

SC-Database

Software version = 5.81 Data version = 4.62
 Experiment list contains 2635 experiments for
 (no ligands specified)
 Metal : Ca++
 (no references specified)
 (no experimental details specified)

e- HL Electron (442)
 Electron;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	EMF	none	25°C	0.00	U				1974LMb (252)	1
K(Ca+2e=CaHg)=-67.730(-2.0034V)										
Ca++	oth	oth/un	25°C	0.0	U	I			1972C0a (253)	2
K(Ca+2e=Ca(s))=-96.79(-2.863)										
Method: Estimated. MeOH: -94.97(-2.809V).EtOH: -92.02(-2.722V).BuOH: -93.48(-2.765).PentOH: -91.28(-2.700V).Me2CO: -92.77(-2.744V)										
Ca++	oth	oth/un	25°C	0.0	U	I			1972C0a (254)	3
K(Ca+2e=Ca(s))=-96.79(-2.863V)										
Method: Estimated. MeCN: -88.37(-2.614V).HCOOH: -103.01(-3.047V). Also NH3,N2H4										
Ca++	EMF	none	25°C	0.00	U				1972KKb (255)	4
K(Ca+2e=Ca/Hg)=-65.93(-1.950V)										
Ca++	EMF	none	25°C	0.00	U	T			1971MPc (256)	5
K(Ca+2e=Ca/Hg)=-67.53(-1.9974V)										
K=-64.59(-2.0065V,40 C), -61.78(-2.0111V,55 C), -59.38(-2.0213V,70 C)										
Ca++	oth	none	25°C	0.0	M				1968BUc (257)	6
K(Ca+2e=CaHg)=-67.48, -1996 mV										
K(Ca+2e=Ca(s))<-94.27,<-2809mV										
Evaluated from literature data										
Ca++	EMF	none	25°C	0.0	M				1967BHd (258)	7
K(Ca+2e=CaHg)=-67.42, -1994 mV										
Ca++	oth	none	25°C	0.0	U	I			1962JTa (259)	8
K(Ca+2e)=-96.97(-2868 mV)										
Method:combination of thermodynamic data. In MeOH: K=-99.03(-2929 mV)										
Ca++	EMF	oth/un	17°C	1.0M	U				1925TAa (260)	9
K(Ca+2e)=-95.7(-2760 mV)										

AsO2- HL Arsenite CAS 14102-45-5 (2616)

Arsenite; As(OH)₄⁻ or AsO₂⁻

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	ISE	NaCl	25°C	0.50M	U			K1=0.2	1995MPb (1081)	10
Method: Ca electrode										

AsO ₄ ⁻⁻⁻		H3L		Arsenate				CAS 7778-39-4	(1557)	
Arsenate;										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	ISE	none	40°C	0	U			K1=4.3 K(Ca+H ₂ AsO ₄)=1.39 K(Ca+HAsO ₄)=2.75	1995MKa (1120)	11

Ca++	oth	oth/un	25°C	0.0	U			*K(Ca ₃ L ₂ (s)+2H=3Ca+2HL)=-1.91	1990SAa (1121)	12
Calculated from thermodynamic data.										

Ca++	sol	NaNO ₃	35°C	0.16M	U	T	H	Kso(Ca ₁₀ (AsO ₄) ₆ (OH) ₂)=-90.40	1987MMd (1122)	13
Kso at 40 C: -90.57; at 45 C: -90.68; at 50 C: -90.92. At 35 C, DH=-52.3 kJ mol ⁻¹ ; DS=-1900										

Ca++	sol	oth/un	20°C	var	U			Kso(Ca ₃ L ₂)=-18.17	1956CHd (1123)	14

AsW11039-----		H7L						(2468)		
alpha-Heteromonoarseno-polytungstate;										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	NaNO ₃	25°C	1.00M	U			K1=4.06	1984COa (1172)	15

As ₂ W17H ₂₀ O ₆₁ -----		H8L						(2469)		
alpha-Heteropolydiarseno-polytungstate;										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	NaNO ₃	25°C	1.00M	U			K1=3.40 K1=4.01 (alpha ₂ isomer)	1984COa (1183)	16

B ₀₄ H ₄ ⁻		HL		Borate				CAS 10043-35-3	(991)	
Borate; B(OH) ₄ ⁻										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	EMF	oth/un	25°C	0.0	C	TIH		K1=1.901	1999SYa (1287)	17
Method: Pt/H ₂ electrode. Data for 5-45 C. Medium: CaCl ₂ , 0.004-0.06 m.										

DH(K1)=1.0 kJ mol⁻¹, DS(K1)=39.7 J K⁻¹ mol⁻¹.

Ca++ gl NaCl 25°C 0.70M U K1=1.06 1988RbBa (1288) 18

Ca++ EMF NaCl04 25°C 3.00M C 1976FRb (1289) 19
K(Ca+HL=CaL+H)=-8.032

Ca++ gl none 25°C 0.0 M TIH 1976REa (1290) 20
K(Ca+H2B03)=1.80

Calculated from data for 0.02-0.16 M CaCl2. Data for 10-50 C.
DH(Ca+H2B03)=3.7 kJ mol⁻¹, DS=46.9 J K⁻¹ mol⁻¹.

Ca++ EMF NaCl 25°C 0.68M U K1=1.11 1974BKd (1291) 21

Ca++ oth NaCl 25°C 0.70M U K1=0.73 1972DH a (1292) 22
Method: estimated value

BrO3- HL Bromate (6017)
Bromate;

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

Ca++ dis NaCl04 25°C 1.00M U H K1=-0.07 1992CKb (2404) 23
DH(K1)=-1.2 kJ mol⁻¹; DS=-5 J K⁻¹ mol⁻¹

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

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

Ca++ cal oth/un 25°C 0.03M C I 1981HWb (2575) 24
DH(Ca + Fe(CN)6)=11.8 kJ mol⁻¹. Fe is Fe(II). Data for I = 0.02-0.08 M.

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

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

Ca++ sol none 25°C 0.0 C 2003DVa (3008) 25
Kso(CaCO3)=-8.485 (calcite)
Kso(CaCO3)=-7.927 (vaterite)
Kso(CaCO3)=-8.331 (aragonite)

Application of Pitzer theory to literature data.

Ca++ gl NaCl04 25°C 0.0 C 1999GPa (3009) 26
K(CdCO3(otavite)+2H=Cd+CO2+H2O)=6.14. Data for 0.15-5.3 m NaCl04
at 25 C and 1.0 m NaCl04 at 25-75 C.

Ca++ sol none 25°C 0 M T 1993BNa (3010) 27
Kso(CaL.6H2O)=-7.461

$$K_{so} = -(7.1199 + 0.011756 \cdot T + 0.000075556 \cdot T^2)$$

 Ca++ sol oth/un 20°C 0.72M C I 19880Ka (3011) 28

Kso(calcite)=-6.16
 Kso(aragonite)=-6.03
 Kso(protodolomite)=-10.30.

Medium: seawater. Data for 0-35% salinity. At I=0.0 M, Kso(calcite)=-8.50,
 Kso(aragonite)=-8.37, Kso(protodolomite*)=-14.91. *=Ca1.06Mg0.94(CO3)2.

 Ca++ sol oth/un 25°C 0.70M M 1984MMF (3012) 29

K(CaL(s)=Ca+L)=-6.59

Solubility of calcite in seawater with various Mg concs. also studied

 Ca++ sol NaCl 25°C 1.0M C I 1984MTb (3013) 30

K(CaL(s)=Ca+L)=-6.79

I=0.1-6 M. Activity coeff. estimated from Pitzer's eq. At I=0 corr:K=-8.46

 Ca++ sol none 25°C 0.0 U K1=4.44 1983Lda (3014) 31

K(Ca+HCO3)=1.14

Kso=-8.48

 Ca++ sol oth/un 25°C 44% U TI 1983MUa (3015) 32

Kso=-6.26 (calcite)

Kso=-6.07 (aragonite)

Data is also available for a range of temperatures (T=5 to 40) and a variety
 of salinities (medium: sea water).

 Ca++ sol none 25°C 0.0 U 1983SMA (3016) 33

Kso=-8.48 (calcite)

Kso=-8.30 (aragonite)

 Ca++ oth none 25°C 0.0 C T H 1982PBb (3017) 34

Kso(CaCO3)=-8.480 (calcite)

Kso(CaCO3)=-8.336 (aragonite)

Kso(CaCO3)=-7.913 (vaterite)

Analysis of literature data. Values for 0-90 C. DH(Kso(calcite))=-
 -9.61 kJ mol⁻¹, DH(Kso(aragonite))=-10.83, DH(Kso(vaterite))=-15.79

 Ca++ gl none 25°C 0.0 M T K1=3.22 1982PBb (3018) 35

K(Ca+HCO3)=1.32

Values for 0-90 C. From solubility of aragonite as a function of pCO2,
 K(Ca+HCO3)=1.11

 Ca++ oth none 25°C 0.0 M K1=3.15 1982PSe (3019) 36

Ks(calcite)=-6.34

Ks(aragonite)=-6.19

Analysis of activity coefficients, based on literature data.

Ks: [Ca]T.[CO3]T. Ks values on molar scale.

 Ca++ sol oth/un 25°C 3.5% U 1980MMc (3020) 37

Kso=-6.18 (aragonite)

Kso=-6.36 (calcite)

Medium: Synthetic sea water; 3.5% salinity.

Ca++ sol oth/un 25°C 35% C IH 1980PJa (3021) 38
Kso(CaCO3)=-6.33

Medium: seawater (35%) and dil seawater. CaCO3: calcite. Data for 5-25 C
Kso: CaCO3(s)=CO3(tot)+CO3(tot). DH(Kso)=-2.37 kJ mol⁻¹. At 5 C, Kso=-6.32

Ca++ sol oth/un 25°C 0.72M C 1980PPb (3022) 39
Kso(CaCO3)=-6.06

CaCO3 is natural oolite (aragonite). Medium: seawater, S=32.6.

Ca++ con none 25°C 0.0 U T 1974JLa (3023) 40
K(Ca+HL)=1.0

K=0.7(0 C), 1.35(50 C)

Ca++ oth none 25°C 0.0 U K1=3.2 1974JLa (3024) 41
Method: Estimated data.

Ca++ oth none 25°C 0.0 U T 1974JLa (3025) 42
Kso=13.870-3059/T-0.04035T

Method: Estimated data. Temperature range 5-50 C, (calcite)

Ca++ sol oth/un 200°C var U T B2=4.5 1974MDa (3026) 43
B2=3.8(300 C), 3.3(350 C). In NaCl(var. conc.): K(Ca+HL)=1.15(150 C),
1.76(225 C)

Ca++ sol none 1°C 0.0 U 1974MNB (3027) 44
Kso=-8.19(p=95atm), -7.98(p=260), -7.86(p=390), -7.64(p=590), -7.52(p=685),
-7.41(p=795), -7.31(p=875)

Ca++ sol none 8°C 0.0 U 1974MNB (3028) 45
Kso=-8.26(p=35atm), -8.08(p=185), -7.88(p=350), -7.76(p=505), -7.59(p=640),
-7.40(p=815)

Ca++ sol none 23°C 0.0 U 1974MNB (3029) 46
Kso=-8.31(p=45atm), -8.32(p=55), -8.16(p=200), -8.17(p=225), -8.10(p=300),
-8.03(p=330), -7.97(p=405), -7.89(p=495), -7.87(p=510), -7.76(p=605)

Ca++ sol none 23°C 0.0 U T 1974MNB (3030) 47
Kso=-7.72(p=640), -7.59(p=790), -7.55(p=845); -8.39(p=25), -8.17(p=250), -8.00
(p=410), -7.87(p=518), -7.68(p=690), -7.45(p=950)(25 C, calcite)

Ca++ EMF oth/un 25°C 0.70M U M 1974PHc (3031) 48
B(MgCaL2)=3.02

Medium: synthetic seawater

Ca++ EMF oth/un 25°C 0.70M U K1=2.21 1974PHc (3032) 49
K(Ca+HL)=0.29

Medium: Synthetic seawater

Ca++ sol none 25°C 0.0 U M K1=8.49 1974PMa (3033) 50
Data also on many Ca:Mg mixtures in $\text{Ca}_x\text{Mg}_{(x-1)}\text{CO}_3$, e.g. B=7.36 when x=0.733

Ca++ gl none 25°C 0.0 U T K1=3.15 1974RLa (3034) 51
K1=-27.393+4114/T+0.0561T

Ca++ sol none 25°C 0.0 U Kso(CaL(H2O))=-7.60 1973HTb (3035) 52

Ca++ sol oth/un 25°C ? U T Kso=-6.34 1973ICa (3036) 53

Medium: synthetic seawater(3.5% salinity); Kso=-6.32(2-13 C)

Ca++ oth NaCl 25°C 0.70M U K1=1.5 1972DHa (3037) 54
K(Ca+HCO3)=0.02

Method: Estimated data.

Ca++ oth none 25°C 0.0 U T Kpso(p)/Kpso(l)=0.48 1972EMa (3038) 55

Method: Estimated data, 0 corr. at 500 bar. Kpso: $\text{CaCO}_3(\text{s})+\text{CO}_2+\text{H}_2\text{O}=\text{Ca}+2\text{HCO}_3$
Kpso(p)/Kpso(l)=0.43(100 C); 0.54(200 C); 0.66(250 C)

Ca++ oth none 25°C 0.0 U T Kpso(p)/Kpso(l)=1.33 1972EMa (3039) 56

Method: Estimated data at 1500 bar. Kpso: $\text{CaCO}_3(\text{s})+\text{CO}_2+\text{H}_2\text{O}=\text{Ca}+2\text{HCO}_3$
Kpso(p)/Kpso(l)=1.19(100 C); 1.54(200 C); 1.92(250 C)

Ca++ ISE none 22°C 0.0 U T K1=4.39 1972MVa (3040) 57
K1=5.34(60 C), 5.55(70 C), 5.74(80 C), 5.82(90 C), 6.00(98 C)

Ca++ EMF none 22°C 0.0 U T K(Ca+HL)=1.27 1972MVa (3041) 58
K(Ca+HL)=1.65(60 C), 1.77(70 C), 1.82(80 C), 1.94(90 C), 2.01(98 C)
K=4.85-1070/T

Ca++ ISE none 25°C 0.0 U Kso=-8.49(ion selective electrode(Ca),glass electrode,Partial pressure CO2),
Kso=-8.43(glass electrode,Partial pressure of CO2) 1972NAe (3042) 59

Ca++ sol none 25°C 0.0 U T M Kso(MgCaL2)=-17.0 1971LAa (3043) 60
Kso=-16.56(0 C), -16.63(5 C), -16.71(10 C), -16.79(15 C), -16.89(20 C)

Ca++ sol none 25°C 0.0 U T Kso=-8.4 1971LAa (3044) 61
Kso=-8.34(0 C), -8.345(5 C), -8.355(10 C,calcite), -8.37(15 C), -8.385(20 C)

Ca++ sol none 22°C 0.0 U T 1971MVa (3045) 62

Kso=-8.36

Kso=-9.17(60 C), -9.38(70 C), -9.54(80 C), -9.70(90 C), -9.82(98 C).

Kso=-15.43+2083/T

Ca++ dis NaCl 25°C 1.00M U K1=1.22 B2=1.38 1970HKa (3046) 63

Ca++ sol none 25°C 0.0 U K1=3.1 1970LAc (3047) 64

Ca++ sol oth/un 150°C ? U T 1970MAb (3048) 65

K(Ca+HL)=1.15

K(Ca+HL)=1.76 at 225 C

Ca++ ISE none 30°C 0.0 U 1969GSb (3049) 66

Kso=-8.0 (resin membrane electrode)

Ca++ oth none 50°C 0.0 U T K1=3.4 1969HEa (3050) 67

Kso=-8.62

Method: Estimated data. K1=3.5, Kso=-8.74(60 C); K1=3.9, Kso=-9.39(100 C);
K1=4.5, Kso=-10.25(150C); K1=5.2, Kso=-11.37(200C); -12.72(250C), -14.10(300C)

Ca++ sol NaCl04 25°C 3.00M U M 1969H0d (3051) 68

K(CaMg(CO3)2(s)+4H=Mg+Ca+2CO2(g)+2H2O)=18.16(dolomite)

Ca++ sol oth/un 22°C ? U 1969HPa (3052) 69

Medium: sea water, Kso(p)/Kso(1)=0.32(p=500atm), 0.63(p=1000)(2 C),
0.26(p=500, 0.50(p=1000)(22 C)(aragonite), also DV(Kso(p)/Kso(1))

Ca++ oth none 25°C 0.0 U T 1968KRa (3053) 70

Kso=-8.22

Method: Estimated data.

Kso=-8.46(50 C), -9.15(100 C), -10.03(150 C), -11.03(200 C)

Ca++ ISE none 25°C 0.0 U M K1=4.48 1968NAa (3054) 71

K(Ca+HL)=1.25

Method: several; Kso=-8.31 (glass electrode, partial pressure of CO2, ion
selective electrode for Ca)

Ca++ sol oth/un 28°C 0.0 U 1966BTa (3055) 72

Kso(aragonite)=-8.10

Ca++ sol oth/un 250°C 0.0 U T 1963ELa (3056) 73

Kso=-12.96

Medium: 0 corr. Kso=-9.62(100 C), -10.06(125 C), -10.54(150 C), -11.62(200 C)
Also data for 0.2, 0.5 and 1.0m NaCl

Ca++ oth oth/un 25°C dil U M 1963HSb (3057) 74

Kso(MgCaL2)=-16.7

Kso(CaL)=-8.29

Method: chemical analysis. K(2CaL(s)+Mg=MgCaL2(s)+Ca)=0.11

Ca++	gl none	25°C	0.0	U		1962GTa (3058)	75
					K(Ca+HL)=1.26		
Ca++	sol none	25°C	0.0	U	K1=3.2	1962GTa (3059)	76
					Kso(CaCO3(s))=-8.35 (calcite)		
					Kso(CaCO3(s))=-8.22(aragonite)		
Ca++	sol none	100°C	0.0	U T		1962SHb (3060)	77
					+Kpso=-7.62		
					I=0 corr. +Kpso: CaCO3(s)+CO2(g)+H2O=Ca+2HCO3. +Kpso=-8.14(125 C),		
					-8.74(150 C), -9.89(200 C), -11.19(250 C). Ks(CaL(s)=CaL)=-4.30 at all temps		
Ca++	sol none	25°C	0.0	U		1960BGB (3061)	78
					Kso(CaCO3(s))=-8.54		
Ca++	sol none	100°C	0.0	U T		1959ELb (3062)	79
					Kso(CaCO3(s))=-9.37		
					+Kpso=-7.40		
					I=0 corr. Kso=-10.42(150 C), -11.54(200 C), -12.77(250 C). +Kpso: CaCO3(s)+		
					CO2(g)+H2O=Ca+2HCO3. +Kpso=-8.45(150 C), -9.56(200 C), -10.72(250 C)		
Ca++	sol oth/un	5°C	3.5%	U TI		1959KRd (3063)	80
					Kso(CaCO3(s))=-5.55 ?		
					Medium: sea water, 3.5% salinity. Kso=-5.40?(at 4.5% salinity), -5.36?(6.0%).		
					At 25 C: Kso=-6.19(3.5%), -5.85(4.5%), -5.74(6.0%)		
Ca++	sol NaClO4	25°C	3.50M	U TI		1958NRa (3064)	81
					Ks(CaCO3(s)+CO2(g))=-5.50		
					Ks: CaCO3(s)+CO2(g)+H2O=Ca+2HCO3. Ks=-5.80(35 C), -6.49(75 C).		
					In 1 M NaClO4: Ks=-4.91(25 C), -5.10(35 C), -5.56(75 C)		
Ca++	sol none	25°C	0.0	U T		1957SEa (3065)	82
					Ks=-2.55		
					I=0 corr. Ks: CaCO3(s)+2OH=Ca(OH)2(s)+CO3. Ks=-2.74(100 C), -2.91(200 C)		
Ca++	sol none	25°C	0.0	U		1957SHa (3066)	83
					Ks(CaCO3+H2CO3=Ca+2HCO3)=-4.41		
Ca++	gl NaCl	22°C	.152M	U		1941GRa (3067)	84
					K(Ca+HL)=0.81		
					K(CaL+H)=7.90		
Ca++	sol none	38°C	0.0	U		1937BHa (3068)	85
					Kso(CaCO3(s) aragonite)=-8.42		
Ca++	sol none	39°C	0.0	U		1935HRa (3069)	86
					Kso(CaCO3(s))=-8.42		
Ca++	sol none	25°C	0.0	U		1935KAa (3070)	87
					Kso(CaCO3(s))=-8.32		

$$K(\text{CaCO}_3(\text{s})+\text{CO}_2(\text{g}))=-5.83$$

I=0 corr. K: $\text{CaCO}_3(\text{s})+\text{CO}_2(\text{g})+\text{H}_2\text{O}=\text{Ca}+2\text{HCO}_3$.

 Ca++ cal oth/un 50°C 2.0M U H 1928RCa (3071) 88
 Medium: HCl. $\text{DH}(\text{CaCO}_3(\text{s})+2\text{H}=\text{Ca}+\text{H}_2\text{O}+\text{CO}_2(\text{g}))=-15.4 \text{ kJ mol}^{-1}$ (calcite)
 $\text{DH}=-15.2$ (aragonite).

Ca++ sol none 25°C 0.0 U 1923MIa (3072) 89
 $K(\text{CaCO}_3(\text{s})+\text{H}_2\text{CO}_3)=-4.28$
 I=0 corr. K: $\text{CaCO}_3(\text{s})+\text{H}_2\text{CO}_3=\text{Ca}+2\text{HCO}_3$.

Ca++ sol none 25°C 0.0 U 19220Sa (3073) 90
 $K_{\text{so}}(\text{CaCO}_3(\text{s}))=-8.14$

Ca++ sol none 25°C 0.0 U T 1921BAa (3074) 91
 $K_{\text{s}}(\text{aragonite})/K_{\text{s}}(\text{calcite})=0.14$
 I=0 corr. $K_{\text{s}}(\text{aragonite})/K_{\text{s}}(\text{calcite})=0.12(9 \text{ C}), 0.15(35 \text{ C})$. $K_{\text{s}}=K_{\text{so}}(\text{CaCO}_3(\text{s}))$

Ca++ sol none 25°C 0.0 U 1917SLb (3075) 92
 $K_{\text{so}}(\text{CaCO}_3(\text{s}))=-8.14$

Ca++ oth oth/un 25°C dil U T 1916JWa (3076) 93
 $K_{\text{so}}(\text{CaCO}_3(\text{s}))=-8.06$
 From thermodynamic data. $K_{\text{so}}=-7.91(0 \text{ C}), -7.94(5 \text{ C}), -7.97(10 \text{ C}), -8.00(15 \text{ C})$
 $-8.03(20 \text{ C}), -8.09(30 \text{ C})$

Ca++ sol none 16°C 0.0 U 1915JOa (3077) 94
 $K_{\text{so}}(\text{CaCO}_3(\text{s}))=-8.01$
 $+K_{\text{so}}=-4.26$
 $+K_{\text{pso}}=-5.62$
 I=0 corr. $+K_{\text{so}}: \text{CaCO}_3(\text{s})+\text{H}_2\text{CO}_3=\text{Ca}+2\text{HCO}_3$, $+K_{\text{pso}}: \text{CaCO}_3(\text{s})+\text{CO}_2(\text{g})+\text{H}_2\text{O}=\text{Ca}+2\text{HCO}_3$

Ca++ sol none 25°C 0.0 U 1911MSa (3078) 95
 $K_{\text{so}}(\text{CaCO}_3(\text{s}))=-8.03$
 $+K_{\text{so}}=-4.29$
 I=0 corr. $+K_{\text{so}}: \text{CaCO}_3(\text{s})+\text{H}_2\text{CO}_3=\text{Ca}+2\text{HCO}_3$

Ca++ sol none 16°C 0.0 U 1900BOa (3079) 96
 $K_{\text{so}}(\text{CaCO}_3(\text{s}))=-8.55$

 C6N6Fe---- H4L (2191)
 Hexacyanoferrate (II); $\text{Fe}(\text{II})(\text{CN})_6$ ----

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	gl	oth/un	25°C	0.10M	C	TIH	$K_1=2.66$ $B(\text{Ca}_2\text{Fe}(\text{CN})_6)=3.28$ $B(\text{CaHFe}(\text{CN})_6)=5.34$	1986CDc (3536)	97

Data for 10-35 C and 0.05-1.0 M CaCl_2 . $\text{DH}(K_1)=11.3 \text{ kJ mol}^{-1}$, $\text{DS}(K_1)=117 \text{ J K}^{-1} \text{ mol}^{-1}$; $\text{DH}(\text{Ca}_2\text{Fe}(\text{CN})_6)=8.8$, $\text{DS}=134$; $\text{DH}(\text{CaHFe}(\text{CN})_6)=15.9$, $\text{DS}=188$

Ca++ ISE oth/un 25°C 0.00 U H K1=3.68 1975JLa (3537) 98
DH=13.0 kJ mol-1

Ca++ EMF oth/un 25°C 3.0M U K1=2.10 1975LMd (3538) 99
Background salt: LiClO4

Ca++ ISE none 15°C 0.00 U T H K1=3.57 1974HIa (3539) 100
K1=3.60(20 C), 3.63(25 C), 3.65(30 C), 3.67(35 C). DH(K1)=8.4 kJ mol-1,
DS=105 J K-1 mol-1. At 25 C: I=0.07 DH(calorimetry)=8.8. I=0.0135, K1=2.85

Ca++ oth oth/un 25°C 0.0 U K1=3.59 1966NSa (3540) 101
Method:electrical migration or transference number.

Ca++ con none 25°C 0.0 U K1=3.77 1949JAa (3541) 102
K(Ca+CaL)=1.43

C6N6Fe--- H3L Ferricyanide (2491)
Hexacyanoferrate (III); Fe(III)(CN)6---

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

Ca++ cal oth/un 25°C 0.10M U K1=1.48 1982ARa (3616) 103

Ca++ EMF oth/un 25°C 3.0M U K1=0.59 1975LMd (3617) 104
Background salt: LiClO4

Ca++ ISE oth/un 25°C 1.30M U TI K1=2.850 1974HIa (3618) 105
At 15 C, I=0: K1=3.57; 20 C, I=0: 3.60

Ca++ ISE oth/un 25°C 0.00 U T K1=2.630 1974HIa (3619) 106
At 15 C: K1=2.60; 35 C: 2.66

Ca++ ISE none 15°C 0.00 U T H K1=2.60 1974HIa (3620) 107
K1=2.60(20 C), 2.63(25 C), 2.65(30 C), 2.66(35 C). DH(K1)=5.9 kJ mol-1
By calorimetry, I=0.07 M) DH(K1)=6.7

Ca++ sol oth/un 25°C 3.0M U K1=0.15 1967RMd (3621) 108
Medium: LiNO3

Ca++ con none 25°C 0.0 U K1=2.83 1952GMb (3622) 109

C6O3 L Benzenetrioxide CAS 264911-91-3 (6002)
cis-Benzenetrioxide;

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

Ca++ nmr alc/w 25°C 100% U K1=1.34 1987BBc (3697) 110

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

Chloride;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	ISE	NaNO3	25°C	0	C	TI		K1=0.42	1998RSa (4194)	111
Method: Cl-ISE, extrapolated to I=0										
Ca++	sol	none	600°C	0.00	C	T		K3=1.32	1995RBa (4195)	112
K(CaAl2Si2O8(s)+2HCl=CaCl2+SiO2(s)+H2O)=7.38 (400 C), 4.173 (500 C), 1.846 (600 C). Method: solubility of anorthite.										
Ca++	ISE	none	25°C	0	C	I		K1=0.43	1995RGa (4196)	113
I=0.16 (Me4N.X) K1=0.07.										
Ca++	cal	none	250°C	0.0	C	TIH		K1=1.85	1992GOa (4197)	114
Calculated from data for 0.24-1.0 m CaCl2. Data for 250-325 C. DH(K1)=82 kJ mol-1, DS(K1)=192 J K-1 mol-1.										
Ca++	con	none	20°C	0	C	TI		K1=0.468	1989PRa (4198)	115
Data for 0-90% CH3CN/H2O. Also data for 10 and 30 C.										
Ca++	sol	oth/un	150°C	var	U	TI		K1=-0.07 B2=0.24	1989WSa (4199)	116
100-360 C, I=0.3-3.0 M Cl-. Constants at I=0										
Ca++	con	alc/w	25°C	100%	C	TH		K1=2.61	1987DWa (4200)	117
Medium: MeOH, DH(K1)=20.6 kJ mol-1, DS(K1)=119 J K-1 mol-1										
Ca++	ISE	alc/w	25°C	100%	U			K1=2.48	1984DMa (4201)	118
Medium: MeOH, 0.05 M NaClO4										
Ca++	gl	KNO3	25°C	3.00M	U	T		K1=-0.17	1982MSb (4202)	119
K1=-0.28(15 C), K1=-0.2(45 C), K1=-0.09(65 C), K1=-0.01(85 C) DH=4.85 kJ mol-1, DS=12.1 J mol-1 K-1										
Ca++	vlt	NaClO4	20°C	1.00M	U			K1=1.44 B2=1.46 B3=1.66	1981TCa (4203)	120
Using convolution voltammetry										
Ca++	sol	oth/un	25°C	0.70M	C			K1=0.08	1975EWa (4204)	121
Mixed medium of NaCl, KCl, MgCl2, NaClO4, Mg(ClO4)2, Na2SO4. Method: solubility of gypsum.										
Ca++	EMF	NaNO3	25°C	0.10M	C	TH		K1=-0.11	1975SCd (4205)	122
Method: Ag,AgCl electrode. Data for 15-60 C. DH(K1)=-7.19 kJ mol-1, DS(K1)=-26.4 J K-1 mol-1.										
Ca++	con	non-aq	25°C	100%	U			K1=2.7	1974KKc (4206)	123
Medium: 50% w/w EtOH/acetone. K1=2.59 to 2.80(depending upon eqn)										

Ca++ ix NaClO4 ? 1.0M U K1=-0.22 1969PSa (4207) 124

Ca++ con non-aq 25°C 100% U I K2=10.39 1960SRb (4208) 125
Medium: 40% BuOH in C6H14. K2=18.41 (12.65% BuOH), 14.28 (25% BuOH)

ClO3- HL Chlorate CAS 7790-93-4 (971)
Chlorate;

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

Ca++ dis NaClO4 25°C 1.00M U H K1=-0.52 1992CKb (6024) 126
DH(K1)=-2.3 kJ mol⁻¹; DS=-18 J K⁻¹ mol⁻¹

ClO4- HL Perchlorate CAS 7001-90-3 (287)
Perchlorate;

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

Ca++ con mixed 25°C 20% C K1=0.72 2003SIa (6131) 127
Medium: 20% w/w propylene carbonate/ethylene carbonate.

Ca++ con non-aq 25°C 100% C K1=1.15 1992STa (6132) 128
Medium: propylene carbonate.

Ca++ con alc/w 30°C 100% C TIH K1=2.27 1990D0d (6133) 129
Medium: MeOH. DH(K1)=14.6 kJ mol⁻¹, DS=96 J K⁻¹ mol⁻¹. Also in MeOH/ethylene glycol mixtures (0, 20, 40, 60, 80, 100%)

Ca++ con alc/w 25°C 100% C T H K1=2.40 1987DWa (6134) 130
Medium: MeOH, DH(K1)=14.8 kJ mol⁻¹, DS(K1)= 96 J K⁻¹ mol⁻¹

Ca++ dis oth/un ? var U Kd(Ca+2L=CaL2(in TBP))=2.3 1968LGa (6135) 131

Medium:HL var. Kd=1.85(Sr), 1.62(Ba)

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

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

Ca++ kin oth/un 300°C 100% U Kso=-4.92(kinetic methods) 1958DIb (6469) 132
Kso=-3.77(solubility)

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

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

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

Ca++ sol NaCl 25°C 0.10M C I 2004GMa (6633) 133
 $K_{so}(\text{CaF}_2) = -9.870$
Spectrophotometric determination of fluoride. Data for 0.00074-0.73 m NaCl and artificial seawater. At I=0, $K_{so}(\text{CaF}_2) = -10.15$. CaF₂: fluorite.

Ca++ ISE none 25°C 0.0 C B2=5.7 2000FGa (6634) 134
Calculated from data for I=0.10 M (TISAB).

Ca++ ISE none 25°C 0.0 C 1993DPd (6635) 135
 $K_{so}(\text{CaF}_2) = -9.73$
Method: double membrane F ion selective electrode.

Ca++ ISE alc/w 25°C 100% C B2=13.7 1988TIa (6636) 136

Ca++ gl KNO3 25°C 3.00M U T H K1=0.68 1982MSb (6637) 137
K1=0.66(15 C), K1=0.76(45 C), K1=0.88(65 C), K1=0.99(85 C)
DH=5.43 kJ mol⁻¹, DS=31.4 J mol⁻¹ K⁻¹

Ca++ sol none 22°C 0.0 C 1981GNa (6638) 138
 $K_{so}(\text{CaF}_2) = -10.60$
Method: F- ion selective electrode.

Ca++ sol none 25°C 0.0 U T 1979RHb (6639) 139
 $K_{so} = -11.9$
Data also available for T=23 to 260.

Ca++ ISE alc/w 25°C 100% C I K1=3.64 1978BBc (6640) 140
Medium: MeOH, 0.05 M Et4NClO4. In H2O, 0.05 M NaClO4
K1=1.52, in 1.0 M K1=1.80. In 0.05 M Et4NClO4 K1=1.56

Ca++ ISE none 25°C 0.0 M 1977MBa (6641) 141
 $K_{so} = -10.51$

Ca++ ISE none 25°C 0.0 C 1977VKb (6642) 142
 $K_{so} = -10.45$
Ca and F ion selective electrodes.

Ca++ sol KCl 25°C 0.0 C K2=0.12 1976SBb (6643) 143
 $K_s(\text{CaF}_2) = \text{ca.} -11.2$
Method: fluoride ISE. Dissolution of CaF₂ in ca 0.6 M acetate buffer, pH 5.9. K_s is an apparent constant which varies with a(F) and a(Ca).

Ca++ sol none 25°C 0.0 U I 1974MNb (6644) 144
 $K_{so}(\text{CaF}_2(\text{s}) = \text{Ca} + 2\text{F}) = -10.66$
At 25 atm. $K_{so} = -10.36(410 \text{ atm}), -10.26(518 \text{ atm}), -10.20(690 \text{ atm}), -9.97(950 \text{ atm})$

Ca++ ISE NaClO4 25°C 1.0M U T K1=0.53 1971BHc (6645) 145
K1=0.43(2 C), 0.74(35 C)

Ca++ ISE NaNO3 25°C 1.0M U T H K1=0.57 1971CVa (6646) 146
DH(K1)=9.6 kJ mol⁻¹, DS=42.7 J K⁻¹ mol⁻¹. K1=0.52(15 C), 0.62(35 C)

Ca++ ISE NaCl 25°C 0.10M U I K1=0.82 1970ELd (6647) 147
K1=0.77(I=0.2), 0.70(I=0.4), 0.64(I=0.6), 0.63(I=0.7), 0.61(I=0.8), 0.59(I=1)

Ca++ ISE NaClO4 25°C 0.50M U K1=0.70 1969ALa (6648) 148

Ca++ ISE NaClO4 25°C 1.0M U T H K1=0.63 1968TWa (6649) 149
DH(K1)=15.9 kJ mol⁻¹, DS(K1)=66.9 J K⁻¹ mol⁻¹. K1=0.41(2 C), 0.79(39 C)

Ca++ cal NaClO4 25°C 1.0M U H 1968TWa (6650) 150
DH(K1)=14.6 kJ mol⁻¹, DS=62.8 J K⁻¹ mol⁻¹

Ca++ sol none 25°C 0.0 U 1962SEa (6651) 151
Kso(CaF2(fluorite))=-10.57

Ca++ sol non-aq 0°C 100% U 1961KCa (6652) 152
Kso(CaF2)=-2.82

Medium: liquid HF corrected to I=0

Ca++ EMF none 25°C 0.0 U I K1=<1.04 1955PAa (6653) 153
At I=0.5 M NaClO4 K1 < 0.51

Ca++ con none 18°C 0.0 U 1937JEa (6654) 154
Kso(CaF2)=-10.5

Ca++ sol none 25°C 0.0 U T 1925AUa (6655) 155
K(CaF2(s)+2H=Ca+2HF)=-2.76
Kso(CaF2)=-10.31

*Kso=-2.83 at 15 C

Ca++ con none 18°C 0.0 U T 1923B0a (6656) 156
Kso(CaF2,fluorspar)=-10.57

Kso=-10.75(0.05 C), -10.44(40 C). Kso=-10.47(18 C), 10.40(26 C) (p'ptation)

GeW11039----- H8L CAS 37369-86-1 (2466)

alpha-Heteromonogermanium-polytungstate;

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

Ca++ gl NaNO3 25°C 1.00M U K1=4.59 1984COa (7464) 157

H2NPO3-- H2L CAS 20171-51-1 (6306)

Amidophosphate; H2NPO3--. Also (H2N)2PO2-, (H2H)2POS-

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

Ca++ oth R4N.X 25°C 1.00M U TIH K1=4.59 1961ICa (7531) 158

K(Ca+HL)=3.15

Ligand:Imidodiphosphate,03PNHPO3 4-, Medium:Me4NBr,Method:tyndallometry,
 At I=0.1: K1=5.59,K(Ca+HL)=3.33; I=0: K1=6.07,K=3.4. DH(K1)=-23.8 kJ mol-1

 Ca++ oth R4N.X 25°C 1.00M U TIH K1=5.66 1961ICa (7532) 159
 K(Ca+HL)=4.16

Ligand:Diimidotriphosphate,P308(NH)2 5-, Medium:Me4NBr,Method:tyndallometry,
 At I=0.1 M: K1=6.74,K(Ca+HL)=4.44; I=0: K1=7.10, K=4.6. Also 37, 50 C

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

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

 Ca++ dis oth/un var U 1968LKa (7796) 160
 Kd(Ca+2I=CaI2(in TBP))=0.39

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

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

 Ca++ gl NaCl04 25°C 3.0M M I K1=-0.13 1995POa (8473) 161
 Kso=-4.671

At I=0: K=0.55

 Ca++ dis NaCl04 25°C 1.00M U H K1=0.52 1992CKb (8474) 162
 DH(K1)=2.6 kJ mol-1; DS=19 J K-1 mol-1

 Ca++ sol NaCl04 25°C 1.00M U K1=1.22 B2=1.84 1985KSb (8475) 163

 Ca++ sol NaCl04 25°C 0.50M U I 1974FRf (8476) 164
 Kso(CaL2(s))=-5.07

Medium: LiCl04; Kso=-4.89(I=1), -4.70(I=2), -4.84(I=3), -5.06(I=4)
 Kso=-6.00 (0 corr)

 Ca++ sol none 25°C 0.0 U T 1969Bma (8477) 165
 Kso(CaL2(H2O)6)=-6.16

Kso'(CaL2(H2O))=-5.57 (40 C)

Kso"(CaL2)=-5.39 (60 C)

Kso=-6.68(14 C), -6.28(22 C), -5.90(30 C), =5.55(38 C). Kso'=-5.48(47 C),
 -5.40(55 C); Kso"=-5.35(70 C), -5.29(79 C), -5.25(86 C)

 Ca++ sol none 25°C 0.0 U T 1953Bgb (8478) 166
 Kso(CaL2(H2O)6)=-6.15

I=0 corr. Kso=-7.54(0 C). Kso(CaL2.H2O)=-5.61(40 C)

 Ca++ sol none 25°C 0.0 U 1949DWa (8479) 167
 Kso(CaL2)=-6.15

 Ca++ con none 18°C 0.0 U K1=0.89 1938Wda (8480) 168

I=0 corr. By solubility, 25 C, Kso(CaL2)=-6.16

Ca++ sol none 25°C 0.0 U T 1934KIa (8481) 169
Kso(CaL2)=-6.13

I=0 corr. Kso=-6.48(18 C), -5.87(30 C)

Ca++ sol none 18°C 0.0 U T 1923B0a (8482) 170
Kso(CaL2)=-6.19

I=0 corr. Kso=-7.31(0 C), -6.65(10 C)

MoO4-- H2L Molybdate (443)

Molybdate;

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

Ca++ sp oth/un 25°C ? U M 1997STa (8702) 171
K(Ca+H2L=CaL+2H)=-2.8

Ligand: nano-Molibdenomanganate, MnMo9032-----

Ca++ sol oth/un 28°C var C I 1992FRa (8703) 172
Kso(CaMoO4)=-7.93

CaMoO4 is powellite. Analyses by ICP(Ca) and ICP-MS(Mo). Kso derived from solubility data up to 1.0 M CaCl2, Ca(NO3) and Na2MoO4.

Ca++ sol none 25°C 0.00 U T 1972ZMa (8704) 173
Kso(CaL2(s))=-8.36

Kso=-8.16(50 C), -8.00(75 C), -8.22(100 C), -8.3(150 C), -8.9(200 C), -9.6(250 C), -10.1(300 C)

Ca++ cal none 25°C 0.0 U H 1958MHa (8705) 174
DH(Kso(CaL))=-2.9 kJ mol-1, DS=-162.8 J K-1 M-1

Ca++ sol none 22°C 0.0 U 1958SSb (8706) 175
Kso(CaL)=-7.38

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

Ammonia

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

Ca++ dis oth/un 25°C 0.5M C TI K1=0.05 B2=-0.28 1990PSb (9050) 176
K3=-0.60

Medium: 0.5 M NH4ClO4; Also for I=1.5 K1=-0.12; K2=-0.49; K3=-0.76; K4=-1.0
For I= 1.0 K1=-0.03; K2=-0.42; K3=-0.69; K4=-0.93

Ca++ gl R4N.X 23°C 2.0M U K1=-0.2 B2=-0.8 1941BJa (9051) 177
K3=-0.8
K4=-1.1
K5=-1.3
K6=-1.7

Medium: NH4NO3.

