4 H2L CAS 601-75-2 (479)
 Ethylpropanedioic acid; H00C.CH(C2H5).C00H

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

Ba++ sp none 25°C 0.0 U T K1=2.26 1976K0a (38236) 272
Also data at 15,30,35 C. Determined colourimetrically

Ba++ gl NaClO4 25°C 0.10M U K1=1.39 19680Va (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
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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
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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
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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
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Ba++ gl KNO3 25°C 0.10M C K1=5.61 2000SDa (39667) 282
K(BaL+H)=7.36

$$K(\text{BaHL}+\text{H})=4.7$$

Ba++ gl KCl 30°C 0.10M U K1=5.1 19580Mb (39668) 283

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

Method: H electrode

C5H1002 HL n-Valeric acid CAS 109-52-4 (3027)
Pentanoic acid; $\text{CH}_3(\text{CH}_2)_3\text{COOH}$

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

C5H1002 HL Pivalic acid CAS 75-98-9 (3026)
Trimethylethanoic acid, 2,2-Dimethylpropanoic acid; $(\text{CH}_3)_3\text{C.COOH}$

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

C5H1005 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

C5H11N02 HL Nor-Valine CAS 760-78-1 (689)
2-Aminopentanoic acid; $\text{CH}_3.\text{CH}_2.\text{CH}_2.\text{CH}(\text{NH}_2).\text{COOH}$

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.

C5H1108P 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

C5H13N07P2 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 K(Ba+HL)=2.36	1983LSa (41754)	290

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 K(Ba+HL)=2.22 K(Ba+BaL)=1.97	1983LSa (41758)	291

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 K(Ba+HL)=2.96	1975SLa (41837)	292

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
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C6H5NO2 HL Picolinic acid CAS 98-98-6 (391)
2-Pyridine-carboxylic acid; C5H4N.CO0H

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
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Ba++	gl	NaNO3	25°C	0.10M	U		K1=2.4	1957SYb (42501)	297
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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					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-Trihydro-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					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		

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*****
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      Tricarballic 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
-----

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Ba++ gl NaClO4 25°C 1.00M M M 1988M0a (45626) 312
K(Ba+H2L+(tartrate))=3.91

Ba++ gl NaClO4 20°C 1.00M M 1983M0a (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; HOOCCCH2.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 1964C0b (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 1946J0a (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									
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									
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									
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									
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; HOO.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	1976K0a (48024)	331

C6H10O4			H2L	Adipic acid			CAS 124-04-9	(401)	
1,6-Hexanedioic acid; HOO.C(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; HOO.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
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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
-------	-----	--------	------	------	-----	-------	-------------	-----------	--------

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-----
Ba++      gl  KNO3   25°C 0.10M C      K1=6.29      1999D0a (51825) 347
              K(BaL+H)=9.57
              K(BaHL+H)=8.32
              K(BaH2L+H)=6.47
              K(BaH3L+H)=4.4

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

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

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```

Ba++      gl  KNO3   25°C 0.10M C      K1=3.12      1999D0a (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

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

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```

Ba++      gl  KNO3   25°C 0.10M C      K1=3.37      1999D0a (51969) 349
              K(BaL+H)=11.07
              K(BaHL+H)=7.8

```

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

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

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Ba++      ISE non-aq 25°C 100% M      K1=3.20      B2=4.49      1988NHa (51978) 350
Medium: MeCN, 0.01 M Et4NClO4

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C6H20N2O12P4      H8L      EDTPA      CAS 1429-50-1 (434)
Ethane-1,2-bis(iminobis(methylenephosphonic acid)); ((H2O3PCH2)2NCH2.)2

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

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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

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

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

```

$$K(\text{BaH}_3\text{L}+\text{H})=6.25$$
$$K(\text{Ba}+\text{H3L})=3.53$$

2,3,5,6-Tetrachloro-1,4-benzoquinone;

$$K(\text{Ba}(\text{SCN})_2 + \text{L}) = 4.48$$

4-Chloropyridine-2,6-dicarboxylic acid; Cl.C₅H₂N(COOH)₂

2,3-Pyridinedicarboxylic acid; $C_5H_3N.(COOH)_2$

2,4-Pyridinedicarboxylic acid; $C_5H_3N.(COOH)_2$

2,6-Pyridinedicarboxylic acid; $C_5H_3N.(COOH)_2$

By ion exchange: $K_2=0.5$

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;									


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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);
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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
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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
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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
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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
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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;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
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Ba++       gl  KCl     25°C 0.10M U        K1=5.16         1969DMd (56939) 384
                        K(Ba+HL)=4.36
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C7H12N2O5 H2L Gly-Glu CAS 7412-78-4 (280)
Glycyl-glutamic acid; H2N.CH2.CO.NH.CH(CH2.CH2.COOH).COOH

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

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

C7H12O4 H2L CAS 534-59-8 (480)
Butylpropanedioic acid (Butylmalonic acid); $\text{HOOC} \cdot \text{CH}(\text{C}_4\text{H}_9) \cdot \text{COOH}$

C7H12O4 H2L CAS 510-20-3 (482)
Diethylpropanedioic acid (Diethylmalonic acid); H00C.C(C2H5)2.C00H

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

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									

Ba++	sp	non-aq	20°C	100%	U		K1=4.46	1992PSa (58489)	396
Medium: DMF, 0.01 M Me4NI									

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).									

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-Thenoylacetone CAS 3151-27-2 (3224)
2-Thenoylacetone, 1-(2'-Thienyl)butane-1,3-dione; C4H3S.CO.CH2.CO.CH3

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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
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ba++       gl  alc/w  25°C 100%  M          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
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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;
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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;
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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
-----
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
-----
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
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 C8H12N2O8 H4L CAS 35039-85-1 (4537)
 1,2-Diaminoethane-N,N'-dimalononic 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
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 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
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 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; HOOCC(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; H₂OC.CH₂.C₄H₈N₂.CH₂.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	cal	NaClO ₄	25°C	0.10M	U	H	K ₁ =1.4	1985EHa (61945)	435
DH(K ₁)=1.8 kJ mol ⁻¹ , DS=33.3 J K ⁻¹ mol ⁻¹									

Ba++	EMF	KCl	20°C	0.10M	U		K ₁ =1.6	1963IPb (61946)	436
Method: H electrode									

 C8H14O7 H2L (241)
 Di(carboxymethoxy)ethyl ether; (H₂OC.CH₂.O.CH₂.CH₂)₂O

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	gl	KNO ₃	25°C	0.10M	U		K ₁ =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	KNO ₃	25°C	0.10M	C		K ₁ =2.66	1993WLa (62527)	438
Ba++	cal	NaClO ₄	25°C	0.10M	U	H	K ₁ =2.5	1983EHa (62528)	439
DH ₁ =-3.8 kJ mol ⁻¹ , DS ₁ =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		K ₁ =2.3	1972DKa (62584)	440
Ba++	gl	KNO ₃	20°C	0.10M	U		K ₁ =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	K ₂ =2.39	1992BCf (62659)	442
Medium: MeOH. DH(K ₂)=-6.3 kJ mol ⁻¹ , DS(K ₂)=25 J K ⁻¹ mol ⁻¹ .									

Ba++	cal	alc/w	25°C	100%	U	H T	K ₁ =2.56	1987BUa (62660)	443
Medium: MeOH. DH(K ₁)=-21.4 kJ mol ⁻¹ ; DS=-23 J K ⁻¹ mol ⁻¹ ; DH(B ₂)=-27.3									

Ba++	cal	non-aq	25°C	100%	C	H	K ₂ =<2	1986BUe (62661)	444
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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
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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-Cyclopentanetetra-carboxylic 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; HOOCH.N(CH2COOH)2CH2CH2COOH										

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										

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
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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	1976K0a (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 K(Ba+HL)=2.16	1984KMa (68311)	489

Ba++	gl	oth/un	25°C	1.00M	U		K1=4.37 K(Ba+HL)=2.16	1982PSc (68312)	490
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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									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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	NaClO ₄	25°C	0.10M	U			K ₁ =2.0	1968SMb (70845)	501

C ₁₀ H ₁₁ N ₀₄			H ₂ L					CAS 1137-73-1	(2567)	
N-Phenyliminodiethanoic acid; C ₆ H ₅ .N(CH ₂ .COOH) ₂										

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

C ₁₀ H ₁₁ N ₀₅			H ₃ L					CAS 100844-86-8	(2108)	
N-(2-Hydroxyphenyl)iminodiethanoic acid; HO.C ₆ H ₄ .N(CH ₂ .COOH) ₂										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ba++	gl	KN ₀₃	20°C	0.10M	U			K ₁ =4.27 K(Ba+HL)=2.50	1963IFb (71038)	503

C ₁₀ H ₁₁ N _{07S}			H ₃ L					(3335)		
N-(2-Sulfophenyl)iminodiethanoic acid; HO ₃ S.C ₆ H ₄ .N(CH ₂ .COOH) ₂										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ba++	EMF	KCl	20°C	0.10M	C			K ₁ =3.48	1947SWa (71066)	504
Method: H electrode										

C ₁₀ H ₁₂ N ₂ O ₂			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		K ₁ =3.00 B ₂ = 4.78 K(BaL+A)=2.73 K(BaL+en)=5.31 K(BaL+pro)=2.02 K(BaL+B)=2.51	1995RRe (71194)	505
Medium: 40% v/v EtOH/H ₂ O, 0.10 M KN ₀₃ . K(BaL+ala)=1.47, K(BaL+gly)=0.65. H ₂ A is catechol, HB is hydroxyproline.										

Ba++	gl	alc/w	30°C	40%	M	M		K(Ba(phe)+L)=2.68 K(BaA+L)=1.50	1995RRe (71195)	506
Medium: 40% v/v EtOH/H ₂ O, 0.10 M KN ₀₃ . H ₂ A is salicylic acid.										

C ₁₀ H ₁₂ N ₂ O ₄			H ₂ L					CAS 16598-05-3	(967)	
2-Pyridylmethyliminodiethanoic acid; C ₅ H ₄ N.CH ₂ .N(CH ₂ .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-ribose 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				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-ribose;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Ba++	nmr	non-aq	21°C	100%	U			1973SFa (72008)	515
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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
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Ba++	gl	NaNO3	25°C	0.10M	M		K1=0.99	1997SSg (72152)	516
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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
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Ba++	gl	R4N.X	25°C	0.10M	C	T	K1=1.76	1991SMa (72184)	517
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IUPAC evaluation

Ba++	gl	NaNO3	25°C	0.10M	U		K1=1.12	1989MSf (72185)	518
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Ba++	gl	KNO3	40°C	0.10M	U T H		K1=1.64	1967TMf (72186)	519
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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
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Ba++	gl	R4N.X	25°C	0.10M	C	T	K1=1.74	1991SMa (72236)	520
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IUPAC evaluation