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

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

Ca++ cal NaClO4 25°C 1.00M U TI K1=-0.22 1985VBa (9526) 178
DH1 = -7.56 kJ mol-1

Ca++ sp oth/un 25°C 5.80M U K1=0.52 B2=0.18 1980BDa (9527) 179

Ca++ sol NaClO4 25°C 0.50M U I K1=0.06 B2=-0.3 1974FRF (9528) 180
Medium: LiClO4. K1=-0.06,B2=-0.5(I=1). K1=-0.02,B2=-0.4(I=2). K1=0.04,
B2=-0.4,B3=-1.1(I=3). K1=0.08,B2=-0.4,B3=-0.7(I=4). θ corr:K1=0.68, B2=0.65

Ca++ con non-aq 25°C 100% U K1=2.75 1974KKc (9529) 181
Medium: 1:1 EtOH/Me2CO K1=2.64 to 2.89 depending upon equation

Ca++ ix NaClO4 25°C 1.0M U K1=-0.22 1969PSa (9530) 182

Ca++ oth oth/un 25°C 0.0 U K1=0.6 1966MBb (9531) 183

Ca++ ix mixed 23°C 90% U K1=0.57 B2=0.85 1966WFa (9532) 184
Medium: 90% i-PrOH, 0.5 M HL

Ca++ oth R4N.X 94°C 25.0M U T K1=-0.85 1964HPb (9533) 185
Method:Raman spectra. Medium:10-40 M NH4ClO4. K1=0.78(26 C), -0.82(48, 70 C)

Ca++ con oth/un 25°C 0.0 U T H K1=0.31 1963VWa (9534) 186
Medium: θ corr. K1=0.41(18 C). DH(K1)=-23.8 kJ mol-1, DS=-75 J K-1 mol-1

Ca++ oth oth/un 26°C var U H K1=-0.8 1962HEa (9535) 187
Method: Raman spectra., Medium:2-13 M CaL2. DH(K1)=0

Ca++ con oth/un 18°C 0.0 U K1=0.28 1930RDa (9536) 188

N2H4 L Hydrazine CAS 302-01-2 (2117)
Hydrazine; H2N.NH2

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

Ca++ dis oth/un 25°C 0.80M U K1=-0.16 B2=-1.80 1954SEa (10069) 189
K3=-1.11

Medium: Ca(NO3)2

OH- HL Hydroxide (57)
Hydroxide;

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

Ca++ oth none 25°C 0.0 U K1=1.15 B2= 3.14 1998GLa (10751) 190
Calculated from literature data. Kso(Ca(OH)2)=-5.35

Ca++ sol none 400°C 0.00 C T K1=1.87 1995Rba (10752) 191
Method: solubility of anorthite.
At 500 C, K1=6.21; at 600 C, K1=9.55

Ca++ sol oth/un 200°C var U T *K1=-8.20 1991SSa (10753) 192
100-350 C.P=500 bars. Constants at I=0

Ca++ oth none 0°C 0.0 U K1=1.22 1987BSb (10754) 193
Calculated values

Ca++ sol oth/un 300°C var U T *Kso=13.45 1986WAa (10755) 194
300-600 C, P=1-3 kbar. Constant at I=0

Ca++ gl KNO3 25°C 0.15M C I K1=0.99 1983DDa (10756) 195

Ca++ gl NaClO4 25°C 3.00M U *K1=-13.36 1973FJa (10757) 196
Kw=-14.22

Ca++ gl none 25°C 0.00 U T K1=1.301 1972Mva (10758) 197
K1=2.796(60 C), 3.056(70 C), 3.503(80 C), 3.564(90 C), 3.876(98 C).
K1=14.36-3877/T

Ca++ gl KNO3 37°C 0.15M U *K1=-11.7 1970CHc (10759) 198

Ca++ oth none 0°C 0.0 U T Kso=-4.97 1968KRa (10760) 199
Method:Estimated data.Temp Range 0-350.Kso=-5.24(50C), -6.00(100C), -6.98(150C),
-8.00(200C), -9.31((250C), -10.60(300C), -11.94(350C)

Ca++ sol none 0°C 0.0 M T H Kso=-4.88 1967YMa (10761) 200
Kso=-5.03(25 C), -5.25(50 C), -5.83(100C), -6.57(150C), -7.43(200C), -8.37(250C),
-9.38(300 C), -10.45(350 C). DH(Kso)=-12.5(25 C), -131.25(300 C) kJ mol-1

Ca++ gl oth/un 75°C ? U *K1=-10.3 1965CTa (10762) 201
Ks=-1 to -1.3
Medium: Ca(NO3)2(H2O)4. Ks: K(0.5Ca(OH)2(s)+0.5Ca=CaOH)

Ca++ cal none 25°C 0.0 M H 1965Hwd (10763) 202
DH(Kso)=-18.2 kJ mol-1, DS=-160 J K-1 mol-1. DH(K1)=8.4

Ca++ EMF NaClO4 25°C 3.0M C K1=0.64 1961COd (10764) 203

Ca++ EMF none 25°C 0.0 C T K1=1.2 1959BBc (10765) 204
K1=1.02-1.14(0 C),1.12-1.24(10 C),1.36-1.45(40 C). Method: H electrode

Ca++ kin none 25°C 0.0 U K1=1.46 1956BPa (10766) 205

Ca++ EMF none 25°C 0.0 C T H K1=1.37 1954GMb (10767) 206
DH(K1)=5.2 kJ mol⁻¹, DS(K1)=47.3(25 C); K1=1.34(15 C), 1.40(35 C).
Method: H electrode

Ca++ sol none 25°C 0.0 U T H K1=1.40 1953BGb (10768) 207
DH(K1)=5.0 kJ mol⁻¹, DS(K1)=43.5(25 C); K1=1.37(0 C), 1.48(40 C)

Ca++ sol none 25°C 0.0 U K1=1.30 1951DHa (10769) 208

Ca++ sol none 0°C 0.0 U K1=1.3 1950BWa (10770) 209
By kinetics K1=1.3

Ca++ kin oth/un 25°C 0.02M U I K1=0.96 1949BPb (10771) 210
Medium:0.02-0.04 M. At I=0 corr K1=1.29

Ca++ sol none 25°C 0.0 U K1=1.51 1938DAa (10772) 211

Ca++ sol none 25°C 0.0 U K1=1.40 1934KIa (10773) 212
Kso(Ca(OH)2)=-5.26

Ca++ sp oth/un 18°C var U K1=1.07 1923KOa (10774) 213

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

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

Ca++ gl NaNO3 25°C 0.10M M K(Ca+HL)=1.64 1996SSa (12995) 214

Ca++ gl NaClO4 25°C 0 M I K1=0.96 B2=1.69 1995POa (12996) 215
In 3.0 M NaClO4: K1=0.40, B2=0.6

Ca++ oth NaCl 25°C 0.15M U T K1=1.3 1993GMa (12997) 216
Method: Coulometric titration. K1=1.4 (37 C)

Ca++ gl NaClO4 25°C 3.0M M I 1991CIa (12998) 217

K(Ca+2H2L)=0.33
K(Ca+2H2L=CaHL+H3L)=-3.61
K(Ca+3H2L=CaH3L2+H3L)=-2.98

In 0 M (extrapolation using SIT): K(Ca+2H2L)=1.36, K(Ca+HL)=2.54,
K(Ca+H2L+HL)=3.18

Ca++ gl oth/un 37°C 0.00 M I K1=6.13 1991ZEa (12999) 218
K(Ca+HL)=2.77
K(Ca+H2L)=1.44

Ca++ gl KCl 37°C 0.15M C 1985DSa (13000) 219
K(Ca+HL)=1.94
K(Ca+H+HL)=7.90

Ca++ gl R4N.X 37°C 0.10M C I 1982DRc (13001) 220
K(Ca+H2PO4)=1.11
K(Ca+HPO4)=2.02

Additional method: Ca ion selective electrode. Data for 0.03-0.50 M Et4NI.
At I=0.0 M, K(Ca+H2PO4)=1.52.

Ca++ ISE NaCl 25°C 0.10M U I 1979CMb (13002) 221
K(Ca+HPO4)=1.87

Ca++ oth none 25°C 0.0 U 1977VLa (13003) 222
B(Ca3L2)=28.92

Ca++ gl oth/un 25°C 0.68M C K1=4.98 1976ACc (13004) 223
K(Ca+HPO4)=1.25
K(Ca+H2PO4)=0.24

Medium: NaCl/CaCl2 and KCl/CaCl2 mixtures.

Ca++ sol none 25°C 0.0 U 1976BAc (13005) 224
Kso(CaHL(H2O)2)=-6.55

Ca++ gl NaClO4 25°C 0.10M U M 1975RMa (13006) 225
K(Ca+HPO4)=6.27
K(Ca+citrate+HPO4)=10.72
K(Ca+Cys+HPO4)=8.49
K(Ca+NTA+HPO4)=14.50

Ca++ sol none 25°C 0.0 U T 1974GMe (13007) 226
Kso=-28.921. -29.012(5 C), -28.775(15 C), -29.548(37 C).
Kso=-45723.26/T+287.4536-0.54763*T (Beta-Ca3(P04)2)

Ca++ sol none 25°C 0.0 U 1974PGa (13008) 227
Kso(Ca(HL)(H2O)2)=-6.60(brushite)

Ca++ sol none 5°C 0.0 U T H 1971MBb (13009) 228
K'(Ca+H2L)=0.7
K''(Ca+HL)=2.38
DH(K')=15.0 kJ mol⁻¹, DS=67 J K⁻¹ mol⁻¹; DH(K'')=13.8, DS=96.0
K''=2.28(15 C), 2.58(25 C), 2.59(37 C). Kso(CaHL)=-6.71. 37 C: -7.04. DH=-17

Ca++ gl KNO3 37°C 0.15M U 1970CHc (13010) 229
K(Ca+H2L)=0.6
K(Ca+HL)=1.3

						$K(\text{CaH}_2\text{L}+\text{HL})=2.5$	
						$K(2\text{CaHL}=(\text{CaHL})_2)=3.7$	
Ca++	sol none	25°C	0.0	U T			1970GMg (13011) 230
						$K'(\text{Ca}+\text{H}_2\text{L})=0.6$	
						$K''(\text{Ca}+\text{HL})=2.41$	
						$K'=1.00, K''=2.67(5\text{ C}). 0.75, 2.44(15\text{ C}). 0.6, 2.61(37.5\text{ C}). K_{\text{so}}(\text{Ca}(\text{HL})(\text{H}_2\text{O})_2)=-6.63(5\text{ C}); -6.60(15\text{ C}), -6.59(25\text{ C}), -6.63(37.5\text{ C})$	
Ca++	gl none	37°C	0.0	U			1970MAa (13012) 231
							$K_{\text{so}}(\text{Ca}(\text{HL})(\text{H}_2\text{O})_2)=-6.646$
						$K(\text{Ca}_4\text{HL}_3(\text{H}_2\text{O})_3(\text{s})+2\text{H}=4\text{Ca}+3\text{HL})=-11.59$	
Ca++	sol none	25°C	0.0	U			1969MNa (13013) 232
							$K_{\text{so}}(\text{Ca}(\text{HL})(\text{H}_2\text{O})_2)=-6.68$
Ca++	gl oth/un	25°C	0.0	U T H		$K_1=6.46$	1968CMc (13014) 233
						$K(\text{Ca}+\text{H}_2\text{L})=1.41$	
						$K(\text{Ca}+\text{HL})=2.74$	
						Medium:0 corr. $K(\text{Ca}+\text{H}_2\text{L})=1.50(37\text{ C}), \text{DH}=14.2\text{ kJ mol}^{-1}, \text{DS}=75.2\text{ J K}^{-1}\text{ mol}^{-1}$	
						$K(\text{Ca}+\text{HL})=2.83(37\text{ C}), \text{DH}=13.8, \text{DS}=96.1, K_1=6.54(37\text{ C}), \text{DH}(K_1)=13.0, \text{DS}=167.2$	
Ca++	oth oth/un	37°C	0.0	U		$K_1=6.3$	1967WBa (13015) 234
Ca++	sol oth/un	38°C	0.0	U			1966MGb (13016) 235
						$K_{\text{s}}(\text{CaHL}(\text{H}_2\text{O})_2)=-6.66$	
						$K(\text{Ca}+\text{H}_2\text{L})=0.87$	
						$K(\text{Ca}+\text{HL})=2.77$	
Ca++	sol oth/un	40°C	0.0	U			1964DRb (13017) 236
						$K_{\text{s}}(\text{Ca}_2(\text{HL})(\text{H}_2\text{O}))=-28$	
						K_{s} for "surface complex" on surface of hydroxyapatite, $\text{Ca}_5\text{L}_3\text{OH}(\text{s})$	
Ca++	sol none	18°C	0.0	U T			1964PCa (13018) 237
						$K_{\text{s}}(\text{CaHL}(\text{H}_2\text{O})_2=\text{Ca}+\text{HL}+2\text{H}_2\text{O})=-6.57(18\text{ C}), -6.62(37\text{ C}).$	
						Solubilities of other mixed Cu/HL/H ₂ O complexes, 18 to 37 C	
Ca++	EMF oth/un	18°C	dil	U			1963GRb (13019) 238
						$K(\text{Ca}+\text{HPO}_4)=2.6$	
						$K(\text{CaPO}_4+\text{H})=8.5$	
						Methods: H electrode, quinhydrone electrode.	
Ca++	sol none	25°C	0.0	U M			1962FEa (13020) 239
						$K_{\text{so}}(\text{Ca}_{10}\text{L}_6\text{F}_2)=-120.86$	
Ca++	sol NaCl	24°C	0.17M	U			1962MEa (13021) 240
						$K_{\text{so}}(\text{Ca}_2(\text{HL})(\text{OH})_2)=-27.0$	
						Surface complexes. $K_{\text{s}}(\text{Ca}_5\text{L}_3(\text{OH})(\text{s})+3\text{H}_2\text{O}=2\text{Ca}_2(\text{HL})(\text{OH})_2(\text{surface})+\text{Ca}+\text{HL})=-8.52$	
Ca++	sol none	25°C	0.0	U T			1962RDa (13022) 241

$$K_{so}(\text{Ca}_2(\text{HL})(\text{OH})_2) = -27.3$$

Solubility of hydroxyapatite determined by surface complex $\text{Ca}_2\text{HL}(\text{OH})_2$
 $K_{so} = -25.1(40\text{ C})$

Ca++	gl	oth/un	21°C	0.08M	U		1961BMb (13023)	242
							$K_s(\text{Ca}_4\text{HL}_3=4\text{Ca}+\text{H}+3\text{L}) = -40.92(\text{gr})$	
							$K_s = -37.83$ (gelatinous)	
Ca++	sol	none	25°C	0.0	U		1960MBA (13024)	243
							$K_{so}(\text{Ca}(\text{HL})(\text{H}_2\text{O})_2) = -6.56$	
							$K_s(\text{Ca}_4\text{HL}_3=4\text{Ca}+\text{H}+3\text{L}) = -46.90$	
							$K_s(\text{Ca}_4(\text{HL})_3\text{H}-2) = -9.93$	
Ca++	sol	none	90°C	0.0	U		1960MMA (13025)	244
							$K_{so}(\text{Ca}(\text{HL})) = -7.9$	
Ca++	cal	none	25°C	0.0	U	HM	1957ELa (13026)	245
							$\text{DH}(K_{so}(\text{Ca}(\text{H}_2\text{L})_2(\text{H}_2\text{O}))) = -12 \text{ to } -16 \text{ kJ mol}^{-1}$	
Ca++	sol	none	25°C	0.0	U		1957SNa (13027)	246
							$K_{so}(\text{Ca}(\text{HL})(\text{H}_2\text{O})_2) = -6.57$	
Ca++	gl	R4N.X	25°C	0.20M	U		1956SAa (13028)	247
							$K(\text{Ca}+\text{HL}) = 1.70$	
							Medium: Pr4NCl	
Ca++	sol	none	25°C	0.0	U		1955CLa (13029)	248
							$K_{so}(\text{Ca}_5\text{L}_3(\text{OH})) = -57.8$	
Ca++	sol	none	25°C	0.0	U		1953DHa (13030)	249
							$K(\text{Ca}+\text{HL}) = 2.70$	
							$K(\text{Ca}+\text{H}_2\text{L}) = 1.08$	
							$K(\text{CaHL}+\text{H}) = 5.59$	
Ca++	ix	NaCl	37°C	0.15M	U		1953GCa (13031)	250
							$K(\text{Ca}+\text{HL}) = 1.86$	
Ca++	sol	oth/un	18°C	var	U T		1951ZAa (13032)	251
							$K_{so}(\text{Ca}_5\text{L}_3(\text{OH})) = -44.51$	
							$K_{so} = -40.64(40\text{ C})$	
Ca++	sol	oth/un	18°C	var	U		1951ZHa (13033)	252
							$K_{so}(\text{Ca}_3\text{L}_2) = -28.70$	
Ca++	sol	none	25°C	0.0	U		1950FAa (13034)	253
							$K_s(\text{Ca}(\text{H}_2\text{L})_2(\text{s}) = \text{Ca}+2\text{H}_2\text{L}) = -1.14$	
							$K_s(\text{CaHL}(\text{s}) = \text{Ca}+\text{HL}) = -6.66$	
							$K_{so}(\text{Ca}_5\text{L}_3\text{OH}) = -55.91$	
Ca++	sol	NaCl	22°C	0.16M	U	M	1945GRa (13035)	254

B(Ca₂(HL)(HCO₃)H-1)=1.33
 K(Ca₂LCO₃+H)=8.3

 Ca++ EMF KCl 25°C 0.20M U I 1940GRa (13036) 255

K(Ca+HL)=1.50

Method: H electrode. K=2.20 (glass electrode, 22 C, I=0.006 M)

 Ca++ sol none 40°C 0.0 U 1931LUB (13037) 256

Ks(CaHL(s)=Ca+HL)=-6.56

 Ca++ sol oth/un 19°C dil U 1925DSa (13038) 257

Ks(CaHL(s)=Ca+HL)=-6.25

 Ca++ sol none 38°C 0.0 U 1925HMa (13039) 258

Kso(Ca₃L₂)=-32.5

Ks(CaHL(s)=Ca+HL)=-6.4

 Ca++ sol oth/un 25°C var U 1917BAa (13040) 259

Kso(Ca₃L₂)=-25

Ks(CaHL(s)=Ca+HL)=-5.3

 PW11039----- H7L (2467)

alpha-Heteromonophospho-polytungstate;

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

 Ca++ gl NaNO₃ 25°C 1.00M U K1=3.84 1984COa (13396) 260

 P206---- H4L Hypophosphate CAS 9803-60-3 (199)

Hypophosphate;

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

 Ca++ gl R4N.X 25°C 0.50M U K1=2.27 1967CMc (13412) 261

Ligand: O3POPHO2---. Medium: Me4NCl

 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

 Ca++ ISE NaCl 25°C 0.10M U K1=4.33 B2=7.21 1979Cmb (13528) 262

 Ca++ kin R4N.X 30°C 0.10M U K1=5.23 1978KHa (13529) 263

Medium: 0.10 M NH₄NO₃

 Ca++ sol oth/un ? var U I 1971WIa (13530) 264

B(Ca₂L)=2.80

Kso=-12.87

Ca++ oth R4N.X 25°C 1.00M U TI K1=4.89 1960ICa (13531) 265
 K(Ca+HL)=2.22
 Medium: Me4NBr, Method:tydallometry. K1=4.63(37 C), 4.31(50 C). In 0.1 M:
 25 C: K1=5.39, K(Ca+HL)=3.32. K1=5.44(37 C), 5.39(50 C).

Ca++ oth none 25°C 0.0 U TIH K1=5.60 1960ICa (13532) 266
 K(Ca+HL)=3.6
 I=0 corr. Method: tydallometry. K1=5.75(37 C), 5.86(50 C).
 DH(K1)=19.2 kJ mol⁻¹, DS=192 J K⁻¹ mol⁻¹

Ca++ gl R4N.X 25°C 1.00M U K1=5.55 1959WLa (13533) 267
 K(Ca+HL)=2.28
 Medium: Me4NCl

Ca++ gl R4N.X 25°C 1.00M U K1=4.95 1959WLa (13534) 268
 K(Ca+HL)=2.30
 Medium: Me4NCl

Ca++ gl none 25°C 0.0 U T K1=6.8 1959W0a (13535) 269
 B(Ca(OH)L)=8.9
 Ks(Ca+CaL)=-7.9
 At 40 C: K1=6.5, Ks=-7.9

Ca++ sp oth/un 19°C var U K1=5.00 1956YVb (13536) 270

Ca++ ix NaCl 37°C 0.15M U K1=3.7 1953GCa (13537) 271
 Method: cation exchange at pH 7.4

 P208---- H4L CAS 13825-81-5 (2402)
 Peroxodiphosphate, also cyclic metaposphates, thiophosphates etc.;

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

Ca++ ix NaCl04 20°C 0.05M U I K1=3.75 1974K0a (13684) 272
 Ligand:metaphosphate,cyclic;(PO3)4 4-, Additional ionic strength:
 K1=3.28(I=0.10),2.98(I=0.15),2.90(I=0.20),5.1(I=0)

Ca++ ix NaCl04 20°C 0.05M U I K1=5.13 1974K0a (13685) 273
 Ligand:metaphosphate,cyclic;(PO3)6 6-, Additional ionic strength:
 K1=4.59(I=0.10),4.31(I=0.15),4.11(I=0.20),6.9(I=0)

Ca++ ix NaCl04 20°C 0.05M U I K1=5.79 1974K0a (13686) 274
 Ligand:metaphosphate,cyclic;(PO3)8 8-, Additional ionic strength:
 K1=5.18(I=0.10),4.84(I=0.15),4.62(I=0.20),8.1(I=0)

 P2W17061----- Polytungstate (2102)
 alpha-Heterodiphospho-polytungstate (usually alpha1 isomer)

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

Ca++ gl NaNO3 25°C 1.00M U K1=2.96 1984COa (13704) 275
 K1=3.89 (alpha2 isomer)

P3010----- H5L CAS 10380-08-2 (1001)

Tripolyphosphate; from (HO)2PO.O.PO(OH).O.PO(OH)2

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

 Ca++ ISE NaCl 25°C 0.10M U K1=5.05 B2=9.41 1979Cmb (13795) 276

Ca++ kin oth/un 30°C 0.10M U I K1=5.69 1978KHa (13796) 277

Ca++ cal oth/un 25°C var C H K1=6.4 1977RLb (13797) 278
 K(Ca+CaL)=3.0
 K(Ca2L+Na)=4.0

Medium 0.02 M CaCl2 or Na5P3010. DH(K1)=14.2 kJ mol⁻¹, DS=172 J K⁻¹ mol⁻¹.
 DH(Ca+CaL)=-6.28, DS(Ca+CaL)=38. DH(Ca2L+Na)=33.5, DS(Ca2L+Na)=188.

 Ca++ gl KNO3 25°C 0.10M U T H K1=4.80 1973TRa (13798) 279
 K(Ca+HL)=3.28

At 2 C: K1=5.80, K(Ca+HL)=3.00; 35 C: K1=5.74, K=3.34. DH(K1)=-27.6 kJ mol⁻¹
 DH(Ca+HL)=-3.3

 Ca++ gl KNO3 45°C 0.10M U K1=4.73 1971TRa (13799) 280
 K(Ca+HL)=3.07

 Ca++ gl R4N.X 20°C 0.10M U H K1=6.31 1965ANa (13800) 281
 K(Ca+HL)=4.02
 K(CaL+H)=6.54

Medium: Me4NNO3. By calorimetry: DH(K1)=13.8 kJ mol⁻¹, DS=167 J K⁻¹ mol⁻¹

 Ca++ gl KCl 25°C 0.10M U K1=5.20 1964EMb (13801) 282
 K(Ca+HL)=3.04
 K(CaL+H)=5.90

 Ca++ gl R4N.X ? 0.10M U K1=4.6 1962RKa (13802) 283
 K(Ca+HL)=3.3

Medium: K,NH4Cl

 Ca++ oth R4N.X 25°C 1.00M U TIH K1=5.36 1960ICa (13803) 284
 K(Ca+HL)=3.30
 K(Ca+H2L)=2.77

Medium: Me4NBr. K1=5.25(37 C), 5.18(50 C). In 0.1 M, 25 C: K1=6.41, K(Ca+HL)
 =3.78. I=0 corr: K1=6.90, 6.80(37 C), 6.72(50 C). DH(K1)=-13 kJ mol⁻¹, DS=88

 Ca++ gl R4N.X 25°C 1.00M U K1=5.44 1959WLa (13804) 285
 K(Ca+HL)=3.01

Medium: Me4NCl

 Ca++ gl none 25°C 0.0 U T K1=8.1 1959WOa (13805) 286

B(Ca(OH)L)=10.4

At 40 C: K1=7.8, B(Ca(OH)L)=9.8

Ca++	gl	KCl	20°C	0.10M	U		K1=4.95 K(Ca+HL)=3.1	1956MSa (13806)	287
Ca++	sol	oth/un	30°C	var	U T		K1=6.51	1954QUa (13807)	288
		K1=6.68(60 C)							
Ca++	ix	NaCl	37°C	0.15M	U			1953GCa (13808)	289
						Keff(Ca+HL)=4,32 pH 7.4			
Ca++	sol	oth/un	25°C	0.02M	U		K1=6.41	1949TOa (13809)	290

P309---		H3L				CAS 13566-25-1 (235)			
Cyclotrimetaphosphate;									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	ix	NaCl04	20°C	0.10M	U	I	K1=2.06	1974K0a (13934)	291
Ionic strength from 0 (K1=3.4) to 0.2 (K1=1.81)									
Ca++	ISE	R4N.X	25°C	1.00M	U		K1=1.64	1969WKa (13935)	292
Medium:Me4NCl									
Ca++	sp	R4N.X	?	0.10M	U		K1=1.68	1962RKa (13936)	293
Medium: NH4Cl									
Ca++	ix	NaCl	37°C	0.15M	U			1953GCa (13937)	294
						K1eff=2.50 at pH 7.4			
Ca++	sol	none	25°C	0.0	U		K1=3.48	1949DMa (13938)	295
Ca++	con	none	25°C	0.0	U		K1=3.45	1949JMa (13939)	296

P4012----		H4L				CAS 13598-74-8 (234)			
Cyclotetrametaphosphate;									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	ix	NaCl04	20°C	0.10M	U	I	K1=3.28	1974K0a (13986)	297
Ionic strength from 0 (K1=5.1) to 0.20 (K1=2.90)									
Ca++	ISE	R4N.X	25°C	1.00M	U		K1=3.10	1969WKa (13987)	298
Medium: Me4NCl. Polarography also used									
Ca++	sp	R4N.X	?	0.10M	U		K1=3.77	1962RKa (13988)	299
Medium: NH4Cl									
Ca++	ix	NaCl	37°C	0.15M	U			1953GCa (13989)	300

K1eff=3.66 pH 7.4

Ca++ con none 25°C 0.0 U K1=5.42 1950JMb (13990) 301
K(CaL+Ca)=2.70
B(CaNaL)=5.7

By solubility K1=5.32, K(CaL+Ca)=2.60

Ca++ sol none 25°C 0.0 U K1=4.89 1949DMa (13991) 302
K(CaL+Ca)=2.66

P4013----- H6L Tetraphosphate (1102)

Tetraphosphate;

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

Ca++ kin oth/un 30°C 0.10M U K1=7.11 1978KHa (14037) 303

Ca++ ISE R4N.X 25°C 1.00M U K1=5.45 1969WKa (14038) 304
K(Ca+CaL)=3.35
K(Ca+HL)=3.31

Medium: Me4NCl

Ca++ gl R4N.X 25°C 1.0M U K1=5.46 1968WMc (14039) 305
K(Ca+HL)=3.54
K(Ca+CaL)=3.07

Medium: Me4NCl

P6012----- H6L CAS 25268-83-1 (6590)

Dodecaoxohexaphosphate(III); anion of (PO.OH)₆

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

Ca++ sp R4N.X 25°C 0.10M C K1=8.8 1999Nwa (14055) 306
Method: competition with EDTA. Medium: 0.10 M Me4NCl, pH 7.

P6018----- H6L (233)

Cyclohexametaphosphate;

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

Ca++ ix NaCl04 20°C 0.10M U I K1=4.59 1974K0a (14067) 307
Ionic strength from 0 (K1=6.9) to 0.23 (K1=2.62)

P8024----- H8L (232)

Cyclooctametaphosphate;

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

Ca++ ix NaCl04 20°C 0.10M U I K1=5.18 1974K0a (14079) 308
Ionic strengths from 0 (K1=8.1) to 0.23 (K1=3.65)

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

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

Ca++ oth none 25°C 0 U 1988LIa (14265) 309

Kso(CaS)=-6.1
*Kso(CaS)=11.2

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

S03-- H2L Sulfite CAS 7782-99-2 (801)
Sulfite;

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

Ca++ sol oth/un RT 0.0 C I K1=2.62 1991RFb (15424) 310

Kso(CaS03.0.5H2O)=-6.64

Calculated from data for 0.0002 to 0.4 M CaCl2 using Pitzer model.

Ca++ sol oth/un ? ? U K1=2.62 1990RFb (15425) 311

Ca++ sol NaCl04 25°C 3.50M U TI 1958FNa (15426) 312

Kso(CaL)=-5.04

Molality units. Kso=-5.05(35 C), -5.57(75 C). At I=1.0: Kso=-4.80(25 C),
-4.87(35 C), -5.17(75 C)

Ca++ sol NaCl04 25°C 3.50M U TI 1958NRa (15427) 313

Kpso=-0.52

Molality units. Kpso: CaL(H2O)0.5+S02(g)+0.5H2O=Ca+2HL. Kpso=-0.91(35 C),
-1.89(75 C). At I=1.0: Kpso=0.09(25 C), -0.26(35 C), -1.30(75 C)

Ca++ sol NaCl04 25°C 1.0M U TI 1958RBa (15428) 314

Kso(CaL)/Kso(CaS04)=-1.88

Molality units. Kso(CaL)/Kso(CaS04)=-1.96(35 C), -2.23(75 C). At I=0 corr.,
25 C: Kso(CaL)=-6.5

Ca++ sol none 25°C 0.0 U 1923BIa (15429) 315

Kso(CaL)=-7.17

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

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

Ca++ oth none 25°C 0.0 C H 1990RAd (15802) 316

Kso(CaS04)=-4.265

K(CaS04.2H2O)=-4.597

Literature review. CaS04: anhydrite; CaS04.2H2O: gypsum. Data for 0-300C
(anhydrite) and 0-120C (gypsum).

Ca++ sol none 25°C 0.0 U K1=2.35 1985LDb (15803) 317

Ca++ oth none 25°C 0.00 U 1985LMa (15804) 318
Kso(CaSO4.H2O)=-4.59
Kso(CaSO4)=-4.36

Derived from literature data. CaSO4.H2O: gypsum. CaSO4: anhydrite.

Ca++ oth none 25°C 0.0 C H K1=2.19 1981YYa (15805) 319
Calcd from published osmotic coefficient data. From UV-spectrometry
(competition with Cu), K1=2.12. From conductivity, DH(K1)=5.92 kJ mol⁻¹

Ca++ ISE NaCl 25°C 0.10M U K1=1.39 1979CMb (15806) 320

Ca++ ISE NaCl 25°C 0.70M C I K1=1.40 1979EWa (15807) 321
Medium: NaCl/Na2SO4/CaCl2 mixtures. Method: Ca ISE.

Ca++ con none 25°C 0.0 C T K1=2.35 1979FFc (15808) 322
Data for 10-30 C. Also data at 1000 and 2000 atm.
K expressed on molal scale.

Ca++ ISE none 25°C 0.0 M T H K1=2.29 1978EFb (15809) 323
Method: divalent cation electrode, dil NaCl medium. At 15 C, K1=2.24; at
at 35 C, K1=2.34. DH(K1)=9.20 kJ mol⁻¹, DS=75 J K⁻¹ mol⁻¹.

Ca++ con mixed 25°C ? U T H K1=2.17 1976KAa (15810) 324
K1=2.10 (0 C); 2.16 (20 C); 2.20 (30 C); 2.25 (40 C); 2.27 (45 C)
Medium: Water-ethylene glycol mixture

Ca++ sol oth/un 25°C 0.70M C K1=1.49 1975EWa (15811) 325
Kso(CaSO4)=-3.54
Mixed medium of NaCl, KCl, MgCl2, NaClO4, Mg(ClO4)2, Na2SO4.
Method: solubility of gypsum.

Ca++ sp none 25°C 0.0 C K1=2.03 1975YYa (15812) 326
By vapour pressure osmometry, K1=2.13

Ca++ ISE oth/un 25°C ? U K1=2.370 1974HIa (15813) 327

Ca++ EMF oth/un 25°C 0.0 U T H K1=2.31 1973AIa (15814) 328
K1=2.38(40 C), 2.44(50 C). DH(K1)=6.3(25 C) to 13(50 C).

Ca++ sol NaClO4 0°C 0.47M U TI K1=1.13 1973KYa (15815) 329
K1=0.90(I=1.95), 0.77(I=5.88). Kso(CaSO4(H2O)2)=-3.38(I=0.47), -3.116(I=1.95),
-3.693(I=5.88)

Ca++ sol NaClO4 25°C 0.47M U TI K1=1.12 1973KYa (15816) 330
K1=0.94(I=2.01), 0.86(I=5.92). Kso(CaSO4(H2O)2)=-3.33(I=0.47), -3.64(I=5.92)
Data also at 150, 250, 350 C

Ca++ cal oth/un 25°C 0.0 U H 1973POa (15817) 331
DH(K1)=7.7-8.0 kJ mol⁻¹

Ca++ con none 15°C 0.0 U T K1=2.15 1972ISa (15818) 332
At p=200 kg/cm². K1=2.11(p=400), 2.09(p=600), 2.00(p=800), 1.92(p=1200).
Also to 40 C. DH=19.6 kJ mol⁻¹

Ca++ oth none 25°C 0.0 C K1=2.49 B2= 2.31 1972PIa (15819) 333
Calculated from published osmotic coefficient data.

Ca++ sol NaNO₃ 25°C 0.50M U I K1=0.76 1972YMa (15820) 334
K1=0.26(I=2.1), 0.13(I=6). In LiCl: K1=0.79(I=0.5), 0.61(I=2.1), 0.43(I=6).
Also Na₂SO₄-NaCl and Li₂SO₄-LiNO₃ mixtures

Ca++ sol oth/un 0°C 0.0 U T 1970GGb (15821) 335
Kso(CaSO₄(H₂O)₂)=-4.68(0 C), -4.62(20 C), -4.67(40 C), -4.76(60 C), -4.89(80 C),
-5.06(100 C), -5.18(110 C). Kso(CaSO₄)=-5.46(100 C), -6.43(150 C), -7.43(200 C)

Ca++ cal none 25°C 0.0 C H 1970LAe (15822) 336
DH(K1)=6.3 kJ mol⁻¹, DS(K1)=65.3 J K⁻¹ mol⁻¹.
Method: heat of dilution measurements.

Ca++ ISE oth/un 25°C 0.0 U K1=2.23 1970LNd (15823) 337
By solubility: Kso(CaSO₄)=-4.6(25 C)

Ca++ sol NaClO₄ 25°C 0.20M U K1=1.54 1969DIa (15824) 338
Kso=-3.78

Ca++ ISE oth/un 30°C 0.0 U 1969GSb (15825) 339
Method: resin membrane electrode. Kso=-4.9

Ca++ cal oth/un 25°C 0.0 U H K1=2.43 1969IEa (15826) 340
DH(K1)=3.4 kJ mol⁻¹, DS=57.3 J K⁻¹ mol⁻¹

Ca++ sol oth/un 0°C 0.0 U T H 1969YMb (15827) 341
Ks=-1.97(0 C), -2.23(25 C), -2.46(50 C), -2.86(100 C), -3.27(150 C),
-3.71(200 C), -4.21(250 C), -5.42(350 C). Ks: K(CaL₂(s))=CaL+L

Ca++ sol oth/un 0°C 0.0 U T H 1969YMb (15828) 342
Kso(CaSO₄(H₂O)₂)=-4.54(0 C), -4.52(25 C). Kso=-3.91(0 C), -4.27(25 C), -5.36
(100 C), -7.07(200 C), -10.3(350 C)(anhydrite)(m unit) also thermod. data

Ca++ ISE oth/un 25°C dil U K1=2.57 1968GFd (15829) 343

Ca++ sol oth/un 115°C 0.0 U T 1968MSd (15830) 344
Medium:0 corr. 30-200 C. Equations for Kso for CaSO₄(H₂O)₂, CaSO₄ and hemi-
hydrate and in seawater at various salinities

Ca++ oth oth/un 25°C 0.0 U H K1=2.31 1967HEb (15831) 345
DH(K1)=8.1 kJ mol⁻¹, DS=71.5 J K⁻¹ mol⁻¹ (or DH=7.4, DS=69)

Ca++ ISE oth/un 25°C 0.0 U K1=2.27 1967NRa (15832) 346
Kso=-4.60

Ca++ sol oth/un 125°C 0.0 U T 1966MJa (15833) 347
Kso(CaSO4(H2O)0.5)=-5.02
Kso=-6.00(150 C), -6.47(175 C), -6.94(200 C), -7.48(225 C), -8.04(250 C),
-8.64(275 C), -9.22(300 C), -9.78(325 C), -10.37(350 C); CaSO4(s,anhydrite)

Ca++ sol oth/un 110°C 0.0 U T 1966MSe (15834) 348
Kso=-4.71
Kso=-4.46(0.5 C), -4.37(25 C), -4.41(50 C), -4.55(80 C). Solid=CaSO4(H2O)2

Ca++ sol oth/un 20°C 0.0 U K1=2.0 1965LIb (15835) 349

Ca++ sol none 25°C C T H 1964MSe (15836) 350
Kso(CaSO4)=-4.20
Kso(CaSO4.2H2O)=-4.37
DH(Kso(CaSO4))=-7.95 kJ mol⁻¹, DH(Kso(CaSO4.2H2O))=6.7 kJ mol⁻¹.
Data at 25-200C for CaSO4 and 25-60 C for CaSO4.2H2O.

Ca++ sol oth/un 25°C 0.0 U T H 1960GCa (15837) 351
Kso(CaL)=-5.04
DH(so)=-13.8 kJ mol⁻¹, DS=-142.3 J K⁻¹ mol⁻¹. Kso=-4.99(20 C), -5.10(30 C),
-5.18(40 C), -5.26(50 C), -5.37(60 C), -5.49(70 C), -5.61(80 C), -5.91(100 C)

Ca++ sol R4N.X 25°C 1.0M U 1959WLa (15838) 352
Kso=-3.16

Ca++ sol NaClO4 25°C 1.0M U TI 1958NRa (15839) 353
Kso(CaL)=-2.92
Kso=-2.91(35 C), -2.94(75 C). In 3.5 M NaClO4 Kso=-3.16(25 C), -3.09(35 C),
-3.34(75 C)

Ca++ sol oth/un 25°C 0.0 U H 1955SIa (15840) 354
Kso(CaL)=-5.92
DH(so)=0.9 kJ mol⁻¹, DS=-110 J K⁻¹ mol⁻¹

Ca++ sol oth/un 25°C 0.0 U T H K1=2.31 1953BGB (15841) 355
K1=2.22(0 C), 2.29(40 C). DH(K1)=6.9 kJ mol⁻¹, DS=67.4 J K⁻¹ mol⁻¹(25 C)
By freezing point, 0 C, K1=2.27-2.48

Ca++ oth oth/un 25°C 0.0 U H 1933LHa (15842) 356
Kso(CaL)=-4.625
From thermodynamic data. DH(so)=1.1 kJ mol⁻¹, DS=-85 J K⁻¹ mol⁻¹

Ca++ con oth/un 18°C 0.0 U K1=2.28 1932MDa (15843) 357

Ca++ cal oth/un 25°C sat U IH 1930LMa (15844) 358
DHso=2.6 kJ mol⁻¹ in saturated CaL; -1.1 kJ mol⁻¹ in I=0 corr.

S203-- H2L Thiosulfate CAS 73686-28-7 (177)
Thiosulfate;

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

Ca++ cal R4N.X 25°C 0.50M U K1=0.68 1997MKa (16756) 359
DH(K1)=2.71 kJ mol-1

Ca++ cal R4N.X 25°C 0.50M U H K1=0.70 1974ARa (16757) 360
DH=2.68 kJ mol-1.

Ca++ ISE oth/un 25°C dil U K1=1.90 B2=3.98 1968GFd (16758) 361

Ca++ con alc/w 25°C 44% U K1=3.49 1956BMa (16759) 362
Medium: 44% EtOH

Ca++ sp none 25°C 0.0 U K1=1.91 1955GMa (16760) 363

Ca++ sol none 25°C 0.0 U K1=1.98 1951DMb (16761) 364

Ca++ sol none 25°C 0.0 U K1=2.05 1949DWa (16762) 365

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

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

Ca++ con oth/un 18°C dil U Kso=-5.74 1968RVa (17028) 366

Ca++ sol oth/un 20°C var U Kso(CaL)=-5.53 1956CHE (17029) 367

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

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

Ca++ cal oth/un 25°C dil U H DH(so(CaL(H2O)2))=-8.5 kJ mol-1 1959SSb (17093) 368

Ca++ sol none 25°C 0.0 U T H Kso(CaL)=-3.09 1958SEb (17094) 369

I=0 corr. T. 0-100 C. DH(so)=-8.2 kJ mol-1(sat. soln)

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

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

 Ca++ EMF NaClO4 25°C 1.0M U K1=3.09 1974SSc (17176) 370
 K(Ca+HL)=0.39
 K(Ca+2HL)=2.89

Method: H electrode

 Ca++ oth none 150°C 0.0 U T 1969HEa (17177) 371
 *Ks(CaAl2Si2O8+8H)=9.79

Method:est.data.(CaAl2Si2O8).*Ks=19.32 (60 C),1.12 (300 C); montmorillonite:
 *Ks=2.89(60 C),-7.73(300 C). Also other data for 60-300 C

 Ca++ sol oth/un 25°C 0.0 U 1965GCa (17178) 372
 Kso(CaL)=-7.0 to -7.3

 Ca++ sol none 25°C 0.0 U T K2=9.83 1960Gcb (17179) 373
 K(CaSiO3(s)=Ca+SiO3)=-7.0

Also glass electrode. I=0 corr. K2=9.7(30 C), 9.6(40 C)

 Ca++ sol oth/un 100°C var U 1958AKa (17180) 374
 K(CaSiO3(s)=Ca+SiO3)=ca.-7

 Ca++ oth none 25°C 0.0 U 1957BAa (17181) 375
 From thermodynamic data. Ks(CaSiO3(s)+H2O=SiO2(s)+Ca+2OH)=-11.08

 Ca++ sol none 30°C 0.0 U 1940REa (17182) 376
 K(CaSiO3(s)=Ca+SiO3)=-7.60
 K(Ca3(HL2)2(s)=3Ca+2HL)=-20.9

 Siw11039----- H8L (2464)
 alpha-Heterosilicon-polytungstate;

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

 Ca++ gl NaNO3 25°C 1.00M U K1=4.09 1984COa (17230) 377
 K(beta1 isomer)=4.24
 K(beta2 isomer)=4.35
 K(beta3 isomer)=4.27

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

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

 Ca++ sol oth/un 20°C var U 1970KBd (17304) 378
 Kso=-13.1
 Kso(3Ca+TeO6)=-15.7

 V04--- H3L CAS 15457-75-7 (1586)
 Vanadate; VO2(OH)3-- or polymers

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	NaCl04	25°C	1.00M	U				1975KIc (17372)	379
									K(Ca+H7PV12036)=3.57	

Ca++	sol	NaCl	20°C	1.00M	U	I			1974IGa (17373)	380
									K(Ca+V4012(4-))=0.43	
									Ks(2Ca(V03)2(H2O)4)=-4.65	
									I=3, K=0.34, Ks(2Ca(V03)2(H2O)4=2Ca + V4012----)=-3.94. I=0.045, Ks=-6.68;	
									I=0.2, Ks=-5.69; I=0.33, Ks=-5.31	

W04--		H2L							CAS 13783-36-3	(445)
Tungstate;										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	con	oth/un	18°C	dil	U				1933BHa (17428)	381
									Kso(CaL)=-8.06	

CH03F3S		HL							CAS 1493-13-6	(6755)
Trifluoromethanesulfonic acid; CF3SO3H										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	ISE	non-aq	25°C	100%	C	I		K1=4.01	1997NMa (17458)	382
Method: polyacrylamide/15-crown-5 sensor. Medium: acetonitrile.										
Also data for DMF (K1=2.53), DMSO (K1=2.24) and PC (K1=2.45).										