Ba++	gl	NaNO3	25°C	0.10M	U		K1=1.08	1989MSf (72237)	521
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Ba++	gl	KNO3	40°C	0.10M	U T H		K1=1.62	1967TMf (72238)	522
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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
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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++ IUPAC evaluation	gl	R4N.X	25°C	0.10M	C	T	K1=1.78	1991SMa (72443)	526
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++ 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	gl	KNO3	40°C	0.10M	U T H		K1=1.66	1967TMf (72446)	529
Ba++	gl	NaClO4	25°C	0.10M	U		K1=1.14	1964SBa (72447)	530
Ba++ ***** C10H14N5O8P Adenosine-5'-monophosphoric acid N(1)-oxide;	gl	KNO3	25°C	0.10M	U		K1=1.73	1962TMa (72448)	531
							CAS 4061-78-3 (3931)		
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 Guanosine-5'-monophosphoric acid;								CAS 85-32-5 (2947)	
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
C10H15N06 N-(1'-Carboxycyclopentyl)iminodiethanoic acid;								(3915)	
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++ ***** C10H15N208P Thymidine-5'-monophosphoric acid, Thymidylic acid;	gl	KCl	20°C	0.10M	U		K1=5.50	1966IMa (72669)	534
								CAS 365-07-1 (2949)	

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										
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.										
Ba++	gl	R4N.X	25°C	0.10M	C		T	K1=2.58 K(Ba+HL)=1.51	1991SMa (72980)	540
IUPAC evaluation										
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										
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, Sequestic 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); ((HOOCC)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 K(Ba+HL)=2.33 1999SSa (74388) 563

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

C10H17N04 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

C10H17N05 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

C10H17N05 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

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	KN03	25°C	0.10M	U		K1=3.13	1990CCa (75232)	575
Ba++	cal	NaCl04	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									

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	NaCl04	30°C	0.10M	U		K1=6.05	1981MMc (75335)	577
Ba++	cal	KN03	25°C	0.10M	U	H		1965WHa (75336)	578
DH(K1)=-22.6 kJ mol ⁻¹ , DS=41.8 J K ⁻¹ mol ⁻¹									
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 K(Ba+HL)=0.65	1959KRa (75338)	580

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	KN03	25°C	0.10M	U		K1=2.29	1974MSa (75618)	581

C10H19N04 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	KN03	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

C10H2002		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		Kso=-8.23	1981HTc (75904)	585

C10H2003S2		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 .									

C10H2005		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 DH1=-4.52 kJ/mol	2000VGa (75974)	589
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 .									

C10H21N04		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

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
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Medium: MeOH

Ba++	cal	alc/w	25°C	100%	U	H	K1=2.72 B2=5.14	1986BUa (76309)	597
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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
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In CH3CN. DH=-35.0 kJ mol-1

Ba++	cal	alc/w	25°C	100%	U	H	K1=2.72	1985BUc (76311)	599
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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.)20

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
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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
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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
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Ba++	gl	oth/un	25°C	0.10M	U		K1=2.87	1959BYa (76757)	604
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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
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Ba++	gl	diox/w	30°C	75%	U		B2=11.4	1953UFe (76985)	605
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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
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Ba++	gl	diox/w	25°C	70%	U		K1=6.46 B2=11.72	1992DAc (77390)	606
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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
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Ba++	gl	NaNO3	25°C	0.50M	M		K1=-0.18	1998KSa (77668)	607
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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
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Ba++	EMF	KCl	20°C	0.10M	U		K1=3.57	1947SWa (77823)	608
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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
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Ba++	EMF	KCl	20°C	0.10M	C		K1=1	1947SWa (77844)	609
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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
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Ba++ EMF KCl 20°C 0.10M C K1=<1 1947SWa (77849) 610
Method: H electrode

C11H1102F 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

C11H12N207 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

C11H1202 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

C11H13N05 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

C11H13N05 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

C11H13N303 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

C11H14N204 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 K(Ba+HL)=0.1	1988SMb (79069)	619

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; <chem>HOOCC6H10.N(CH2.COOH)2</chem>										

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			K(Ba+HL)=2.67	1984RFd (79175)	622

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
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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; ((H00C.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 1964LAa (79423) 627
K(Ba+HL)=2.21

Ba++ EMF KCl 20°C 0.10M C K1=4.24 1948SAa (79424) 628
K(Ba+HL)=2.11

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 1966TKa (79541) 629
K(BaL+H)=7.34

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 1974KGa (79590) 634
K(Ba+HL)=1.14

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

C12H11N09 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

C12H12N06Cl 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

C12H13N06 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

C12H15N04 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

C12H15N05 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

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	1972GBE (82058)	659
							K(Ba+HL)=1.66		
							K(Ba+BaL)=2.66		

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	1964LAa (82212)	662
							K(Ba+HL)=2.58		

Ba++	EMF	KCl	20°C	0.10M	U			1948SAa (82213)	663
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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
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Ba++	gl	KCl	25°C	0.10M	U			1970AIa (82283)	664
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K1=8.53(DL)

K1=8.51(D)

Ba++	gl	KCl	20°C	0.10M	U		K1=8.49	1966IPa (82284)	665
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Ba++	oth	KNO3	20°C	0.10M	U		K1=11	1965JMb (82285)	666
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Method: electrophoresis

Ba++	gl	KCl	20°C	0.10M	U		K1=8.53	1963MDa (82286)	667
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C12H20N2O8 H4L CAS 63818-08-6 (2584)

meso-2,3-Diaminobutane-N,N,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
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Ba++	gl	KNO3	25°C	0.10M	U		K1=3.31	1978SGc (82351)	668
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K(Ba+HL)=1.23

K(Ba+BaL)=1.04

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
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Ba++	gl	KCl	20°C	0.10M	U		K1=6.45	1966IPa (82384)	669
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Ba++	oth	KNO3	20°C	0.10M	U		K1=7	1965JMb (82385)	670
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Method: electrophoresis

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

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
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Ba++	gl	KCl	20°C	0.10M	U		K1=5.34	1964PCa (82448)	672
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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

Ba++	gl	KCl	20°C	0.10M	U		K1=8.15 K(Ba+HL)=3.85	1964PCa (82524)	675
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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.

Ba++	cal	alc/w	25°C	100%	U	H	K1=3.1	1980LIb (82649)	678
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Medium: MeOH. DH=-1.70 kJ mol⁻¹.

Ba++	cal	alc/w	25°C	100%	U	H	K1=3.1	1977ILa (82650)	679
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Medium: MeOH. DH(K1)=-1.90 kJ mol⁻¹

C12H20O8N2 H4L (6908)

2-Methyl-1,2-diaminopropane-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

C12H21N06 H3L (7209)									
1-Carboxy-1-aminoheptane-N,N-diethanoic acid; H00C.CH(C6H13)N(CH2.COOH)2									
Ba++	gl	KNO3	20°C	0.10M	U		K1=4.4	1985LBc (82692)	681

C12H21N305 L CAS 106724-75-8 (8231)									
3,6,9,12,15-Pentaoxa-18,19,20-triazabicyclo[15.2.1]eicosa-1(19),17-diene;									
Ba++	cal	none	25°C	0.0	C H		K1=1.7	1986BNb (82713)	682
DH(K1)=-8.41 kJ mol-1.									

C12H21N306 H3L NOTA (5589)									
1,4,7-Triazacyclononane-N,N',N''-triethanoic acid;									
Ba++	gl	NaN03	25°C	0.10M	C T H		K1=5.10	1987BGc (82729)	683
DH(K1)=-5.8 kJ mol-1									

C12H22N206 H2L (6394)									
1,7-Dioxa-4,10-diazacyclododecan-4,10-diethanoic acid;									
Ba++	gl	R4N.X	25°C	0.10M	C		K1=6.652	1992ADa (82791)	684
Medium: 0.1 M Me4NN03									

C12H22N206 H2L (6641)									
7,10-Diaza-1,4-Dioxacyclododecane-7,10-diethanoic acid;									
Ba++	gl	R4N.X	25°C	0.10M	C		K1=6.68	1992ADa (82805)	685
Medium: 0.1 M Me4NN03									

C12H23N05 L (6793)									
10-Methoxycarbonylethyl-1,4,7-trioxa-10-azacyclododecane;									
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;

Medium: 0.1 M Me₄NNO₃

C12H24O2 HL Lauric acid CAS 143-07-7 (2540)
Dodecanoic acid, CH3.(CH2)10.COOH

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

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;

C12H24O6 L 18-Crown-6 CAS 17455-13-9 (577)
1,4,7,10,13,16-Hexaoxacyclooctadecane;

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 Et4NClO4.
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 5-40°C. 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

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 1985BP a (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 1982HL a (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 Et₄NC104. 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 Et₄NC104

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.O.CH₂.O.CH₂.O.CH₂.O.CH₃)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-diylldimethylenediphosphonic 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-Benzylnitritotriethanoic 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 K(Ba+HL)=1.38	1971KTl (85980)	756

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 K(Ba+HL)=3.91	1959KRa (86112)	758

C13H22N2O8 H4L CAS 1798-14-7 (921)

(Pentamethylenedinitrilo)tetraethanoic acid; ((HOOCH2)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; (HOOCCCH2)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	1981NSc (86249)	761
K(BaL+H)=2.06									

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.									

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	1957SSa (86395)	765
K(Ba+HL)=2.61									
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	1998CCd (86410)	766
*K(BaL)=-11.24									
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

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/H2O, 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; H00C.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; ((H00C.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;
(H00CCH2)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-0,0'-bis(2-aminoethyl ether)-N,N,N',N'-tetraethanoic acid; H4L

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

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.

Ba++	gl	R4N.X	25°C	0.10M	C		K1=7.412	1987DDb (90177)	813
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Ba++	gl	R4N.X	25°C	0.10M	M		K1=7.31	1986COb (90178)	814
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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
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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 Kso=-14.17 1981HTc (90508) 824

C14H28O7 L 21-Crown-7 CAS 33089-36-0 (2264)
1,4,7,10,13,16,19-Heptaoxacycloheptadecane;

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 2004KV a (90572) 826
Medium: 95% MeOH/H2O, 0.01 M Et4NClO4.

Ba++ gl oth/un 25°C ? C K1=3.54 1991DM a (90573) 827

Ba++ ISE alc/w 25°C 100% U H K1=6.9 1983CF b (90574) 828
Medium: MeOH, 0.05 M Et4NClO4

Ba++ gl alc/w 25°C 93% U K1=5.95 1978WW a (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 1988CF a (90609) 830
Medium: MeOH

Ba++ ISE alc/w 25°C 100% U H K1=5.39 1986BU a (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 1985BU c (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 1995LL a (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 1990WH a (90658) 834

C14H30O7 L CAS 1072-40-8 (2499)
2,5,8,11,14,17,20-Heptaoheneicosane; CH3.0.(CH2.CH2.0)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 1993BD b (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 1992BS c (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-diylldimethylenediphosphonic 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 K(Ba+HL)=4.95 K(Ba+H2L)=1.74	1996BJa (90759)	837