CH202		HL							CAS 64-18-6	(37)
Methanoic acid; H.COOH										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	ISE	NaCl	25°C	0.03M	U	TIH		K1=0.75	1981EFa (17561)	383
At 35 C: I=0.045: K1=0.87; 45 C, I=0.45: 0.38; 25 C. I=0.45: 0.92										
DH=13.2 kJ mol-1, DS=62.7 J K-1 mol-1										

Ca++	sol	NaCl04	25°C	0.5M	U	I		K1=0.26	1976KFa (17562)	384
For I=1.0 M K1= 0.45; I=6.0 M K1=0.48										

Ca++	gl	NaNO3	30°C	0.40M	U			K1=0.27	1970BTa (17563)	385
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Ca++	vlt	NaCl04	25°C	2.0M	U			K1=0.48 B2=1.11 B3=1.34 B4=1.20	1957HBa (17564)	386
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Ca++	gl	oth/un	25°C	0.0	U	T H		K1=1.43	1956NAa (17565)	387
Medium: 0 corr. K(35 C)=1.46, DH(K1)=4.09 kJ mol-1, DS1=41.8 J K-1 mol-1										

Ca++	sol	none	25°C	0.0	U			K1=0.80	1952CMF (17566)	388
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Ca++ gl oth/un 25°C 0.0 U K1=1.43 1948SCa (17567) 389

CH2O3Cl3P H2L CAS 5994-41-2 (1970)

Trichloromethylphosphonic acid; Cl3C.PO3H2

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

Ca++ gl KNO3 25°C 0.10M U K1=1.25 1979WNa (17666) 390

CH3O3Cl2P H2L CAS 13113-88-7 (1972)

Dichloromethylphosphonic acid; Cl2CH.PO3H2

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

Ca++ gl KNO3 25°C 0.10M U K1=1.26 1979WNa (17688) 391

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

Ca++ gl KCl 25°C 0.10M C K1=3.57 1994SCa (17694) 392
K(Ca+HL)=1.71
K(CaL+H)=5.71

Ca++ ISE R4N.X 25°C 0.05M C K1=3.55 1981FHa (17695) 393
K(Ca+HL)=1.84

Medium: 0.05 M Et4NClO4. Method: Ca ion selective electrode.

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

Carbamide, Urea; (H2N)2CO

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

Ca++ sp NaClO4 23°C 2.00M U I K1=-0.28 B2=-0.89 1970Klf (17711) 394

Temperature range 20 - 23C

Ionic strength 4.0: K1=-0.05, B2=-0.60

CH4O3BrP H2L CAS 7582-40-3 (1974)

Bromomethylphosphonic acid; Br.CH2.PO3H2

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

Ca++ gl KNO3 25°C 0.10M U K1=1.34 1979WNa (17915) 395

CH4O3ClP H2L CAS 2565-58-4 (1973)

Chloromethylphosphonic acid; Cl.CH2.PO3H2

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

Ca++ gl KNO3 25°C 0.10M U K1=1.38 1979WNa (17923) 396

Ca++ EMF NaNO3 25°C 0.10M U K1=1.47 1970TNa (17924) 397

CH403IP H2L CAS 13298-02-7 (1976)
Iodomethylphosphonic acid; I.CH2.PO3H2

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

Ca++ gl KNO3 25°C 0.10M U K1=1.37 1979WNa (17933) 398

CH406Cl2P2 H4L CAS 10596-23-3 (2370)
Dichloromethanediphosphonic acid; Cl2.C(P03H2)2

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

Ca++ gl KNO3 25°C 0.10M C I R K1=5.9 2001PRa (17946) 399
K(Ca+HL)=3.15

IUPAC Recommended values

Ca++ gl R4N.X 25°C 0.10M C H K1=5.77 1993KLa (17947) 400
K(Ca+HL)=3.09

DH(K1)=5.1 kJ mol⁻¹, DS=128 J K⁻¹ mol⁻¹

Ca++ gl R4N.X 25°C 0.10M U K1=5.95 1984CLb (17948) 401
K(Ca+HL)=3.2
K(CaL+Ca)=3.0

Medium: Me4NNO3

Ca++ ISE oth/un 25°C 0.10M M I K1=4.49 1983FBa (17949) 402
K(Ca+HL)=3.74

For 0.1 M NH4Cl medium

Ca++ gl KCl 25°C 0.10M U K1=4.71 1976DGe (17950) 403
K(Ca+HL)=2.86

CH406F2P2 H4L CAS 10596-32-4 (7848)
Difluoromethylenediphosphonic acid;

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

Ca++ ISE oth/un 25°C 0.10M M K1=4.36 1983FBa (17956) 404
K(CaL+Ca)=1.56

For 0.1 M NH4Cl medium

CH503P H2L CAS 13590-71-1 (1752)
Methylphosphonic acid; CH3.PO3H2

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

Ca++ gl KNO3 25°C 0.10M C I R K1=1.6 2001PRa (18113) 405
IUPAC Recommended values

Ca++ gl NaNO3 25°C 0.10M M K1=1.64 1992SCa (18114) 406

Ca++ gl KCl 25°C 0.10M U K1=1.79 1986NIa (18115) 407

Ca++ gl KNO3 25°C 0.10M U K1=1.51 1979WNa (18116) 408

CH5O4P H2L CAS 2617-47-2 (1977)
Hydroxymethylphosphonic acid; HO.CH2.PO3H2

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

Ca++ gl KNO3 25°C 0.10M U K1=1.68 1979WNa (18143) 409

Ca++ gl R4N.X 25°C 0.10M U K1=1.87 1972WFa (18144) 410
Medium: (CH3)4NCl

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

Ca++ gl NaNO3 25°C 0.10M M K1=1.49 1996SSa (18164) 411

Ca++ gl NaCl 25°C 0.15M U K1=1.394 1990KLb (18165) 412
B(CaH-1L)=-7.09

Ca++ sp oth/un 20°C 0.10M U T K1=1.49 1965BRb (18166) 413
K1(65 C)=1.74

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

Ca++ gl KNO3 25°C 0.10M C I R K1=1.67 2001PRa (18211) 414
K(Ca+HL)=1.06
IUPAC Recommended values

Ca++ gl NaNO3 25°C 0.10M C K1=1.62 1994SCa (18212) 415
K(Ca+HL)=1.03
K(CaL+H)=9.49

Ca++ gl KNO3 25°C 0.10M U K1=1.71 1979WNb (18213) 416
B(CaHL)=11.14

Ca++ gl KNO3 25°C 0.10M U K1=1.84 1971Wnc (18214) 417

B(CaHL)=11.01

CH606P2 H4L Medronic acid CAS 1984-15-2 (2384)
Methanediphosphonic acid; CH₂(PO₃H₂)₂

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

Ca++ gl NaCl 37°C 0.15M C K1=4.86 1997ZJa (18261) 418
K(CaL+H)=7.83
K(CaL+Ca)=3.53

Ca++ gl R4N.X 25°C 0.10M U K1=5.97 1984CLb (18262) 419
K(Ca+HL)=2.89
K(CaL+Ca)=3.84

Medium: Me4NNO₃

Ca++ gl R4N.X 25°C 0.50M U K1=4.70 1968CIa (18263) 420
K(Ca+HL)=2.46

Medium: (CH₃)₄NCl

Ca++ gl KCl 25°C 0.10M U K1=6.03 1967KLa (18264) 421
K(Ca+HL)=3.88

Ca++ gl oth/un 25°C 0.10M U K1=5.51 1963KEa (18265) 422
K(Ca+HL)=2.76
K(Ca+CaL)=3.31

Ca++ oth R4N.X 25°C 1.0M U IH K1=5.01 1962IMb (18266) 423
Method: nephelometric. Medium: 0-1 M Me4NBr. K1=6.5(I=0), 6.02(I=0.1)
At I=0 corr: DH(K1)=0 kJ mol⁻¹, DS=92 J K⁻¹ mol⁻¹

Ca++ oth R4N.X 50°C 1.0M U I K1=4.77 1962IMb (18267) 424
Method: nephelometric. Medium: 0.1-1 M Me4NBr. K1=5.93(I=0.1)

CH607P2 H3L CAS 56399-35-0 (7664)
Methyldiphosphoric acid;

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

Ca++ gl NaNO₃ 25°C 0.10M M K1=2.87 1999SSa (18305) 425

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

Ca++ ISE NaCl 25°C 0.10M U TI 1998STa (18662) 426
Kso(monohydrate)=1.15
Kso(dihydrate)=1.88
Kso(trihydrate)=2.17

Atomic absorption also used. At 37 C $K_{so}(\text{mono})=1.38$, $K_{so}(\text{di})=2.58$,
 $K_{so}(\text{tri})=2.98$. Data for 20-40 C, $I=0.02-0.2$ M

 Ca++ EMF none 37°C 0 C TI 1997KTa (18663) 427
 $K_{so}=-8.02$

$I=0$ to 0.2 M and urine models. At 25 C: $K_{so}=8.24$, 40 C: $K_{so}=7.97$. For mono-
 hydrate: $K_{so}=8.77(25\text{ C}), 8.65(37\text{ C}), 8.62(40\text{ C})$. For dihydrate: 8.34, 8.17, 8.13

 Ca++ oth NaCl 25°C 0.15M U T $K_1=1.46$ 1993GMa (18664) 428
 Method: Coulometric titration. $K_1=1.47$ (37 C)

 Ca++ sol NaCl 37°C dil C I 1989SIb (18665) 429
 $K_{so}(\text{CaL.H}_2\text{O})=-8.66$

Calculated from data for 0.0-0.15 M NaCl solutions.

 Ca++ gl KCl 37°C 0.15M C $K_1=2.36$ 1985DSa (18666) 430

 Ca++ vlt NaNO3 25°C 1.00M U $K_1=2.69$ B2=4.04 1985KIa (18667) 431
 B3=5.16

By linear sweep voltammetry

 Ca++ gl KNO3 35°C 0.10M C M $K_1=4.85$ 1985RRc (18668) 432
 $B(\text{CaL}(\text{cytidine}))=8.80$

 Ca++ gl KNO3 35°C 0.10M C $K_1=4.85$ 1985RRh (18669) 433

 Ca++ ISE oth/un 37°C 0.10M U I $K_1=2.46$ 1982DMa (18670) 434
 Medium: 0.03-0.5 M Et4NI

 Ca++ ISE none 37°C 0.0 C $K_1=3.39$ 1982RAB (18671) 435
 Method: Ca ion selective electrode. At $I=0.0015$ M, $K_1=3.24$

 Ca++ ISE NaCl 25°C 0.10M U I $K_1=2.54$ 1979CMb (18672) 436

 Ca++ dis R4N.X 25°C 0.50M U $K_1=1.95$ 1976MKa (18673) 437

 Ca++ ix oth/un 25°C 0.10M U 1973ADa (18674) 438
 $K(\text{Ca+HL})=1.38$
 $B(\text{Ca+2HL})=1.85$

 Ca++ sp oth/un ? ? U $K_1=3.37$ 1973FSb (18675) 439

 Ca++ ix NaClO4 25°C 0.02M U I $K_1=2.08$ 1972ADa (18676) 440
 $K_1(0.06)=2.11$, $K_1(0.10)=2.10$, $K_1(0.20)=2.06$

 Ca++ sol oth/un 20°C 0.10M U B2=3.49 1971PSf (18677) 441
 Medium : 0.1 - 1.5 HNO3

 Ca++ oth KNO3 25°C 0.10M U $K_1=2.30$ 1970SPg (18678) 442
 Method : ionic migration

Ca++ dis NaClO4 25°C 1.0M U K1=1.66 B2=2.69 1967HMa (18679) 443

Ca++ dis oth/un 20°C 0.10M U 1963STc (18680) 444
Kso=-7.9

Medium: KClO4

Ca++ gl oth/un 25°C 0.10M U K1=3.0 1958GHc (18681) 445

Ca++ con none 18°C 0.0 U K1=3.00 1932MDa (18682) 446

C2H3NO4 HL CAS 625-75-2 (2968)

Nitroacetic acid; O2N.CH2.COOH

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

Ca++ kin oth/un 18°C 0.20M U K1=-0.30 1949PEa (19202) 447

Medium: Ba(NO3)2

C2H3N3 HL 1,2,4-Triazole CAS 288-88-0 (381)
1,2,4-Triazole; cyclo(-NH.N:CH.N:CH-) C2H3N3

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

Ca++ gl none 25°C 0.0 U 1991ASa (19225) 448

K(Ca+HL)=0.76
B(CaHL)=9.8

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

Ca++ sol oth/un 25°C ->0 U K1=0.41 1952CMf (19275) 449

Ca++ sol oth/un 25°C ->0 U K1=0.55 1949DWa (19276) 450

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

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

Ca++ gl NaNO3 30°C 0.40M U K1=0.14 1970BTa (19344) 451

C2H4N2O4 H2L CAS 1687-60-1 (2969)
Oxalldihydroxamic acid; (CO.NH.OH)2

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

Ca++ gl oth/un 25°C 0.10M U 1957MJa (19446) 452

Kso=7.75

C2H4N4 HL CAS 61-82-5 (1265)
3-Amino-1,2,4-triazole; C2H2N3.NH2

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

Ca++ gl KNO3 25°C 0.10M U I 1997DBa (19472) 453
K(Ca+HL)=1.41

Data also for I=0.5 and 1.0 M

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

Ca++ ISE none 25°C 0 C I K1=1.12 1995RGa (19792) 454
I=0.15 (CaCl) K1=0.76.

Ca++ oth none 25°C 0 U T H K1=1.71 1994SHd (19793) 455
Data also at 35, 45 55 C. DH(K1)=3.1 KJ mol⁻¹, DS=43.3 J K⁻¹ mol⁻¹

Ca++ oth NaCl 25°C 0.15M U T K1=0.48 1993GMa (19794) 456
Method: Coulometric titration. K1=0.57(37 C)

Ca++ sol oth/un 80°C var U K1=1.2 1991FEa (19795) 457
Portlandite(Ca(OH)2) solubility measurements.Constants at I=0

Ca++ sol oth/un 200°C var U T K1=2.53 1991SSa (19796) 458
100-350 C.P=500 bars. Constants at I=0

Ca++ gl alc/w 25°C 100% M K1=4.7 B2=7.2 1988PPa (19797) 459
Medium: MeOH

Ca++ gl R4N.X 25°C 0.25M C TIH K1=0.57 1985DRa (19798) 460
I=0.02-1 M Et4NI. 10-45 C. DH = 3.5 kJ mol⁻¹

Ca++ gl R4N.X 25°C 0.16M U I K1=0.57 1985RSa (19799) 461
At 10 C: K1=0.68 (I=0.04); 35 C: 0.61 (0.25); 45 C: 0.70 (0.49)

Ca++ gl KNO3 25°C 0.15M C I K1=0.59 1983DDa (19800) 462

Ca++ ISE NaCl 25°C 0.03M U TIH K1=0.87 1981EFa (19801) 463
At 35 C, I=0.045: K1=0.88; 45 C, I=0.3: 0.61; 45 C, I=0.45: 0.40
DH=7.3 kJ mol⁻¹, DS=45.1 J K⁻¹ mol⁻¹

Ca++ ISE NaCl 25°C 0.11M C T K1=0.74 1979EFc (19802) 464
Method: divalent ion selective electrode. Data for 15-35 C and for
I=0.025-0.105 M NaCl. At I=0, K1=1.04.

Ca++ sol NaClO4 25°C 0.5M U I K1=0.26 1976KFa (19803) 465
 For I=1.0 M K1= 0.39; I=6.0 M K1=0.45

 Ca++ dis R4N.X 25°C 0.50M U K1=0.74 1976MKa (19804) 466

 Ca++ gl NaNO3 30°C 0.40M U K1=0.50 1970BTa (19805) 467

 Ca++ gl none 25°C 0.0 U K1=1.12 1964AMa (19806) 468

 Ca++ gl non-aq 25°C 100% U K2=6.77 1964KLa (19807) 469
 Medium: ethanoic acid

 Ca++ gl oth/un 25°C 0.0 U T H K1=1.24 1956NAa (19808) 470
 Medium: 0 corr. K1(35 C)=1.26, DH(K1)=3.8 kJ mol⁻¹, DS=36.4 J K⁻¹ mol⁻¹

 Ca++ sol oth/un 25°C 0.0 U K1=0.77 1952CMe (19809) 471

 Ca++ ix oth/un 25°C 0.16M U K1=0.62 1952SLa (19810) 472

 Ca++ EMF oth/un 25°C 0.15M U K1=0.53 1946JOa (19811) 473

 Ca++ EMF KCl 20°C 0.20M U K1=0.53 1938CKa (19812) 474
 Method: H electrode

 Ca++ con oth/un 18°C 0.0 U K1=0.0 1938DAa (19813) 475

 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

 Ca++ gl NaClO4 25°C 0.50M C K1=0.92 1995PLa (20467) 476

 Ca++ ISE KNO3 25°C 0.70M U K1=1.11 1986HAe (20468) 477

 Ca++ sol oth/un 25°C 0.0 U T H K1=1.65 1975DNa (20469) 478
 DH=35.52 kJ mol⁻¹ and DS=150.75 J mol⁻¹ K⁻¹.
 Data also at 30, 35, 40 and 45 C. Medium: glycolate buffer, pH 3.8

 Ca++ EMF oth/un 25°C ->0 U K1=1.59 1954DMa (20470) 479
 Method: H electrode

 Ca++ EMF KCl 20°C 0.20M U K1=1.11 1938CKa (20471) 480
 Method: H electrode

 Ca++ sol oth/un 25°C ->0 U K1=1.59 1938DAa (20472) 481

 C2H4O6F4P2 H4L (2457)
 Tetrafluoroethane-1,2-diphosphonic acid;

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

Ca++ gl KCl 25°C 0.20M C K1=2.45 1999FEa (21797) 496

C2H5O5P H2L CAS 590-54-5 (1764)
Acetylphosphoric acid; CH3.CO.O.PO3H2

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

Ca++ gl KNO3 37°C 0.15M M K1=3.18 B2=4.38 1979SPb (21869) 497
K(Ca+HL)=1.62

Ca++ kin oth/un 39°C 0.45M U K1=1.08 1971KSa (21870) 498
Ionic strength=0.45-0.75

Ca++ sp KCl 25°C 1.00M U K1=1.70 1970BSg (21871) 499
pH 8.0 buffer

Ca++ kin oth/un 39°C 0.60M U K1=0.89 19660Ja (21872) 500

C2H5O5P H3L CAS 4408-78-0 (4225)
Phosphonoethanoic acid; HOOC.CH2.PO3H2

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

Ca++ ISE R4N.X 25°C 0.05M C H K1=3.67 1981FHa (21887) 501
K(Ca+HL)=2.10
Medium: 0.05 M Et4NClO4. Data for 0.10-0.25 M.
At I=0.0 M, K1=4.68, DH(K1)=2.5 kJ mol⁻¹, DS(K1)=89.5 J K⁻¹ mol⁻¹.

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

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

Ca++ ISE non-aq 25°C 100% C K1=2.72 1997NMa (22087) 502
Method: polyacrylamide/15-crown-5 sensor. Medium: acetonitrile.

C2H6S L CAS 75-18-3 (151)
Dimethyl sulfide; CH3.S.CH3

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

Ca++ nmr alc/w 34°C 50% C K1=-1.6 1980SSa (22186) 503
Also in D2O, K1=-1.4

C2H7NO3S HL Taurine CAS 107-35-7 (2214)
2-Aminoethane sulfonic acid; H2N.CH2.CH2.SO3H

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	nmr	oth/un	40°C	0.75M	U		K1=0.217 B(CaHL)=8.426	1980IHa (22437)	504

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
Ca++	gl	KNO3	25°C	0.10M	U		K1=2.21	1963TAa (22474)	505

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	gl	NaNO3	25°C	0.10M	M		K1=1.61	1992SCa (22561)	506

Ca++	gl	KNO3	25°C	0.10M	U		K1=1.54	1979WNa (22562)	507

C2H8NO3P		H2L					CAS 6323-97-3	(1862)	
1-Aminoethanephosphonic acid; CH3.CH(NH2).PO3H2									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	gl	KNO3	25°C	0.20M	C		K1=1.43 K(Ca+HL)=1.02	1978MAb (22608)	508

C2H8NO3P		H2L					CAS 2041-14-7	(1863)	
2-Aminoethanephosphonic acid; H2N.CH2.CH2.PO3H2									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	gl	KNO3	25°C	0.10M	U		K1=1.74 B(CaHL)=12.22	1979WNb (22628)	509

Ca++	gl	KNO3	25°C	0.20M	C		K1=1.43 K(Ca+HL)=1.09	1978MAb (22629)	510

C2H8NO4P		H2L					CAS 1071-23-4	(1864)	
2-Aminoethyl-dihydrogenphosphoric acid; H2N.CH2.CH2.OPO3H2									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	gl	KCl	20°C	0.10M	U		K1=1.48	1987BPb (22658)	511

Ca++	gl	KNO3	25°C	0.20M	C		K1=1.54 K(Ca+HL)=1.16	1978MAb (22659)	512

Ca++ gl KNO3 25°C 0.20M C K1=1.54 1978MAc (22660) 513
K(Ca+HL)=1.16
K(CaL+H)=9.74

Ca++ gl R4N.X 20°C 0.10M U T K1=2.0 1965HFb (22661) 514
K(Ca+HL)=1.4

Medium: (C3H7)4NI

Ca++ gl KCl 25°C 0.15M U K1=1.57 19620Sa (22662) 515
K(Ca+HL)=1.11

C2H8N2 L Ethylenediamine CAS 107-15-7 (23)
1,2-Diaminoethane; H2N.CH2.CH2.NH2

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

Ca++ gl NaCl 25°C 0.0 C K1=0.15 1999SFc (23052) 516
K(Ca+HL)=-0.28

Extrapolated from data for 0.03-0.96 M NaCl using the Pitzer equation.

Ca++ sp alc/w 25°C 95% U K1=1.1 1993GSa (23053) 517
Medium: 95% w/w EtOH/H2O, 0.05 M Et4NClO4, by competitive spectrophotometry

Ca++ gl oth/un 25°C 0.10M C I K1=0.03 1990CDb (23054) 518
Medium: 0.10 M CaCl2. Data for I=0.25-1.0 M.

C2H8O6P2 H4L CAS 6145-31-9 (2579)
1,2-Ethylenediphosphonic acid; H2O3P.CH2.CH2.PO3H2

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

Ca++ gl R4N.X 25°C 1.0M U K1=2.80 1962IMb (23257) 519
K(Ca+HL)=2.60

Medium: Me4NBr

C2H8O6P2 H4L CAS 6145-33-1 (3543)
Ethane-1,1-diphosphonic acid; CH3.CH(PO3H2)2

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

Ca++ gl R4N.X 25°C 0.50M U K1=5.21 1968CIa (23264) 520
K(Ca+HL)=2.74

Medium: (CH3)4NCl

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

Ca++ gl R4N.X 25°C 0.10M C I T K1=6.4 2001PRa (23323) 521

K(Ca+HL)=3.3
K(Ca+CaL)=4.6

IUPAC Provisional values

Ca++	gl	KNO3	25°C	0.10M	C	K1=6.2 K(CaL+H)=7.67 K(CaL+Ca)=4.5	1997DBb (23324)	522
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Ca++	gl	NaCl	37°C	0.15M	C	K1=5.34 K(CaL+H)=7.83 K(CaL+Ca)=4.19	1997ZJa (23325)	523
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Ca++	cal	NaCl	25°C	0.50M	U H	DH(Ca2L)=2 kJ mol ⁻¹ , DS=204 J K ⁻¹ mol ⁻¹	1986VKa (23326)	524
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Ca++	cal	R4N.X	25°C	0.50M	U H	K1=5.7 Medium: Et4N.Cl. DH1=0.1 kJ mol ⁻¹ , DS1=109 J K ⁻¹ mol ⁻¹	1986VKb (23327)	525
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Ca++	gl	NaCl	25°C	0.02M	U	K1=7.50 K(Ca+HL)=4.73 B(Ca2L)=12.02	1986VZa (23328)	526
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Ca++	gl	R4N.X	25°C	0.10M	M	K1=6.18 K(Ca+HL)=3.12 K(CaL+Ca)=4.63	1984CLb (23329)	527
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Ca++	cal	KCl	25°C	0.02M	U T H	K(Ca+HL)=3.30 DH=11.00 kJ mol ⁻¹ ; DS=99.6 J mol ⁻¹ K ⁻¹ .	1984VKd (23330)	528
<hr/>								
Ca++	ISE	oth/un	25°C	0.10M	M I	K(Ca+HL)=5.37	1983FBa (23331)	529
<hr/>								
For 0.1 M NH4Cl medium								
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Ca++	gl	KNO3	25°C	0.10M	U	K1=6.48 K(Ca+HL)=4.20 K(Ca+H2L)=2.63	1980ZRC (23332)	530
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Ca++	gl	KCl	25°C	0.10M	U	K1=6.0 K(Ca+HL)=3.0	1976DGe (23333)	531
<hr/>								
Ca++	gl	R4N.X	25°C	0.10M	U	K1=6.6 K(Ca+HL)=3.54 B(2Ca+L)=12.2	1972WFa (23334)	532
<hr/>								
Medium: (CH3)4NCl								
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Ca++	gl	R4N.X	25°C	0.10M	U	K1=5.52 B(3Ca+2L)=18.78 B(4Ca+3L)=29.0 B(7Ca+4L)=48.2	1971GCa (23335)	533

Medium: (CH3)4NC1

Ca++ gl R4N.X 25°C 0.50M U K1=5.74 1968CIa (23336) 534
K(Ca+HL)=3.58

Medium: (CH3)4NC1

Ca++ gl KCl 25°C 0.10M U K1=6.04 1967KLa (23337) 535
K(2Ca+H-1L)=15.59
K(2Ca+L)=9.67

C2H9NO6P2 H4L (6773)
(Aminoethylene)diphosphonic acid, 1-Aminoethane-1,1-di(phosphonic acid);
H2N.C(CH3)(PO3H2)2

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

Ca++ gl KCl 25°C 0.10M C K1=4.31 1980KLa (23419) 536

C2H9NO6P2 H4L IDPA CAS 32545-63-4 (1335)
Imino-N,N-bis(methylenephosphonic acid); HN(CH2PO3H2)2

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

Ca++ gl KCl 25°C 0.20M C K1=3.11 1999MKa (23442) 537
B(CaHL)=12.42
B(CaH2L)=17.09
B(CaH-1L)=-8.68

Ca++ gl KNO3 25°C 0.1M C K1=3.85 1985MMa (23443) 538

B(CaHL)=13.22
B(CaH2L)=18.58

Ca++ gl KNO3 25°C 1.00M M K1=2.79 1982BGB (23444) 539

K(Ca+HL)=1.57

C2H9NO6P2 H4L (6889)
N-Methylaminomethylenedi(phosphonic acid); CH3.NH.CH(PO3H2)2

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

Ca++ gl KCl 25°C 0.10M M K1=4.66 1978GMf (23462) 540

K(Ca+HL)=4.65

C3H3NO2 HL Cyanoacetic CAS 372-09-8 (38)
Cyanoethanoic acid; NC.CH2.COOH

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

Ca++ gl oth/un 25°C ->0 U K1=0.55 1938DAa (23508) 541

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

Ca++ gl NaNO3 25°C 0.50M M K1=-0.17 1998KSa (23795) 542

Ca++ gl oth/un 25°C 0.15M C TI K1=-0.14 1989DDb (23796) 543
 Medium: CaCl2. Also data for I=0.3-1.0 M. By Ca ion selective electrode,
 at 25 C, I=0.04, K1=-0.08; at 37 C, I=0.04, K1=-0.05.

C3H4O3 HL Pyruvic acid CAS 127-17-3 (1152)
 2-Oxopropanoic acid; CH3.CO.COOH

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

Ca++ gl NaClO4 30°C 1.0M U M K1=2.23 1988GMd (24034) 544
 K(Ca(cit)+L)=2.56

Ca++ gl NaClO4 25°C 3.00M C I K1=0.59 1978FGa (24035) 545

Ca++ ix oth/un 25°C 0.16M U K1=0.8 1950SRa (24036) 546

Ca++ sol oth/un 25°C ->0 U K1=1.08 1938DAa (24037) 547

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

Ca++ sol none 35°C 0.00 C T K1=2.4 1995FYa (24316) 548
 Method: atomic absorption and ion chromatography.
 Also data at 80 C (K1=2.9) and 25 C (K1=2.4).

Ca++ ISE none 25°C 0 C I K1=2.50 1995RGa (24317) 549
 I=0.1 (Me4N.X) K1=1.83; I=0.16 (Me4N.X) K1=1.76.

Ca++ gl NaCl 25°C 1.00M C K1=1.15 1988BSa (24318) 550

Ca++ gl R4N.X 25°C 0.25M C TIH K1=1.64 1985DRa (24319) 551
 B(CaHL)=5.90

I=0.02-1 M Et4NI.T=10-45. DH(K1)=7;DH(CaHL)=5 kJ mol⁻¹. DS1=69; DS(CaHL)=143

Ca++ ISE NaCl 25°C 0.10M U K1=1.52 1979CMB (24320) 552

Ca++ ISE NaClO4 25°C 0.1M U K1=1.42 1976KMd (24321) 553

Ca++ sp none 25°C 0.0 U T K1=2.50 1976K0a (24322) 554
 Also data at 15,30,35 C. By competition with bromocresol purple

Ca++ sol KCl 25°C 0.10M U T K1=2.50 1970Gnc (24323) 555
30 C: K1=2.58; 35 C: K1=2.66; 40 C: K1=2.74

Ca++ gl NaCl04 25°C 0.10M U K1=1.51 19680Va (24324) 556

Ca++ gl NaCl04 20°C 0.10M U K1=1.85 1963CAa (24325) 557
K(Ca+HL)=0.80

Ca++ EMF oth/un 25°C 0.04M U K1=2.49 1949SDa (24326) 558

Ca++ EMF KCl 25°C 0.20M U K1=1.46 1938CKa (24327) 559
K(Ca+HL)=0.47

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

Ca++ gl NaCl04 20°C 0.10M U K1=2.27 1963CAa (24610) 560
K(Ca+HL)=1.30

C3H5N04 H2L Aminomalonic ac CAS 1068-84-4 (2980)
2-Aminopropanedioic acid; HOOC.CH(NH2).COOH

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

Ca++ EMF oth/un 20°C ->0 U K1=2.51 1945SKa (24668) 561
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

Ca++ oth none 25°C 0 U T H K1=2.39 1994SHd (24958) 562
Data also at 35, 45 55 C. DH(K1)=1.7 KJ mol-1, DS=51.5 J K-1 mol-1

Ca++ ISE NaCl 25°C 0.03M U TIH K1=1.21 1981EFa (24959) 563
At 35 C, I=0.045: K1=1.17; 45 C, I=0.45: 0.48; 25 C, I=0.45: 1.33
DH=3.4 kJ mol-1, DS=36.4 J K-1 mol-1

Ca++ sol NaCl04 25°C 0.5M U I K1=0.12 1976KFa (24960) 564
For I=1.0 M K1= 0.32; I=6.0 M K1=0.11

Ca++ sol oth/un 25°C ->0 U K1=0.68 1952CMf (24961) 565

Ca++ EMF KCl 20°C 0.20M U K1=0.50 1938CKa (24962) 566
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
Ca++	gl	NaCl04	25°C	0.5M	C			K1=1.05	1995PLa (25359)	567
Ca++	oth	NaCl	25°C	0.15M	U T			K1=0.48	1993GMa (25360)	568
Method: Coulometric titration. K1=0.61 (37 C)										
Ca++	ISE	NaCl	25°C	0.50M	U			K1=0.92 B2=1.62	1981MVa (25361)	569
Ca++	EMF	alc/w	25°C	10%	M TIH			K1=1.51	1977SGa (25362)	570
Method: Pt/H ₂ electrode. Medium: 10% w/w MeOH/H ₂ O. Data for 15-40 C and for 10-90% w/w MeOH/H ₂ O and EtOH/H ₂ O. DH(K1)=29.92 kJ mol ⁻¹										
Ca++	sol	KCl	25°C	0.10M	U			K1=1.55	1970GNc (25363)	571
30 C: K1=1.69. 35 C: 1.78. 40 C: 1.94. 45 C: 2.05										
Ca++	EMF	oth/un	25°C	1.0M	U			K1=0.90 B2=1.24	1965VTa (25364)	572
Method: quinhydrone electrode.										
Ca++	EMF	oth/un	25°C	->0	U			K1=1.42	1954DMb (25365)	573
Method: H electrode										
Ca++	ix	oth/un	25°C	0.16M	U			K1=0.8	1952SLa (25366)	574
Ca++	EMF	oth/un	25°C	0.15M	U			K1=0.82	1946JOa (25367)	575
Ca++	EMF	KCl	20°C	0.20M	U			K1=1.07	1938CKa (25368)	576
Method: H electrode										
Ca++	sol	oth/un	25°C	->0	U			K1=1.47	1938DAa (25369)	577

C3H6O3 HL Methoxyacetic CAS 625-45-6 (29)										
Methoxyethanoic acid; CH ₃ .O.CH ₂ .COOH										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	sol	oth/un	25°C	->0	U			K1=1.12	1938DAa (25593)	578

C3H6O4 HL Glyceric acid CAS 473-81-4 (2520)										
2,3-Dihydroxypropanoic acid; HO.CH ₂ .CH(OH).COOH										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	EMF	KCl	20°C	0.20M	U			K1=1.18	1938CKa (25625)	579
Method: H electrode										

C3H7NO L DMF CAS 68-12-2 (598)										
N,N-Dimethylformamide; HCO.N(CH ₃) ₂										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	ISE	non-aq	25°C	100%	C		K1=1.88	1997NMa (25651)	580
Method: polyacrylamide/15-crown-5 sensor. Medium: acetonitrile.									
Ca++	ISE	non-aq	25°C	100%	C		K1=1.88	1997NMa (25652)	581
Method: polyacrylamide/15-crown-5 sensor. Medium: acetonitrile.									

C3H7NO2		HL			Alanine		CAS 56-41-7	(86)	
2-Aminopropanoic acid; H2N.CH(CH3).COOH									
Ca++	gl	NaCl	37°C	0.15M	U	M	K1=2.06	1995ZWb (26059)	582
B(CaH2(gly)L)=22.86									
Ca++	gl	none	25°C	0.0	C	TIH	K1=1.36	1989CDc (26060)	583
B(CaHL)=10.21									
Calculated from data for protonation of alanine in 0.04-1.0 M CaCl2. Data for 10-50 C. DH(K1)=12 kJ mol ⁻¹ , DS=67 J K ⁻¹ mol ⁻¹ . DH(B(CaHL))=6, DS=27									
Ca++	gl	oth/un	25°C	->0	U	T	K1=1.24	1950DWa (26061)	584

C3H7NO2		HL			B-Alanine		CAS 107-95-9	(575)	
3-Aminopropanoic acid; H2N.CH2.CH2.COOH									
Ca++	ISE	NaCl	37°C	0.15M	C		K1=1.639	1990MOe (26426)	585

C3H7NO2		HL			DL-Alanine		CAS 302-72-7	(189)	
DL-2-Aminopropanoic acid; H2N.CH(CH3).COOH									
Ca++	ISE	NaCl	37°C	0.15M	C		K1=1.309	1990MOe (26533)	586

C3H7NO2		HL					(6927)		
N-Methylacetohydroxamic acid; CH3.CO.N(OH)CH3									
Ca++	gl	KCl	25°C	0.20M	C		K1=1.59	2000FEc (26618)	587

C3H7NO2S		H2L			Cysteine		CAS 52-90-4	(96)	
2-Amino-3-mercaptopropanoic acid; H2N.CH(CH2.SH)COOH									
Ca++	ISE	NaCl	37°C	0.15M	C		K1=1.309	1990MOe (26533)	586

C3H7NO2		HL					(6927)		
N-Methylacetohydroxamic acid; CH3.CO.N(OH)CH3									

Ca++ gl KNO3 37°C 0.15M M K1=2.98 1979ZJa (26734) 588

Ca++ gl NaClO4 25°C 0.10M U M K1=1.92 1975RMa (26735) 589
B(CaL(citrate))=5.58
B(CaL(NTA))=8.44
B(CaL(tartrate))=4.43
K(Ca+L+HPO4)=8.49

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

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

Ca++ gl KNO3 25°C 0.10M U I K1=3.59 1990RAB (27067) 590
B(CaH-1L)=-5.25
Data for 10% w/w EtOH/H2O (K1=3.67; B(CaH-1L)=-5.11) and 25% (3.39; -5.13)

Ca++ gl NaCl 25°C 3.00M M K1=1.00 1988BFa (27068) 591

Ca++ gl NaCl 25°C 3.00M C K1=1.0 1985PBb (27069) 592
D-, L- and DL-serine studied.

Ca++ ix oth/un 25°C 0.16M U K1=0.5 1954SCa (27070) 593

Ca++ sol oth/un 25°C ->0 U K1=1.43 1950DWa (27071) 594

C3H7O5P H3L CAS 5962-42-5 (522)
3-Phosphonopropanoic acid; HOOC.CH2.CH2.PO3H2

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

Ca++ ISE R4N.X 25°C 0.05M C K1=2.38 1981FHa (27308) 595
K(Ca+HL)=1.64
Medium: 0.05 M Et4NClO4. Method: Ca ion selective electrode

Ca++ gl KNO3 25°C 0.10M U K1=1.7 1981WNa (27309) 596

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

Ca++ gl NaNO3 25°C 0.10M U K1=1.38 1992LCb (27318) 597

C3H8NO5P H3L 3-Phosphono-Ala CAS 20263-06-3 (1509)
2-Amino-3-phosphonatopropanoic acid; (H2O3P)CH2.CH(NH2).COOH

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

Ca++ gl KNO3 25°C 0.20M C K1=1.82 1978MAb (27346) 598

Ca++ gl R4N.X 20°C 0.10M U K1=3.2 1965HFa (27450) 608
K(Ca+HL)=2.5

Medium: (C3H7)4NI

Ca++ gl KCl 25°C 0.15M U K1=2.2 19590Sa (27451) 609
K(Ca+HL)=1.43

Ca++ gl oth/un 25°C 0.15M U K1=2.3 19570Sa (27452) 610

C3H9O3P L (6342)
Dimethoxy-P-methylphosphine oxide; (CH3O)2PO.CH3

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
Ca++ oth non-aq 25°C 100% U K1=2.69 B2=4.30 1989SSc (27995) 611
B4=6.04

Medium: CH3CN. Ca as Ca(NCS)2. Method: IR-spectroscopy
For diphenoxy-P-methylphosphine oxide: K1=1.92, B2=3.84

C3H9O3PS H2L CAS 69639-94-3 (545)
(Ethylthiomethyl)phosphonic acid; CH3.CH2.S.CH2.PO3H2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
Ca++ gl KNO3 25°C 0.10M U K1=1.70 1981WNa (28007) 612

C3H9O4P H2L (6694)
(Phosphonylmethoxy)ethane; H2O3P.CH2.O.CH2.CH3

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
Ca++ gl NaNO3 25°C 0.10M M K1=1.70 1992SCa (28016) 613

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
Ca++ gl NaNO3 25°C 0.10M U K1=1.43 1992LCb (28040) 614

Ca++ gl KCl 20°C 0.10M U K1=1.66 1957SAa (28041) 615

C3H10NO3P H2L CAS 13138-33-5 (1982)
3-Aminopropylphosphonic acid; H2N.CH2.CH2.CH2.PO3H2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
Ca++ gl KNO3 25°C 0.10M U K1=1.68 1979WNb (28086) 616
B(CaHL)=12.37

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

Ca++ gl KNO3 25°C 0.10M C K1=1.7 1993SKc (28096) 617

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

Ca++ gl KCl 20°C 0.10M U K1=2.65 1951SRa (28385) 618
K(Ca+HL)=1.7

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

Ca++ gl oth/un 25°C 0.10M U K1=2.6 1962IMb (28390) 619

Ca++ gl KCl 20°C 0.10M U K1=2.58 1951SRa (28391) 620
K(Ca+HL)=1.8

C3H10O6P2 H4L (3556)
Propane-2,2-diphosphonic acid; CH3.C(PO3H2)2.CH3

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

Ca++ gl R4N.X 25°C 0.50M U K1=6.33 1968CIa (28397) 621
K(Ca+HL)=3.14

Medium: Me4NCl

C3H11NO6P2 H4L (6772)
(Dimethylamino)-N-methylenediphosphonic acid; (CH3)2N.CH(PO3H2)2

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

Ca++ gl KCl 25°C 0.10M M K1=4.78 1978GMf (28408) 622
K(Ca+HL)=4.78

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

Ca++ gl KCl 25°C 0.20M C K1=4.11 1999MKa (28434) 623
B(CaHL)=14.03
B(CaH2L)=19.13

B(CaH-1L)=-8.66

Ca++ gl KNO3 25°C 0.10M C K1=4.61 1993SKc (28435) 624
K(CaL+H)=10.13
K(CaHL+H)=5.1

Ca++ gl NaClO4 25°C 0.10M U K1=4.52 1988Lda (28436) 625

C3H11NO7P2 H4L CAS 40291-99-9 (1346)
1-Hydroxy-3-aminopropyl-1,1-diphosphonic acid; (H2O3P)2C(OH).CH2.CH2.NH2

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

Ca++ gl NaCl 37°C 0.15M C 1999ZJa (28456) 626
K(Ca+H+L)=17.27
K[Ca(HL)+H]=6.31
K(Ca2L+H)=9.92
K(2Ca+L)=10.79

Ca++ gl KCl 25°C 0.10M M 1978KMa (28457) 627
K(Ca+H2L)=2.85

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

Ca++ gl KCl 25°C 0.10M C I R 2001PRa (28533) 628
K(Ca+HL)=4.0
K(CaL+H)=8.85
K(CaHL+H)=6.2
K(CaH2L+H)=5.0

IUPAC Recommended values. K(CaH3L+H)=4.1

Ca++ gl KNO3 25°C 0.10M C K1=7.6 1997DBb (28534) 629
K(CaL+H)=8.9
K(CaH2L+H)=5.1
K(CaHL+H)=6.30
K(CaH3L+H)=4.1

K(CaL+Ca)=2.9

Ca++ gl KNO3 25°C 0.10M C H K1=7.86 1993SMa (28535) 630
K(CaL+H)=8.80
K(CaHL+H)=6.11
DH(K1)=-0.6, DH(CaHL)=-19.7, DH(CaH2L)=5.0 kJ mol⁻¹.