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		B(BaHL)=18.75 B(BaH2L)=29.64 B(BaH3L)=37.90 B(BaH4L)=45.43	1990DSa (90870)	838

Medium: Me4NN03

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		K(Ba+HL)=4.32 K(Ba+H2L)=2.30	1964STa (91725)	841

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;

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

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

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

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;									
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;									
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;									
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;									
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;									
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;									

1-(4-Sulfophenylazo)-2-hydroxynaphthalene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Ba++	gl	mixed	25°C	75%	U			K1=3.0	1972Mcb (92996)	864
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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
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Ba++	gl	KNO3	25°C	0.10M	U				1971KMb (93061)	865
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K(Ba+HL)=1.84

Ba++	gl	KNO3	25°C	0.10M	U				1968NMb (93062)	866
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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
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Ba++	gl	KNO3	25°C	0.10M	U				1968NMb (93075)	867
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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
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Ba++	gl	KNO3	25°C	0.10M	U				1968NMb (93082)	868
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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
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Ba++	gl	KNO3	25°C	0.10M	U				1968NMb (93086)	869
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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
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Ba++	gl	KNO3	25°C	0.10M	U				1968NMb (93092)	870
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K(Ba+HL)=1.58

C16H13N2O10AsS2 H5L Thorin I CAS 3688-92-4 (2609)
1-((2-Arsonophenyl)azo)-2-hydroxy-3,6-naphthalylidysulfonic acid;

C16H13N2O10AsS2 H5L (5204)
2-(2-Arsonophenylazo)-1-hydroxynaphthalene-3,6-disulfonic acid;

C16H13N2O11AsS2 H6L Arsenazo I CAS 520-10-5 (277)
2-(2'-Arsonophenylazo)chromotropic acid;

C₁₆H₁₄N₄O₂ H₂L (3467)
5-Hydroxy-4-(2-hydroxyphenylazo)-3-methyl-1-phenylpyrazole;

C16H14N4O4S HL (5184)
5-Methyl-1-phenyl-4-(2-sulfophenylazo)-3-pyrazolone;

C16H20N2O8	H4L	CAS 6411-02-5	(1919)
1-Phenyl-ethylenediamine-N,N,N',N'-tetraethanoic acid (DL)			

Ba++ gl KNO3 20°C 0.10M U K1=8.39 1969NDb (94032) 878

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	1988ZHa (94064)	880

B(Ba2L)=9.14

C16H24N2O8 H4L CAS 38557-30-1 (1256)
Ethylene-bis(N,N'-(2,6-dicarboxy)piperidine); ((HOOCC2.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/H2O, 0.005 M acetate buffer, pH 5.5.

Ba++	cal	non-aq	25°C	100%	C	H	K1=2.68	1999WBa (94380)	883
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Medium: N,N-dimethylformamide. DH(K1)=-23.4 kJ mol⁻¹.

Ba++	cal	non-aq	25°C	100%	U	H	K1=5.80	1993BDb (94381)	884
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Medium: acetone. DH=-49.3 kJ mol⁻¹; TDS=-16.4 Calorimetric titration

Ba++	con	none	25°C	0.0	U		K1=2.90	1989TKa (94382)	885
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Ba++	cal	non-aq	25°C	100%	C	H	K1=5.48	1986ICa (94383)	886
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Medium: MeOH. DH(K1)=-37.2 kJ mol⁻¹, DS(K1)=-19.9 J K⁻¹ mol⁻¹.

Ba++	sp	alc/w	25°C	100%	U		K1=5.35	1981EMb (94384)	887
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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;
(HOOCCCH2)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
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Ba++	gl	R4N.X	25°C	0.10M	U		K1=7.63	1983CRb (95029)	906
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C16H30N4O8 H4L (3473)

N,N'-Dimethyl-2,2'-ethylenedi-iminobis(ethylenediethanoic acid);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Ba++	gl	KCl	20°C	0.10M	U		K1=6.24	1964PCa (95082)	907
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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
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Ba++	gl	alc/w	25°C	95%	M		K1=3.34	1990LNa (95116)	908
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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
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Ba++	ISE	non-aq	25°C	100%	C	H	K1=6.60	1999WBa (95176)	909
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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
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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
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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
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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
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Medium: DMF, 0.01 M Me4NI

Ba++	cal	alc/w	25°C	100%	U	H		1986BUa (95181)	914
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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
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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;									
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;									
Ba++	gl	KNO3	25°C	0.10M	U		K(Ba+HL)=2.81	1971KMb (95719)	927
Ba++	gl	KNO3	25°C	0.10M	U		K(Ba+HL)=2.81	1968NMb (95720)	928

C17H14N2O		HL					CAS 2046-17-5	(5214)	
1-(2-Methylphenylazo)-2-hydroxynaphthalene;									
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;									
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;									
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:Me4NN03									

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 2004KVc (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
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Ba++	gl	KNO3	25°C	0.10M	U		K(Ba+HL)=2.43	1971KMb (96939)	947
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C18H14N2O11S2 H5L (4132)
 2-(2'-(Carboxyhydroxymethyl)phenylazo)chromotropic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Ba++	gl	KNO3	25°C	0.10M	U		K(Ba+HL)=3.12	1971KMb (96945)	948
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C18H14N2O11S2 H5L (4133)
 2-(2'-(Carboxymethoxy)phenylazo)chromotropic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Ba++	gl	KNO3	25°C	0.10M	U		K(Ba+HL)=3.00	1971KMb (96952)	949
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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
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Ba++	gl	diox/w	30°C	75%	U		K1=3.1	1962SCc (97210)	950
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C18H18O8 H2L (5631)
 1,4-bis(2-Carboxymethoxyphenyl)-1,4-dioxabutane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Ba++	gl	alc/w	25°C	90%	M		K1=4.95	1998KLa (97303)	951
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Medium: 90% v/v MeOH/H2O, 0.1 M Me4NC1