Ca++ gl KNO3 25°C 0.10M C K1=7.86 1987SAa (28536) 631
K(CaL+H)=8.80
K(CaHL+H)=6.11
K(CaH2L+H)=4.9

C4H4N6 L 8-Azaadenine CAS 1123-54-2 (1884)
8-Aza-6-aminopurine;

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

Ca++ gl KNO3 45°C 0.10M U K1=3.8 1973TKa (28949) 639

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

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

Ca++ gl R4N.X 25°C 0.25M C TI K1=1.76 1985DRa (29031) 640
B(CaHL)=6.67

I=0.02-1 M Et4NI

Ca++ cal NaNO3 25°C 0.50M C H 1984ARa (29032) 641
DH(K1)=5.11 kJ mol-1, DS(K1)=39 J K-1 mol-1.

Ca++ gl KNO3 25°C 0.15M C I K1=1.40 1983DDa (29033) 642
K(Ca+HL)=0.75

Ca++ ISE NaClO4 25°C 0.1M U K1=1.42 1976K Md (29034) 643

Ca++ sp none 25°C 0.0 U T K1=2.47 1976K0a (29035) 644
Also data at 15,30,35,40,45 C. Determined colourimetrically

Ca++ ix oth/un 25°C 0.16M U K1=1.10 1952SLa (29036) 645

Ca++ con oth/un 25°C ->0 U K1=2.43 1940TDa (29037) 646

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

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

Ca++ cal NaNO3 25°C 0.50M C H 1984ARa (29175) 647
DH(K1)=4.90 kJ mol-1, DS(K1)=30 J K-1 mol-1.

Ca++ ix oth/un 25°C ->0 U K1=0.48 1952SLa (29176) 648

Ca++ con oth/un 25°C ->0 U K1=2.00 1940TDa (29177) 649

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

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

Ca++ gl oth/un 25°C 0.10M U K1=2.6 1958GHc (29255) 650

K(CaL+Ca)=2

Ca++ ix oth/un 25°C 0.16M U K1=1.6 1952SLa (29256) 651

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

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

Ca++ gl NaNO3 25°C 0.50M M K1=-0.01 1998KSa (29331) 652

C4H5N3O HL Cytosine CAS 71-30-7 (1096)
2-Oxy-6-aminopyrimidine;

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

Ca++ gl KNO3 35°C 0.10M U M 1986RRe (29395) 653
K(Ca+HL+HA)=8.22
K(Ca(HL)A+H)=3.40
K(Ca+HL+D)=8.49
K(Ca+HL+HC)=7.21
HA is glycine; H2D is oxalic acid; C is histamine.
K(Ca(HL)C+H)=3.22

Ca++ gl KNO3 35°C 0.10M U T H 1983KSa (29396) 654
K(Ca+HL)=21.4
K(Ca+2HL)=3.01

Ca++ gl KNO3 45°C 0.10M U K1=2.5 1974KKa (29397) 655
K(Ca+HL)=2.2

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

Ca++ gl NaNO3 25°C 0.50M M K1=-0.2 1998KSa (29558) 656

C4H6N2O5 H2L CAS 25081-31-6 (3003)
N-Nitrosoiminodiethanoic acid; O:N.N(CH2.COOH)2

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

Ca++ gl KCl 30°C 0.10M U K1=1.3 1957TBb (29629) 657

C4H6N2O6 H2L CAS 25081-33-8 (3004)
N-Nitroiminodiethanoic acid; O2N.N(CH2.COOH)2

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

Ca++ gl KCl 30°C 0.10M U K1=1.6 1957TBb (29635) 658

C4H6N4O L CAS 56-06-4 (5994)
2,4-Diamino-6-hydroxypyrimidine;

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

Ca++ gl KNO3 45°C 0.10M C K1=2.5 1986KZa (29670) 659

C4H6N4O L CAS 1672-50-0 (5993)
4,5-Diamino-6-hydroxypyrimidine;

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

Ca++ gl KNO3 45°C 0.10M C K1=2.93 1986KZa (29680) 660

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

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

Ca++ gl NaClO4 37°C 0.10M U K1=1.33 1992GHa (29885) 661
Method: coulometric titration

Ca++ gl R4N.X 25°C 0.25M C TIH K1=1.45 1985DRa (29886) 662
B(CaHL)=5.96
I=0.02-1M Et4NI.T=15-45 C. DH(K1)=10; DH(CaHL)=11 kJ M-1.DS1=76;DS(CaHL)=165

Ca++ cal NaNO3 25°C 0.50M C H 1984ARa (29887) 663
DH(K1)=7.70 kJ mol-1, DS(K1)=40 J K-1 mol-1.

Ca++ gl R4N.X 25°C 0.10M C TIH K1=1.55 1984DDa (29888) 664
B(CaHL)=6.02
Medium: Et4NI. Data for 0.05-1.0 M and 15-45 C.DH(K1)=7.5 kJ mol-1, DS(K1)
=54 J K-1 mol-1; DH(CaHL)=8.4, DS=142. At I=0, K1=2.26, B(CaHL)=6.71.

Ca++ gl KNO3 25°C 0.15M C I K1=0.95 1983DDa (29889) 665
K(Ca+HL)=0.58

Ca++ ISE NaClO4 25°C 0.1M U K1=1.15 1976KMd (29890) 666

Ca++ gl NaClO4 20°C 0.10M U K1=1.20 1963CAa (29891) 667
K(Ca+HL)=0.54

Ca++ gl oth/un 25°C ? U K1=1.9 1958GHc (29892) 668

Ca++ ix NaCl 25°C 0.16M U K1=1.0 1952SLa (29893) 669

Ca++ EMF oth/un 25°C 0.15M U K1=1.16 1946JOa (29894) 670

Ca++ con oth/un 25°C ->0 U K1=2.00 1940TDa (29895) 671

Ca++ EMF KCl 25°C 0.20M U K1=1.20 1938CKa (29896) 672
K(Ca+HL)=0.52

C4H6O4 HL Acetoxyacetic a CAS 13831-30-6 (4249)
Acetoxyethanoic acid; CH3.CO2.CH2.COOH

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

Ca++ gl NaNO3 30°C 0.40M U K1=0.32 1970BTa (30083) 673

C4H6O4 H2L Me-Malonic Acid CAS 516-15-2 (816)
Methylpropanedioic acid; HOOC.CH(CH3).COOH

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

Ca++ gl NaClO4 25°C 0.10M U K1=1.65 19680Va (30110) 674

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

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

Ca++ gl KCl 30°C 0.10M U K1=1.4 1957TBb (30201) 675

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

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

Ca++ gl KNO3 37°C 0.15M M T K1=2.79 1979ZJa (30307) 676

At 20 C, 0.15 M KNO3, K1=2.84.

C4H6O4Se H2L CAS 6228-62-2 (984)
Selenodiethanoic acid; HOOC.CH2.Se.CH2.COOH

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

Ca++ gl NaClO4 25°C 0.10M U K1=2.3 1966SYa (30446) 677

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

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

Ca++ gl R4N.X 25°C 0.25M C TIH K1=1.95 1985DRa (30553) 678

B(CaHL)=5.72

0.02-1 M NEt4I. 10-37 C. DH1=-7; DH(CaHL)=-9 kJ mol⁻¹. DS1=30; DS(CaHL)=94

Ca++ cal NaNO3 25°C 1.00M U H K1=1.67 1980ARa (30554) 679
DH(K1)=-1.8 kJ mol-1

Ca++ ISE NaCl 25°C 0.10M U K1=2.00 1979CMb (30555) 680

Ca++ ISE NaCl04 25°C 0.1M U K1=2.08 1976KMd (30556) 681

Ca++ sol KCl 25°C 0.10M U T H K1=3.01 1975DNc (30557) 682
DH=36.0 kJ mol-1 and DS=179 J mol-1 K-1. Values also at 35 and 45 C

Ca++ gl NaCl04 20°C 0.10M U 1963CAa (30558) 683
K(Ca+H2L)=1.06
K(Ca+HL)=1.96

Ca++ ix NaCl 25°C 0.16M U K1=2.06 1952SCa (30559) 684

Ca++ kin oth/un 25°C ->0 U K1=2.24 1951BWa (30560) 685
K(Ca+HL)=1.10

Ca++ con oth/un 25°C ->0 U K1=2.66 1940TDa (30561) 686

Ca++ EMF KCl 25°C 0.20M U K1=1.80 1938CKa (30562) 687
K(Ca+HL)=1.02

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

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

Ca++ gl oth/un 25°C 0.0 C I K1=4.28 1999DGa (30831) 688
B(CaHL)=7.12

Medium: artificial seawater. Extrapolated from data for 5-45% salinity.

Ca++ gl R4N.X 25°C 0.25M C TIH K1=3.46 1985DRa (30832) 689
B(CaHL)=6.38
0.02-1 M NEt4I. 12.5-48 C. DH(K1)=-10 kJ mol-1, DS=48; DH(CaHL)=-15, DS=86

Ca++ gl KCl 25°C 0.10M C K1=3.36 1984MMg (30833) 690
K(CaL+H)=1.94

Ca++ gl KNO3 25°C 0.10M C K1=3.54 1975FCc (30834) 691
B(CaHL)=6.56

Ca++ gl KNO3 25°C 0.10M U K1=3.39 1974MSa (30835) 692

Ca++ gl KCl 30°C 0.10M U K1=3.4 1957TBb (30836) 693

C4H6O6 H2L DL-Tartaric acid CAS 133-37-9 (94)
DL-Tartaric acid,DL-2,3-Dihydroxybutanedioic acid; HOOC.CH(OH).CH(OH).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Ca++	gl	R4N.X	25°C	0.25M	C	TIH	K1=2.10 B(CaHL)=5.02	1985DRa (31000)	694
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0.02-1 M NEt4I. 10-37 C. DH(K1)=-9 kJ mol⁻¹, DS=27; DH(CaHL)=-12, DS=71

Ca++	oth	oth/un	25°C	dil	C		K1=2.895	1982HKa (31001)	695
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Method: isotachophoresis. Medium: 0.006-0.019 M tartrate buffer, pH 5.1.

Ca++	ISE	NaCl04	25°C	0.1M	U		K1=1.89	1976K Md (31002)	696
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C4H6O6 H2L L-Tartaric acid CAS 87-69-4 (92)
L-Tartaric acid, L-2,3-Dihydroxybutanedioic acid; HOOC.CH(OH).CH(OH).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Ca++	gl	NaCl04	25°C	0.50M	C		K1=1.66 B(CaH2L2)=10.84	1995PLa (31147)	697
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Ca++	nmr	KNO3	25°C	1.50M	U		K1=1.6	1994PRa (31148)	698
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Keff(Ca+B04(H-1L)2=CaB04(H-1L)2)=4.57, Keff(CaL+B04(H-1L)2=CaB04(H-1L)2+L)=3
At pH 11.5

Ca++	gl	NaCl04	37°C	0.10M	U		K1=1.83	1992GHa (31149)	699
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Method: coulometric titration

Ca++	ix	oth/un	30°C	dil	C	T	K1=2.20	1992LHb (31150)	700
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Medium: 0.2-5.0 mM tartaric acid eluent. At 40 C, K1=2.22

Ca++	gl	NaCl04	25°C	0.10M	U	M	K1=2.83 B(CaL(Cys))=4.35 K(Ca+L+HP04)=9.69	1975RMa (31151)	701
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Ca++	gl	NaCl04	37°C	0.09M	U		K1=2.17	1965TPa (31152)	702
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Ca++	dis	NaCl04	20°C	0.10M	U		K1=<2.0	1963STc (31153)	703
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Ca++	oth	oth/un	?	?	U		K1=2.98	1958TIa (31154)	704
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Ca++	ix	oth/un	25°C	0.16M	U		K1=1.78	1952SLa (31155)	705
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Ca++	gl	oth/un	25°C	->0	U		K1=2.98 B2=6.03	1951HEb (31156)	706
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Ca++	con	oth/un	25°C	->0	U		K1=2.80	1940TDa (31157)	707
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Ca++	EMF	KCl	25°C	0.20M	U		K1=1.80 K(Ca+HL)=1.11	1938CKa (31158)	708
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C4H6O6 H2L meso-Tartaric CAS 147-73-9 (91)
meso-2,3-Dihydroxybutanedioic acid; HOOC.CH(OH).CH(OH).COOH

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

Ca++ nmr KNO3 25°C 1.50M U K1=1.72 1994PRa (31423) 709
Keff(Ca+B04(H-1L)2=CaB04(H-1L)2)=4.65, Keff(CaL+B04(H-1L)2=CaB04(H-1L)2+L)=
2.93. At pH 11.5

C4H7N02S HL Thioproline CAS 444-27-9 (1183)
Thiazolidine-4-carboxylic acid; C3H6NS.COOH

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

Ca++ gl NaCl 37°C 0.15M C K1=1.657 1981HMa (31470) 710

C4H7N03 HL CAS 543-24-8 (3586)
N-Acetylglycine; CH3.CO.NH.CH2.COOH

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

Ca++ gl NaNO3 30°C 0.40M U K1=0.29 1970BTa (31495) 711

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

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

Ca++ gl NaNO3 25°C 0.10M C M K1=4.13 2000KAb (31750) 712
K(CaA+L)=4.35
B(CaAL)=8.85

H2A=Dipicolinic acid.

Ca++ gl NaCl 25°C 0.0 C TIH K1=2.52 1991DDc (31751) 713
B(CaHL)=11.44
B(CaH2L)=14.33

DH(K1)=1 kJ mol⁻¹, DS(K1)=53 J K⁻¹ mol⁻¹; DH(CaHL)=-44, DS(CaHL)=71,
DH(CaH2L)=-54, DS=92. Data for 10-45 C, 0.1-1.0 M NaCl, CaCl2, EtNI

Ca++ ISE NaCl 37°C 0.15M C K1=1.989 1990MOe (31752) 714
B(CaHL)=10.567

Ca++ gl NaCl04 37°C 0.15M C K1=1.135 B2=3.855 1987BBd (31753) 715
B(CaH2L)=14.128
B(CaHL)=10.590
B(CaH-1L)=-9.241

Ca++ gl KNO3 25°C 0.10M M K1=2.77 1981GVa (31754) 716

Ca++ gl KCl 25°C 0.10M U K1=1.60 1953LMa (31755) 717

C4H7N04 H2L IDA CAS 142-73-4 (118)

Iminodiethanoic acid; HN(CH₂.COOH)₂

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	oth/un	25°C	0.10M	C			K1=3.32 B2=6.02	1975MRb (32155)	718
Ca++		oth R4N.X	?	0.10M	U			K1=4.0	1969ASb (32156)	719
Method: chromatography. Medium: NH ₄ Cl										
Ca++	gl	KNO ₃	25°C	1.00M	U			K1=2.09	1968KSa (32157)	720
Ca++	gl	KNO ₃	20°C	0.10M	U	H		K1=2.59	1964ANa (32158)	721
By calorimetry: DH(K1)=1.3 kJ mol ⁻¹ , DS=53.1 J K ⁻¹ mol ⁻¹										
Ca++		EMF KCl	20°C	0.10M	U			K1=2.59	1964PCa (32159)	722
Method: H electrode										
Ca++	gl	oth/un	30°C	0.10M	U			K1=2.7	1957TBb (32160)	723
Ca++		EMF oth/un	20°C	->0	U			K1=3.41	1945SKa (32161)	724
Method: H electrode										

C₄H₇N₅ H₂L (1234)
 N-Hydroxyiminodiethanoic acid; HO.N(CH₂.COOH)₂

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	KNO ₃	25°C	0.10M	C			K1=3.0	1987AKa (32422)	725
Ca++	gl	KNO ₃	25°C	0.10M	U			K1=3.0	1987BKa (32423)	726

C₄H₇N₃ L Creatinine CAS 60-27-5 (3005)
 1-Methyl-2-imino-imidazolidine-4-one;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	ix	oth/un	25°C	0.16M	U			K1=0	1954SCa (32438)	727

C ₄ H ₈ N ₂ O ₃		HL		Asparagine				CAS 70-47-3	(17)	
2-Aminobutanedioic acid 4-amide; H ₂ N.CH(CH ₂ .CO.NH ₂).COOH										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	NaCl	25°C	1.00M	C			K1=0.87	1996BFb (32655)	728

C ₄ H ₈ N ₂ O ₃		HL		Gly-Gly				CAS 556-50-3	(54)	
Glycyl-glycine; H ₂ N.CH ₂ .CO.NH.CH ₂ .COOH										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Ca++ gl KCl 20°C 0.20M U K1=2.04 1982RRc (32974) 729

Ca++ sol oth/un 25°C ->0 U K1=1.24 1950DWa (32975) 730

C4H8N2O4 H2L HDA CAS 19247-05-3 (1025)
Hydrazine-N,N'-diethanoic acid; HOOC.CH2.NH.NH.CH2.COOH

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

Ca++ gl KCl 30°C 0.10M U K1=2.9 1957TBb (33078) 731

C4H8O2 HL Isobutyric acid CAS 79-31-2 (573)
2-Methylpropanoic acid; CH3.CH(CH3).COOH

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

Ca++ sol oth/un 25°C ->0 U K1=0.51 1952CMf (33220) 732

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

Ca++ oth none 25°C 0 U T H K1=2.40 1994SHd (33311) 733
Data also at 35, 45 55 C. DH(K1)=1.9 KJ mol⁻¹, DS=52.2 J K⁻¹ mol⁻¹

Ca++ ISE NaCl 25°C 0.03M U TIH K1=1.21 1981EFa (33312) 734
At 35 C, I=0.045: K1=1.17; 45 C, I=0.45: 0.48; 25 C, I=0.45: 1.29
DH=3.3 kJ mol⁻¹ DS=36.4 J K⁻¹ mol⁻¹

Ca++ sol NaClO4 25°C 0.5M U I K1=0.03 1976KFa (33313) 735
For I=1.0 M K1= 0.11

Ca++ sol none 25°C 0.0 U K1=0.54 1952CMf (33314) 736

Ca++ EMF KCl 25°C 0.20M U K1=0.51 1938CKa (33315) 737
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

Ca++ gl NaClO4 25°C 0.50M C K1=1.09 1995PLa (33437) 738

Ca++ EMF NaClO4 25°C 1.0M U K1=0.92 B2=1.42 1965VTa (33438) 739
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
Ca++	dis	NaNO3	20°C	0.15M	C		K1=0.5	1973APa (33610)	740
Method: ion exchange using 45Ca isotope									
Ca++	EMF	KCl	25°C	0.20M	U		K1=0.60	1938CKa (33611)	741
Method: H electrode									
Ca++	sol	none	25°C	0.0	U		K1=0.82	1938DAa (33612)	742

C4H8O3			HL				CAS 591-81-1	(39)	
4-Hydroxybutanoic acid; HO.CH2.CH2.CH2.COOH									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	dis	NaNO3	20°C	0.15M	C		K1=0.7	1973APa (33649)	743
Method: ion exchange using 45Ca isotope									

C4H8S			L				CAS 110-01-0	(150)	
Tetrahydrothiophene; cyclo(-CH2.CH2.S.CH2.CH2-)									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	sp	alc/w	25°C	50%	C		K1=-0.30	1979SRa (33731)	744
Medium: 50% EtOH/H2O, 1.0 M NaClO4									

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
Ca++	ISE	non-aq	25°C	100%	C		K1=2.60	1997NMa (33760)	745
Method: polyacrylamide/15-crown-5 sensor. Medium: acetonitrile.									

C4H9NO3			HL	Threonine			CAS 72-19-5	(48)	
2-Amino-3-hydroxybutanoic acid; H2N.CH(CH(OH)).CH3)COOH									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	gl	NaCl	37°C	0.15M	U			1986XHa (34261)	746
							B(CaH-1L2)=-5.859		
							B3=6.045		

C4H9NO7P2			H4L				CAS 56269-30-8	(2397)	
1-Pyrrolidone-5,5-diphosphonic acid; (O)C4H5N(P03H2)2									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	gl	R4N.X	25°C	0.10M	M			1984CLb (34403)	747

K(Ca+HL)=6.86
K(Ca+H2L)=3.73

C4H10N06P H2L CAS 6401-59-8 (2399)
O-Phospho-2-methylserine;

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

Ca++ gl KNO3 25°C 0.20M C K1=1.82 1978MAc (34473) 748
K(Ca+HL)=1.09
K(CaL+H)=9.34

C4H10N06P H2L CAS 1114-81-4 (2400)
O-Phospho-threonine;

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

Ca++ gl KNO3 25°C 0.20M C K1=2.23 1978MAc (34481) 749
K(Ca+HL)=1.53
K(CaL+H)=8.97

C4H10N204S HL ACES CAS 7365-82-4 (7488)
N-(2-Acetamido)-2-aminoethanesulfonic acid;

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

Ca++ gl KNO3 25°C 0.10M C M K1=4.86 2001AAa (34617) 750
Also data for ternary complexes with 5'-GMP, 5'-IMP and 5'-CMP.

Ca++ gl KNO3 25°C 0.10M C K1=3.38 2000ADa (34618) 751

Ca++ gl NaClO4 37°C 0.10M U T K1=0.2 1992GHa (34619) 752
Method: coulometric titration. At 25 C, K1=0.4.

C4H1002S 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

Ca++ sp NaClO4 25°C 1.0M C K1=-0.09 1979SRa (34679) 753

C4H1003 L CAS 111-46-6 (3579)
2,2'-Oxydiethanol; (HO.CH2.CH2)2.0 (Diethylene glycol)

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

Ca++ con non-aq 25°C 100% C K1=3.2 1992MSe (34699) 754
Medium: 100% MeOH. Anion: picrate. Also data for nitrophenolate anions.

C4H1006C12P2 CAS 134757-52-1 (5246)

Clodronic acid monoisopropyl ester; H3L

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

Ca++ gl R4N.X 25°C 1.0M C K1=3.29 1995RLa (34715) 755
Medium: 1.0 M Me4NCl

C4H11N03 L Tris buffer CAS 77-86-1 (550)
2-Amino-2-(hydroxymethyl)-propan-1,3-diol; (HO.CH2)3C.NH2

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

Ca++ gl R4N.X 25°C 1.00M C I K1=0.25 1982SSf (35045) 756
In 90 % (v/v) DMSO/water mixture: K1=0.25 (I=0.25 M)

C4H11N08P2 H5L CAS 2439-99-8 (2129)
N-Carboxymethyl-N,N-bis(methylenephosphonic acid); HOOC.CH2.N(CH2.PO3H2)2

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

Ca++ gl KNO3 25°C 0.10M C K1=7.90 2000SDa (35096) 757
K(CaL+H)=7.22
K(CaHL+H)=5.46
K(CaH2L+H)=3.7

Ca++ ix NaNO3 RT 0.10M U K1=7.0 1985PMc (35097) 758

Ca++ gl KNO3 25°C 0.10M U K1=6.17 1965WRa (35098) 759

C4H1103P H2L CAS 4923-84-6 (524)
Butylphosphonic acid; C4H9PO3H2

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

Ca++ gl KNO3 25°C 0.10M U K1=1.69 1981WNa (35243) 760

C4H1104P H2L (5867)
n-Butyl phosphoric acid; C4H9.O.PO(OH)2

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

Ca++ gl NaNO3 25°C 0.10M C K1=1.56 1988MSa (35282) 761

C4H12N03P H2L AMPPH CAS 18108-24-2 (222)
1-Amino-2-methylpropylphosphonic acid; (CH3)2.CH.CH(NH2).PO3H2

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

Ca++ gl KNO3 24°C 0.10M U K1=3.42 1989YKa (35306) 762

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

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

Ca++ gl oth/un 25°C 0.10M U K1=2.5 1962IMb (35573) 763

Ca++ gl KCl 20°C 0.10M U K1=2.54 1951SRa (35574) 764
K(Ca+HL)=1.7

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

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

Ca++ gl NaNO3 25°C 0.10M M K1=3.00 1999SSa (35581) 765

C4H13NO3P+ HL (1971)
Trimethylammonium-methylphosphonic acid; +N(CH3)3.CH2.PO3H2

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

Ca++ gl KNO3 25°C 0.10M U K1=0.93 1979WNa (35590) 766

C4H13NO6P2 H4L CAS 5995-26-6 (1336)
N-Ethyliminobis(methylenephosphonic) acid; C2H5N(CH2PO3H2)2

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

Ca++ gl KCl 25°C 0.20M C K1=3.71 1999MKa (35600) 767
B(CaHL)=14.59
B(CaH2L)=19.88

Ca++ gl KNO3 25°C 1.00M M K1=3.14 1982BGb (35601) 768
K(Ca+HL)=1.66

Ca++ gl KNO3 25°C 1.0M U K1=3.36 1967CCb (35602) 769
K(Ca+HL)=1.29
K(Ca+H2L) < 1

C4H13NO7P2 H4L CAS 63132-40-1 (1347)
1-Hydroxy-4-aminobutyl-1,1-diphosphonic acid; (PO3H2)2C(OH).CH2.CH2.CH2.NH2

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

Ca++ gl KCl 25°C 0.10M M K1=6.10 1978KMa (35617) 770
K(Ca+HL)=6.01
K(Ca+H2L)=5.37

C4H13N3 L Dien CAS 111-40-0 (584)

1,4,7-Triazaheptane, 2,2'Iminobis(ethylamine), diethylenetriamine;
 NH2.(CH2)2.NH.(CH2)2.NH2

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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  NaCl   25°C  0.0  C           K1=0.42      1999SFc (35737) 771
                (Ca+HL)=0.10
                (Ca+H2L)=-0.32
Extrapolated from data for 0.03-0.96 M NaCl using the Pitzer equation.
-----
```

```
Ca++      gl  KCl    25°C  0.0  C           K1=-0.01    1992DDa (35738) 772
                (Ca+HL)=<-0.2
                (Ca+H2L)=<-0.4
-----
```

 C4H14N2O6P2 H2L EDDPO CAS 1733-49-9 (2435)
 1,2-Diaminoethane-N,N'-bis(methylenephosphonic) acid; (H2O3P.CH2.NH.CH2)2

```
-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      EMF KCl    25°C  0.10M C           B(CaHL)=14.3
                B(CaH2L)=24.4
                B(CaH3L)=30.6
                B(Ca2L)=19.6
-----
```

```
Ca++      gl  KCl    25°C  0.10M U           K1=>2      1965DKb (35859) 774
-----
C5H205                    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
-----
Ca++      sol KCl    25°C  0.30M U           K1=1.29    1965CDa (35936) 775
                Kso=-4.05
-----
```

 C5H3N4Cl L 6-Chloropurine CAS 87-42-3 (3032)
 6-Chloropurine;

```
-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  KNO3   45°C  0.10M U           K1=6.2     1971TKc (35986) 776
-----
C5H4NBr                    L                            CAS 1120-87-2 (8780)
4-Bromopyridine;
-----
```