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
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Ba++	gl	diox/w	24°C	50%	U		K1=4.3	1979ACa (97560)	952
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C18H26N6 L (6628)
 3,6,14,17,23,24-Hexaazatricyclo[17.3.1.1]tetracos-1(23),8,10,12(24),19,21-hexaene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Ba++	gl	KCl	25°C	0.10M	M		K1=<2	1996MBb (97712)	953
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C18H27N2O3F L CAS 173417-90-8 (6571)
23-Fluoro-4,7,20-trioxa-1,10-diazatricyclo[8.7.5.1,12,16]tricos-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)20 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-hexaoxacyclooctadeca-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 (OE0AcAcOE)2 CAS 62950-36-1 (2254)
1,4,10,13,16,22-Hexaoxacyclotetracos-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;((HOOCH2)2NCH2CH2N(CH2COOH)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	1963GHa (98012)	961
								K(Ba+H2L)=1.7		
								K(Ba+HL)=5.55		
								K(BaL+Ba)=3.41		

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	KN03	25°C	0.10M	C	H			1984DFa (98190)	963
DH(K1)=10.5 kJ mol-1, DS(K1)=109 J K-1 mol-1.										

Ba++	gl	KN03	25°C	0.10M	C			K1=3.854	1982DSa (98191)	964
								K(Ba+HL)=2.519		

Ba++	EMF	KCl	20°C	0.10M	C			K1=4.3	1981SFa (98192)	965
Method: Pt/H2 electrode.										

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	1999CDb (98255)	968
								K(BaL+Ba)=3.01		

2-Carboxy-3-N-butylformamide-1,4,7,10,13,16-hexaoxacyclooctadecane;

Medium: 90% v/v MeOH/H₂O, 0.05 M R4NX

1,4,7,10-Tetraazacyclododecane-1-(2-hydroxy-3-methoxypropyl)-4,7,10-triethanoic acid:

Medium: 0.1 M Me₄NCI

10-[2,3-Dihydroxy-(1-hydroxymethyl)-propyl]-1,4,7,10-tetraazacyclododecane-1,4,7-triethanoic ac.;

1,10-Diaza-4,7,14,20,23-Pentaoxabicyclo[8.8.7]pentacosane:

Medium: 95% MeOH, 0.05 M Bu₄NBr. For the 12,16-dihydroxy- analogue: K₁=3.63

5,8,15,18,23-Pentaoxa-1,12-diazabicyclo[10.8.5]pentacosane:

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
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Ba++	cal	KCl	25°C	0.10M	U	IH	K1=7.21	1997Zia (98418)	975
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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
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Ba++	ISE	non-aq	25°C	100%	C	H	K1=8.01	1999Wba (98514)	976
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Medium: N,N-dimethylformamide. Method: competitive titration against
Ag⁺, using Ag⁺ ISE. By calorimetry: DH(K1)=-54.8 kJ mol⁻¹.

Ba++	EMF	non-aq	25°C	100%	C	I	K1=17.90	1997DKb (98515)	977
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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.

Ba++	gl	R4N.X	25°C	0.05M	C	H	K1=9.5	1996BCh (98516)	978
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Medium: 0.05 M Et₄NClO₄. By calorimetry: DH(K1)=-62.8 kJ mol⁻¹.

Ba++	EMF	non-aq	25°C	100%	C	H	K1=6.21	1995CDb (98517)	979
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Medium: DMSO, 0.1 M Et₄NClO₄. DH=-48.1 kJ mol⁻¹, DS=-42.5 J K⁻¹ mol⁻¹.

Ba++	sp	non-aq	25°C	100%	U	T H	K1=5.02	1994GSb (98518)	980
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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

Ba++	cal	non-aq	25°C	100%	C	H		1992BSc (98519)	981
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Medium: propylene carbonate. DH(K1)=-105.1 kJ mol⁻¹, DS(K1)=-27 J K⁻¹
mol⁻¹.

Ba++	cal	alc/w	25°C	100%	U	H		1986BUa (98520)	982
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B(Ba₂L₂) >12
Medium: MeOH. DH=-68.9 kJ mol⁻¹; DS=15

Ba++	ISE	non-aq	25°C	100%	U	H	K1=>9	1986BUb (98521)	983
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In CH₃CN. DH=-108.8 kJ mol⁻¹

Ba++	con	none	25°C	0.0	C		K1=ca. 9	1986KHe (98522)	984
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Method: conductance stopped-flow. Medium pH 11.3.

Ba++	ISE	alc/w	25°C	100%	U	H	K1=12.2	1985BUc (98523)	985
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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-diylldimethylenediphosphonic 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++	g1	R4N.X	25°C	0.10M	U		K1=9.0 K(Ba+HL)=2.9	1978LMa (99489)	998

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			K1eff=1.75	1978BRb (99725)	1001

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/H2O, 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)tetraethiafulvalen

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
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Medium: 20% w/w propylene carbonate/ethylene carbonate.