```
-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  NaNO3  25°C  0.50M C           K1=-0.01   2002KSb (35999) 777
-----
C5H4NCl                    L                            CAS 626-60-8 (322)
```


3-Chloropyridine; C5H4N.Cl

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	NaNO3	25°C	0.50M	C			K1=-0.08	2002KSb (36017)	778

C5H4N2O3S			H2L					Thioorotic acid (4335)		
1,2,3,6-Tetrahydro-2-thio-6-oxo-4-pyrimidinecarboxylic acid;										
Ca++	gl	NaCl	20°C	0.15M	U			K1=2.95 K(Ca+HL)=2.15	1979DZe (36072)	779

C5H4N2O4			H2L					Orotic acid CAS 65-86-1 (624)		
1,2,3,6-Tetrahydro-2,6-dioxo-4-pyrimidinecarboxylic acid;										
Ca++	gl	NaClO4	25°C	0.50M	U	I		K(Ca+H2L)=2.34 K(Ca+HL)=3.42 K(Ca+H2L)=2.54 (0.1 NaClO4)	1983MDa (36101)	780

Ca++	gl	NaCl	20°C	0.15M	U			K1=3.15 K(Ca+HL)=2.26	1979DZe (36102)	781

C5H4N4O			HL					Hypoxanthine CAS 68-94-0 (1174)		
6-Hydroxypurine;										
Ca++	gl	KNO3	25°C	0.10M	U	T H		K(Ca+HL)=2.20 K(Ca+2HL)=4.11	1983KSa (36180)	782

Ca++	gl	KNO3	45°C	0.10M	U			K1=6.45	1971TKc (36181)	783

C5H4N4S			HL					6-Purinethiol CAS 6112-76-1 (115)		
6-Mercaptopurine, 6-Thiohypoxanthine;										
Ca++	gl	KNO3	45°C	0.10M	U			K1=6.4	1971TKc (36222)	784

C5H4O2S			HL					2-Thenoic acid CAS 527-72-0 (2312)		
Thiophene-2-carboxylic acid; C4H3S.CO0H										
Ca++	gl	KNO3	45°C	0.10M	U			K1=6.4	1971TKc (36222)	784

C5H4O2S			HL					2-Thenoic acid CAS 527-72-0 (2312)		
Thiophene-2-carboxylic acid; C4H3S.CO0H										

Ca++ gl NaClO4 30°C 0.20M U T H K1=2.01 1976SSd (36247) 785

Ca++ gl oth/un 25°C ->0 U K1=1.33 1960LUB (36248) 786

C5H4O3 HL 2-Furoic acid CAS 88-14-2 (2492)
Furan-2-carboxylic acid; C4H3O.COOH

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

Ca++ gl oth/un 25°C ->0 U K1=-1.0 1960LUB (36290) 787

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

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

Ca++ gl NaNO3 25°C 0.50M C K1=-0.12 2002KSb (36526) 788

Ca++ gl KCl 25°C 1.00M U I K1=-0.45 1986CCd (36527) 789
K=-0.24 if values calculated by allowing for both CaCl+ and H(py)Cl species.

C5H5NO2 HL CAS 13161-30-3 (5582)
1-Hydroxypyridin-2(1H)-one, 2-Hydroxypyridine 1-oxide;

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

Ca++ gl KCl 25°C 0.20M C K1=2.47 B2= 3.50 2000FEc (36747) 790

C5H5NO2 HL CAS 16867-04-2 (2316)
2,3-Dihydroxypyridine, 3-Hydroxypyridin-2(1H)-one; C5H3N(OH)2

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

Ca++ gl KNO3 37°C 0.15M C K1=2.68 1980SHb (36774) 791

C5H5NO2 HL CAS 1121-23-9 (2315)
3-Hydroxypyridin-4(1H)-one;

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

Ca++ gl KNO3 37°C 0.15M C K1=3.12 B2=4.72 1980SHb (36824) 792

C5H5NO2 HL CAS 634-97-9 (2877)
Pyrrole-2-carboxylic acid; C4H4N.COOH

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

Ca++ cal NaNO3 25°C 1.00M U H 1981ARb (36835) 793

DH(K1)=-0.54 kJ mol-1; DS(K1)=28.0.

Ca++ gl none 25°C 0.00 U K1=2.36 1972LUc (36836) 794

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

Ca++ gl NaNO3 25°C 0.50M C K1=-0.21 2002KSb (36855) 795

C5H5N5 L Adenine CAS 73-24-5 (237)
6-Aminopurine; H2N.C5H3N4

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

Ca++ gl KNO3 35°C 0.10M U T H 1983KSa (36951) 796
K(Ca+HL)=1.86
K(Ca+2HL)=3.35

Ca++ gl KNO3 45°C 0.10M U K1=2.95 1971TKc (36952) 797

C5H5N5S H3L 6-Thioguanine CAS 3647-48-1 (4307)
2-Amino-6-mercaptapurine;

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

Ca++ gl KNO3 45°C 0.10M U K1=2.9 1973TKa (37009) 798
K(Ca+H2L)=2.7

C5H5N5S H3L CAS 154-42-7 (4308)
2-Mercapto-6-aminopurine;

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

Ca++ gl KNO3 45°C 0.10M U 1973TKa (37017) 799
K(Ca+H2L)=2.8
K(CaH2L=CaHL+H)=2.9

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

Ca++ gl NaNO3 25°C 0.50M C K1=-0.19 2002KSb (37116) 800

Ca++ sp alc/w 25°C 95% U K1=0.98 1993GSa (37117) 801
Medium: 95% w/w EtOH/H2O, 0.05 M Et4NClO4, by competitive spectrophotometry

C5H6N2O HL (3035)
2-Aminopyridine 1-oxide; C5H4N(-O)(NH2)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	sp	NaClO4	25°C	0.50M	U			K(Ca+HL)=0.01	1963SBd (37200)	802

C5H6N2O2		HL		Thymine				CAS 65-71-4	(413)	
2,4-Dihydroxy-5-methylpyrimidine; C4HN2(CH3)(OH)2										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	KNO3	25°C	0.10M	U	T H		K1=2.92	1983Ksa (37265)	803
Ca++	gl	KNO3	35°C	0.10M	U			K1=2.86	1982TSa (37266)	804
Ca++	gl	KNO3	45°C	0.10M	U			K1=2.6	1974KKa (37267)	805

C5H6N6		HL		Diaminopurine				CAS 1904-98-9	(4290)	
2,6-Diaminopurine;										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	KNO3	45°C	0.10M	U			K1=2.8	1973TKa (37335)	806

C5H6O4		H2L		Citraconic acid				CAS 498-23-7	(3021)	
Citraconic acid; CH3.C(COOH):CH.COOH										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	ix	oth/un	25°C	0.16M	U			K1=1.3	1952SLa (37354)	807

C5H6O4		H2L		Itaconic acid				CAS 97-65-4	(398)	
Methylenesuccinic acid; HOOC.CH2.C(:CH2).COOH										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	cal	NaNO3	25°C	0.50M	C	H			1984ARa (37406)	808
DH(K1)=5.73 kJ mol-1, DS(K1)=38 J K-1 mol-1.										
Ca++	ix	oth/un	25°C	0.16M	U			K1=1.2	1952SLa (37407)	809

C5H6O5		H2L		Ketoglutaric				CAS 328-50-7	(1146)	
2-Ketoglutaric acid; HOOC.CH2.CH2.CO.COOH										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	ix	oth/un	25°C	0.16M	U			K1=1.29	1952SLa (37472)	810

C5H6O7		H3L						(8107)		
Carboxymethyltartronic acid;										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	KCl	25°C	0.10M	C			K1=4.62 K(CaL+H)=2.65	1984MMg (37485)	811

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
Ca++	gl	diox/w	28°C	70%	U			K1=6.34 B2=11.80	1992ZHa (37874)	812
Ca++	gl	NaNO3	25°C	0.10M	C			K1=2.32	1982HNa (37875)	813
Ca++	gl	diox/w	24°C	50%	U			K1=3.1	1979ACa (37876)	814
Ca++	gl	diox/w	20°C	17%	C			K1=5.59 B2=9.97	1976JWa (37877)	815

C5H8O4		H2L						CAS 595-46-0	(1144)	
Dimethylmalonic acid; HOOC.C(CH3)2.COOH										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	NaClO4	25°C	0.10M	U			K1=1.52	19680Va (38203)	816

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	sp	none	25°C	0.0	U T			K1=2.47	1976K0a (38230)	817
Also data at 15,30,35 C. Determined colourimetrically										
Ca++	gl	NaClO4	25°C	0.10M	U			K1=1.59	19680Va (38231)	818

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
Ca++	ix	oth/un	25°C	0.16M	U			K1=0.55	1952SLa (38301)	819
Ca++	EMF	KCl	25°C	0.20M	U			K1=1.06 K(Ca+HL)=0.50	1938CKa (38302)	820

C5H9NO		L		NMP				CAS 826-41-5	(7823)	
N-Methylpyrrolidone;										

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

Ca++ ISE non-aq 25°C 100% C K1=2.53 1997NMa (38459) 821
Method: polyacrylamide/15-crown-5 sensor. Medium: acetonitrile.

C5H9NO3 HL Hydroxyproline CAS 51-35-4 (416)
4-Hydroxy-2-pyrrolidinecarboxylic acid; C4H7N(OH)(COOH)

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

Ca++ gl KCl 20°C 1.0M U K1=9.58 1959PEc (38711) 822

Ca++ ix oth/un 25°C 0.16M U K1=0.48 1954SCa (38712) 823

C5H9NO3S H2L N-Acetyl-Cys CAS 616-91-1 (1187)
N-Acetylcysteine; CH3.CO.NH.CH(CH2.SH)COOH

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

Ca++ gl oth/un 25°C 0.10M U K1=2.8 1975IMa (38811) 824
Medium not stated.

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

Ca++ gl NaNO3 25°C 0.10M C M K1=2.95 2000KAb (39000) 825
K(CaA+L)=3.05
B(CaAL)=7.55

H2A=Dipicolinic acid.

Ca++ gl NaCl 25°C 1.00M C K1=0.60 1988BSa (39001) 826

Ca++ gl NaCl04 37°C 0.15M C K1=1.474 1987BBd (39002) 827
B(CaH2L)=14.020
B(CaHL)=10.377
B(CaH-1L)=-9.071

Ca++ gl KNO3 25°C 0.10M M K1=2.63 1981GVa (39003) 828

Ca++ gl KCl 25°C 0.10M U K1=1.43 1953LMa (39004) 829

Ca++ sol oth/un 25°C ->0 U K1=2.05 1950DWa (39005) 830

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

Ca++ gl oth/un 25°C 0.10M C K1=4.40 B2=7.30 1975MRb (39213) 831

Ca++ vlt NaClO4 25°C 0.10M U K1=3.88 1969VPa (39214) 832

Ca++ gl KCl 25°C 0.10M U H K1=3.85 B2=6.57 1968NPb (39215) 833
By calorimetry:DH(K1)=-5.0 kJ mol⁻¹, DS=56.8 J K⁻¹ mol⁻¹, DH(K2)=-2.9, DS=42

Ca++ cal KNO3 20°C 0.10M U H 1965ANa (39216) 834
DH(K1)=-6.9 kJ mol⁻¹, DS=48.9 J K⁻¹ mol⁻¹

Ca++ gl KCl 20°C 0.10M U K1=3.75 1955SAa (39217) 835

Ca++ EMF oth/un 20°C ->0 U K1=4.51 1945SKa (39218) 836
Method: H electrode

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

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

Ca++ gl NaNO3 25°C 0.10M U K1=5.5 B2= 9.80 1993GAa (39506) 837

Ca++ gl KNO3 35°C 0.10M C M 1985RRc (39507) 838
K(Ca+HL)=2.32
K(CaL(cytidine)+H)=3.13
K(Ca+HL+cytidine)=8.63

C5H10N07P 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

Ca++ gl KNO3 25°C 0.10M C K1=7.41 2000SDa (39651) 839
K(CaL+H)=6.19
K(CaHL+H)=4.0

Ca++ ix NaNO3 RT 0.10M U K1=7.2 1985PMc (39652) 840

Ca++ oth KNO3 RT 0.10M C 1980MVa (39653) 841
K(Ca+HL)=2.2

Method: paper electrophesis.

Ca++ gl KCl 30°C 0.10M U K1=7.1 19580Mb (39654) 842

Ca++ EMF KCl 20°C 0.10M U K1=7.18 1949SAa (39655) 843
K(Ca+HL)=2.43

Method: H electrode

C5H10N2O2 HL CAS 2762-32-5 (3041)
Piperazine-2-carboxylic acid; C4H9N2.COOH

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

Ca++ gl KCl 22°C 0.10M U K1=<1 1960REb (39720) 844

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

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

Ca++ gl NaCl 37°C 0.15M U M K1=2.17 1997NZa (39796) 845
B(CaH2(glu)L)=21.65

C5H10N2O3 HL Ala-Gly CAS 687-69-4 (55)
Alanyl-glycine; H2N.CH(CH3).CO.NH.CH2.COOH

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

Ca++ gl KCl 20°C 0.20M U K1=1.87 1982RRc (39882) 846

Ca++ sol oth/un 25°C ->0 U K1=0.66 1950DWa (39883) 847

C5H10N2O3 HL Gly-DL-Ala CAS 926-77-2 (66)
Glycyl-DL-alanine; H2N.CH2.CO.NH.CH(CH3).COOH

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

Ca++ gl KCl 20°C 0.20M U K1=2.02 1982RRc (39931) 848

C5H10O2 HL IsoValeric acid CAS 503-74-2 (1311)
3-Methyl-butanoic acid, Isovaleric acid; (CH3)2CH.CH2.COOH

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

Ca++ sol oth/un 25°C ->0 U K1=0.20 1952CMf (40183) 849

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

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

Ca++ sol oth/un 25°C ->0 U K1=0.30 1952CMf (40199) 850

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

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

Ca++ sol oth/un 25°C ->0 U K1=0.55 1952CMf (40214) 851

C5H10O5 L D-Arabinose CAS 10323-20-3 (3606)
D-Arabinose;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	ISE	KNO3	25°C	0.70M	U			K1=-0.82	1986HAe (40331)	852

C5H10O5				L				CAS 1114-34-7	(6113)	
D-Lyxose										
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	ISE	KNO3	25°C	0.70M	U			K1=-0.80	1986HAe (40338)	853

C5H10O5				L		D-Ribose		CAS 50-69-1	(512)	
D-Ribose;										
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	cal	none	25°C	0.0	U	H		K1=0.28	1991MLa (40342)	854
DH(K1)=-17 kJ mol-1										
Ca++	cal	none	25°C	0.0	U	H			1989MMb (40343)	855
DH(CaL)=-16.6 kJ mol-1; TDS=-14.9.										
Ca++	ISE	KNO3	25°C	0.70M	U			K1=-0.34	1986HAe (40344)	856
Ca++	ISE	KCl	25°C	0.10M	U			K1=0.93	1985MLb (40345)	857
Ca++	nmr	none	-9°C	0.0	U			K1=4.6	1982SBb (40346)	858
a-furanose form; data also for a-pyranose and b-pyranose forms.										

C5H10O5				L		D-Xylose		CAS 58-86-6	(3607)	
D-Xylose;										
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	ISE	KNO3	25°C	0.70M	U			K1=<-1	1986HAe (40359)	859

C5H10O5				L		L-Arabinose		CAS 5328-37-0	(1616)	
L-Arabinose										
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	ISE	NaClO4	25°C	1.00M	C	I		K1=0.21	1977EOa (40364)	860
Data also for D-Xylose and D-Ribose										

C5H10O10P2				H6L				CAS 51395-42-7	(2396)	
2,3-Dicarboxypropane-1,1-diphosphonic acid; CH2(COOH)CH(COOH)CH(PO3H2)2										
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo

Ca++ gl R4N.X 25°C 0.10M M K1=4.1 1984CLb (40381) 861
K(Ca+HL)=4.15
K(CaL+Ca)=2.91
K(CaHL+Ca)=3.83

C5H11N02 HL Nor-Valine CAS 760-78-1 (689)
2-Aminopentanoic acid; CH3.CH2.CH2.CH(NH2).COOH

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

Ca++ gl NaNO3 25°C 0.10M C M K1=4.92 2000KAb (40821) 862
K(CaA+L)=3.70
B(CaAL)=8.20

H2A=Dipicolinic acid.

C5H11N02S H2L D-Penicillamine CAS 52-67-5 (1323)
D-2-Amino-3-mercapto-3-methylbutanoic acid; (CH3)2C(SH)CH(NH2)COOH

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

Ca++ gl KNO3 37°C 0.15M M T K1=3.01 1979ZJa (41175) 863
At 20 C, 0.15 M KNO3, K1=3.15

C5H11N207P H3L (3635)
Glycyl-O-phosphoryl-D,L-serine;

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

Ca++ gl KCl 25°C 0.15M U K1=1.77 19620Sa (41376) 864
K(Ca+HL)=1.48

C5H11N207P H3L CAS 6665-42-5 (3636)
O-Phosphorylserylglycine;

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

Ca++ gl KCl 25°C 0.15M U K1=1.85 19620Sa (41381) 865
K(Ca+HL)=1.30

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

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

Ca++ gl NaNO3 25°C 0.10M C K1=1.48 1988MSa (41415) 866

C5H12N04P HL CAS 51276-47-2 (5704)
2-Amino-4-(methylhydroxyphosphoryl)butanoic acid;

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

 Ca++ gl NaClO4 23°C 0.10M U K1=2.43 1990YTa (41441) 867

 C5H12N2O2 HL Ornithine CAS 1069-31-4 (46)
 2,5-Diaminopentanoic acid; H2N.CH2.CH2.CH2.CH(NH2)COOH

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

Ca++ gl KNO3 25°C 0.10M U I K(Ca+HL)=1.52 1970CMc (41558) 868

I=1.0 M, K(Ca+HL)=1.68

 C5H12O5 L Arabitol CAS 488-82-4 (5403)
 Arabitol; HO.CH2.HOCH.HCOH.HCOH.CH2.OH

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

Ca++ ISE KNO3 25°C 0.70M U K1=-0.65 1986HAe (41674) 869

C5H12O5 L Ribitol CAS 488-81-3 (3009)
 Ribitol, Adonitol; HO.CH2.HCOH.HCOH.HCOH.CH2.OH

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

Ca++ ISE KNO3 25°C 0.70M U K1=-0.80 1986HAe (41678) 870

C5H12O5 L Xylitol CAS 87-99-0 (2139)
 Xylitol; HO.CH2.HCOH.HOCH.HCOH.CH2.OH

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

Ca++ ISE KNO3 25°C 0.70M U K1=-0.54 1986HAe (41682) 871

C5H13NO6P2 H4L CAS 56152-35-3 (8890)
 N-Pyrrolidinomethane-1,1-diphosphonic acid;

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

Ca++ gl KCl 25°C 0.20M C B(CaH2L)=23.40
 B(CaHL)=17.30
 B(CaHL2)=21.02

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

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

Ca++ gl KNO3 30°C 0.15M U K1=6.56 B2=10.46 1983LSa (41752) 873
 K(Ca+HL)=2.85

K(Ca+CaL)=1.73

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
Ca++	gl	KNO3	30°C	0.15M	U			K1=6.81 B2=10.04 K(Ca+HL)=2.80 K(Ca+CaL)=2.16	1983LSa (41756)	874

C5H13NO7P2 H4L CAS 32545-75-8 (6890)
N-Methylenedi(phosphonic acid)tetrahydrooxazine; OC4H8N.CH(P03H2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	KCl	25°C	0.10M	M			K1=4.18 K(Ca+HL)=4.05	1978GMf (41763)	875

C5H13NO8P2 H4L (3714)
N-(2'-Carboxyethyl)iminobis(methylenephosphonic acid)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	KNO3	25°C	0.10M	U			K1=4.88	1965WRa (41768)	876

C5H14NO3P H2L CAS 82101-93-7 (544)
2-(2-Dimethylaminopropyl)phosphonic acid; (CH3)2N.C(CH3)2.P03H2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	KNO3	25°C	0.10M	U			K1=1.2 B(CaHL)=13.25	1981WNa (41826)	877

C5H14NO3P H2L CAS 72696-97-0 (1990)
Diethylaminomethylphosphonic acid; (C2H5)2N.CH2.P03H2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	KNO3	25°C	1.0M	U			K1=1.3 K(Ca+HL) < 1	1967CCa (41831)	878

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	NaClO4	25°C	0.1M	U			K1=3.85 K(Ca+HL)=2.88	1975SLa (41835)	879

C5H15N06P2 H4L CAS 195000-13-6 (8888)
N-(1-Methylpropyl)aminomethane-1,1-diphosphonic acid;

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

Ca++ gl KCl 25°C 0.20M C 2002MKc (41941) 880
B(CaH2L)=22.30
B(CaHL)=16.69

C5H15N07P2 H4L AMOK CAS 63132-39-8 (1350)
1-Hydroxy-3-N,N-dimethylaminopropane-1,1-diphosphonic acid;
Me2N.CH2.CH2.C(OH)(PO3H2)2

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

Ca++ gl R4N.X 25°C 0.15M U M K1=6.11 1988MNa (41950) 881
B(CaHL)=17.59
B(CaH2L)=25.56
B(Ca2L)=11.05
B(CaNaL)=8.82

Ca++ sol KCl 22°C 0.10M U 1985Ksa (41951) 882
K(Ca+HL)=5.24

Ca++ gl KCl 25°C 0.10M M K1=5.71 1978KMa (41952) 883
K(Ca+HL)=5.57
K(Ca+H2L)=3.38

C5H15N07P2 H4L (1348)
1-Hydroxy-3-N-ethylaminopropylydenediphosphonic acid;
CH3.CH2.NH.CH2.CH2.C(OH)(PO3H2)2

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

Ca++ gl KCl 25°C 0.10M M K1=6.17 1978KMa (41961) 884
K(Ca+HL)=6.09
K(Ca+H2L)=4.21

C5H17N013P4 H5L ADOPPH CAS 82372-37-0 (228)
1-Hydroxy-3-(N,N-bis(methylenephosphonic)-aminopropylydene-1,1-diphosphonic acid;

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

Ca++ gl KNO3 25°C 1.0M U K1=7.40 1982SBa (42017) 885
K(Ca+HL)=6.23
K(Ca+H2L)=4.33
K(Ca+H3L)=2.9
K(Ca+H4L)=2.34

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
Ca++	con	alc/w	30°C	100%	U	I M		K2=2.92	1979PSa (42083)	886
Medium: iso-PrOH. K(CaL2+diethyleneglycol)=2.84; K(CaL2=triethyleneglycol)=2.75 In H2O: K2=1.65, K(CaL2+tetraethyleneglycol)=1.59										

Ca++	sp	oth/un	25°C	->0	U			K1=3.74	1960KAb (42084)	887
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Ca++	sp	oth/un	21°C	0.40M	U			B2=2.48	1955BKa (42085)	888
Medium:0.2-0.6(some EtOH)										

 C6H4N2O5 HL CAS 50-28-5 (505)
 2,4-Dinitrophenol; HO.C6H3(NO2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	sp	oth/un	21°C	0.40M	U			B2=2.17	1955BKa (42220)	889
Medium:0.2-0.6(some EtOH)										

 C6H4N2O6 H2L CAS 7659-29-2 (2694)
 1,2-Dihydroxy-3,5-dinitrobenzene; (HO)2.C6H2(NO2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	KCl	25°C	0.10M	M			K1=3.21 B2=5.88	1987HAb (42260)	890

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	NaNO3	20°C	0.10M	U			K1=1.81	1960ANb (42471)	891
Ca++	gl	oth/un	25°C	0.0	U			K1=2.22 B2=3.79	1957LUa (42472)	892
Ca++	gl	NaNO3	25°C	0.10M	U			K1=2.5	1957SYb (42473)	893

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
Ca++	gl	KCl	25°C	0.10M	M			K1=4.42 B2=7.50	1986HAc (42851)	894

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
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Ca++ gl KCl 25°C 0.10M M K1=5.79 B2=6.4 1985HAa (42902) 895

C6H5N2O8P H2L CAS 2566-76-9 (6146)

2,4- Dinitrophenylphosphoric acid; (NO2)2C6H3.O.PO3H2

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

Ca++ kin KCl 39°C 1.00M C K1=6.0 1987HJb (42981) 896

C6H6NBr L (8782)

5-Bromo-2-methylpyridine;

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

Ca++ gl NaNO3 25°C 0.50M C K1=-0.05 2002KSb (43190) 897

C6H6NCl L CAS 10445-91-7 (8781)

4-(Chloromethyl)pyridine;

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

Ca++ gl NaNO3 25°C 0.50M C K1=-0.06 2002KSb (43206) 898

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

Ca++ gl NaNO3 25°C 0.10M C K1=1.26 1988MSa (43240) 899

Ca++ kin KCl 39°C 1.00M C K1=7.5 1987HJb (43241) 900

C6H6N2O2 HL (8281)

3-Hydroxy-2-amidocarboxypyridine, Hydroxypicolinamide;

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

Ca++ gl KNO3 25°C 0.10M C K1=2.68 1990ARa (43369) 901

C6H6N2O4 HL Methylrotic CAS 706-36-2 (2611)

3N-Methyl-2,4-dihydroxypyrimidine-6-carboxylic acid, methylrotic acid;

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

Ca++ sp oth/un 20°C var C K1=3.40 1981LGc (43466) 902

Medium: phosphate (0.1 M) or borax (0.01 M) buffers.

Ca++ gl NaCl 20°C 0.15M U K1=3.45 1979DZc (43467) 903

K(Ca+HL)=2.05

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

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

Ca++ ix oth/un 20°C .016M U T H K1=1.93 1979VMb (43533) 904
 K(Ca+HL=CaL+H)=-8.10

DH= 53.5 kJ mol⁻¹. Dta also available for T=30 and 40.

C6H6O2 H2L Catechol CAS 120-80-9 (534)
 1,2-Dihydroxybenzene, pyrocatechol; HO.C6H4.OH

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

Ca++ sp alc/w 25°C 95% U K1=1.7 1993GSa (43694) 905
 Medium: 95% w/w EtOH/H2O, 0.05 M Et4NClO4, by competitive spectrophotometry

 Ca++ gl KNO3 35°C 0.10M C K1=3.64 1985RRh (43695) 906

C6H6O3 HL Maltol CAS 118-71-8 (2442)
 3-Hydroxy-2-methyl-4H-pyran-4-one;

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

Ca++ gl diox/w 30°C 50% U K1=4.84 B2=7.25 1957Cwa (44069) 907

C6H6O4 HL Kojic acid CAS 501-30-4 (1800)
 5-Hydroxy-2-(hydroxymethyl)-4H-pyran-4-one;

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

Ca++ EMF KCl 21°C 0.10M U K1=2.5 19590Kb (44177) 908
 Method: H electrode

 Ca++ gl diox/w 30°C 50% U K1=4.4 B2=7.1 1954BFa (44178) 909

C6H6O5S H3L CAS 7134-09-0 (3687)
 3,4-Dihydroxybenzenesulfonic acid; (HO)2.C6H3.SO3H

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

Ca++ gl KNO3 30°C 0.10M U K1=4.40 B2=7.99 1963Mnc (44277) 910

C6H6O6 H3L trans-Aconitic CAS 4023-65-8 (3065)
 trans-1,2,3-Propenetricarboxylic acid; HOOC.CH:C(COOH)CH2.COOH

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

Ca++ ix oth/un 25°C 0.16M U K1=1.50 1952SLa (44304) 911

Ca++ gl KNO3 25°C 0.10M U K1=1.43 1981WNa (45198) 918

 C6H7O4P H2L CAS 701-64-4 (5866)
 Phenyl phosphoric acid; C6H5O.P(O)(OH)2

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

Ca++ gl NaCl 25°C 0.15M U K1=1.44 1990KLb (45225) 919

Ca++ gl NaNO3 25°C 0.10M C K1=1.45 1988MSa (45226) 920

 C6H8N2 L CAS 95-54-5 (2899)
 1,2-Diaminobenzene, 1,2-Phenylenediamine; C6H4(NH2)2

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

Ca++ sp alc/w 25°C 95% U K1=1.4 1993GSa (45267) 921
 Medium: 95% w/w EtOH/H2O, 0.05 M Et4NClO4, by competitive spectrophotometry

 C6H8N2O4 H2L (3100)
 Cyanomethyliminodiethanoic acid; NC.CH2.N(CH2.COOH)2

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

Ca++ gl KCl 20°C 0.10M U K1=2.75 1955SAa (45412) 922

 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

Ca++ gl NaClO4 25°C 0.10M U K1=1.54 19660Cb (45500) 923

 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

Ca++ ISE none 25°C 0 C I K1=3.17 1995RGa (45553) 924
 B(Ca2L)=4.5
 I=0.16 (Me4N.X) K1=2.05, B(Ca2L)=3.0; I=0.25 (Me4N.X) K1=2.03, B(Ca2L)=3.0.

 Ca++ gl oth/un 25°C 0.0 C I K1=3.284 1994DFc (45554) 925
 B(CaHL)=8.674
 B(CaH2L)=12.449
 B(Ca2L)=4.458

Values at I=0 calculated from data for 0.05-0.25 M CaCl2.

 Ca++ gl NaClO4 20°C 0.10M U K1=2.17 1964COB (45555) 926
 K(Ca+HL)=1.46

$$K(\text{Ca}+\text{H}_2\text{L})=0.88$$

 Ca++ ix oth/un 25°C 0.16M U K1=1.82 1952SLa (45556) 927

 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

 Ca++ gl mixed 25°C 80% U K(Ca+HL)=1.3 1980KKd (45612) 928
 Medium: 80% DMF

Ca++ ix oth/un 25°C 0.16M U K1=0.19 1952SLa (45613) 929

 C6H8O7 H3L Isocitric acid CAS 1637-73-6 (2527)
 2-Hydroxy-3-carboxypentanedioic acid; HOOC.CH(OH).CH(COOH).CH2.COOH

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

 Ca++ ix oth/un 25°C 0.16M U K1=2.47 1952SLa (45726) 930

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

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

 Ca++ gl NaClO4 25°C 0 C I Kso(Ca3L2.4H2O)=-17.81 2001CTc (45925) 931
 Extrapolated over the range 3.5 to 0.1 mol kg-1

Ca++ gl oth/un 25°C 0.0 C I K1=4.91 1999DGa (45926) 932
 K(Ca+H+L)=9.23
 K(Ca+2H+L)=12.3
 Medium: artificial seawater. Extrapolated from data for 5-45% salinity.

Ca++ gl R4N.X 25°C 0.0 C Kso(CaHL)=-11.35, Kso(Ca3L2)=-16.95 (I=0.2-0.54 M NaCl or Et4NI). 1995DGb (45927) 933

Ca++ gl NaClO4 25°C 0.50M C K1=2.71 1995PLa (45928) 934
 B(CaHL)=6.70

Ca++ oth NaCl 25°C 0.15M U T K1=3.17 1993GMa (45929) 935
 Method: Coulometric titration. K1=3.28 (37 C)

Ca++ gl NaClO4 37°C 0.10M U K1=3.5 1992GHa (45930) 936
 Method: coulometric titration

Ca++ gl NaClO4 37°C 0.10M U K1=3.5 1992GHa (45931) 937
 Method: coulometric titration

Ca++ ISE NaCl 37°C 0.0 C TI K1=4.845 1991SYb (45932) 938
Method: Calcium ISE. Data for 18 to 45 C and 0.02 to 0.17 M NaCl. DH(K1)=
-1.71 kJ mol⁻¹, DS(K1)=87.4 J K⁻¹ mol⁻¹. In 0.15 M NaCl, K1=4.850.

Ca++ gl NaClO4 30°C 1.0M U K1=3.02 1988GMd (45933) 939

Ca++ gl NaClO4 37°C 0.15M C K1=3.364 B2=4.965 1987BBd (45934) 940
B(CaH2L)=11.005
B(CaHL)=7.614
B(CaH-1L)=-8.395
B(CaH-2L2)=-16.808

Ca++ gl KNO3 37°C 0.10M U I K1=3.485 1982ADa (45935) 941
B(CaHL)=7.81
Ionic strength range: 0.03-0.3.

Ca++ gl oth/un 25°C 0.00 U H K1=4.91 1982ADa (45936) 942
K(Ca+HL)=2.81
DH1=-6.44 kJ mol⁻¹, DS1=71.9 J mol⁻¹ K⁻¹.

Ca++ oth oth/un 25°C dil C K1=4.850 1982HKa (45937) 943
K(Ca+HL)=2.786
Method: isotachopheresis. Medium: 0.006-0.019 M citrate buffer, pH 5.1.

Ca++ gl KCl 25°C 0.10M M I K1=3.63 1980PEa (45938) 944
K(Ca+HL)=2.03
K(Ca+H2L)=1.04
Extrapolated to I=0.0 M: K1=4.87; K(CaHL)=3.03.

Ca++ ISE NaCl 25°C 0.10M U K1=3.42 1979CMb (45939) 945

Ca++ dis R4N.X 25°C 0.50M U K(Ca+HL)=2.52 1976MKa (45940) 946

Ca++ gl KNO3 25°C 0.10M C K1=3.50 1975FCc (45941) 947
B(CaHL)=8.02

Ca++ gl NaClO4 25°C 0.10M U M K1=3.54 1975RMa (45942) 948
B(CaL(Cys))=5.58
K(Ca+L+HPO4)=10.72

Ca++ gl NaCl 37°C 0.15M C K1=3.27 1974MEa (45943) 949
K(Ca+HL)=1.83

Ca++ EMF oth/un ? ? U K1=3.24 1969BMb (45944) 950

Ca++ gl NaClO4 20°C 0.10M U K1=3.55 1964COb (45945) 951
K(Ca+HL)=2.10
K(Ca+H2L)=1.05

Ca++	gl	NaClO4	33°C	0.25M	U	K1=3.4	1961PPa (45946)	952
Ca++	sp	R4N.X	25°C	0.10M	C	K1=3.15	1961WAa (45947)	953
Medium: 0.16 M Me4NCl.								
Ca++	gl	NaCl	28°C	0.15M	U	K1=3.20	1957LEa (45948)	954
Ca++	ix	oth/un	25°C	->0	U	K1=4.68 K(Ca+HL)=3.09 K(Ca+H2L)=1.10	1955DHb (45949)	955
Ca++	ix	oth/un	25°C	0.16M	U	K1=3.15	1954SCa (45950)	956
Ca++	sol	oth/un	25°C	->0	U	K1=4.90 K(Ca+HL)=3.05 K(Ca+H2L)=1.15	1953DHa (45951)	957
Ca++	gl	oth/un	25°C	->0	U	K1=4.84 B2=8.02 K(Ca+HL)=3.29 K(Ca+2HL)=6.79	1951HEb (45952)	958

Ca++	oth	oth/un	25°C	0.15M	U	K1=3.17	1946JOa (45953)	959
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Ca++	oth	oth/un	22°C	0.16M	U	K1=3.22	1934HMa (45954)	960
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Ca++	sol	oth/un	25°C	->0	U	K1=4.85	1929BUa (45955)	961

C6H8O7P2		H3L				CAS 101378-64-7	(7666)	
Phenyldiphosphoric acid;								

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	gl	NaNO3	25°C	0.10M	M		K1=2.90	1999SSa (46341)	962

C6H9NO6		H3L					(6054)	
3-Carboxyglutamic acid; H2N.CH(CH(COOH).CH2.COOH)COOH								

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	gl	NaCl	25°C	1.00M	C		K1=0.60	1988BSa (46356)	963

C6H9NO6		H3L					CAS 41035-84-1	(4367)
N-Carboxymethyl-L-aspartic acid;								

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	gl	KNO3	25°C	0.10M	U		K1=3.71	1975GNb (46371)	964

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
Ca++	gl	KNO ₃	25°C	0.05M	C	I		K1=6.72 B2= 9.31	1995AKa (46604)	965
Data for 0.05-2.50 m KNO ₃ and Me ₄ NNO ₃ . At I=0.0 M, K1=7.699, B2=9.66.										
Ca++	gl	NaCl	37°C	0.15M	U			K1=6.24 B2= 8.62	1992FDa (46605)	966
B(CaHL)=11.74 B(CaNdL2)=20.68										
Ca++	gl	NaClO ₄	37°C	0.10M	U			K1=6.3	1992GHa (46606)	967
Method: coulometric titration										
Ca++	gl	KNO ₃	20°C	0.10M	C	TIH	R	K1=6.45	1982ANa (46607)	968
IUPAC evaluation										
Ca++	ISE	NaCl	25°C	0.10M	U			K1=6.31	1979CMb (46608)	969
Ca++	gl	NaClO ₄	25°C	0.10M	U		M T	K1=6.44	1975RMa (46609)	970
B(CaL(Cys))=8.44 K(Ca+L+HPO ₄)=14.50										
Ca++	dis	R4N.X	?	0.10M	U			K1=6.6	1969ASb (46610)	971
Method: chromatography. Medium: NH ₄ Cl										
Ca++	gl	KCl	20°C	0.10M	U		T	K1=6.46	1966IMb (46611)	972
Ca++	cal	KNO ₃	20°C	0.10M	U		H		1964HDa (46612)	973
DH(K1)=-5.7 kJ mol ⁻¹ , DS=103.2 J K ⁻¹ mol ⁻¹										
Ca++	gl	KNO ₃	25°C	0.10M	U		T H	K1=6.57	1962MFb (46613)	974
K1=6.59(15 C), 6.56(20 C), 6.57(30 C), 6.53(35,40 C). DH(K1)=-3.4 kJ mol ⁻¹ , DS=115 J K ⁻¹ mol ⁻¹										
Ca++	gl	KNO ₃	25°C	0.10M	U		T H	K1=6.33	1960BMb (46614)	975
K1=6.61(0.5 C), 6.35(42.5 C). DH(K1)=-8.4 kJ mol ⁻¹ , DS=92 J K ⁻¹ mol ⁻¹										
Ca++	EMF	oth/un	30°C	0.0	U		T H	K1=7.595	1956HMa (46615)	976
Method: H electrode. K1=7.704(0 C), 7.652(10 C), 7.608(20 C) DH(K1)=0, DS=146 J K ⁻¹ mol ⁻¹										
Ca++	EMF	oth/un	25°C	0.0	U		H		1956MAa (46616)	977
Method:H electrode. DG(K1)=-43.51 kJ mol ⁻¹ , DH=-4.2, DS=134										
Ca++	gl	KCl	20°C	0.10M	U		T	K1=6.41	1955SAa (46617)	978
Ca++	EMF	oth/un	20°C	0.0	U			K1=8.17 B2=11.60	1945SKb (46618)	979
Method: H electrode										

C6H9N07 H3L CAS 3055-17-2 (3694)
Nitritotriethanoic acid N-oxide; O-N(CH2.COOH)3

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

Ca++ gl KNO3 25°C 0.10M U K1=2.46 1967CCc (47133) 980

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

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

Ca++ gl NaCl 25°C 0.0 C TIH K1=1.55 1991DDc (47459) 981
B(CaHL)=9.95
B(CaH2L)=15.43

DH(K1)=-3 kJ mol⁻¹, DS(K1)=18 J K⁻¹ mol⁻¹; DH(CaHL)=-39, DS(CaHL)=59;
DH(CaH2L)=-46, DS=141. Data for 10-45 C, 0.1-1.0 M NaCl, CaCl2, Et4NI

Ca++ gl R4N.X 25°C 0.25M C TIH K1=0.95 1985DRa (47460) 982
B(CaHL)=9.35
B(CaH2L)=15.4

0.02-1 M NEt4I.10-37 C.DH(K1)=5 kJ mol⁻¹, DS=44; DH(CaHL)=-36, DS=61;
DH(CaH2L)=-66, DS=66

Ca++ gl KNO3 35°C 0.10M C M K(Ca+HL)=3.10 1985RRc (47461) 983
K(CaL(cytidine)+H)=2.79
K(Ca+HL+cytidine)=8.72

Ca++ gl KNO3 35°C 0.10M C K(Ca+HL)=3.10 1985RRh (47462) 984

Ca++ gl KNO3 35°C 0.10M C M K1=2.72 1983KSc (47463) 985
K(Ca+HA+L)=3.19
K(Ca+HB+L)=2.73

A is adenine; HB is cytosine.

C6H10N2O4 H2L (3104)
Piperazine-2,6-dicarboxylic acid;

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

Ca++ gl KCl 22°C 0.10M U K1=<1 1964PCa (47732) 986

C6H10N2O4 H2L CAS 89601-09-2 (3102)
trans-Piperazine-2,3-dicarboxylic acid;

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

Ca++ gl KCl 22°C 0.10M U K1=<1 1964PCa (47744) 987

 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

 Ca++ gl KNO3 25°C 0.10M C K1=4.01 1983LRc (47819) 988

Ca++ gl KCl 20°C 0.10M U K1=3.96 1955SAa (47820) 989

C6H10N2O6P2 H4L (6893)
 N-(2-Pyridyl)aminomethylenedi(phosphonic acid); C5H4N.NH.CH(PO3H2)2

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

 Ca++ gl KNO3 25°C 0.10M U K1=5.89 1990GKa (47868) 990

K(Ca+HL)=5.43
 K(Ca+H2L)=3.84

 C6H10N4O5 L (2622)
 4,5-Dimethyl-2,4,6,8-tetraazabicyclo[3,3,0]-octane-3-one-7-thione;

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

 Ca++ gl KNO3 25°C 0.10M U K1=3.33 1986KKa (47888) 991

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

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

 Ca++ sp none 25°C 0.0 U K1=3.17 1976K0a (48022) 992

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

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

 Ca++ con oth/un 25°C ->0 U K1=2.19 1940TDa (48051) 993

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

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

 Ca++ gl oth/un 20°C 0.10M U K1=1.74 196150b (48229) 994

K(Ca+HL)=1.16

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


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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  KNO3   25°C 0.10M U      K1=3.15      1974MSa (48326) 995
-----
Ca++      gl  oth/un 25°C 0.10M U      K1=4.12      1961KEa (48327) 996
*****
C6H10O7          HL   Galacturonic      CAS 685-73-4 (290)
D-Galacturonic acid;
-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      ISE KNO3 25°C 0.70M U      K1=1.31      1986HAe (48381) 997
Data also for many other mono- and disaccharide acids
-----
Ca++      gl  NaClO4 25°C 1.00M C      B(CaH-1L)=-10.15
                                           K(Ca+H-1L)=2.09
*****
C6H10O7          HL   Glucuronic acid  CAS 6556-12-3 (599)
D-Glucuronic acid;
-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  R4N.X  25°C  0 M I      K1=1.17      1996GMb (48410) 999
At I=0.16 M: K1=0.78
-----
Ca++      ISE KNO3 25°C 0.70M U      K1=1.03      1986HAe (48411)1000
Data also for many other mono- and disaccharide acids
-----
Ca++      gl  NaClO4 25°C 1.00M C      B(CaH-1L)=-10.40
                                           K(Ca+H-1L)=1.64
*****
C6H11NO4          H2L                               (1232)
2,2'-Iminodipropanoic acid; HN(CH(CH3)COOH)2
-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  KNO3   25°C 0.10M C      K1=2.0       1987AKa (48573)1002
-----
Ca++      gl  KNO3   25°C 0.10M U      K1=2.0       1987BKa (48574)1003
*****
C6H11NO4          H2L                               CAS 5336-17-4 (345)
N-Ethyliminodiethanoic acid; C2H5.N(CH2.COOH)2
-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  oth/un 25°C 0.10M C      K1=3.92      1975MRb (48599)1004
*****

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C6H11N04S 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

Ca++ gl KCl 20°C 0.10M U K1=4.88 1955SAa (48606)1005
K(Ca+HL)=2.77

C6H11N05 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

Ca++ gl oth/un 25°C 0.10M C K1=4.58 1975MRa (48667)1006

Ca++ dis R4N.X ? 0.10M U K1=5.3 1969ASb (48668)1007
Method: chromatography. Medium: NH4Cl

Ca++ gl KCl 20°C 0.10M U K1=4.63 1955SAa (48669)1008

Ca++ gl KCl 30°C 0.10M U K1=4.83 1952CCa (48670)1009

C6H11N05 H2L (1233)
N-Hydroxyimino-2,2'-dipropanoic acid; HO.N(CH(CH3)COOH)2

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

Ca++ gl KNO3 25°C 0.10M C K1=2.7 1987AKa (48835)1010

Ca++ gl KNO3 25°C 0.10M U K1=2.7 1987BKa (48836)1011

C6H11N07S 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

Ca++ EMF KCl 20°C 0.10M U K1=4.15 1949SAa (48844)1012
Method: H electrode

C6H11O4P H2L CAS 85931-58-4 (5652)
Ethylphosphinediethanoic acid;

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

Ca++ gl NaClO4 25°C 0.10M U K1=6.10 B2= 8.86 1983NPa (49008)1013
K3=0.9
K3 by spectrophotometry in 1.0 M HCl/KCl.

Ca++ gl NaClO4 25°C 0.10M U 1983NPa (49009)1014
K(Ca+HL)=0.73

 C6H12N07P 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

 Ca++ EMF KCl 20°C 0.10M U K1=5.44 1949SAa (49032)1015
 K(Ca+HL)=2.05

Method: H electrode

 C6H12N203 HL DL-Ala-DL-Ala CAS 2867-20-1 (67)
 DL-Alanyl-DL-alanine; H2N.CH(CH3).CO.NH.CH(CH3).COOH

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

 Ca++ gl KCl 20°C 0.20M U K1=2.15 1982RRc (49126)1016

 C6H12N204 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

 Ca++ cal NaClO4 25°C 0.10M U H K1=2.9 1983EHa (49208)1017
 DH1=2.9 kJ mol⁻¹, DS1=57.6 J K⁻¹ mol⁻¹

 C6H12N204 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

 Ca++ gl KCl 20°C 0.10M U K1=4.63 1955SAa (49294)1018

 C6H1205 L CAS 22416-73-5 (8237)
 Methyl-alpha-D-lyxofuranoside;

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

 Ca++ kin non-aq 25°C 100% C K1=1.70 1980LVc (49510)1019
 Medium: methanol.

 Ca++ ISE KCl 25°C 0.10M C K1=-0.05 1980LVd (49511)1020
 Method: Ca ion selective electrode.

 C6H1205 L CAS 52485-92-4 (8236)
 Methyl-alpha-D-ribofuranoside;

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

 Ca++ kin non-aq 25°C 100% C K1=2.08 1980LVc (49513)1021
 Medium: methanol. For methyl-beta-D-ribofuranoside, K1<1.0

Ca++ ISE KCl 25°C 0.10M C K1=0.08 1980LVd (49514)1022
Method: Ca ion selective electrode. For methyl-beta-D-ribofuranoside,
K1=-0.52

C6H12O5 L CAS 1824-96-0 (8238)
Methyl-alpha-D-xylofuranoside;

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

Ca++ kin non-aq 25°C 100% C K1=<1.0 1980LVc (49517)1023
Medium: methanol. For methyl-beta-D-xylofuranoside, K1<1.0

Ca++ ISE KCl 25°C 0.10M C K1=-1.0 1980LVd (49518)1024
Method: Ca ion selective electrode.

C6H12O5S HL (691)
1-Thio-beta-D-glucopyranose;

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

Ca++ gl KNO3 37°C 0.15M M K1=1.58 1979ZJa (49523)1025

C6H12O6 L D(+)-Allose CAS 2595-97-3 (2898)
D(+)-Allose;

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

Ca++ cal none 25°C 0.0 U H 1989MMb (49530)1026
DH(CaL)=-15.9 kJ mol⁻¹; TDS=-13.0.

C6H12O6 L D(+)-Talose CAS 2595-98-4 (2897)
D(+)-Talose;

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

Ca++ cal none 25°C 0.0 U H 1989MMb (49531)1027
DH(CaL)=-18.6 kJ mol⁻¹; TDS=-17.7.

C6H12O6 L D-Fructose CAS 57-48-7 (1561)
D-Fructose

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

Ca++ ISE KNO3 25°C 0.70M U K1=<-1 1986HAe (49534)1028

C6H12O6 L D-Galactose CAS 59-23-4 (1559)
D-Galactose

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

 Ca++ ISE KNO3 25°C 0.70M U K1=<-1 1986HAe (49556)1029

 C6H12O6 L D-Glucose CAS 492-62-6 (1560)
 D-Glucose

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

 Ca++ ISE KNO3 25°C 0.70M U K1=<-1 1986HAe (49573)1030

 C6H12O6 L D-Mannose CAS 3458-28-4 (1562)
 D-Mannose

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

 Ca++ ISE KNO3 25°C 0.70M U K1=<-1 1986HAe (49597)1031

 C6H12O6 L Sorbose CAS 87-79-6 (930)
 L(-)-Sorbose;

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

 Ca++ ISE KNO3 25°C 0.70M U K1=<-1 1986HAe (49610)1032

 C6H12O6 HL a-ISA CAS 1518-54-3 (5925)
 a-Isosaccharinic acid;

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

 Ca++ ISE NaCl 22°C 0.20M C K1=1.78 2004VGa (49618)1033
 Method: Ca ion selective electrode. Medium pH 6.1 (1 mM morphinoethane-
 sulfonic acid). By ion exchange, K1=1.80.

 Ca++ sol oth/un 25°C var C K1=1.44 2003RHa (49619)1034
 Kso(CaL2)=-6.26
 Solubility of CaL2 in 0.01-0.2 M NaL, pH 8.3.

 Ca++ sol none 20°C 0.0 C 1999LGa (49620)1035
 Kso(CaL2)=-6.53. Also data for 2.6-50.4 C.
 DH(Kso)=40 kJ mol-1, DS(Kso)=17 J K-1 mol-1

 Ca++ sol none 25°C 0.0 C K1=1.70 1999VGa (49621)1036
 K(Ca+HL=CaL+H)=-10.4
 Kso(CaL2)=-6.36.

 Ca++ sol oth/un 23°C 0.0 C 1998RRa (49622)1037
 Media: 0.03-0.52 m Ca, pH 1-14. At I=0.0 m, Ks(CaL2(s)+2H=Ca +2HL)=1.30
 Ks(CaL2(s)=CaL2)=-2.22, K(H+L)=4.46.

 C6H12O6 L CAS 576-63-6 (2284)

cis-Inositol, cyclohexane-1,2,3,4,5,6-hexol;

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

Ca++ ISE none 25°C 0.0 C K1=0.95 B2=2.65 1975AHa (49625)1038

C6H12O6 L CAS 488-58-4 (2283)

epi-Inositol;

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

Ca++ ISE none 25°C 0.0 C K1=0.34 1975AHa (49629)1039

C6H12O6 L Inositol CAS 87-89-8 (2285)

myo-Inositol, meso-Inositol;

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

Ca++ ISE KNO3 25°C 0.70M U K1=-0.89 1986HAe (49634)1040

Ca++ ISE none 25°C 0.0 C K1=-0.7 1975AHa (49635)1041

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

Ca++ sol none 20°C 0.0 C 1999LGA (49679)1042
Kso(cal2)=-4.19. Also data for 2.6-50.4 C.
DH(Kso)=37 kJ mol⁻¹, DS(Kso)=60 J K⁻¹ mol⁻¹

Ca++ ISE KNO3 25°C 0.70M U K1=1.31 1986HAe (49680)1043

Data also for many other mono- and disaccharide acids

Ca++ ISE NaCl 25°C 0.50M U K1=1.05 B2=1.88 1981MVA (49681)1044

Ca++ ix oth/un 25°C 0.16M U K1=1.22 1952SLa (49682)1045

Ca++ gl oth/un 25°C ->0 U K1=2.16 B2=4.64 1951HEa (49683)1046

Ca++ EMF KCl 20°C 0.20M U K1=1.21 1938CKa (49684)1047

Method: H electrode

C6H13NO2 HL Leucine CAS 61-90-5 (47)

2-Amino-4-methylpentanoic acid; H2N.CH(CH2.CH(CH3)2)COOH

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

Ca++ gl KNO3 25°C 0.10M U I K1=3.96 1990RAB (50031)1048

B(CaH-1L)= -5.09

Data also for 10% w/w EtOH/H2O (B1=4.07; B(CaH-1L)=-5.1) and 25% EtOH/H2O (4.25; -5.04).

C6H13N04 HL Bicine CAS 150-25-4 (2124)
 N,N-Bis(2-hydroxyethyl)glycine; (HO.CH2.CH2)2N.CH2.COOH

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

Ca++ gl KNO3 25°C 0.10M C K1=2.66 1991KNa (50323)1049

C6H13N04S HL MES CAS 4432-31-9 (7807)
 4-Morpholineethanesulfonic acid;

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

Ca++ gl NaClO4 37°C 0.10M U T K1=0.3 1992GHa (50428)1050
 Method: coulometric titration. At 25 C, K1=0.5.

C6H13N303 HL Citrulline (579)
 2-Amino-5-ureidovaleric acid; H2N.CO.NH.CH2.CH2.CH2.CH(NH2).COOH

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

Ca++ gl KNO3 25°C 0.10M U K1=1.65 B2=1.85 1970CMc (50566)1051

C6H1303P H2L CAS 1005-23-8 (520)
 Cyclohexylphosphonic acid; C6H11.PO3H2

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

Ca++ gl KNO3 25°C 0.10M U K1=1.65 1981WNa (50599)1052

C6H1309P H2L CAS 26177-86-6 (7139)
 Fructose-6-phosphoric acid; C6H1105.H2PO4

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

Ca++ gl NaClO4 25°C 0.10M C K1=3.30 1996GCa (50603)1053

Ca++ gl KCl 20°C 0.10M U K1=1.47 1957SAa (50604)1054

C6H1309P H2L CAS 59-56-3 (3049)
 alpha-D-Glucose-1-phosphoric acid; Glucopyranose-1-phosphoric acid;

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

Ca++ gl NaCl 25°C 0.15M U K1=1.773 1990KLb (50616)1055

Ca++ EMF oth/un 25°C ? U T H K1=2.495 1956CDb (50617)1056
 Method: H electrode. K1=2.418(10 C), 2.468(20 C), 2.528(30 C), 2.590(40 C),

2.677(50 C), 2.573(37 C). DH(K1)=10.05 kJ mol⁻¹, DS(K1)=81.6 J K⁻¹ mol⁻¹

C6H14N02P HL (6465)
Piperidinemethylphosphinic acid; C5H10N.CH2.PO2H2

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

Ca++ gl NaClO4 25°C 0.10M C K1=3.05 1992LBa (50632)1057

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

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

Ca++ gl KNO3 25°C 0.10M U K1=2.21 1970CMc (50990)1058

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

Ca++ cal non-aq 25°C 100% C H 1992BSc (51044)1059
Medium: propylene carbonate. DH(K1)=-19.1 kJ mol⁻¹.

Ca++ con non-aq 25°C 100% C K1=2.8 1992MSe (51045)1060
Medium: 100% MeOH. Anion: picrate. Also data for nitrophenolate anions.

C6H14O4 L CAS 112-27-6 (5663)
2,2'-(1,2-Ethanediy)bis(oxy))bisethanol;

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

Ca++ con non-aq 25°C 100% C K1=3.2 1992MSe (51054)1061
Medium: 100% MeOH. Anion: picrate. Also data for nitrophenolate anions.

C6H14O6 L D-Dulcitol CAS 608-66-2 (3663)
D-Galactitol;

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

Ca++ ISE KNO3 25°C 0.70M U K1=-0.51 1986HAe (51058)1062

C6H14O6 L D-Mannitol CAS 69-65-8 (3664)
D-Mannitol;

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

Ca++ ISE KNO3 25°C 0.70M U K1=-0.62 1986HAe (51066)1063

C6H14O6 L Glucitol CAS 50-70-4 (2878)

D-Sorbitol;

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

Ca++ ISE KNO3 25°C 0.70M U K1=-0.52 1986HAe (51093)1064

Ca++ nmr none 36°C 0.0 U T K1=-0.22 1981BKc (51094)1065
In D2O. At 4 C, K1=0.08.

C6H14O8P2 H4L CAS 36011-96-8 (4391)
trans-1,2-Cyclohexanediol diphosphate; C6H10(OP03H2)2

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

Ca++ gl R4N.X 20°C 0.10M U K1=3.74 1969HRa (51115)1066
K(Ca+HL)=2.15

Medium: (C3H7)4NI

C6H14O12P2 H4L CAS 488-69-7 (3705)
Fructose-1,6-diphosphoric acid;

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

Ca++ gl NaClO4 25°C 0.10M C K1=3.59 1996GCa (51121)1067

C6H14O12P2 H4L CAS 84364-89-6 (7140)
Fructose-2,6-diphosphoric acid; C6H10O4.(H2P04)2

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

Ca++ gl NaClO4 25°C 0.10M C K1=4.14 1996GCa (51127)1068

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

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

Ca++ gl R4N.X 25°C 1.00M C I K1=0.78 1982SSf (51274)1069

In 90 % (v/v) DMSO/water mixture: K1=0.82 (I=0.25 M)

C6H15NO6P2 H4L (6891)
Piperidine-N-Methylenedi(phosphonic acid); C5H10N.CH(P03H2)2

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

Ca++ gl KCl 25°C 0.10M M K1=4.53 1978GMf (51320)1070

K(Ca+HL)=3.64

C6H15NO7P2 H4L CAS 126104-92-5 (8889)
N-2-Methylenetetrahydrofuryloaminomethane-1,1-diphosphonic acid;

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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  KCl      25°C 0.20M C          K1=6.08  B2= 9.28  2002MKc (51341)1071
                                     B(CaH2L)=22.20
                                     B(CaHL)=16.76
                                     B(CaH2L2)=30.92
                                     B(CaHL2)=21.55

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*****
C6H15O15P3      H6L      Ins(1,2,6)P3      CAS 28841-62-5 (6479)
D-myo-Inositol 1,2,6-trisphosphoric acid;
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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  R4N.X  25°C 0.10M U TI      K1=4.59          1992SSa (51529)1072
                                     B(CaHL)=12.20
                                     B(CaH2L)=18.44
                                     B(Ca2L)=7.22

```

in 0.2 M KCl, 25 C: B1=3.12, B(CaHL)=10.14

```

-----
Ca++      gl  KCl      37°C 0.20M U I      K1=4.06          1990BJb (51530)1073
                                     B(Ca2HL)=13.95

```

In But4NBr 0.1 M: K1=5.80, B(CaHL)=13.57, B(CaH2L)=19.33, B(Ca2LH2)=22.15, B(Ca3L)=11.58

```

*****
C6H16NO4P      H2L          (8073)
1-Amino-2-hydroxy-4-methylpentane-2-phosphonic acid;
-----

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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  NaClO4  25°C 0.1M U          K1=3.85          1975SLa (51560)1074
                                     K(Ca+HL)=2.88

```

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*****
C6H16NO4P      HL          CAS 387383-55-3 (8776)
N,N,N-Trimethyl-2-(phosphonomethoxy)ethylamine;
-----

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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  NaNO3  25°C 0.10M M          K1=1.17          2002FGb (51569)1075

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*****
C6H16O4P2      H2L          CAS 55743-51-6 (1359)
1-Diethylphosphinyl-2-dihydroxyphosphinyethane;
-----

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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  KCl      25°C 0.10M U          K1=2.18          1974KMb (51781)1076

```

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*****
C6H16O6P2      H4L          CAS 4721-22-6 (3708)
Hexane-1,6-diphosphonic acid; H2O3P(CH2)6PO3H2
-----

```

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	g/l	KCl	25°C	0.10M	U			K1=<3	1967KLa (51788)	1077

C6H17NO6P2			H4L					CAS 71066-28-9	(8887)	
N-(3-Methylbutyl)aminomethane-1,1-diphosphonic acid;										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	g/l	KCl	25°C	0.20M	C			B(CaH2L)=22.79	2002MKc (51801)	1078

C6H17NO6P2			H4L					CAS 71066-29-0	(8886)	
N-Pentylaminomethane-1,1-diphosphonic acid;										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	g/l	KCl	25°C	0.20M	C			B(CaH2L)=22.70 B(CaHL)=17.06	2002MKc (51805)	1079

C6H17NO6P2								CAS 5995-28-8	(1339)	
N-t-Butyliminobis(methylenephosphonic) acid; (CH3)3CN(CH2PO3H2)2 H4L										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	g/l	KNO3	25°C	1.00M	M			K(Ca+HL)=2.91	1982BGb (51810)	1080

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
Ca++	g/l	KNO3	25°C	0.10M	C			K1=7.77 K(CaL+H)=9.04 K(CaHL+H)=7.87 K(CaH2L+H)=5.91 K(CaH3L+H)=4.5	1999D0a (51819)	1081

C6H18N2O4P2			H2L					(7261)		
1,2-Diaminoethane-N,N'-bis-(dimethylenemethylphosphinic acid); (CH2NHCH2PO(OH)CH3)2										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	g/l	R4N.X	25°C	0.10M	M			K1=3.85	1996BCa (51928)	1082

C6H18N2O6P2			H4L					(1363)		
Medium: 0.1 M Me4NNO3.										

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
-----
Ca++      gl  KNO3   25°C 0.10M C           K1=4.27      1999D0a (51943)1083
                               K(CaL+H)=9.94
                               K(CaHL+H)=7.0
```

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

```
-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  KNO3   25°C 0.10M C           K1=4.85      1999D0a (51963)1084
                               K(CaL+H)=10.32
                               K(CaHL+H)=7.4
```

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

```
-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      ISE non-aq 25°C 100% C           K1=3.81      1997NMa (51976)1085
Method: polyacrylamide/15-crown-5 sensor. Medium: acetonitrile.
```

 C6H18N4 L Trien-tetramine CAS 112-24-3 (11)
 1,4,7,10-Tetraazadecane; H2N.CH2.CH2.NH.CH2.CH2.NH.CH2.CH2.NH2

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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  NaCl   25°C 0.0 C           K1=1.4       1999SFc (52066)1086
                               K(Ca+HL)=0.8
                               K(Ca+H2L)=0.2
                               K(Ca+H3L)=-0.5
```

Extrapolated from data for 0.03-0.96 M NaCl using the Pitzer equation.

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

```
-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  KCl    25°C 0.10M C I R           2001PRa (52291)1087
                               K(Ca+HL)=5.75
                               K(CaL+H)=9.44
                               K(CaHL+H)=8.3
                               K(CaH2L+H)=6.65
```

IUPAC Recommended values. $K(\text{CaH3L}+\text{H})=5.2$

Ca++ gl NaCl 37°C 0.15M C K1=6.41 1995JWa (52292)1088
 K(CaL+H)=8.94
 K(CaL+OH)=3.33
 K(CaHL+H)=8.06

 Ca++ gl KNO3 25°C 0.10M C H K1=9.29 1993SMa (52293)1089
 K(CaL+H)=9.45
 K(CaHL+H)=8.24
 K(CaH2L+H)=6.74
 K(CaH3L+H)=5.49
 DH(K1)=-5.7, DH(CaHL)=-8.1, DH(CaH2L)=-7.9, DH(CaH3L)=-7.7, DH(CaH4L)=-1.8
 kJ mol⁻¹.

 Ca++ gl KCl 25°C 0.10M U K1=6.93 1980RZa (52294)1090
 K(CaL+H)=10.33
 K(CaH2L+H)=7.50
 K(CaHL+H)=9.59
 K(CaH3L+H)=6.78

 Ca++ gl KNO3 25°C 0.10M U K1=6.34 1979RZa (52295)1091
 K(Ca+HL)=4.48
 K(Ca+H2L)=3.85
 K(Ca+H3L)=3.22

 Ca++ gl KNO3 25°C 0.10M C K1=9.36 1976MMa (52296)1092
 K(CaL+H)=9.42
 K(CaHL+H)=8.44
 K(CaH2L+H)=6.59
 K(CaH3L+H)=5.25

 Ca++ dis R4N.X 20°C 0.10M U K1=6.09 1970TIa (52297)1093
 Method: chromatography. Medium: NH4Cl

 Ca++ EMF KCl 20°C 0.10M U K1=6.28 1970TIa (52298)1094
 K(Ca+HL)=5.30
 K(Ca+H2L)=3.39
 K(CaL+Ca)=3.01

 Ca++ gl KCl 25°C 0.10M U K1=9.33 1967KDa (52299)1095
 K(Ca+HL)=7.00
 K(Ca+H2L)=4.95
 K(Ca+H3L)=3.87
 K(Ca+H4L)=2.17

 Ca++ gl KNO3 25°C 0.10M U K1=5.74 1965WRa (52300)1096

 Ca++ gl oth/un 25°C 0.10M U K1=6.09 1956WMe (52301)1097

C7H4N04Cl H2L CAS 4722-94-5 (3780)
 4-Chloropyridine-2,6-dicarboxylic acid; Cl.C5H2N(COOH)2

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

Ca++ gl NaClO4 22°C 0.10M U K1=3.61 1964BBe (52382)1098

C7H5N04 H2L Quinolinic acid CAS 89-00-9 (567)
2,3-Pyridinedicarboxylic acid; C5H3N.(COOH)2

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

Ca++ gl KNO3 25°C 0.10M U K1=2.1 1958YYa (52616)1099

C7H5N04 H2L CAS 499-80-9 (566)
2,4-Pyridinedicarboxylic acid; C5H3N.(COOH)2

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

Ca++ gl KNO3 25°C 0.10M U K1=2.1 1958YYa (52645)1100

C7H5N04 H2L Dipicolinic aci CAS 449-83-2 (418)
2,6-Pyridinedicarboxylic acid; C5H3N.(COOH)2

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

Ca++ gl NaNO3 25°C 0.10M C K1=4.50 2000KAb (52728)1101

Ca++ gl NaCl 30°C 0.10M M K1=4.59 B2=7.28 1985RAa (52729)1102

Ca++ EMF KNO3 25°C 1.0M U K1=4.39 1968TRa (52730)1103
K(Ca+2HL)=2.25

Ca++ gl oth/un 25°C 0.10M U K1=4.60 B2=7.20 1966BSe (52731)1104
By ion exchange: K2=2.98

Ca++ gl NaNO3 20°C 0.10M U K1=4.40 1960ANb (52732)1105

Ca++ gl KNO3 25°C 0.10M U K1=4.2 1957SYb (52733)1106

Ca++ gl KCl 30°C 0.10M U K1=4.6 B2=7.2 1957TBb (52734)1107

C7H5N04 HL CAS 5274-70-4 (3148)
3-Nitrosalicylaldehyde; HO.C6H3(NO2).CHO

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

Ca++ sp NaClO4 25°C 0.10M U K1=1.0 1966PMa (52882)1108

C7H5N04 HL CAS 97-51-8 (1887)
5-Nitrosalicylaldehyde; O2N.C6H3(OH).CHO

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	sp	NaCl04	25°C	0.10M	U		K1=0.8	1966PMa (52934)	1109

C7H5N05			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
Ca++	gl	NaCl04	22°C	0.10M	U		K1=5.40	1964BBa (53068)	1110
Ca++	gl	oth/un	20°C	0.10M	U		K1=5.6 K(CaL+H)=6.51	1963ANd (53069)	1111

C7H5O2Cl			HL				CAS 118-91-2	(2519)	
2-Chlorobenzoic acid; Cl.C6H4.COOH									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	ISE	NaCl	25°C	0.03M	U	TIH	K1=1.06	1982EFa (53142)	1112
At 35 C, I=0.045 M: K1=1.02; 45 C, I=0.45 M: 0.389. Further data available									

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	sp	NaCl04	25°C	0.10M	U		K1=1.74	1966PMa (53155)	1113

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	sp	NaCl04	25°C	0.10M	U		K1=0.7	1966PMa (53187)	1114

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	sp	NaCl04	25°C	0.10M	U		K1=1.1	1966PMa (53206)	1115

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	sp	NaCl04	25°C	0.10M	U		K1=0.9	1966PMa (53221)	1116

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

Ca++ gl KNO3 20°C 0.10M U K1=5.18 1965ABa (53499)1117

Ca++ gl NaClO4 22°C 0.10M U K1=5.28 1964BBa (53500)1118

C7H6O2 HL Salicylaldehyde CAS 90-02-8 (193)
2-Hydroxybenzaldehyde, Salicylaldehyde; HO.C6H4.CHO

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

Ca++ sp NaClO4 25°C 0.10M U K1=1.1 1966PMa (53608)1119

C7H6O2 HL Tropolone CAS 533-75-5 (3129)
2-Hydroxycyclohepta-2,4,6-trien-1-one;

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

Ca++ sp NaClO4 25°C 0.10M U K1=3.06 1970HOa (53656)1120

Ca++ gl diox/w 30°C 50% U K1=4.8 B2=8.0 1953BFa (53657)1121

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

Ca++ gl alc/w 25°C 100% M K1=4.7 B2=7.3 1988PPa (53807)1122
Medium: MeOH

Ca++ ISE NaCl 25°C 0.03M U TIH K1=1.27 1982EFa (53808)1123
At 35 C, I=0.045 M: K1=1.24; at 45 C, I=0.45: K1=0.446

Ca++ gl KNO3 30°C 0.40M U K1=0.2 1970BTa (53809)1124

C7H6O2S2 H2L CAS 89677-36-1 (5448)
3-(2-Thiophene)-2-mercaptopropenoic acid; C4H3S.CH:C(SH).COOH

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

Ca++ gl diox/w 25°C 0.10M U K1=3.28 1977WVa (53928)1125

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

Ca++ cal R4N.X 25°C 0 U IH K1=1.73 1997MAa (54104)1126
 Medium: Me4NCl. I=0.025 M: K1=1.57, DH(K1)=2.0 kJ mol⁻¹. I=0.050: K1=1.48,
 DH(K1)=2.0. I=0.075 M: K1=1.38 DH(K1)=3.1. I->0: DH(K1)=1.5 kJ/mol

Ca++ sp NaCl 25°C 0.50M U T 1990DOa (54105)1127
 K(Ca+HL=CaL+H)=-10.19
 K(Ca+HL)=-0.58

Ca++ gl alc/w 25°C 100% M 1988JTa (54106)1128
 K(Ca+HL)=4.5
 K(Ca+2HL)=7.0

Medium: MeOH

Ca++ cal alc/w 25°C 100% U H 1988PPa (54107)1129
 Medium: MeOH. DH(CaL)=21.2 kJ mol⁻¹; DS=157. DH(CaL2)=28; DS=235

Ca++ gl R4N.X 25°C 0.25M C TIH T 1985DRa (54108)1130
 K(Ca+HL)=0.63
 I=0.02-1 M Et4NI. 10-45 C. DH = 5 kJ mol⁻¹

Ca++ ISE NaCl 25°C 0.03M U TIH 1982EFa (54109)1131
 K(Ca+HL)=1.50
 At 35 C, I=0.045 M: K1=1.42; at 45 C, I=0.045 M: K1=1.44

Ca++ gl NaCl04 37°C 0.15M C T K1=4.290 1978AKa (54110)1132

Ca++ ix NaCl 25°C 0.16M U 1954SCa (54111)1133
 K(Ca+HL)=0.15

Ca++ kin oth/un 25°C ->0 U 1951BWa (54112)1134
 K(Ca+HL)=0.36

Ca++ ISE NaCl 25°C 0.15M U 1946JOa (54113)1135
 K(Ca+HL)=0.14

Ca++ sol oth/un 25°C ->0 U 1938DAa (54114)1136
 K(Ca+HL)=0.55

 C7H6O3 H2L CAS 99-06-9 (1370)
 3-Hydroxybenzoic acid; HO.C6H4.COOH

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

Ca++ EMF NaCl 25°C 0.0 C T H 1984EFa (54373)1137
 K(Ca+HL)=1.51

Method: Ca selective electrode. Extrapolated from data for 0.15-0.30 M
 NaCl. DH(K)=2.34 kJ mol⁻¹, DS(K)=36.7 J K⁻¹ mol⁻¹. Data for 35 and 45 C.

 C7H6O4 H3L Protocatechuic CAS 99-50-3 (875)
 3,4-Dihydroxybenzoic acid; C6H3(OH)2.COOH

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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  KNO3   30°C 0.10M U          K1=3.71 B2=6.36  1963Mnc (54650)1138
*****
C7H6O4      H3L                      CAS 99-10-5 (4409)
3,5-Dihydroxybenzoic acid; C6H3(OH)2.COOH
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      EMF NaCl  25°C 0.0 C T H          1984EFa (54713)1139
                      K(Ca+H2L)=1.435
Method: Ca selective electrode. Extrapolated from data for 0.15-0.30 M
NaCl. DH(K)=2.34 kJ mol-1, DS(K)=35.4 J K-1 mol-1. Data for 35 and 45 C.
*****
C7H6O5      H4L Gallic acid      CAS 149-91-7 (446)
3,4,5-Trihydroxybenzoic acid; C6H2(OH)3.COOH
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      EMF KNO3  25°C 0.10M U          1985SCd (54744)1140
                      B(Ca2L)=11.5
Method: divalent cation liquid ion exchange electrode
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-----
Ca++      EMF R4N.X 25°C 0.0 C T H          1984EFa (54745)1141
                      K(Ca+H3L)=1.649
Method: Ca selective electrode. Extrapolated from data for 0.15-0.30 M
Et4NCl. DH(K)=2.17 kJ mol-1, DS(K)=38.9 J K-1 mol-1. Data for 35, 45 C.
*****
C7H6O6S      H3L                      CAS 5965-83-3 (399)
5-Sulfosalicylic acid, 2-Hydroxy-5-sulfobenzoic; HO3S.C6H3(OH).COOH
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  NaNO3  25°C 0.10M C          K1=3.07      1982HNa (54917)1142
*****
C7H7NO2      HL Anthranilic      CAS 118-92-3 (1589)
2-Aminobenzoic acid, Anthranilic acid; H2N.C6H4.COOH
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  oth/un 25°C ->0 U          K1=0.67      1958LUa (55198)1143
*****
C7H7NO2      H2L Salicylaldehyde   CAS 94-67-7 (1486)
2-Hydroxybenzaldehyde oxime; HO.C6H4.CH:N.OH
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  oth/un 25°C ->0 U          1958LUa (55299)1144
                      K(Ca+HL)=0.92
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K(Ca+2HL)=3.72

C7H7NO2 HL CAS 3222-47-7 (3154)
6-Methylpyridine-2-carboxylic acid; CH3.C5H3N.CO0H

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

Ca++ gl NaNO3 20°C 0.10M U K1=2.25 1960ANb (55421)1145

C7H7NO2 HL CAS 495-18-1 (184)
Benzohydroxamic acid; C6H5.CO.NH.OH

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

Ca++ gl KCl 25°C 0.20M C K1=2.135 2000FEc (55484)1146

Ca++ gl NaNO3 25°C 0.10M M K1=2.81 1996KSc (55485)1147

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

Ca++ gl NaNO3 25°C 0.10M C K1=3.24 2000KHa (55579)1148

Ca++ gl NaNO3 25°C 0.10M M K1=3.35 1996KSc (55580)1149

C7H8N4 L (1928)
Bis(imidazol-2-yl)methane; C3H3N2.CH2.C3H3N2

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

Ca++ gl KNO3 35°C 0.20M U K1=1.80 1989RVa (55990)1150

C7H8O8P2 H4L (6892)
1,2-((Phenylenedioxy)methylene)diphosphonic acid; C6H4O2C(P03H2)2

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

Ca++ gl R4N.X 25°C 0.50M U K1=5.44 1985GMb (56163)1151

K(Ca+HL)=2.83

Medium: 0.5 M Me4NCl

C7H9N L 3,5-Lutidine (323)
3,5-Dimethylpyridine; C5H3N.(CH3)2

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

Ca++ gl NaNO3 25°C 0.50M C K1=-0.11 2002KSb (56277)1152

C7H9NO8 H4L (8068)
2-Aminopropane-1,3-dioic-N,N-bis(ethanoic acid);

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

Ca++ gl KNO3 25°C 0.1M U K1=7.10 1976NGb (56465)1153

C7H9NO8 H4L CAS 4379-32-2 (5702)
2-Aminopropane-1,3-dioic-N-2-butane-1,4-dioic acid; (HOOC)2CH.NH.CH(COOH)CH2.COOH

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

Ca++ gl KNO3 25°C 0.10M U K1=4.46 1988KMa (56470)1154

C7H9O6ClP2 H4L CAS 53818-08-9 (4342)
4-Chlorophenylmethane diphosphonic acid; Cl.C6H4.CH(PO3H2)2

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

Ca++ gl R4N.X 25°C 0.10M M K1=5.87 1984CLb (56526)1155
K(Ca+HL)=2.6
K(CaL+Ca)=3.0

C7H9O6ClP2S H4L CAS 89987-48-4 (2395)
4-Chlorophenylthiomethylene-diphosphonic acid; Cl.C6H4.S.CH(PO3H2)2

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

Ca++ ISE NaNO3 20°C 0.04M U K1=6.55 1988BLa (56529)1156
K(Ca+HL)=3.7

C7H10NO6ClP2 H4L (6895)
N-(4-Chlorphenyl)aminomethylenedi(phosphonic acid); ClC6H4.NH.CH(PO3H2)2

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

Ca++ gl KNO3 25°C 0.10M U K1=6.7 1990GKa (56553)1157
K(Ca+HL)=4.3

C7H10N2O8P2 H5L CAS 195000-06-7 (8891)
N-(3-Carboxy-2-pyridyl)aminomethane-1,1-diphosphonic acid;

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

Ca++ gl KCl 25°C 0.20M C 2002MKc (56701)1158
B(CaH2L)=20.17
B(CaHL)=13.97

C7H11NO4 H2L CAS 16598-06-4 (965)
N-(Prop-2-enyl)iminodiethanoic acid; CH2:CH.CH2.N(CH2.COOH)2

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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  KCl    25°C 0.10M U      K1=3.4   B2=5.31   1966SIb (56784)1159
*****
C7H11N04      H2L                      CAS 499-82-1 (3163)
Piperidine-2,6-dicarboxylic acid; C5H9N(COOH)2
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  KCl    30°C 0.10M U      K1=2.2                      1957TBb (56800)1160
*****
C7H11N05      H2L                      (3164)
1-Amino-2-propanone-N,N-diethanoic acid; CH3.CO.CH2.N(CH2.COOH)2
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  KNO3   25°C 0.10M U      K1=4.08                      1963ANa (56824)1161
*****
C7H11N06      H3L                      (2926)
2-Aminobutanoic-N-propane-1,3-dioic acid; HOOC.CH(C2H5)NH.CH(COOH)2
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  KNO3   25°C 0.10M U      K1=3.43                      1982KKa (56837)1162
*****
C7H11N06      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
-----
Ca++      EMF KCl    20°C 0.10M U      K1=5.04                      1949SAa (56868)1163
Method: H electrode
*****
C7H11N06      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
-----
Ca++      gl  KNO3   20°C 0.10M U      K1=6.97                      1974RMf (56898)1164
-----
Ca++      gl  KCl    20°C 0.10M U      K1=6.97                      1966IMa (56899)1165
*****
C7H11N06P2      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
-----
Ca++      gl  KCl    25°C 0.10M U      K1=6.56                      1969DMd (56935)1166
K(Ca+HL)=4.82
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Ca++ gl diox/w 24°C 50% U K1=3.1 1979ACa (57285)1173

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

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

Ca++ sp none 25°C 0.0 U K1=2.49 1976K0a (57330)1174

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

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

Ca++ sp none 25°C 0.0 U T K1=2.55 1976K0a (57353)1175
 Also data at 15,20,30,35,40 C. Determined colourimetrically

 C7H13NO2 HL (3170)
 1-Aminocyclohexanecarboxylic acid; H2N.C6H10.COOH

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

Ca++ gl KCl 20°C 0.10M U K1=1.2 1963IPa (57429)1176

 C7H13NO4 H2L CAS 5394-32-1 (340)
 N-(1-Methylethyl)iminodiethanoic acid; (CH3)2.CH.N(CH2.COOH)2

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

Ca++ gl oth/un 25°C 0.10M C K1=3.77 1975MRb (57509)1177

 C7H13NO4 H2L CAS 16578-07-5 (341)
 N-Propyliminodiethanoic acid; CH3.CH2.CH2.N(CH2.COOH)2

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

Ca++ gl oth/un 25°C 0.10M C K1=3.71 1975MRb (57523)1178

 Ca++ gl KCl 25°C 0.10M U K1=3.4 B2=5.40 1966SIb (57524)1179

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

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

Ca++ gl KCl 20°C 0.10M U K1=3.34 1955SAa (57541)1180

 C7H13NO5 H2L CAS 59881-61-0 (336)
 N-(2-Hydroxypropyl)iminodiethanoic acid; CH3.CH(OH).CH2.N(CH2.COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	gl	oth/un	25°C	0.10M	C		K1=4.94 B2=8.04	1975MRa (57562)	1181

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
Ca++	gl	oth/un	25°C	0.10M	C		K1=4.68 B2=7.58	1975MRa (57568)	1182

C7H13NO5			H2L				CAS 59881-62-1	(339)	
N-(3-Hydroxypropyl)iminodiethanoic acid; HO.(CH2)3.N(CH2.COOH)2									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	gl	KCl	20°C	0.10M	U		K1=4.53	1955SAa (57569)	1183

C7H13NO5			H2L				CAS 41433-03-8	(4451)	
N-(Carboxymethyl)-N-(2'-hydroxyethyl)alanine;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	EMF	KNO3	20°C	0.10M	U		K1=4.70	1968MRb (57593)	1185

C7H13NO6			H2L				CAS 32013-58-4	(6079)	
N-(2,3-Dihydroxypropyl)iminodiethanoic acid; HO.CH2.CH(OH).CH2.N(CH2.COOH)2									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	gl	KNO3	20°C	0.10M	U		K1=4.41	1980MRc (57603)	1186

Ca++	gl	oth/un	25°C	0.10M	C		K1=4.34	1975MRa (57604)	1187

C7H13NO6			H2L				CAS 58144-30-2	(6066)	
N-(2-Hydroxy-(1-hydroxymethyl)ethyl)iminodiethanoic acid; (HO.CH2)2CH.N(CH2.COOH)2									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	gl	oth/un	25°C	0.10M	C		K1=4.97 B2=8.47	1975MRa (57624)	1188

Ca++	gl	oth/un	25°C	0.10M	C		K1=3.73	1975MRb (57625)	1189

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
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Ca++ cal NaClO4 25°C 0.10M U H K1=2.4 1983EHa (57814)1190
DH1=3.8 kJ mol⁻¹, DS1=57.9 J K⁻¹ mol⁻¹

C7H14N3O8P H3L (3788)

Glycyl-O-phosphoryl-DL-serylglycine;

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

Ca++ gl KCl 25°C 0.15M U K1=1.81 19620Sa (57831)1191

K(Ca+HL)=1.45

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

Ca++ gl NaNO3 25°C 0.10M M K1=1.20 2003FHa (57838)1192

C7H14O6 L CAS 56782-15-1 (2286)

3-O-Methyl-epi-Inositol;

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

Ca++ ISE none 25°C 0.0 C K1=0.2 1975AHa (57884)1193

C7H15NO4 HL CAS 41244-51-3 (4459)

N,N-Bis(2'-hydroxyethyl)alanine; (HO.CH2.CH2)2.N.CH(CH3)COOH

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

Ca++ EMF KNO3 20°C 0.10M U K1=2.26 1968MRb (57929)1194

C7H16O6Cl2P2 H2L CAS 133918-05-5 (5250)

Clodronic acid P,P'-diisopropyl ester;

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

Ca++ gl R4N.X 25°C 1.0M C K1=1.91 1995RLa (58090)1195

Medium: 1.0 M Me4NCl.

C7H17NO6S HL DIPSO (1097)

3-[N,N-Bis(2-hydroxyethyl)amino]-2-hydroxypropane sulfonic acid;

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

Ca++ gl KNO3 25°C 0.10M C K1=3.47 2000ADa (58132)1196

C7H17NO7P2 HL CAS 220491-02-1 (7714)

N-2-Methyltetrahydrofuryliminodi(methylenephosphonic acid);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	gl	KCl	25°C	0.20M	C		K1=6.03 B2= 9.03 B(CaHL)=14.01 B(CaH2L)=19.00	1999MKa (58149)	1197

C7H17N07S HL TAPSO CAS 68399-81-5 (167)
3-[N-(Tris(hydroxymethyl)methyl)amino]-2-hydroxypropane sulfonic acid

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	gl	KNO3	25°C	0.10M	C	M	K1=4.21	2001AAa (58170)	1198

Also data for ternary complexes with 5'-GMP, 5'-IMP and 5'-CMP.

Ca++	gl	KNO3	25°C	0.10M	C		K1=3.50	2000ADa (58171)	1199
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C7H19N06P2 H4L (7464)
N-(3-Methylbutyl)imino-bis(methylenephosphonic acid);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	gl	KCl	25°C	0.20M	C		K1=3.77 B(CaHL)=14.89 B(CaH2L)=20.36	1999MKa (58269)	1200

C7H19N07P2 H4L CAS 63161-30-8 (1349)
1-Hydroxy-3-N,N-diethylaminopropylidenediphosphonic acid;
(C2H5)2N.CH2.CH2.C(OH)(PO3H2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	gl	KCl	25°C	0.10M	M		K1=5.73 K(Ca+HL)=5.62 K(Ca+H2L)=3.37	1978KMa (58277)	1201

C7H20N204P2 H2L (7263)
1,3-Diaminopropane-N,N'-bis(methylenemethylphosphinic acid);
CH2(CH2NHCH2PO(OH)CH3)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	gl	R4N.X	25°C	0.10M	M		K1=3.40	1996BCa (58328)	1202

Medium: 0.1 M Me4NNO3.

C7H21N2010P3 H6L (7004)
N-(2-Hydroxyethyl)-1,2-diaminoethane-N,N'N'-trimethylenephosphonic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	gl	KCl	25°C	0.10M	U		K1=5.62	1974KRd (58370)	1203

K(Ca+HL)=3.78

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

Ca++ ISE KNO3 25°C 0.1M U K1=4.90 1985SNd (58382)1204
B(CaHL)=16.00
B(CaH3L)=33.76
B(CaH2L)=25.73
B(CaH4L)=40.58

B(CaH5L)=45.96

B(Ca2L)=7.68

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

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

Ca++ sp none 25°C dil C K1=5.46 2004AZa (58468)1205
H-point standard addition method.

Ca++ sp non-aq 25°C 100% U T H K1=4.73 1994GSb (58469)1206
At 35 C: K1=4.66; 45 C: K1=4.62; 55 C: K1=4.58. DH(K1)=-8.8 kJ mol⁻¹, DS=61
Medium: DMSO

Ca++ sp alc/w 25°C 95% U K1=6.52 1993GSa (58470)1207
Medium: 95% w/w EtOH/H2O, 0.05 M Et4NC104

Ca++ sp non-aq 20°C 100% U K1=5.55 1992PSa (58471)1208
Medium: DMF, 0.01 M Me4NI

Ca++ sp alc/w 25°C 100% U I K1=6.09 1988KGa (58472)1209
Medium: MeOH. Also in DMF (K1=4.98) and DMSO (4.64).

Ca++ sp alc/w 25°C 100% U I K1=6.09 1987GKb (58473)1210
Medium: MeOH. Also in DMF (K1=3.98) and DMSO (K1=4.64)

Ca++ sp non-aq 25°C 100% U K1=4.57 1983PSc (58474)1211
Medium: DMSO

Ca++ vlt oth/un 30°C ? U T K1=3.69 1982GWb (58475)1212
Medium: (CH2)6N4-HCl buffer solution. pH=7.02

Ca++ sp NaClO4 30°C 0.10M C K1eff=2.803 1978BKd (58476)1213

Medium pH 5.4 (acetate).

Ca++ sp oth/un 25°C 0.10M U 1961NAa (58477)1214
K(Ca+H2L)=2.68

Medium: CaCl2

Ca++ sp oth/un rt 0.10M U 1949SGa (58478)1215
K(Ca+H2L)=2.6
K(CaHL+H)=8.2
K(CaL+H)=9.5

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

Ca++ gl diox/w 20°C 17% C K1=7.09 B2=12.65 1976JWa (58592)1216

C8H6O3Cl2 HL CAS 94-75-7 (8292)
2,4-Dichlorophenoxyethanoic acid;

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

Ca++ gl oth/un 25°C 0.0 C TIH K1=0.66 1988CDb (58812)1217

Derived from ligand protonation data in 0.06-0.78 M CaCl2.

Data for 10-45 C. DH(K1)=2.4 kJ mol⁻¹.

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

Ca++ gl NaCl 25°C 0.10M U K1=2.45 1989SKa (58919)1218

Ca++ ISE R4N.X 25°C 0.20M C TIH K1=1.50 1986FWb (58920)1219

Method: Ca ion selective electrode. Data for 25-45 C and I=0.15-0.30 M

Me4NCl. At 45 C, K1=1.50. At I=0.0 M, K1=1.93. DH(K1)=1.0 kJ mol⁻¹

Ca++ gl R4N.X 25°C 0.25M C TI K1=1.71 1985DRa (58921)1220

B(CaHL)=5.70

0.02-1 M NEt4I.

Ca++ gl NaClO4 25°C 0.02M U K1=2.43 1985GMc (58922)1221

Ca++ con none 25°C 0.0 U K1=2.47 1984TWa (58923)1222

Ca++ gl KNO3 25°C 0.15M C I K1=1.35 1983DDa (58924)1223

K(Ca+HL)=0.54

Ca++ EMF oth/un 25°C 0.07M M T H K1=2.64 1976PAa (58925)1224

Method: quinhydrone electrode. Medium: 0.07 M CaCl2.

Data for 20 and 35 C. DH(K1)=13.1 kJ mol⁻¹, DS(K1)=91.2 J K⁻¹ mol⁻¹.

Ca++ sol KCl 25°C 0.10M U T K1=2.41 1970Gnc (58926)1225
K1(30 C)=2.49, K1(35 C)=2.59, K1(40 C)=2.66, K1(45 C)=2.75

Ca++ EMF oth/un 25°C 0.15M U K1=1.07 1946J0a (58927)1226

Ca++ con oth/un 25°C 0.0 U K1=2.43 1940TDa (58928)1227

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

Ca++ con oth/un 25°C 0.0 U K1=2.00 1940TDa (59046)1228

C8H6O4 H2L Terephthalic Ac CAS 199-21-0 (518)
Benzene-1,4-dicarboxylic acid; C6H4(COOH)2

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

Ca++ ISE R4N.X 25°C 0.20M C TIH K1=1.38 1986FWb (59069)1229
Method: Ca ion selective electrode. Data for 25-45 C and I=0.15-0.30 M
Me4NCl. At 45 C, K1=1.39. At I=0.0 M, K1=1.80. DH(K1)=1.34 kJ mol-1

Ca++ con none 25°C 0.0 U K1=2.05 1984TWa (59070)1230

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

Ca++ gl NaClO4 22°C 0.10M U K1=5.37 1964BBa (59350)1231

C8H8O2 HL p-Toluic acid CAS 99-94-5 (1372)
4-Methylbenzoic acid; CH3.C6H4.COOH

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

Ca++ ISE NaCl 25°C 0.03M U TIH K1=1.27 1982EFa (59498)1232
At 35 C, I=0.045 M: K1=1.24; at 45 C, I=0.45: K1=0.389

C8H8O2 HL CAS 1004-72-4 (3190)
alpha-Methyltropolone;

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

Ca++ gl diox/w 30°C 50% U K1=5.1 B2=8.5 1954BFb (59578)1233

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

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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  diox/w 30°C  50% U      K1=5.3   B2=8.9   1954BFb (59589)1234
*****
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
-----
Ca++      gl  alc/w  25°C 100% M      K(Ca+HL)=4.5
                                           K(Ca+2HL)=7.0
Medium: MeOH
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*****
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
-----
Ca++      sol oth/un 25°C  0.0 U T H   K1=1.46      1975DNa (59801)1236
DH=32.05 kJ mol-1 and DS=135.56 J mol-1 K-1.
Data also at 30, 35, 40 and 45 C. Medium: glycolate buffer, pH 3.8
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Ca++      kin oth/un 25°C  0.0 U      K1=1.29      1951BWa (59802)1237
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Ca++      sol oth/un 25°C  0.0 U      K1=1.45      1938DAa (59803)1238
*****
C8H8O3      HL  Phenoxyacetic  CAS 122-59-8 (1153)
Phenoxyethanoic acid; C6H5.O.CH2.COOH
-----

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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  none  25°C  0.0 C TIH  K1=1.04      1985CDb (60034)1239
Calculated from protonation data for I=0.04-0.9 M CaCl2. Data for 10-45 C.
DH(K1)=7.1 kJ mol-1, DS(K1)=43 J K-1 mol-1.
*****

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C8H8O4      HL  CAS 520-45-6 (4478)
3-Acetyl-2-hydroxy-6-methylpyran-4-one, Dehydroethanoic acid;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  diox/w 35°C  50% U      K1=2.23   B2=4.20   1971MAa (60078)1240
Medium: 50% dioxan, 0.1 M NaClO4
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*****
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
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Ca++ gl mixed 24°C 50% U K1=2.84 B2=5.35 1993ZMa (60104)1241
Medium: 50% v/v acetone/H2O

C8H8O5 H2L CAS 5629-08-3 (679)

7-Oxy-bicyclo[2.2.1]-hept-5-ene-2,3-dicarboxylic acid;

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

Ca++ gl NaCl 37°C 0.15M U K1=2.62 1988HYa (60122)1242

C8H9NO2 HL (2591)

N-Phenyl-N-acetohydroxamic acid; CH3.CO.N(OH)C6H5

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

Ca++ gl KCl 25°C 0.20M C K1=1.64 2000FEc (60279)1243

C8H9NO4 H2L (4520)

Dehydroethanoic acid oxime;

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

Ca++ gl diox/w 35°C 50% U 1971MAa (60484)1244

K(Ca+HL)=2.42

K(Ca+2HL)=4.44

Medium: 50% dioxan, 0.01 M NaClO4

C8H9N3O7 H2L Uramildiacetic CAS 13055-06-5 (185)

5-Amino-2,4,6-trioxo-1,3-perhydrodiazimino-N,N-diethanoic acid;

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

Ca++ cal KNO3 25°C 0.1M C H 1981CSb (60601)1245

DH(K1)=-10.5 kJ mol⁻¹, DS=117 K J mol⁻¹

Ca++ gl KNO3 25°C 0.10M U T K1=8.15 1977SVa (60602)1246

Ca++ cal R4N.X 20°C 0.1M C 1976ANb (60603)1247

DH1= -13.5 kJ/mol

in Me4NCl

Ca++ gl R4N.X 25°C 0.10M C K1=8.40 B2=13.90 1975JTa (60604)1248

Ca++ gl KNO3 20°C 0.10M U K1=8.31 B2=13.58 1963IFb (60605)1249

Ca++ ISE oth/un 20°C 0.0 U K1=8.77 B2=13.0 1948SBa (60606)1250

C8H9O3P H2L CAS 1707-08-0 (1969)

2-Styrylphosphonic acid; C6H5.CH:CH.PO3H2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	KNO3	25°C	0.12M	U			K1=2.05	1979RZb (60669)	1251

C8H10N2O4			H2L			Mimosine		CAS 2116-55-4	(2308)	
2-Amino-3-(3-hydroxy-4-oxo-1,4-dihydropyridin-1-yl)propanoic acid;										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	KNO3	37°C	0.15M	C			K1=3.24 B2=5.09 B(CaHL)=10.49 B(CaHL2)=13.1	1980SHb (60754)	1252

C8H10N2O4			H2L			Isomimosine		CAS 60384-61-4	(2314)	
2-Amino-3-(5-hydroxy-4-oxo-1,4-dihydropyridin-2-yl)propanoic acid;										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	KNO3	37°C	0.15M	C			K1=3.32 B2=5.0 B(CaHL)=11.39 B(CaHL2)=14.0	1980SHb (60761)	1253

C8H10O8			H4L					CAS 1703-58-8	(7339)	
1,2,3,4-Butanetetracarboxylic; HOOC.CH2.CH(COOH).CH(COOH).CH2.COOH										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	R4N.X	25°C	0.0	C				1995DGb (60891)	1254
Kso(Ca2L)=-14.53 (I=0-0.6 M Et4NI). *****										
C8H10O9			H4L					CAS 137172-86-2	(6612)	
SS-0xydisuccinic acid; O(CH(COOH)CH2.COOH)2										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	KCl	25°C	0.10M	C			K1=5.42 K(CaL+H)=4.35 K(CaHL+H)=3.53 K(CaH2L+H)=2.72 K(Ca+HL)=3.81	1992MMa (60899)	1255
K(Ca+H2L)=2.55, K(Ca+H3L)=1.87 *****										
C8H10O9			H4L					CAS 84852-72-2	(6611)	
meso-0xydisuccinic acid; O(CH(COOH)CH2.COOH)2										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	KCl	25°C	0.10M	C			K1=5.82 K(CaL+H)=4.43 K(CaHL+H)=3.53	1992MMa (60911)	1256

K(CaH2L+H)=3.41

K(Ca+HL)=4.27

K(Ca+H2L)=2.95, K(Ca+H3L)=2.39

C8H10O10 H4L (5894)

1-Hydroxy-3-oxapentane-1,2,4,5-tetracarboxylic acid;

HO.CH(COOH).CH(COOH).O.CH(COOH).CH2(COOH)

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

Ca++ gl KCl 25°C 0.10M C K1=5.20 1989MMd (60923)1257

K(CaL+H)=4.43

K(CaHL+H)=2.94

C8H11NO L CAS 20819-02-5 (5524)

4-Methoxy-2,6-dimethylpyridine;

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

Ca++ gl NaNO3 25°C 0.50M U K1=0.8 1983BEb (61032)1258

C8H11NO2 H2L Dopamine CAS 579-59-9 (251)

2-(3',4'-Dihydroxyphenyl)ethylamine; (HO)2.C6H3.CH2.CH2.NH2

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

Ca++ gl KCl 25°C 0.10M U T H 1986CVb (61067)1259

K(Ca+HL)=4.10

K(Ca+2HL)=5.85

Data for 0-37 C. At 37 C, K(Ca+HL)=4.00, K(Ca+2HL)=5.60.

DH(Ca+HL)=-24.9 kJ mol⁻¹, DS=4.56 J K⁻¹ mol⁻¹; DH(Ca+2HL)=-15.6, DS=18.5

C8H11NO3 H2L Noradrenaline CAS 138-65-8 (253)

Norepinephrine, 3,4-Dihydroxyphenylethanolamine; (HO)2C6H3.CH(CH2.NH2).OH

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

Ca++ gl KCl 25°C 0.10M U T H K1=5.11 B2= 6.52 1982CVa (61152)1260

Data for 0 and 37 C. DH(K1)=-28.7 kJ mol⁻¹, DS(K1)=-12 J K⁻¹ mol⁻¹;

DH(K2)=-9.3, DS(K2)=8.0.