Ba++	nmr	non-aq	27°C	100%	C I		K1=6.65	2001KZa (100627)	1017
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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
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Ba++	gl	alc/w	25°C	95%	M		K1=7.53	1990LNa (100783)	1021
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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
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Ba++	gl	alc/w	25°C	95%	M		K1=5.21	1990LNa (100792)	1022
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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
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Ba++	gl	alc/w	25°C	90%	M		K1=10.40	1977LSc (100807)	1023
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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
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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
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Ba++	gl	NaNO3	25°C	0.10M	C		K1=2.73	1991DHa (100861)	1025
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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
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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 2004KV a (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 K(?)=5.66 1969PMb (101535)1037
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 B(BaH2L)=25.9 1965BV a (101536)1038

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

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-----
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;
((HOOCH2)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
-----

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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/H2O, 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-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 (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-diazabicyclo[8:8:8]hexacosane-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]dotriacontane;

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

Ba++ cal alc/w 25°C 95% U H K1=5.37 1997ZIIa (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)-quinoline;									

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					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-Ethanediybis(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-octaoxacyclotetracos-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.									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	oth	alc/w	35°C	3.0%	C		K1=1.20	1999MTd (103110)	1076
Method: capillary zone electrophoresis. Medium: 3% v/v EtOH/H2O, 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=4.04	1986ICa (103111)	1077
Medium: MeOH. DH(K1)=-24.6 kJ mol ⁻¹ , DS(K1)=-5.0 J K ⁻¹ mol ⁻¹ .									

C24H35N2O9		L					CAS 330462-64-1	(8032)	
6,7-Dimethoxy-4-(1,4,7,10,13-pentaoxa-16-azacyclooctadec-16-ylmethyl)-2H-1-benzopyran-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-diazacyclooctadecane;

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	2004KV a (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	NaNO ₃	25°C	0.10M	C		K1=4.14	1989HB a (103554)	1086

C₂₅H₃₀N₃O₅Cl HL CAS 172033-66-8 (8619)
 5-Chloro-2-(3,6,12,15-tetraoxa-9,21-diazabicycloheptacos-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		1997ZB b (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-diazabicycloheptacos-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		1997ZB b (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)
 Penta-oxa-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	R ₄ N.X	25°C	0.10M	U		K1=5.3	1981GL a (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	2004KV a (103842)	1090

Medium: 95% MeOH/H₂O, 0.01 M Et₄NClO₄.

C₂₆H₂₅N₉O₉S 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	KN03	25°C	0.10M	U		K1=4.75 B(BaHL)=12.72	1974Y0a (103943)	1091

C26H27N3O10		H4L					(7231)		
2-((2-Amino-5-methylphenoxy)-methyl)-6-methoxy-8-aminoquinoline-N,N,N',N'-tetraethanoic acid;									
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									
Ba++	gl	diox/w	24°C	50%	U		K1=6.4	1979ACa (104020)	1093

C26H31N08S2		L					CAS 136195-71-6 (6832)		
Crown Ether Styryl Dye;									
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;									
Ba++	sp	diox/w	25°C	40%	C		K1=5.26 K(BaL+Ba)=2.37	2003GHb (104038)	1095
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;									
Ba++	sp	non-aq	25°C	100%	C		K1=3.46 K(BaL+Ba)=2.72	2003GHa (104044)	1096
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 K(BaL+Ba)=3.44	2003GHa (104073)	1097

Method: fluorescence spectroscopy. Medium: acetonitrile, 0.05 M Et4NClO4.

C26H34N6O8 H4L CAS 132709-65-0 (8941)
3,6,14,17,23,24-Hexaazatricyclotetracos-1,8,10,12,19,21-hexaene-3,6,14,17-tetraacetic 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-diazacyclooctadecane;

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-diene;

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
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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
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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
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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-Hepta-1,4,6,18,20,23-hexaazabicyclo[21.8.8]nonatridecane-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.

C27H32N5S+ 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 K(BaP+L=LiPL)=5.16 2001LFa (104623)1113

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-13-ylstyryl)-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-benzotriazolium;

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									
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									
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)									
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;									
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;									
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]dotetratricontane-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.

C29H35N05 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 K(Ba(SCN)2+L)=4.35 1997KKa (105098)1127

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)-dibenzotetraoxaazacycloheneicosine;

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									

C30H30N2O010		L					CAS 259886-49-2	(8959)	
Cucurbit[5]uril;									
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;									
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.C6H4.0.(C2H4)2)									
Ba++	gl	alc/w	25°C	93%	U		K1=2.55	1978WVa (105309)	1132
Medium: 93% MeOH/H2O									

C30H57N08		HL		18NH15-C5A			CAS 79145-86-1	(5405)	
2-Carboxy-3-N-octadecanylformamide-1,4,7,10,13-pentaoxycyclopentadecane;									
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;									
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'-dimethylfuchstone-2''-sulfonic 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 K(BaL+H)=10.86 K(BaL+Ba)=3.45 K(Ba2L+H)=9.30	1998GBa (105453)	1135

Ba++	sp	KNO3	25°C	0.10M	U		K1=6.67 K(Ba+HL)=5.04 K(Ba+H2L)=2.02 K(Ba+BaL)=4.57 K(Ba+BaHL)=2.0	1974Y0a (105454)	1136
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C31H46N2O6 L (2446)
Bicyclo-NcN'-1,10-Diaza-4,7,13,16-tetraoxaoctadecane;(c=(CH2.C6H4.0.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 B(BaHL)=18.17 B(Ba2L)=11.65	1981GMd (105609)	1140

Ba++	gl	KCl	20°C	0.1M	U		K1=6.2	1954AGb (105610)	1141
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K(Ba+HL)=4.8
K(Ba+H2L)=2.3
K(Ba+H3L)=1.3
K(Ba+BaL)=5.2