C8H11NO7 H3L (6055)

N-Acetyl-3-carboxyglutamic acid; CH3.CO.NH.CH(CH(COOH).CH2.COOH)COOH

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

Ca++ gl NaCl 25°C 1.00M C K1=1.06 1988BSa (61178)1261

C8H11NO8 H4L CAS 24868-49-3 (2572)

2-Amino(N,N-diethanoic)-1,4-butanedioic acid;HOOCCCH(N(CH2COOH)2)CH2COOH

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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  KNO3   25°C 0.10M U      K1=5.81      1975NGa (61183)1262
*****
C8H11NO8      H4L      CAS 7408-20-0 (2608)
Amino-di(butanedioic acid);HN(CH(COOH)CH2.COOH)2
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  KNO3   25°C 0.1M C      K1=4.63      1999VZb (61196)1263
-----
Ca++      gl  KNO3   25°C 0.1M U      K1=4.42      1978MNa (61197)1264
*****
C8H11NO8P2     H5L      (6894)
N-(4-Carboxyphenyl)aminomethylenedi(phosphonic acid); HOOC.C6H4.NH.CH(PO3H2)2
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  KNO3   25°C 0.10M U      K1=6.89      1990GKa (61225)1265
                    K(Ca+HL)=2.91
*****
C8H12N2O8      H4L      CAS 35039-85-1 (4537)
1,2-Diaminoethane-N,N'-dimalonic acid; (HOOC)2.CH.NH.CH2.CH2.NH.CH(COOH)2
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  KNO3   20°C 0.10M U      K1=5.18      1973DSc (61484)1266
                    K(Ca+HL)=1.9
-----
Ca++      gl  KNO3   25°C 0.10M U      K1=5.45      1973MAb (61485)1267
                    K(Ca+HL)=2.02
-----
Ca++      gl  KNO3   25°C 0.10M U      K1=4.80      1972GBd (61486)1268
                    K(Ca+HL)=2.61
                    K(Ca+CaL)=2.26
*****
C8H12N5O4P     H2L      CAS 106941-25-7 (6693)
9-(2-(Phosphonylmethoxy)ethyl)adenine; H2O3P.CH2.O.CH2.CH2.adenine
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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  NaNO3  25°C 0.10M M      M  K1=1.01      2000KLb (61643)1269
                    K(PtLA+Ca)=1.01
A=diethylenetriamine
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-----
Ca++      gl  NaNO3  25°C 0.10M M      K1=1.65      1992SCa (61644)1270
*****
C8H13NO6      H3L      (3835)
2-Amino-2-carboxypropane-N,N-diethanoic acid; HOCC(CH3)2N(CH2COOH)2
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  KNO3   20°C 0.10M U          K1=5.19      1974RMf (61752)1271
-----
Ca++      gl  KCl    20°C 0.10M U          K1=8.32      1966IMa (61753)1272
*****
C8H13NO6          H3L                      (5681)
2-Aminobutanoic-N,N-diethanoic acid; CH3CH2CH(COOH)N(CH2COOH)2
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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  KNO3   20°C 0.10M U          K1=6.46      1974RMf (61779)1273
*****
C8H13NO6S        H3L                      (5675)
2-Mercapto-1-aminoethane-N,N,S-triethanoic acid; HOOC.CH2.S.CH2.CH2.N(CH2COOH)2
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  NaClO4 25°C 0.10M U          K1=4.56      1975POa (61814)1274
                        K(Ca+HL)=1.75
*****
C8H13N6O4P        H2L                      (7462)
9-[2-(Phosphonomethoxy)ethyl]-2,6-diaminopurine;
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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  NaNO3  25°C 0.10M M          K1=1.67      1999BSa (61871)1275
                        K(Ca+HL)=0.4
*****
C8H14N2O3          HL      Pro-Ala          CAS 6422-36-2 (263)
Prolyl-alanine; C4H8N.CO.NH.CH(CH3).COOH
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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  KCl    20°C 0.20M U          K1=1.77      1982RRc (61926)1276
*****
C8H14N2O4          H2L                      CAS 124099-98-5 (5607)
1,4-Piperazine-N,N'-diethanoic acid; HOOC.CH2.C4H8N2.CH2.COOH
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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      cal NaClO4 25°C 0.10M U  H      K1=2.0      1985EHa (61941)1277
DH(K1)=1.7 kJ mol-1, DS=44.4 J K-1 mol-1
-----
Ca++      EMF KCl   20°C 0.10M U          K1=2.5      1963IPb (61942)1278
Method: H electrode
*****
C8H14N2O6P2        HL                      (7465)
N-(3-Pyridylmethyl)imino-bis(methylphosphonic acid);
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  KCl    25°C 0.20M C          K1=3.69      1999MKa (61965)1279
                    B(CaHL)=12.87
                    B(CaH2L)=18.33
                    B(CaH3L)=22.83
                    B(CaH-1L)=-8.49

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*****
C8H14O4      H2L    Suberic acid      CAS 505-48-6 (517)
Octanedioic acid; HOOC.(CH2)6.COOH
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
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Ca++      con none 25°C 0.0 U          K1=1.66      1984TWa (62093)1280
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C8H14O7      H2L                                (241)
Di(carboxymethoxy)ethyl ether; (HOOC.CH2.0.CH2.CH2)20
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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
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Ca++      gl  KNO3   25°C 0.10M U          K1=2.40      1974MSa (62144)1281
*****

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```

C8H15NO4      H2L                                CAS 56004-49-0 (343)
N-(iso-Butyl)iminodiethanoic acid; (CH3)2.CH.CH2.N(CH2.COOH)2
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
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Ca++      gl  oth/un 25°C 0.10M C          K1=3.40      1975MRb (62175)1282
*****

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C8H15NO4      H2L                                CAS 56004-50-3 (344)
N-(tert-Butyl)iminodiethanoic acid; (CH3)3C.N(CH2.COOH)2
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----

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Ca++      gl  oth/un 25°C 0.10M C          K1=3.71      1975MRb (62179)1283
*****

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C8H15NO4      H2L                                CAS 33994-68-7 (347)
N-Butyliminodiethanoic acid; C4H9.N(CH2.COOH)2
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
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Ca++      gl  oth/un 25°C 0.10M C          K1=4.01      1975MRb (62187)1284
*****

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C8H15NO5      H2L                                CAS 62130-86-3 (6073)
N-(2-Hydroxy-(1-ethyl)ethyl)iminodiethanoic acid; HO.CH2.CH(CH2.CH3)N(CH2.COOH)2
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
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Ca++      gl  oth/un 25°C 0.10M C          K1=5.45      B2=7.75      1975MRa (62191)1285

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C8H15N05 H2L CAS 5344-77-4 (332)
N-(2-Hydroxy-1,1-dimethylethyl)iminodiethanoic acid; HO.CH2.C(CH3)2.N(CH2.COOH)2

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

Ca++ gl oth/un 25°C 0.10M C K1=4.67 B2=7.97 1975MRa (62194)1286

C8H15N05 H2L CAS 59881-66-2 (6076)
N-(3-Methoxypropyl)iminodiethanoic acid; CH3.O.(CH2)3.N(CH2.COOH)2

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

Ca++ gl oth/un 25°C 0.10M C K1=3.98 B2=6.78 1975MRa (62203)1287

C8H15N05 H2L CAS 62117-04-8 (337)
N-(4-Hydroxybutyl)iminodiethanoic acid; HO.(CH2)4.N(CH2.COOH)2

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

Ca++ gl oth/un 25°C 0.10M C K1=4.12 B2=7.72 1975MRa (62206)1288

C8H15N06 H2L CAS 92511-22-3 (6074)
N-(1,1-Di(hydroxymethyl)ethyl)iminoethanoic acid; (HO.CH2)2C(CH3).N(CH2.COOH)2

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

Ca++ gl NaClO4 25°C 1.0M C K1=4.85 1981ASb (62212)1289

Ca++ gl oth/un 25°C 0.10M C K1=6.00 B2=9.30 1975MRa (62213)1290

C8H15N209P H4L (3847)
O-Phosphoryl-L-seryl-L-glutamic acid;

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

Ca++ gl KCl 25°C 0.15M U K1=2.14 19620Sa (62234)1291
K(Ca+HL)=1.64
K(Ca+CaL)=1.46
K(Ca+CaHL)=1.0
K(Ca2L+H)=7.29

K(Ca+H2L)=1.08

C8H16N203 HL Gly-Leu CAS 869-19-2 (255)
Glycyl-leucine; H2N.CH2.CO.NH.CH(CH2.CH(CH3)2).COOH

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

Ca++ gl KCl 20°C 0.20M U K1=1.93 1982RRc (62377)1292

C8H16N2O3 HL Leu-Gly CAS 686-50-0 (1248)
Leucyl-glycine; H2N.CH(CH2.CH(CH3)2).CO.NH.CH2.COOH

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

Ca++ gl KCl 20°C 0.20M U K1=1.74 1982RRc (62423)1293

Ca++ sol oth/un 25°C 0.0 U K1=0.70 1950Dwa (62424)1294

C8H16N2O4 H2L (267)
1,2-Diaminoethane-N,N'-di(2-propanoic acid); ((CH3)(COOH).CH.NH.CH2)2

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

Ca++ cal NaClO4 25°C 0.10M U H K1=2.1 1983EHa (62462)1295
DH1=8.7 kJ mol-1, DS1=77.0 J K-1 mol-1

Ca++ gl KNO3 20°C 0.10M U K1=1.74 1966MKb (62463)1296

Ca++ gl KCl 20°C 0.10M U K1=1 1958ISa (62464)1297

C8H16N2O4 H2L CAS 13288-40-9 (3237)
1,2-Diaminoethane-N,N'-di(3-propanoic acid); (HOOCCH2CH2NHCH2.)2

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

Ca++ gl KCl 20°C 0.10M U K1=1 1958ISa (62491)1298

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

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

Ca++ gl KNO3 25°C 0.10M C K1=3.91 B2=5.51 1993WLa (62520)1299
K(Ca+HL)=2.5

Ca++ cal NaClO4 25°C 0.10M U H K1=6.0 1983EHa (62521)1300
DH1=-4.8 kJ mol-1, DS1=99.0 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

Ca++ EMF oth/un 20°C 0.10M U K1=3.26 1972DKa (62576)1301

Ca++ gl KNO3 20°C 0.10M U K1=3.26 1970DKa (62577)1302

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
Ca++	nmr	non-aq	27°C	100%	C			K1=4.36	2000SMg (62649)	1303
Medium: acetonitrile. Method: competitive 7Li nmr technique.										
Ca++	cal	non-aq	20°C	100%	U	H		K1=1.85	1988SVb (62650)	1304
Medium: EtOH, CaCl2. DH(K1)=-28.1 kJ mol-1; for Ca(NO3)2: K1=1.16; DH=-21.1										
Ca++	cal	alc/w	25°C	100%	U	H	T	K1=2.53	1987BUa (62651)	1305
Medium: MeOH. DH(K1)=-2.3 kJ mol-1; DS=40.6 J K-1 mol-1; DH(B2)=-6.6										
Ca++	EMF	non-aq	25°C	100%	U		T	K1=5.53 B2=9.51	1982MRb (62652)	1306
Medium: anhydrous propylene carbonate, 0.1M Et4NClO4										

C8H17NO3S		HL			CHES			CAS 103-47-9	(7489)	
2-(N-Cyclohexylamino)ethanesulfonic acid;										
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	KNO3	25°C	0.10M	C			K1=3.86	2000ADa (62774)	1307

C8H17NO4		H2L						CAS 6353-68-6	(3238)	
N,N-Di-(2-Hydroxypropyl)glycine; (HO.CH2.CH2)2N.CH2.COOH										
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	oth/un	30°C	0.10M	U			K1=2.65	1957FCa (62780)	1308

C8H17N3O4		H2L						CAS 100585-61-3	(1588)	
3,6,9-Triazaundecanedioic acid; (HOOC.CH2.NH.CH2.CH2)2NH										
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	NaCl	25°C	0.15M	C			K1=2.64	1990JKa (62807)	1309
B(CaH-1L)=-8.53										

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
Ca++	sp	alc/w	25°C	100%	C			K1=4.65	2002NFa (62839)	1310
Medium: 100% MeOH. Method: electrospray ionization mass spectrometry.										

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

Ca++ gl NaCl 25°C 0.10M C K1=2.03 1999HLb (62856)1311

C8H18N2O10P2 H6L EDDADPO CAS 2310-83-0 (2436)
1,2-Diaminoethane-N,N'-diethanoic-N,N'-dimethylphosphonic acid;
(-CH2.N(CH2.COOH)(CH2.PO3H2))2

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

Ca++ gl KCl 25°C 0.10M U K1=7.91 1965DKb (62893)1312

Ca++ ix oth/un 20°C 0.10M U K1=8.88 1965TIc (62894)1313
Medium: NH4+. By glass electrode: I=0.1 M KCl: K1=8.9

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

Ca++ cal non-aq 25°C 100% C H 1992BSc (62978)1314
Medium: propylene carbonate. DH(K1)=-29.9 kJ mol-1.

Ca++ con non-aq 25°C 100% C K1=3.7 1992MSe (62979)1315
Medium: 100% MeOH. Anion: picrate. Also data for nitrophenolate anions.

C8H18O5 L Tetra-Et-Glycol CAS 112-60-7 (5664)
2,2'-(Oxybis(2,2-ethanedioxy))-bis-ethanol; O(CH2.CH2.O.CH2.CH2.OH)2

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

Ca++ con non-aq 25°C 100% C K1=4.0 1992MSe (63000)1316
Medium: 100% MeOH. Anion: picrate. Also data for nitrophenolate anions.

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

Ca++ gl mixed 25°C 90% C I K1=1.64 1982SSf (63048)1317
Medium: 90% DMSO/H2O

Ca++ gl KNO3 25°C 1.0M C K1=2.25 1980SAb (63049)1318
K(Ca(ATP)+L)=1.85

C8H19NO6P2 H4L CAS 5995-40-4 (1338)
N-Cyclohexyliminobis(methylenephosphonic) acid; C6H11.N(CH2PO3H2)2

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

Ca++ gl KCl 25°C 0.20M C K1=3.39 1999MKa (63080)1319
B(CaHL)=15.09

B(CaH2L)=20.30

C8H19N3O L (4430)

1-Oxa-4,7,10-triazacyclododecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Ca++	gl	NaNO3	25°C	0.10M	U			K1=2.03	1988HSb (63129)	1320
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Ca++	gl	NaNO3	25°C	0.10M	U			K1=2.3	1986TSa (63130)	1321
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C8H20N4 L Cyclen CAS 294-90-6 (10)

1,4,7,10-Tetraazacyclododecane; cyclo(-(NH.CH2.CH2.)4-)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Ca++	gl	NaNO3	25°C	0.10M	U			K1=3.12	1988HSb (63277)	1322
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Ca++	gl	NaNO3	25°C	0.10M	U			K1=3.1	1986TSa (63278)	1323
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C8H22N2O6P2 H4L CAS 13516-59-1 (3850)

2,2'-(Ethylenedi-imino)bis(propylphosphonic acid);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Ca++	gl	KCl	25°C	0.10M	U			K1=<2	1965DKb (63331)	1324
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C8H23N5 L Tetren CAS 112-57-2 (715)

1,4,7,10,13-Pentaazatridecane (Tetraethylenepentamine);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Ca++	gl	NaCl	25°C	0.0	C			K1=1.85	1999Sfc (63454)	1325
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K(Ca+HL)=1.30

K(Ca+H2L)=0.7

K(Ca+H3L)=0.0

K(Ca+H4L)=-0.6

Extrapolated from data for 0.03-0.96 M NaCl using the Pitzer equation.

K(Ca+CaL)=-0.2

C8H24N2O12P4S H8L CAS 33424-58-7 (2648)

1,7-Diaza-4-thiaheptane-1,1,7,7-tetra(methylphosphonic acid);

S(CH2.CH2.N(CH2.PO3H2)2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Ca++	gl	KCl	20°C	0.10M	U			K1=5.10	1971TIa (63483)	1326
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K(Ca+H2L)=2.44

K(Ca+HL) =3.77

K(Ca+CaL)=1.60

By ion exchange K1=5.36

C8H24N2O13P4 H8L CAS 25007-19-4 (2647)

1,7-Diaza-4-oxaheptane-1,1,7,7-tetra(methylphosphonic acid);

O(CH2.CH2.N(CH2.PO3H2)2)2

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

Ca++ gl oth/un 20°C 0.10M U K1=6.59 1969TIIa (63491)1327

K(Ca+HL)=4.70

K(Ca+H2L)=2.96

K(Ca+CaL)=2.96

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

Ca++ gl NaNO3 25°C 0.50M M K1=-0.12 1998K5a (63501)1328

C9H6NOCl HL CAS 130-16-5 (1268)

5-Chloro-8-hydroxyquinoline;

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

Ca++ gl diox/w 25°C 60% U K1=4.02 B2=7.17 1973SCd (63656)1329

Medium: 60% dioxan, 0.1 M NaClO4

C9H6NO4IS H2L Ferron CAS 547-91-1 (275)

7-Iodo-8-hydroxyquinoline-5-sulfonic acid; (HO)(HO3S)C9H4NI

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

Ca++ gl KNO3 28°C 0.10M U K1=2.60 1971LSb (63762)1330

Ca++ gl oth/un 25°C 0.0 U K1=3.07 B2=4 1953NEa (63763)1331

C9H6N2O3 HL CAS 5437-99-0 (3865)

5-Nitro-8-hydroxyquinoline;

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

Ca++ gl diox/w 25°C 60% U K1=3.24 B2=5.76 1973SCd (63858)1332

Medium: 60% dioxan, 0.1 M NaClO4

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

Ca++ gl oth/un 25°C 0.0 U K1=2.26 B2=4.50 1955NUa (63904)1333

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

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

Ca++ gl NaCl 25°C 0.0 C K1=4.28 1995DGB (63963)1334
B(CaHL)=9.35
B(CaH2L)=13.05
B(Ca2HL)=6.57

Calculated from data for 0-0.7 M NaCl and 0.2-0.4 M Et4NI.

Kso(CaHL)=-12.95 (I=0-0.39 M NaCl).

C9H6O6 H3L Trimellitic aci CAS 528-44-9 (1622)
1,2,4-Benzenetricarboxylic acid; C6H3.(COOH)3

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

Ca++ gl NaCl 25°C 0.0 C K1=3.58 2003CDB (63989)1335
B(CaHL)=8.04
B(CaH2L)=11.31
B(Ca2L)=5.4
Kso(CaHL)=-11.7

Extrapolated from values for 0.2-0.4 M Et4NI or 0-0.8 M NaCl.

C9H6O6 H3L CAS 554-95-0 (1623)
1,3,5-Benzenetricarboxylic acid; C6H3.(COOH)3

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

Ca++ gl NaCl 25°C 0.0 C K1=3.08 2003CDB (63998)1336
B(CaHL)=8.01
B(CaH2L)=11.45
Kso(Ca3L2)=-13.6

Extrapolated from values for 0.2-0.4 M Et4NI or 0-0.8 M NaCl.

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

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

Ca++ sp alc/w 25°C 95% U K1=2.13 1993GSA (64192)1337
Medium: 95% w/w EtOH/H2O, 0.05 M Et4NClO4, by competitive spectrophotometry

Ca++ sp non-aq 25°C 100% U I K1=3.42 B2=5.80 1992GSA (64193)1338
Medium: MeCN. In acetone:K1=2.17, K2=1.19; in MeOH:K1=1.77, K2=1.08.
By fluorimetry

Ca++ gl diox/w 25°C 60% U K1=4.40 B2=8.01 1973SCD (64194)1339

Medium: 60% dioxan, 0.1 M NaClO4

Ca++ gl diox/w 30°C 75% U K1=7.3 B2=13.2 1954UFa (64195)1340

Ca++ gl oth/un 20°C 0.0 U K1=3.27 1952NAa (64196)1341

C9H7NO2 HL CAS 1477-50-5 (4610)
2-Indolecarboxylic acid;

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

Ca++ gl oth/un 25°C 0.0 U K1=1.38 1972LPa (64391)1342

C9H7NO4S H2L Sulfoxine CAS 84-88-8 (448)
8-Hydroxyquinoline-5-sulfonic acid;

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

Ca++ gl diox/w 25°C 60% U K1=4.53 B2=8.01 1973SCd (64507)1343
Medium: 60% dioxan, 0.1 M NaClO4

Ca++ sp oth/un 25°C 0.0 U K1=3.52 1954NUa (64508)1344

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

Ca++ gl alc/w 25°C 50% U K(Ca+HL)=3.5 1967NPb (64688)1345

Medium: 50% MeOH, 0.1 M NaClO4

C9H8N2 L CAS 578-66-5 (503)
8-Aminoquinoline;

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

Ca++ gl KCl 20°C 0.10M U K1=1.49 1957WSa (64776)1346

C9H8N2O2S HL (8279)
Dehydroxydemethylidesferrithiocin;

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

Ca++ gl KNO3 25°C 0.10M C K1=2.5 1990ARa (64800)1347

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

Ca++ vlt NaClO4 25°C 0.50M C T H K1=6.59 1989GRb (64891)1348
Method: polarography. Medium: 0.50 M NH4ClO4, pH 4.8. Data for 25-45 C.
DH(K1)=-32.3 kJ mol⁻¹, DS(K1)=17.4 J K⁻¹ mol⁻¹.

Ca++ gl NaClO4 37°C 0.15M C K1=2.946 1978AKa (64892)1349

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

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

Ca++ sp NaClO4 ? 0.20M U K1=3.05 1967GDb (64929)1350

C9H9NO3 HL Hippuric acid CAS 495-69-2 (1184)
Benzoylaminoethanoic acid, N-benzoylglycine; C6H5.CO.NH.CH2.COOH

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

Ca++ sol oth/un 25°C 0.0 U K1=0.43 1950DWa (65053)1351

C9H9NO3I2 H2L Iodogorgoic acid CAS 300-39-0 (2726)
2-Amino-3-(3,5-diiodo-4-hydroxyphenyl)propanoic acid, Diiodotyrosine;

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

Ca++ sol oth/un 25°C 0.0 U K1=1.54 1950DWa (65070)1352

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

Ca++ gl alc/w 30°C 40% M M K1=2.83 B2= 4.31 1995RRd (65145)1353
K(CaL+A)=4.26
K(CaL+en)=6.10
K(CaL+pro)=3.30
K(CaL+B)=2.93
Medium: 40% v/v EtOH/H2O, 0.10 M KNO3. K(CaL+ala)=2.64, K(CaL+gly)=1.37;
H2A is catechol, HB is hydroxyproline.

Ca++ gl alc/w 30°C 40% M M 1995RRd (65146)1354

K(Ca(phen)+L)=2.70
K(CaA+L)=1.46
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

 Ca++ gl alc/w 30°C 40% M M K1=3.24 B2= 4.99 1995RRd (65212)1355
 K(CaL+A)=4.25
 K(CaL+en)=6.00
 K(CaL+pro)=3.20
 K(CaL+B)=2.86

Medium: 40% v/v EtOH/H2O, 0.10 M KNO3. K(CaL+ala)=2.55, K(CaL+gly)=1.34;
 H2A is catechol, HB is hydroxyproline.

Ca++ gl alc/w 30°C 40% M M 1995RRd (65213)1356
 K(Ca(phen)+L)=2.80
 K(CaA+L)=1.50

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

Ca++ gl NaCl04 22°C 0.10M U K1=5.42 1964BBa (65264)1357

 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

Ca++ gl diox/w 25°C 50% U 1969ZSa (65272)1358
 K(Ca+H2L)=2.38
 K(Ca+HL)=4.68

 C9H10O8 H4L CAS 3724-52-5 (1264)
 cis-1,2,3,4-Cyclopentanetetracarboxylic acid; C5H6.(COOH)4

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

Ca++ gl NaCl04 25°C 0.19M U K1=6.15 B2= 9.05 1986MSc (65635)1359

 C9H11NO3 H2L Tyrosine CAS 60-18-4 (4)
 2-Amino-3-(4-hydroxyphenyl)propanoic acid; HO.C6H4.CH2.CH(NH2).COOH

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

Ca++ sol oth/un 25°C 0.0 U 1950DWa (66192)1360
 K(Ca+HL)=1.48

 C9H11NO4 H3L DOPA CAS 59-92-7 (5)
 2-Amino-3-(3,4-dihydroxyphenyl)propanoic acid;H2NCH(CH2C6H3(OH)2)COOH

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

Ca++ gl NaCl 25°C 0.12M U M K1=2.74 1978RMc (66381)1361
K(Ca(ATP)+L)=2.32

C9H11N05 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

Ca++ gl KNO3 20°C 0.10M U K1=3.58 1963IFa (66448)1362

C9H11N307 H3L (3877)
N-(1-Methyl-2,4,6-trioxo-perhydropyrimidinyl)iminodiethanoic acid;

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

Ca++ gl KNO3 20°C 0.10M U K1=8.22 B2=13.60 1963IFb (66521)1363

C9H12N206 HL Uridine CAS 58-96-8 (828)
Uracil-1-beta-D-ribofuranoside;

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

Ca++ gl KNO3 25°C 0.10M C T HM K1=3.05 1987KRa (66682)1364

Ca++ gl KNO3 35°C 0.10M U M K1=2.62 1986RRa (66683)1365
Ternary complexes with glycine, oxalate, histidine and histamine

C9H12N2010 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

Ca++ gl KNO3 25°C 0.1M U K1=7.60 1982KBe (66727)1366

C9H13N02 H2L Phenylephrine CAS 61-76-7 (2759)
3-Hydroxy-alpha-(methylaminomethyl)benzyl alcohol; HO.C6H4.CH(CH2.NH.CH3)OH

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

Ca++ gl KNO3 22°C 0.25M U 1984GKa (66809)1367

K(Ca+HL)=2.25

C9H13N03 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

Ca++ gl KCl 25°C 0.10M U T H K1=5.45 B2= 6.78 1983CVa (66848)1368

Data for 0 and 37 C. DH(K1)=-34.3 kJ mol⁻¹, DS(K1)=-28.2 J K⁻¹ mol⁻¹;
 DH(K2)=-27.4, DS(K2)=-47.6.

C9H13N06 H3L (3881)

2,6-Dicarboxypiperidyl-N-ethanoic acid;

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

Ca++ gl KNO3 25°C 0.10M U K1=5.41 1968KTd (66876)1369

C9H13N08 H4L (7012)

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

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

Ca++ gl KNO3 25°C 0.10M U K1=5.18 1977GNb (66902)1370

Ca++ gl KNO3 25°C 0.1M U K1=5.93 1976NGb (66903)1371

C9H13N209P H3L UMP-5 CAS 58-97-9 (2948)

Uridine-5'-monophosphoric acid;

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

Ca++ gl KNO3 35°C 0.10M U M 1992RAd (66952)1372

K(Ca+HL)=1.70
 K(Ca+HL+Gly)=2.04
 K(Ca+HL+His)=7.05
 K(Ca+HL+histamine)=6.42

Ca++ gl R4N.X 25°C 0.10M C T 1991SMa (66953)1373

K(Ca+HL)=1.90

IUPAC evaluation

 Ca++ gl NaNO3 25°C 0.10M C 1988MSa (66954)1374

K(Ca+HL)=1.44

C9H13N305 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

Ca++ gl NaNO3 25°C 0.50M C K1=0.18 1992KJa (67035)1375

Ca++ gl KNO3 35°C 0.10M C M K1=2.47 1985RRc (67036)1376

B(CaHL(Gly))=11.87
 B(CaL(oxalate))=8.80
 B(CaHL(His))=11.51
 B(CaHL(histamine))=11.76

Ca++ gl KNO3 45°C 0.10M U K1=2.56 1981TKa (67037)1377

C9H14N04P H2L (8075)
2-Amino-3-hydroxy-3-phenylpropane-3-phosphonic acid;

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

Ca++ gl NaClO4 25°C 0.1M U K1=1.52 1975SLa (67109)1378

C9H14N209 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

Ca++ gl KNO3 25°C 0.10M U K1=3.08 1975KGa (67133)1379
K(Ca+HL)=2.05

C9H14N2012P2 H4L UDP CAS 58-98-0 (3288)
Uridine-5'-diphosphoric acid;

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

Ca++ gl NaNO3 25°C 0.10M M K1=2.90 1999SSa (67150)1380
K(Ca+H2L)=1.5
K(CaHL+H)=5.0

Ca++ gl KNO3 25°C 0.10M U K1=2.90 1995SBa (67151)1381

C9H14N308P 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

Ca++ gl KNO3 25°C 0.10M C M K1=2.40 2001AAa (67226)1382
Also data for ternary complexes with MOPSO, TAPSO and ACES.

Ca++ gl R4N.X 25°C 0.10M C T K1=1.86 1991SMa (67227)1383
IUPAC evaluation

Ca++ gl NaNO3 25°C 0.10M C K1=1.40 1988MSa (67228)1384

Ca++ gl KNO3 35°C 0.10M U M 1986RRe (67229)1385
K(Ca+HL+HA)=5.87
K(Ca+HL+E)=6.40
K(Ca+L+HC)=5.57
K(CaLC+H)=2.63

K(Ca+L+HD)=5.43. HA is glycine; H2E is oxalic acid;
C is histamine; HD is histidine.

C9H14N403 HL Carnosine CAS 305-84-0 (272)

3-Alanyl-histidine; H2N.CH2.CH2.CO.NH.CH(CH2.C3H3N2).COOH

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

Ca++ nmr none 25°C 0.0 U 1990GVb (67305)1386
Keff=1.40

Medium: D20 at pH 7.0

Ca++ gl KNO3 25°C 0.10M U K1=3.22 1964LMa (67306)1387

C9H14N5O3P H2L CAS 121149-93-7 (2512)
9-(4-Phosphonobutyl)adenine;

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

Ca++ gl NaNO3 25°C 0.10M M K1=1.57 2000GKa (67353)1388
K(Ca+HL)=0.2
*K(CaHL)=-6.3

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

Ca++ gl KNO3 20°C 0.10M U K1=6.40 1974RMf (67399)1389

C9H15NO6P2 H4L (6888)
N-Benzyl-N-methylaminomethylenedi(phosphonic acid); C6H5.CH2.N(CH3)CH(PO3H2)2

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

Ca++ gl KCl 25°C 0.10M M K1=4.20 1978GMf (67445)1390
K(Ca+HL)=4.03

C9H15NO6P2 H4L CAS 6056-53-7 (1337)
N-Benzyliminobis(methylenephosphonic) acid; C6H5CH2N(CH2PO3H2)2

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

Ca++ gl KCl 25°C 0.20M C K1=3.88 1999MKa (67456)1391
B(CaHL)=13.91
B(CaH2L)=19.05
B(CaH-1L)=-8.68

Ca++ gl KNO3 25°C 1.00M M K1=3.05 1982BGb (67457)1392
K(Ca+HL)=1.67

C9H15N2O15P3 H5L UTP CAS 63-39-8 (407)
Uridine-5'-triphosphoric acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	gl	R4N.X	25°C	0.10M	C	T	K(Ca+HL)=4.14 K(Ca+H2L)=2.70	1991SMa (67506)	1393

IUPAC evaluation

Ca++	gl	NaNO3	25°C	0.10M	C		K(Ca+HL)=3.94 K(CaL+H)=5.25 K(Ca+H2L)=2.74	1987STb (67507)	1394
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Ca++	gl	KNO3	25°C	0.10M	U T H		K1=5.20	1983RRe (67508)	1395
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Also data for 35 and 45 C. At 45 C: K1=5.01.
DH(K1)=-17.1 kJ mol⁻¹, DS(K1)=41 J K⁻¹ mol⁻¹.

Ca++	gl	NaClO4	25°C	0.10M	C		K1=3.66 K(Ca+HL)=3.66	1977SIc (67509)	1396
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Ca++	gl	KNO3	35°C	0.10M	U		K(Ca+HL)=5.12	1976KRa (67510)	1397
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Ca++	ix	NaCl	23°C	0.10M	U		K(Ca+HL)=3.71	1958WAa (67511)	1398
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C9H15N3O11P2 H3L CDP CAS 63-38-7 (2187)
Cytidine-5'-diphosphoric acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	gl	NaNO3	25°C	0.10M	M		K1=2.87 K(Ca+HL)=1.5 K(CaL+H)=5.02	1999SSa (67579)	1399

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
Ca++	gl	KCl	20°C	0.10M	U		K1=2.99	1955SAa (67623)	1400

C9H16N3O14P3 H4L CTP CAS 65-47-4 (406)
Cytidine-5'-triphosphoric acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	gl	R4N.X	25°C	0.10M	C	T	K1=4.13 K(Ca+HL)=2.17	1991SMa (67681)	1401

IUPAC evaluation

Ca++ gl NaNO3 25°C 0.10M C K1=3.85 1987STb (67682)1402
K(Ca+HL)=2.21
K(CaL+H)=4.91

Ca++ gl KNO3 25°C 0.10M U T H K1=4.16 1983RRe (67683)1403
K(Ca+HL)=3.84

Also data for 35 and 45 C. At 45 C: K1=4.03, K(Ca+HL)=3.70.
DH(K1)=-12.1 kJ mol⁻¹, DS(K1)=40 J K⁻¹ mol⁻¹; DH(Ca+HL)=-13.0, DS=30

Ca++ gl NaClO4 25°C 0.10M C K1=3.72 1977SIc (67684)1404

Ca++ gl KNO3 35°C 0.1M C I K1=4.13 1975TRc (67685)1405
K(Ca+HL)=3.81

Ca++ ix NaCl 23°C 0.10M U K1=3.81 1958WAa (67686)1406

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

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

Ca++ sp none 25°C 0.0 U T K1=2.55 1976K0a (67766)1407

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

C9H16O4 H2L CAS 57218-62-9 (484)
Ethyl(2-methylpropyl)propanedioic acid; H0OC.C(C2H5)(CH2.CH(CH3)2).COOH

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

Ca++ sp none 25°C 0.0 U T K1=3.02 1976K0a (67783)1408

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

C9H16O4 H2L CAS 2085-15-6 (483)
Ethylbutylpropanedioic acid; H0OC.C(C2H5)(C4H9).COOH

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

Ca++ sp none 25°C 0.0 U T K1=2.62 1976K0a (67786)1409

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

C9H17N04 H2L CAS 56004-51-4 (346)
N-Pentyliminodiethanoic acid; C5H11.N(CH2.COOH)2

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

Ca++ gl oth/un 25°C 0.10M C K1=4.22 1975MRb (67807)1410

C9H17N05 H2L CAS 60470-38-4 (338)
N-(5-Hydroxypentyl)iminodiethanoic acid; HO.(CH2)5.N(CH2.COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	oth/un	25°C	0.10M	C			K1=4.22 B2=7.72	1975MRa (67819)	1411

C9H17NO6			H2L					CAS 58144-32-4	(6077)	
N-(1,1-Di(hydroxymethyl)propyl)iminodiethanoic acid; (HO.CH2)2C(CH2.CH3).N(CH2.COOH)2										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	NaCl04	25°C	1.0M	C			K1=4.84	1981ASb (67825)	1412

Ca++	gl	oth/un	25°C	0.10M	C			K1=5.49 B2=8.59	1975MRa (67826)	1413

C9H18N2O3			HL	Ala-Leu				CAS 1999-42-4	(264)	
Alanyl-leucine; H2N.CH(CH3).CO.NH.CH(CH2.CH(CH3)2).COOH										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	KCl	20°C	0.20M	U			K1=1.74	1982RRc (67900)	1414

C9H18N2O4			H2L					CAS 18992-11-5	(5913)	
N,N-Dihydroxynonanediamide; HN(OH).CO.(CH2)7.CO.NH(OH)										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	KCl	25°C	0.20M	C			K1=2.78 B(CaHL)=12.07	1999FEa (67934)	1415

C9H19N2O4+			H2L					(3277)		
2-Di(carboxymethyl)aminoethyltrimethylammonium cation +										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	KCl	20°C	0.10M	U			K1=1.88	1955SAa (67997)	1416

C9H20N3O7P			H3L					CAS 88794-71-2	(3887)	
O-Phosphoryl-L-seryl-L-lysine;										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	KCl	25°C	0.15M	U			K1=1.53	19620Sa (68074)	1417

C9H20O14P2			H3L					(4662)		
1-(Glycerylphosphoryl)-L-myoinositol-5-phosphate;										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	R4N.X	20°C	0.10M	U			K1=2.07	1969HRa (68127)	1418

Medium: 0.1 (C3H7)4NI

C9H21O17P3 H5L CAS 98975-41-8 (3885)

1'-Glycerylphosphorylinositol-3,4-diphosphoric acid;

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

Ca++ gl R4N.X 20°C 0.10M U K1=3.27 1969HRa (68222)1419
K(Ca+HL)=2.22

Medium : 0.1 (C3H7)4NI

Ca++ gl R4N.X 20°C 0.10M U K1=3.3 1965HFb (68223)1420
K(Ca+HL)=2.2

Medium: (C3H7)4NI

C9H24N3O6P3 H3L (7110)

1,4,7-Triazacyclononane-1,4,7-triyltrimethylenetris(phosphinic acid);

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

Ca++ gl KNO3 25°C 0.10M C K1=4.29 1995BLa (68288)1421
B(CaH-1L)=-7.41

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

Ca++ gl KCl 25°C 1.0M U K1=6.38 1984KMa (68301)1422
K(Ca+HL)=2.67

Ca++ gl oth/un 25°C 1.00M U K1=6.38 1982PSc (68302)1423
K(Ca+HL)=2.67

C9H28N3O15P5 10L DTPPH CAS 15827-60-8 (2921)

Diethylenetriamine-N,N,N',N'',N''-penta(methylphosphonic acid);

H2O3PCH2.N(CH2CH2.N(CH2PO3H2)2)2 H

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

Ca++ gl NaClO4 25°C 0.10M M 1987ZGa (68398)1424
K(Ca+H2L)=4.39
K(Ca+H3L)=3.47
K(Ca+H4L)=2.91
K(Ca+H5L)=2.59

K(Ca+H6L)=1.99

Ca++ gl oth/un 25°C 0.10M U 1984ZGa (68399)1425

K(Ca+H2L)=4.39
K(Ca+H3L)=3.47

Ca++ gl oth/un 25°C 0.0 U K1=1.42 B2=2.99 1955LUa (68692)1432

C10H7NO2 HL CAS 86-59-9 (873)

Quinoline-8-carboxylic acid;

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

Ca++ gl oth/un 25°C 0.0 U K1=1.20 B2=3.93 1955LUa (68747)1433

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

Ca++ cal KCl 25°C 0.25M U H K1=-0.04 1997MKb (69460)1434

DH(K1)=-17 kJ mol⁻¹; DS=-57 J K⁻¹ mol⁻¹

Ca++ gl oth/un 25°C 0.20M U TIH K1=0.0 1993DGa (69461)1435

DH(K1)=21 kJ mol⁻¹, DS(K1)=71 J K⁻¹ mol⁻¹. Data for 5-45 C, 0.20-
0.75 M CaCl₂

Ca++ sp alc/w 25°C 95% U K1=1.97 1993GSa (69462)1436

Medium: 95% w/w EtOH/H₂O, 0.05 M Et₄NClO₄, by competitive spectrophotometry

Ca++ sp non-aq 25°C 100% U I K1=2.71 B2=4.81 1992GSa (69463)1437

K3=1.00

Medium: MeCN. In acetone:K1=2.00, K2=0.66; in MeOH:K1=1.66, K2=0.90

Ca++ gl KCl 25°C 0.25M U T H K1=-0.05 1985CRa (69464)1438

K1=0.09(10 C);K1=-0.19(40 C).

DH=-15.9 kJ mol⁻¹,DS=-54 J mol⁻¹ K⁻¹

C10H8O5S H3L DHNSA (877)

2,3-Dihydroxynaphthalene-6-sulfonic acid;

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

Ca++ gl NaNO₃ 25°C 0.10M U K1=5.21 B2=7.92 1984NHa (69829)1439

C10H9NO3S H2L CAS 49608-51-7 (8280)

4,5-Dihydro-2-(2-hydroxyphenyl)-4-thiazolecarboxylic acid,
Deazademethyldeferrithiocin;

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

Ca++ gl KNO₃ 25°C 0.10M C K1=3.56 1990ARa (70164)1440

C10H9NO₈ H2L CAS 83785-11-9 (685)

2-Nitro-1,4-di(carboxymethoxy)benzene; O₂N.C₆H₃.(OCH₂COOH)₂


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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
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Ca++      con oth/un 25°C 0.10M U          K1=3.46      1985TZa (70229)1441
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Ca++      gl  oth/un 30°C   ?  U          K1=3.49      1985TZa (70230)1442
*****
C10H9O2Br          HL          CAS 4023-81-8 (1182)
4-Bromo-1-phenyl-1,3-butanedione; Br.C6H4.CO.CH2.CO.CH3
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  diox/w 20°C 75% M T          K1=7.93  B2=13.09  1980GMd (70430)1443
*****
C10H9O4P          H2L          CAS 1136-89-6 (1931)
1-Naphthyl-phosphoric acid;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  NaCl  25°C 0.15M U          K1=1.223      1990KLb (70460)1444
*****
C10H10N2O3S          H2L          CAS 76045-30-2 (7218)
Desferriferrithiocin,
2-(3-Hydroxypyridin-2-yl)-4-methyl-4,5-dihydrothiazole-4-carboxylic acid;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  KNO3  25°C 0.10M C          K1=4.65  B2= 7.25  1990ARa (70554)1445
*****
C10H10O2          HL  Benzoylacetone  CAS 93-91-4 (197)
1-Phenylbutane-1,3-dione; C6H5.CO.CH2.CO.CH3
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  diox/w 20°C 17% C          K1=6.03  B2=10.65  1976JWa (70693)1446
*****
C10H10O6          H2L          CAS 5411-14-3 (2394)
1,2-Phenylenedioxodiethanoic acid; C6H4(O.CH2.COOH)2
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  NaClO4 25°C 0.10M U          K1=3.1        1968SMb (70841)1447
*****
C10H11NO4          H2L          CAS 1137-73-1 (2567)
N-Phenyliminodiethanoic acid; C6H5.N(CH2.COOH)2
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      cal KNO3  25°C 0.1M C  H          DH(K1)=6.7 kJ mol-1  1991ANa (70986)1448
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Ca++ cal KNO3 25°C 0.10M U K1=1.5 1991Aa (70987)1449
DH(K1)=6.69 kJ mol⁻¹, DS(K1)=50.21 J K⁻¹ mol⁻¹

Ca++ gl KCl 30°C 0.10M U K1=1.5 1957TBc (70988)1450

Ca++ gl KCl 20°C 0.10M U K1=1.5 1955SAa (70989)1451

Ca++ EMF KCl 20°C 0.10M U K1=0.6 1947SWa (70990)1452

Method: H electrode

C10H11N04S H3L (3928)
N-(2'-Mercaptophenyl)iminodiethanoic acid; HS.C6H4.N(CH2.COOH)2

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

Ca++ gl KNO3 20°C 0.10M U K1=2.79 ? 1963IFb (71020)1453

C10H11N05 H3L CAS 100844-86-8 (2108)
N-(2-Hydroxyphenyl)iminodiethanoic acid; HO.C6H4.N(CH2.COOH)2

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

Ca++ gl KNO3 20°C 0.10M U K1=6.27 1963IFb (71033)1454
K(Ca+HL)=3.21

C10H11N05S H2L (3929)
N-(2-Thenylmethyl)iminodiethanoic acid; C4H3S.CO.CH2.N(CH2.COOH)2

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

Ca++ gl KNO3 25°C 0.10M U K1=4.26 1965AUa (71058)1455

C10H11N07S H3L (3335)
N-(2-Sulfophenyl)iminodiethanoic acid; HO3S.C6H4.N(CH2.COOH)2

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

Ca++ EMF KCl 20°C 0.10M C K1=4.57 1947SWa (71064)1456

Method: H electrode

C10H11N07S H3L (3336)
N-(3-Sulfophenyl)iminodiethanoic acid; HO3S.C6H4.N(CH2.COOH)2

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

Ca++ EMF KCl 20°C 0.10M C K1=1.26 1947SWa (71071)1457

Method: H electrode

C10H11N07S H3L (3337)

N-(4-Sulfophenyl)iminodiethanoic acid; H₃S.C₆H₄.N(CH₂.COOH)₂

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Ca++	EMF	KCl	20°C	0.10M	C			K1=0.95	1947SWa (71074)	1458
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Method: H electrode

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Ca++	gl	alc/w	30°C	40%	M	M		K1=3.79 B2= 6.20	1995RRe (71188)	1459
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K(CaL+A)=4.07
 K(CaL+en)=5.76
 K(CaL+pro)=3.05
 K(CaL+B)=2.75

Medium: 40% v/v EtOH/H₂O, 0.10 M KNO₃. K(CaL+ala)=2.40, K(CaL+gly)=1.25.
 H₂A is catechol, HB is hydroxyproline.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Ca++	gl	alc/w	30°C	40%	M	M		K(Ca(phe)+L)=2.88 K(CaA+L)=2.00	1995RRe (71189)	1460
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Medium: 40% v/v EtOH/H₂O, 0.10 M KNO₃. H₂A is salicylic acid.