K(Ba+BaHL)=1

C32H37N09S 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 B(BaHL)=13.41	1974Y0a (105664)	1142

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 K(Ba+HL)=12.2	1995ZBa (105677)	1143

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-diazacyclooctadecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ba++	cal	alc/w	25°C	100%	U	H		K(Ba+H2L)=3.60	1996BBf (105689)	1144

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)]bisquinoline;

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-diazacyclooctadecane;

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

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: 90% v/v MeOH/H₂O, 0.05 M R4NX

3,11-Bis-carboxy-2,12-bis(octanylformamide)-18-crown-6 (syn);

$$B(\text{BaHL}) = 12.1$$

4,10,13,19,25,28,33,36,41,44-Decaoxa-1,7,16,22-tetraazatricyclo[20.8.8.8.16]hexatetracontane;

$$K(\text{BaL}+\text{Ba})=6.3$$

1,10-Didecyl-1,10-diaza-4,7,13,16-tetraoxacyclooctadecane;

Medium: MeOH, 0.05 M Et₄NClO₄. DH=-32.9 kJ mol⁻¹

1,4,12,15,18,26,31,39,42,43,44-Undecaazapentacyclo[13.13.13.1.1.1]tetratetracontapentadecane;

Medium: CH₃CN

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)
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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
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Ba++	con	alc/w	25°C	100%	M	H		K1=2.45	2000BSe (106055)	1158
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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)
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3,18-Dichlorooctahydro-5H,16H-6,15-(ethanoxyethanoxyethano)tribenzotetraoxadiazacyc
lodocosine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Ba++	cal	non-aq	25°C	100%	C	H		K1=4.03	1998ZBc (106056)	1159
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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)
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5-Bromolasalocid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Ba++	gl	alc/w	25°C	100%	M				1988JTa (106096)	1160
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K(Ba+HL)=6.62

K(Ba+2HL)=5.8

Medium: MeOH

C34H54O8	H2L	Lasalocid	CAS 25999-20-6	(2335)
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Lasalocid acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Ba++	nmr	non-aq	20°C	100%	C				1998MLa (106123)	1161
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K(Ba+HL)=1.8

Medium: CD3OD. Method: 13C nmr.

Ba++	dis	non-aq	25°C	100%	U				1993LPa (106124)	1162
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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
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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 B(BaHL)=14.1	1984FWa (106177)	1166

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 K(BaL+H)=7.9 K(BaHL+H)=8.60 K(BaH2L+H)=6.00	2001BBa (106201)	1167

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;

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);

C36H62O11	HL	Monensin	CAS 17090-79-8	(737)
Monensin, 1,6-dioxaspiro[4,5]decane derivative;				

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	KN03	25°C	0.10M	U		K1=6.93 B(BaHL)=18.03 B(BaH2L)=26.19 K(Ba+BaL=Ba2L)=4.65 K(Ba+BaHL=Ba2HL)=1.9	1974Y0a	(106586)1175

C40H36O4P2 HL CAS 126763-08-4 (7791)
1,2-Bis[2-(diphenylphosphinylmethyl)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-trioxasheptane; Ph2P0.C6H4.0.C2H4.0.C2H4.0.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

Ba++		EMF non-aq	25°C	100%	C		K1=8.91 B2=13.42	1997PKc (106743)	1178
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Medium: nitrobenzene

C40H50N20010 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.

C40H64012 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

C41H66012 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

C42H4005P2 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

C42H52N406 L CAS 405917-44-4 (9250)

Tetraoxadiazacyclooctadecane-7,16-diylbis(methylene)bis-methyl-4-pyridinylidenecycl ohexadienone;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++		sp R4N.X	25°C	0.10M	C			2004COa (106961)	1183

$$K(\text{Ba}+\text{H}_2\text{L}=\text{BaL}+2\text{H})\Rightarrow 15.30$$

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 B(BaHL2)=23.63 B(Ba2HL2)=28.61	2000ABb (107141)	1188

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 K(BaL+Ba)=6	1977LSc (107192)	1190
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-0(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 B(BaHL)=19.6 B(BaH2L)=31.8 B(BaH3L)=41.4	1993ABb (107295)	1193
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]arene dicarboxylic 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]arene;

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)calix[4]arene;									
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;									
Ba++	sp	non-aq	20°C	100%	C		K1=3.03	20030Aa (107522)	1202
Medium: 100% acetonitrile, 0.01 M Et4NClO4.									

C54H90N6O18		L			Valinomycin		CAS 2001-95-8	(2142)	
Valinomycin, Potassium Ionophore									
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;									
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;									
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]arene;									

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)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=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-butylcalix[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-Butyldihomooxcalix[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-butyldihomooxcalix[4]arene tetraphenylketone;

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-β-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 K(Ba+HL)=3.81 K(Ba+H2L)=3.04	2003WWa (107972)	1218

Medium: 0.10 M Et₄NClO₄.

C114H198N6O73 L CAS 571203-66-2 (9254)
4,13-Bis(8-(6-deoxy-β-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 K(Ba+HL)=4.54 K(Ba+H2L)=4.10	2003WWa (107999)	1219

Medium: 0.10 M Et₄NClO₄.

C120H192O24 L CAS 175349-58-3 (7495)
C-Undecylcalix[4]resorcinarene octa-α-(tert-butyl ethanoate);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	dis	non-aq	25°C	100%	U		K=5.34	1995FDa (108005)	1220

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-α-(N,N-diethyl acetamide);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ba++	dis	non-aq	25°C	100%	U		K=8.75	1995FDa (108016)	1221

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
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 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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