C10H12N2O4		H2L						CAS 16598-05-3	(967)	
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2-Pyridylmethyliminodiethanoic acid; C₅H₄N.CH₂.N(CH₂.COOH)₂

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Ca++	gl	NaNO ₃	20°C	0.10M	C	H		K1=4.91	1981ANb (71237)	1461
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DH1=-6.3 kJ mol⁻¹ DS1=72.4 J K⁻¹ mol⁻¹

Ca++	gl	KCl	25°C	0.10M	U			K1=4.80 B2=7.72	1966SIb (71238)	1462
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Ca++	gl	KNO ₃	20°C	0.10M	U			K1=4.92	1963IFc (71239)	1463
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C10H12N4O6		H2L	Xanthosine					CAS 5968-90-1	(1176)	
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3,9-Dihydro-9-ribofuranosyl-1H-purine-2,6-dione;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Ca++	gl	KNO ₃	25°C	0.10M	U	M		K(Ca(Histidine)+H+L)=2.82 B(CaH ₂ L(histamine))=7.90 B(CaH ₂ L(catechol))=5.62 K(Ca(Gly)+H+L)=2.72	1990RRa (71457)	1464
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Ca++	gl	NaNO ₃	25°C	0.10M	C				1989Kta (71458)	1465
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K(Ca+H-1L) < 0.6

 Ca++ gl KNO3 35°C 0.10M C M 1985RRh (71459)1466
 K(Ca+HL)=2.21
 K(Ca(gly)+HL)=2.6
 K(Ca(his)+HL)=2.76
 K(Ca+HL+HA)=5.45
 K(Ca+HL+B)=8.22. H2A is catechol, H2B is oxalic acid.

Ca++ gl KNO3 35°C 0.10M U M 1983RRb (71460)1467
 K(Ca+HL)=2.21
 K(Ca+2HL)=5.15
 K(CaGly+H2L=CaHLGly+H)=2.6

Ca++ gl KNO3 25°C 0.10M U T H 1983RRc (71461)1468
 K(Ca+2HL)=5.16
 At 5 C: K=6.01; 35 C: 5.15; 45 C: 5.56

Ca++ gl KNO3 45°C 0.10M U M 1979RRb (71462)1469
 K(Ca+HL+TetraMeen)=5.21
 K(Ca+HL+Sulphosalicylate)=2.22

Ca++ gl KNO3 45°C 0.10M U M 1979RRb (71463)1470
 K(Ca+HL+bpy)=6.42

Ca++ gl KNO3 25°C 0.10M U T 1978RRa (71464)1471
 K(Ca+HL)=2.37

 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

Ca++ sp NaCl04 25°C 0.10M U K1=1.5 1965SIa (71506)1472

 C10H12O2 HL CAS 1946-74-3 (202)
 3-Isopropyltropolone;

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

Ca++ dis NaCl04 25°C 0.10M U K1=2.77 B2=4.54 1962DYa (71560)1473

Ca++ gl diox/w 30°C 50% U K1=5.2 B2=8.8 1954BFb (71561)1474

Ca++ gl diox/w 30°C 50% U K1=5.4 B2=9.0 1954BFb (71562)1475

 C10H13N2O11P H3L Orotidylic acid CAS 68244-58-6 (6665)
 Orotidine-5'-monophosphoric acid, uridine-5-carboxylic acid-5-monophosphoric acid;

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

Ca++ gl NaNO3 25°C 0.10M M K1=1.76 1991BSc (71786)1476
K(CaH-1L+H)=8.77

Ca++ gl NaNO3 25°C 0.10M M I 1991BSd (71787)1477
K(CaL+H)=8.77
K(Ca+HL)=1.76

In 30% v/v dioxan/H2O: K(Ca+HL)=2.36, K(CaL+H)=9.15.
In 50% v/v dioxan/H2O: K1=2.76, K(CaL+H)=9.27

C10H13N3O7 H3L (3912)
1,3-Dimethyluramil-N,N-diethanoic acid;

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

Ca++ gl KNO3 20°C 0.10M U K1=8.13 B2=13.53 1963IFb (71801)1478

C10H13N4O8P H3L IMP CAS 131-99-7 (843)
Inosine-5'-monophosphoric acid;

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

Ca++ gl KNO3 25°C 0.10M C M K1=1.52 2001AAa (71845)1479
Also data for ternary complexes with MOPSO, TAPSO and ACES.

Ca++ gl NaNO3 25°C 0.10M M 1994SMb (71846)1480
K(Ca+HL)=1.50
*K(CaHL)=-8.62

C10H13N4O9P H3L (3930)
Inosine-5'-monophosphoric acid N(1)-oxide;

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

Ca++ sp NaClO4 25°C 0.10M U 1965SIa (71881)1481
K(Ca+HL)=2.0

C10H13N5O4 L Adenosine CAS 58-61-7 (2154)
Adenosine, Adenine-9-beta-D-ribofuranoside;

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

Ca++ nmr non-aq 21°C 100% U K1=0.81 1973SFa (71934)1482
Medium : (CH3)2SO

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

Ca++ gl KNO3 25°C 0.10M C T HM 1988KR a (71995)1483

K(Ca+HL)=1.75
K(CaHL+HL)=3.54

Also data at 15, 35 and 45 C. DH(CaHL)=+13; DS=76. DH(CaH2L2)=+9.5; DS=100
Also ternary complexes with bpy, phen and 5-sulfosalicylic acid

Ca++ nmr non-aq 21°C 100% U 1973SFa (71996)1484
K(Ca+HL)=1.06

Ca++ nmr oth/un 37°C var U 1972JMa (71997)1485
K(Ca+HL)=1.23

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

Ca++ gl NaNO3 25°C 0.10M M K1=1.27 1997SSg (72145)1486

Ca++ gl KNO3 25°C 0.10M U K1=1.27 1995SSe (72146)1487

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

Ca++ gl R4N.X 25°C 0.10M C T K1=1.88 1991SMa (72173)1488
IUPAC evaluation

Ca++ gl NaNO3 25°C 0.10M U K1=1.43 1989MSf (72174)1489

Ca++ gl KNO3 40°C 0.10M U T H K1=1.81 1967TMf (72175)1490
K1=1.87(0.4 C),1.85(12 C),1.83(25 C). At 25 C: DH(K1)=-2.5 kJ mol⁻¹, DS=27

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

Ca++ gl R4N.X 25°C 0.10M C T K1=1.85 1991SMa (72220)1491
IUPAC evaluation

Ca++ gl NaNO3 25°C 0.10M U K1=1.36 1989MSf (72221)1492

Ca++ gl KNO3 40°C 0.10M U T H K1=1.78 1967TMf (72222)1493
K1=1.86(0.4 C),1.84(12 C),1.80(25 C). At 25 C: DH(K1)=-2.5 kJ mol⁻¹, DS=27

Ca++ gl KNO3 25°C 0.10M U K1=1.80 1962TMa (72223)1494

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
Ca++	gl	NaNO3	25°C	0.10M	M		K1=1.48 K(CaL+H)=4.5 K(Ca+HL)=-0.2	2003BSa (72364)	1495
Ca++	gl	KNO3	25°C	0.10M	C	M	K1=1.85 K(CaL+A)=1.35 B(CaLA)=3.20 K(CaL+B)=2.82 B(CaLB)=4.67 K(CaL+C)=3.89, B(CaLC)=5.74, K(CaL+D)=2.35, B(CaLD)=4.20. HA=MOPS, HB=POPSO, HC=HEPPSO and HD=AMPSO.	2001A0a (72365)	1496
Ca++	gl	KNO3	25°C	0.10M	C	M	K1=1.85 K(CaL+A)=4.26 B(CaLA)=6.11 K(CaL+B)=4.03 B(CaLB)=5.88 HA=ACES, HB=MOPSO. Also data for CHES, TAPSO and DIPSO.	2000ADa (72366)	1497
Ca++	gl	NaNO3	25°C	0.10M	M		K1=1.48	1996SSd (72367)	1498
Ca++	gl	R4N.X	25°C	0.10M	C	TIH R	K1=1.92 IUPAC evaluation. DH(K1)=4.2 kJ mol ⁻¹ (tentative). 37 C, I=0.15 M: K1=1.68	1991SMa (72368)	1499
Ca++	gl	NaNO3	25°C	0.10M	U		K1=1.46	1989MSf (72369)	1500
Ca++	gl	KNO3	25°C	0.10M	U	M	K1=2.30	1988MBa (72370)	1501
Ca++	gl	NaNO3	25°C	0.10M	C		K1=1.46	1988SMb (72371)	1502
Ca++	gl	NaClO4	25°C	0.10M	C	H	K1=2.03 DH(K1)=4.23 kJ mol ⁻¹ , DS=53 J K ⁻¹ mol ⁻¹	1987SCa (72372)	1503
Ca++	ISE	oth/un	25°C	0.0	C		K1=2.59 Method: Ca ion selective electrode. Self medium, pH 9.1.	1976KRb (72373)	1504
Ca++	gl	KNO3	40°C	0.10M	U	T H	K1=1.83 K1=1.88(0.4 C), 1.87(12 C), 1.85(25 C). At 25 C: DH(K1)=-2.5 kJ mol ⁻¹ , DS=27 J	1967TMf (72374)	1505
Ca++	gl	NaClO4	25°C	0.10M	U		K1=1.39	1964SBa (72375)	1506
Ca++	gl	KNO3	25°C	0.10M	U		K1=1.85	1962TMa (72376)	1507
Ca++	ix	NaCl	23°C	0.10M	U		K1=1.76	1958WAa (72377)	1508
Ca++	gl	KCl	20°C	0.10M	U		K1=1.41	1956MSa (72378)	1509

Ca++ gl R4N.X 25°C 0.20M U K1=1.43 1956SAa (72379)1510
Medium: 0.2 M n-Pr4NCl

C10H14N5O8P H2L CAS 4061-78-3 (3931)

Adenosine-5'-monophosphoric acid N(1)-oxide;

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

Ca++ gl NaClO4 25°C 0.10M U 1964SBa (72519)1511

K(Ca+HL)=1.43
K(CaL+H) > 10.93

By spectrophotometry: K1 < 3.00

C10H14N5O8P H3L GMP-5 CAS 85-32-5 (2947)

Guanosine-5'-monophosphoric acid;

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

Ca++ gl KNO3 25°C 0.10M C M K1=1.54 2001AAa (72568)1512

Also data for ternary complexes with MOPSO, TAPSO and ACES.

Ca++ gl NaNO3 25°C 0.10M M 1994SMb (72569)1513

K(Ca+HL)=1.53
*K(CaHL)=-9.01

Ca++ gl NaNO3 25°C 0.10M C K1=1.53 1988MSd (72570)1514

K(Ca+HL)=1.53

C10H15N06 H3L (3915)

N-(1'-Carboxycyclopentyl)iminodiethanoic acid;

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

Ca++ gl KCl 20°C 0.10M U K1=8.22 1966IMa (72667)1515

C10H15N2O8P H2L TMP-5 CAS 365-07-1 (2949)

Thymidine-5'-monophosphoric acid, Thymidylic acid;

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

Ca++ gl R4N.X 25°C 0.10M C T 1991SMa (72690)1516

K(Ca+HL)=1.86

IUPAC evaluation

Ca++ gl NaNO3 25°C 0.10M C 1988MSa (72691)1517

K(Ca+HL)=1.40

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

Inosine 5'-triphosphoric acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	NaNO3	25°C	0.10M	C				2001SBc (72744)	1518

K(Ca+HL)=3.93
K(CaHL+H)=4.95
K(Ca+H2L)=2.4

For pyrimidine nucleoside 5'-triphosphoric acid, K1=3.84, K(Ca+HL)=2.2, K(CaL+H)=4.85

Ca++	gl	R4N.X	25°C	0.10M	C	T			1991SMa (72745)	1519
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K(Ca+HL)=4.14

IUPAC evaluation

Ca++	gl	NaClO4	25°C	0.10M	C				1977SIc (72746)	1520
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K(Ca+HL)=3.73

Ca++	gl	KNO3	25°C	0.10M	U T				1973TRb (72747)	1521
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K(Ca+HL)=3.41

K(35 C)=3.59, K(45 C)=3.37

Ca++	ix	NaCl	23°C	0.10M	U				1958WAa (72748)	1522
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K(Ca+HL)=3.76

C10H15N5O10P2 H3L ADP CAS 20398-34-9 (2181)
Adenosine-5'-diphosphoric acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	NaNO3	25°C	0.10M	M				2003BSa (72906)	1523

K1=2.95
K(CaL+H)=4.95
K(Ca+HL)=1.5

Ca++	gl	KNO3	25°C	0.10M	C	M			2001A0a (72907)	1524
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K1=2.86
K(CaL+A)=3.05
B(CaLA)=5.91
K(CaL+B)=3.72
B(CaLB)=6.58

K(CaL+C)=2.16, B(CaLC)=5.02.
HA=POPSO, HB=HEPPSO and HC=AMPSO.

Ca++	gl	KNO3	25°C	0.10M	C	M			2000ADa (72908)	1525
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K1=2.86
K(CaL+A)=6.90
B(CaLA)=9.76
K(CaL+B)=3.78
B(CaLB)=6.64

K(CaL+C)=3.60, B(CaLC)=6.46. HA=ACES, HB=MOPSO, HC=CHES.
Also data for TAPSO and DIPSO.

Ca++	gl	NaNO3	25°C	0.10M	C	M			2000KHa (72909)	1526
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K1=2.86
K(CaL+A)=3.06

B(CaLA)=5.92

H2A=salicylhydroxamic acid.

Ca++	gl	KNO3	25°C	0.10M	U		K1=2.96	1995SBa (72910)1527
Ca++	gl	R4N.X	25°C	0.10M	C	TIH R	K1=3.08 K(Ca+HL)=1.65	1991SMa (72911)1528
IUPAC evaluation. 37 C, 0.15 NaCl, K1=2.85, K(Ca+HL)=1.52								
Ca++	gl	KNO3	25°C	0.10M	U	M	K1=2.91	1988MBa (72912)1529
Ca++	gl	NaClO4	25°C	0.10M	C	H	K1=2.90 B(CaHL)=7.00	1987SCa (72913)1530
DH(K1)=13.80 kJ mol ⁻¹ , DS=101 J K ⁻¹ mol ⁻¹								
Ca++	gl	KNO3	22°C	0.25M	U		K1=2.18	1984GKa (72914)1531
Ca++	gl	KNO3	40°C	0.10M	U	T H	K1=2.80 K(Ca+HL)=1.54	1967TMF (72915)1532
K1=2.91(0.4 C), 2.88(12 C), 2.86(25 C); K=1.61(0.4 C), 1.60(12 C), 1.58(25 C). At 25 C: DH(K1)=-5.0 kJ mol ⁻¹ , DS=38 J K ⁻¹ mol ⁻¹ ; DH(Ca+HL)=-2.5, DS=21								
Ca++	sp	oth/un	30°C	0.10M	U		K1=3.34	1964OPa (72916)1533
Medium: 0.1 M buffer N-ethylmorpholine+HCl								
Ca++	oth	R4N.X	23°C	0.06M	U		K1=2.93	1962AMa (72917)1534
Method: interferometer. Medium: 0.06 M Me4NCl, 0.05(HOCH2)3.CNH2 In 0.06 Me4NCl, 0.05 CH3COO ⁻): K(Ca+HL)=1.52								
Ca++	gl	KNO3	25°C	0.10M	U		K1=2.86 K(Ca+HL)=1.58	1962TMa (72918)1535
Ca++	sp	R4N.X	25°C	0.10M	U		K1=2.86	1959BUa (72919)1536
Medium: Bu3EtNBr								
Ca++	ix	NaCl	23°C	0.10M	U		K1=2.82	1958WAa (72920)1537
Ca++	ix	oth/un	23°C	0.10M	U		K1=2.84	1957NAc (72921)1538
Ca++	gl	KCl	20°C	0.10M	U		K1=2.78	1956MSa (72922)1539
Ca++	gl	R4N.X	25°C	0.20M	U		K1=2.81 K(Ca+HL)=1.52	1956SAa (72923)1540
Ca++	ix	oth/un	37°C	0.10M	U		K1=3.74	1953SNa (72924)1541

C10H16N2O2 L (7408)								
N-(2-Pyridylmethyl)iminodiethanol; C5H4N.CH2.N(CH2CH2.OH)2								

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

 Ca++ gl KNO3 25°C 0.10M C K1=1.0 1986DSa (73033)1542

 C10H16N2O3S HL Vitamin H CAS 58-85-5 (410)
 D-Biotin (Coenzyme R);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	nmr	NaClO4	27°C	3.00M	U		K1=-1.4	1982SSb (73046)	1543
Medium: D20 *****									
		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
Ca++	gl	KNO3	25°C	0.50M	U		K1=4.40 K(Ca+HL)=1.05	1990KLa (73093)	1544
DH(K1)=3 kJ mol ⁻¹ , DS=94.3 J K ⁻¹ mol ⁻¹									

Ca++	gl	KNO3	25°C	0.10M	U		K1=4.58 K(Ca+HL)=1.44	1989VZc (73094)	1545
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Ca++	gl	KNO3	25°C	0.10M	U		K1=4.23 K(Ca+HL)=2.45 K(Ca+CaL)=1.95	1971GBc (73095)	1546
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Ca++	gl	KNO3	20°C	0.10M	U		K1=4.72 K(Ca+HL)=1.65	1968MJa (73096)	1547

		H4L		EDTA			CAS 60-00-4 (120)		
1,2-Diaminoethane-N,N,N',N'-tetraethanoic acid, Sequestric acid;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	gl	NaClO4	37°C	0.10M	U		K1=10.75	1992GHa (73445)	1548
Method: coulometric titration									

Ca++	gl	NaCl	37°C	0.15M	C		K1=9.36	1984DMb (73446)	1549
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Ca++	gl	R4N.X	25°C	0.15M	C T H		K1=10.75	1983AMb (73447)	1550
Medium: 0.15-0.77 M Me4NCl. At 10 C, K1=11.03. DH(K1)=-25.1 kJ mol ⁻¹ , DS(K1)=121 J K ⁻¹ mol ⁻¹ .									

Ca++	EMF	KCl	20°C	0.10M	C		K1=11.0	1981SFa (73448)	1551
Method: Pt/H2 electrode.									

Ca++	ISE	NaCl	25°C	0.10M	U		K1=10.93	1979CMb (73449)	1552
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Ca++	gl	KNO3	20°C	0.10M	U		K1=10.69	1978NLb (73450)	1553
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Ca++ dis none 25°C 0.0 U K1=11.0 1977MFb (73451)1554
Measured by liquid chromatography on a chelating resin

Ca++ cal KNO3 25°C 0.5M U IH K1=9.95 1976VBc (73452)1555
DH1= 29.46 kJ/mol
For 15 C: K1=10.15, DH1=30.84; 35 C: K1=9.81, DH1=28.12
for 25 C and I=0.3 M K1=10.03; for 25 C and I=1.0 M K1=9.75

Ca++ cal KNO3 25°C 0.3M U TI 1976VBe (73453)1556
DH(K1)=-29.0 kJ mol⁻¹
For 1.0 M KNO3 DH1=-30.9 kJ/mol;
For 0.3 M KNO3 and 35 C DH1=-27.4 kJ/mol 15 C DH1=-30.4;

Ca++ gl KNO3 25°C 0.10M U K1=10.73 1975APc (73454)1557
K(Ca+HL)=3.42

Ca++ gl R4N.X 25°C 0.50M M K1=10.28 1975CSb (73455)1558
K(Ca+HL)=3.53
K(CaL+H)=3.47

Ca++ ISE KNO3 25°C 0.10M U K1=10.78 1973HRa (73456)1559

Ca++ gl NaClO4 20°C 0.10M U K1=10.85 1970AMa (73457)1560

Ca++ gl KNO3 25°C 1.0M U K1=9.68 1968KSa (73458)1561

Ca++ nmr oth/un 20°C 0.20M U 1968LWa (73459)1562
K(CaL+Ca)=1.1
K(Ca3L=Ca+Ca2L)=0.4
Medium: EDTA. Method: NMR

Ca++ oth KNO3 20°C 0.10M U K1=11 1965JMb (73460)1563
Method: electrophoresis

Ca++ gl KNO3 20°C 0.10M U 1964ANa (73461)1564
K(Ca+HL)=3.51

Ca++ EMF KCl 25°C 0.10M U K1=10.57 1964PCa (73462)1565
Method: H electrode

Ca++ cal KNO3 20°C 0.10M U H 1963ANf (73463)1566
DH(K1)=-27.4 kJ mol⁻¹, DS=113 J K⁻¹ mol⁻¹

Ca++ gl KCl 30°C 0.10M U K1=10.59 1963GHa (73464)1567

Ca++ gl KNO3 25°C 0.10M U T H K1=10.42 1960BMc (73465)1568
K1=10.94(0.5 C), 10.62(13.4 C), 10.11(42.4 C). DH(K1)=-33 kJ mol⁻¹, DS=92

Ca++ ix oth/un ? 0.30M U K1=10.45 1960MSb (73466)1569

B(Ca2L)=12.52

Ca++ cal none 25°C 0.0 U H K1=11.0 1957JAb (73467)1570
DH(K1)=-23.8 kJ mol-1, DS=130 J K-1 mol-1

Ca++ ix none ? 0.0 U K1=11.31 1957KFa (73468)1571

Ca++ ISE NaNO3 22°C 0.10M U T K1=10.85 1957SAb (73469)1572

Ca++ gl oth/un 20°C 0.17M U H 1956CSb (73470)1573
DH(K1)=-27.0 kJ mol-1; DG=-60.00 to -61.46; DS=115 J K-1 mol-1

Ca++ EMF oth/un 25°C 0.0 U H 1956MAa (73471)1574
Method: H electrode. DH(K1)=-13 kJ mol-1; DG=-62.8; DS=176 J K-1 mol-1

Ca++ EMF NaClO4 25°C 0.10M U K1=10.7 1956SRb (73472)1575

Ca++ cal oth/un 25°C 0.05M U H 1954CHa (73473)1576
Medium: Ca(NO3)2. DH(K1)=-24.2 kJ mol-1, DS=130 J K-1 mol-1

Ca++ EMF oth/un 20°C 0.0 U H K1=11.0 1954CMb (73474)1577
Method: H electrode. DH(K1)=-10.5 kJ mol-1, DS=176 J K-1 mol-1

Ca++ EMF KCl 20°C 0.10M U T K1=10.59 1954SGa (73475)1578
K(Ca+HL)=3.51

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

Ca++ gl KNO3 25°C 0.10M U K1=5.70 1978SGc (74358)1579
K(Ca+HL)=1.72
K(Ca+CaL)=2.05

C10H16N2O9 H4L CAS 616-90-0 (2615)

Bis-(2-aminoethylether)-N,N'di(1,3-propanedioic acid); ((HOO)2CH.NH.CH2.CH2)2O

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

Ca++ gl KNO3 25°C 0.10M U K1=5.13 1979KBd (74371)1580
K(Ca+HL)=2.79

C10H16N2O11P2 H4L CAS 491-97-4 (7674)

Thymidine-5'-diphosphoric acid;

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

Ca++ gl NaNO3 25°C 0.10M M 1999SSa (74384)1581

Ca++ sp oth/un 25°C 0.02M U K1=3.9 1971HRa (74593)1603
K(Ca+HL)=1.0
Medium: 0.015 M CaCl2, 0.02 M H4L. Raman spectra

Ca++ ix KCl 25°C 0.10M U K1eff=3.26 1971YBa (74594)1604
pH=7.4. At pH 8.5: K1eff=3.73

Ca++ gl KNO3 40°C 0.10M U T H K1=3.94 1966TMb (74595)1605
K(Ca+HL)=2.13
K1=4.10(0.4 C),3.99(12 C),3.97(25 C); K=2.34(0.4 C),2.21(12 C),2.13(25 C).
At 25 C:DH(K1)=-3.8(?) kJ mol-1,DS=50(?) J K-1 mol-1; DH(Ca+HL)=-1.3, DS=37

Ca++ gl R4N.X 30°C 0.10M U K1=4.51 19640Pa (74596)1606
Medium: Et4NBr

Ca++ sp oth/un 30°C 0.10M U K1=4.49 19640Pa (74597)1607
Medium: N-ethylmorpholine buffer

Ca++ oth R4N.X 23°C 0.06M U K1=3.88 1962AMa (74598)1608
Method: interferometer. Medium: 0.06 M Me4NCl,0.05(HOCH2)3.CNH2
With 0.06 Me4NCl,0.05 CH3COO-: K(Ca+HL)=1.45

Ca++ gl KNO3 25°C 0.10M U K1=3.97 1962TMb (74599)1609
K(Ca+HL)=2.13

Ca++ sp NaCl 25°C 0.10M U K1=3.90 1961NAa (74600)1610

Ca++ gl R4N.X 25°C 0.10M U K1=3.92 1961NAa (74601)1611
Medium: Et4NBr. By ion exchange: K1=3.97

Ca++ sp R4N.X 25°C 0.10M U K1=3.45 1959BUa (74602)1612
Medium: Bu3EtNBr

Ca++ ix NaCl 23°C 0.10M U K1=3.77 1958WAa (74603)1613

Ca++ ix oth/un 23°C 0.10M U H K1=3.14 1957NAc (74604)1614
DH(K1)=19.1 kJ mol-1, DS=120 J K-1 mol-1

Ca++ gl KCl 20°C 0.10M U K1=3.60 1956MSa (74605)1615
K(Ca+HL)=1.8

Ca++ gl R4N.X 25°C 0.20M U K1=3.29 1956SAa (74606)1616
K(Ca+HL)=1.61
Medium: 0.2 M n-Pr4NCl

Ca++ ix oth/un 37°C 0.10M U K1=4.06 1953SNa (74607)1617

C10H16N5O14P3 H5L GTP CAS 86-01-1 (404)
Guanosine-5'-triphosphoric acid;


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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  NaNO3  25°C 0.10M C                K(Ca+HL)=3.96
                                         K(CaHL+H)=5.15
                                         K(Ca+H2L)=2.6
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Ca++      gl  R4N.X  25°C 0.10M C                T
                                         K(Ca+HL)=4.14
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IUPAC evaluation

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Ca++      gl  NaClO4 25°C 0.10M C                K(Ca+HL)=3.73
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Ca++      gl  KNO3   25°C 0.10M U T                K(Ca+HL)=4.92
K(35 C)=5.01, K(45 C)=4.85
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Ca++      ix  NaCl   23°C 0.10M U                K(Ca+HL)=3.58
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*****
C10H16O8P2          H4L                      (6907)
1,2-Diphosphinoethane-P,P,P'P'-tetraethanoic acid;
(HOOC.CH2)2P.CH2.CH2.P(CH2.COOH)2
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  NaClO4 25°C 0.10M C                K1=3.20
                                         B(CaHL)=8.58
                                         B(CaH2L)=12.80
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-----
Ca++      gl  NaClO4 25°C 0.10M C                K1=3.20
                                         B(CaHL)=8.58
                                         B(CaH2L)=12.80
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*****
C10H17N04          H2L                      CAS 2848-06-8 (3916)
N-(Cyclohexyl)iminodiethanoic acid; C6H11.N(CH2.COOH)2
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  KNO3   20°C 0.10M U                K1=3.34
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*****
C10H17N05          H2L                      CAS 6243-06-7 (3326)
N-(2-Hydroxycyclohexyl)iminodiethanoic acid; HO.C6H10.N(CH2.COOH)2
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  KCl    20°C 0.10M U                K1=5.19
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C10H17N05 H2L (3917)
N-(Tetrahydropyran-2-ylmethyl)iminodiethanoic acid;

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

Ca++ gl KNO3 20°C 0.10M U K1=4.86 1963IFa (74996)1627

C10H17N08S HL (1735)
2-(5-Carboxy-1,2,3,4-tetrahydroxypentyl)4-carboxythiazolidine,
Galactocarboxythiazolidine;

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

Ca++ gl NaClO4 25°C 0.10M C K1=1.61 1992GNa (75011)1628

C10H17N2014P3 H3L TTP CAS 365-08-2 (402)
Thymidine-5'-triphosphoric acid;

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

Ca++ gl R4N.X 25°C 0.10M C T K(Ca+HL)=4.16 1991SMa (75043)1629

IUPAC evaluation

Ca++ gl NaNO3 25°C 0.10M C K(Ca+HL)=3.85 1987STb (75044)1630

Ca++ gl NaClO4 25°C 0.10M U K(Ca+HL)=3.78 1977SIc (75045)1631

C10H17N306S H3L Glutathione CAS 70-18-8 (333)
Glutamyl-cysteinyl-glycine;

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

Ca++ gl NaClO4 25°C 0.10M U TIH K1=6.245 2001SGd (75100)1632
Data for 0.05-0.2 M NaClO4 and 15-45 C. DH(K1)=-28.4 kJ mol⁻¹, DS(K1)=-31
J K-1 mol⁻¹. At I=0, K1=6.580. Also data for MeOH/H2O, EtOH/H2O, DMF/H2O.

Ca++ gl NaClO4 37°C 0.15M U M K1=3.84 1976TWa (75101)1633
B(CaHL)=12.89
B(CaH2L)=20.68
B(CaH-1L)=-6.46
*K1=-9.40

B(CaZnH-1L)=4.0

C10H17N6012P3 H4L CAS 4209-30-7 (4795)
Adenyl-5'-yl-imidodiphosphoric acid; adenosine-0.PO(OH).O.PO(OH).NH.PO(OH)2

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

 Ca++ gl R4N.X 20°C 0.10M M T H K1=4.58 1976PSe (75166)1634
 K(Ca+HL)=2.68
 Medium: 0.1 M Me4NClO4. At 0 C: K1=4.83, K(Ca+HL)=2.86. DH(K1)=-19 kJ mol-1,
 DS=7 J K-1 mol-1; DH(Ca+HL)=-14, DS=1

Ca++ ix KCl 25°C 0.10M U 1971YBa (75167)1635
 K1eff=4.07

pH=8.5

 C10H18N2O4 H2L CAS 124125-60-6 (914)
 1,5-Diazacyclooctane-N,N'-diethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Ca++	cal	NaClO4	25°C	0.10M	U	H	K1=5.0	1985EHa (75198)1636	
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DH(K1)=-5.8 kJ mol-1, DS=85.5 J K-1 mol-1

 C10H18N2O4S H2L (6638)
 1-Thia-4,7-diazacyclononane-N,N'-diethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Ca++	gl	KNO3	25°C	0.10M	C		K1=5.01	1993WLa (75212)1637	
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 C10H18N2O5 H2L (5608)
 1-Oxa-4,7-diazacyclononane-N,N'-diethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Ca++	gl	KNO3	25°C	0.10M	U		K1=5.36	1990CCa (75226)1638	
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Ca++	cal	NaClO4	25°C	0.10M	U	H	K1=5.0	1985EHa (75227)1639	
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DH(K1)=-11.3 kJ mol-1, DS=58.8 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
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Ca++	gl	NaClO4	30°C	0.10M	U		K1=7.88	1981MMc (75304)1640	
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Ca++	gl	NaClO4	20°C	0.10M	U		K(Ca+HL)=8.55	1970AMa (75305)1641	
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Ca++	cal	KNO3	25°C	0.10M	U	H		1965WHa (75306)1642	
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DH(K1)=-27.2 kJ mol-1, DS=62.7 J K-1 mol-1

Ca++	gl	KNO3	15°C	0.10M	U	T H	K1=8.56	1961MFb (75307)1643	
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K1=8.51(20 C), 8.43(25 C), 8.35(30 C), 8.30(35 C), 8.24(40 C)

DH(K1)=-22.6 kJ mol⁻¹(25C), DS=83.7 J K⁻¹ mol⁻¹

Ca++ gl KCl 20°C 0.10M U K1=8.14 1959KRa (75308)1644
K(Ca+HL)=1.38

Ca++ gl KCl 30°C 0.10M U K1=8.0 1955CMA (75309)1645

C10H18N4O6 H2L (4504)
Hexanoic acid bis(3-hydroxycarbamoyl-methyl)amide; HONHCOCH2NHCO(CH2)4CONHCH2CONHOH

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

Ca++ gl KCl 25°C 0.20M C K1=2.68 1999FEa (75565)1646
B(CaHL)=11.08

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

Ca++ gl KNO3 25°C 0.10M U K1=2.14 1974MSa (75615)1647

C10H18O8 HL CAS 172606-56-3 (7617)
Methyl-3-O-(2-carboxyethyl)-alpha-D-glucopyranoside;

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

Ca++ ISE KCl 25°C 0.10M C K1=1.89 1995BBf (75623)1648
Method: calcium ion selective electrode.

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

Ca++ gl KCl 20°C 0.10M U K1=3.68 1955SAa (75634)1649

C10H19N04 H2L CAS 56024-52-5 (6065)
N-Hexyliminodiethanoic acid; CH3.(CH2)5.N(CH2.COOH)2

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

Ca++ gl oth/un 25°C 0.10M C K1=4.60 B2=8.00 1975MRb (75644)1650

C10H19N05 H2L CAS 62117-06-0 (6064)
N-(6-Hydroxyhexyl)iminodiethanoic acid; HO.(CH2)6.N(CH2.COOH)2

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

Ca++ gl oth/un 25°C 0.10M C K1=4.0 B2=7.10 1975MRa (75646)1651

C10H19N3O4 H2L (8095)
1,4,7-Triazacyclononane-1,4-diethanoic acid;

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

Ca++ gl KCl 25°C 1.0M U K1=5.30 2000LKc (75653)1652

C10H20N2O4 H2L CAS 5578-84-7 (5914)
N,N-Dihydroxydecanediamide; HN(OH).CO.(CH2)8.CO.NH(OH)

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

Ca++ gl NaNO3 25°C 0.10M C K1=4.94 1989EHa (75794)1653

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

Ca++ gl KNO3 20°C 0.10M U K1=3.45 1970DKa (75830)1654

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

Ca++ sp oth/un 20°C 0.10M U K1=3.45 1972DKa (75841)1655

C10H20N2O6 H2L CAS 5616-21-7 (3330)
N',N'-Di-(2-hydroxyethyl)diaminoethane-N,N-diethanoic acid;

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

Ca++ gl oth/un 25°C 0.10M U K1=5.7 1953KPb (75850)1656

C10H20O5 L 15-Crown-5 CAS 33100-27-5 (576)
1,4,7,10,13-Pentaoxacyclopentadecane; cyclo(-(O.CH2.CH2)5-)

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

Ca++ ISE alc/w 25°C 100% C IH T K1=2.2 2003ADa (75948)1657
IUPAC Tentative. Medium: 0-0.1 M various. DH(K1)=-8 kJ mol-1

Ca++ con mixed 25°C 20% C K1=4.10 2003SIa (75949)1658
Medium: 20% w/w propylene carbonate/ethylene carbonate.

Ca++ nmr non-aq 27°C 100% C K1=5.41 2000SMg (75950)1659
Medium: acetonitrile. Method: competitive 7Li nmr technique.

Ca++ cal non-aq 25°C 100% U H T K1=4.01 1993BDb (75951)1660
Medium: acetone. DH=-35.2 kJ mol⁻¹; TDS=-12.4

Ca++ cal non-aq 25°C 100% C H K1=>5 1992BSc (75952)1661
Medium: propylene carbonate. DH(K1)=-33.9 kJ mol⁻¹.

Ca++ cal alc/w 20°C 100% U H K1=2.46 1988SVb (75953)1662
Medium:EtOH, CaCl₂. DH(K1)=-26.8 kJ mol⁻¹; for Ca(NO₃)₂: K1=2.06; DH=-14.7

Ca++ con alc/w 25°C 100% C K1=2.42 1987CBd (75954)1663
Medium: methanol.

Ca++ ISE alc/w 25°C 100% U K1=2.36 1983GGa (75955)1664
Medium: MeOH

Ca++ cal alc/w 25°C 100% U H T K1=2.18 1980LIa (75956)1665
Medium: MeOH. DH=-6.07 kJ mol⁻¹.

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

Ca++ sp non-aq 20°C 100% U K1=4.82 1992PSa (76293)1666
Medium: DMF, 0.01 M Me₄NI

Ca++ ISE alc/w 25°C 100% U K1=3.1 1988CFa (76294)1667
Medium: MeOH

Ca++ cal alc/w 25°C 100% U H K1=2.56 1986BUa (76295)1668
Medium: MeOH. DH(K1)=-4.3 kJ mol⁻¹; DS=34 J K⁻¹ mol⁻¹

C10H22N4O4 H2L CAS 66650-98-4 (1587)
3,6,9,12-Tetraazatetradecanedioic acid; (HOOC.CH₂.NH.CH₂.CH₂.NH.CH₂-)₂

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

Ca++ gl NaCl 25°C 0.15M C K1=3.17 1990JKa (76429)1669
B(CaH-1L)=-8.19

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

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

Ca++ cal non-aq 25°C 100% U H K1=2.49 1993BDb (76434)1670
Medium: acetone. DH=-26.8 kJ mol⁻¹; TDS=-12.7

Ca++ con non-aq 25°C 100% C H K1=2.43 1992BSc (76435)1671
Medium: propylene carbonate. By calorimetry, DH(K1)=-30.6 kJ mol⁻¹,

DS(K1)=-56.4 J K-1 mol-1.

Ca++ con non-aq 25°C 100% C K1=3.0 1992MSe (76436)1672
Medium: 100% MeOH. Anion: picrate. Also data for nitrophenolate anions.

C10H24O6P2 H4L CAS 5943-21-5 (3920)
Decane-1,10-diphosphonic acid; H2O3P.(CH2)10.PO3H2

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

Ca++ gl R4N.X 25°C 1.0M U K1=<1 1962IMb (76713)1673
K(Ca+HL) < 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

Ca++ gl oth/un 25°C 0.10M U K1=5.49 1959BYa (76753)1674

C10H26N4 L Spermine CAS 71-44-3 (291)
4,9-Diazadodecane-1,12-diamine; (H2N.CH2.CH2.CH2.NH.CH2.CH2.)2

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

Ca++ gl NaCl 25°C 0.0 C K1=1.07 1999SFC (76790)1675
K(Ca+HL)=0.23
K(Ca+H2L)=-0.15
K(Ca+H3L)=-0.8

Extrapolated from data for 0.03-0.96 M NaCl using the Pitzer equation.

C10H26N4O6P2 H4L CAS 200951-96-8 (7643)
1,4,7,10-Tetraazacyclododecane-1,7-bis(methanephosphonic acid);

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

Ca++ gl KCl 25°C 0.10M C K1=9.0 1998BRa (76800)1676
*K(CaL)=-8.5

C10H26N4S4 L CAS 55677-43-5 (1178)
1,1,2,2-Tetramercaptoethylamine-ethane; (CH(S.CH2.CH2.NH2)2)2

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

Ca++ gl NaClO4 25°C 0.10M U 1976CJa (76814)1677
K(Ca+H2L)=3.86

C11H8O3 H2L CAS 92-70-6 (1130)
2-Hydroxy-3-naphthoic acid (3-Hydroxy-2-naphthoic acid);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	gl	KNO3	30°C	0.15M	U	IH	K1=3.25	1976SSc (77106)	1678

C11H8O3S		HL					CAS 32267-05-3	(3353)	
2-Furoyl-2-thenoylmethane; C4H3O.CO.CH2.CO.C4H3S									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	gl	diox/w	30°C	75%	U		K1=6.72 B2=12.70	1953UFe (77152)	1679

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	gl	diox/w	35°C	50%	U		K1=1.96 B2=3.69	1971MAa (77166)	1680

C11H9NO2		HL					CAS 92609-55-3	(4827)	
5-Acetyl-8-hydroxyquinoline;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	gl	diox/w	25°C	60%	U		K1=3.71 B2=6.75	1973SCd (77325)	1681

C11H9NO2S		HL					CAS 29556-13-6	(1450)	
N-Phenyl-2-thenoylhydroxamic acid; C4H3SCON(C6H5)OH									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	gl	diox/w	25°C	70%	U		K1=6.92 B2=12.69	1992DAc (77344)	1682

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
Ca++	gl	diox/w	25°C	70%	U		K1=6.70 B2=12.24	1992DAc (77386)	1683

C11H9NO4		H2L					CAS 4321-82-7	(4829)	
3-Acetyl-4-hydroxycoumarin oxime;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	gl	diox/w	35°C	50%	U			1971MAa (77408)	1684

K(Ca+HL)=2.33
K(Ca+2HL)=4.35

Medium: 50% dioxan, 0.01 M NaClO4

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

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

Ca++ gl NaNO3 25°C 0.50M M K1=-0.09 1998KSa (77664)1685

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

Ca++ EMF KCl 20°C 0.10M U K1=5.06 1947SWa (77812)1686

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

Ca++ EMF KCl 20°C 0.10M C K1=1.46 1947SWa (77842)1687

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

Ca++ EMF KCl 20°C 0.10M C K1=1.3 1947SWa (77847)1688

Method: H electrode

C11H11N2O2Br HL (9228)
3-[4-Bromophenylazo]penta-2,4-dione;

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

Ca++ gl alc/w 25°C 0.1M U K1=6.38 2004GMc (77872)1689

Medium: 0.1 mol/L KCl in 3:7 EtOH/H2O mixture

C11H11N2O2Cl HL (9229)
3-[4-Chlorophenylazo]penta-2,4-dione;

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

Ca++ gl alc/w 25°C 0.1M U K1=6.23 2004GMc (77884)1690

Medium: 0.1 mol/L KCl in 3:7 EtOH/H2O mixture

 C11H11N202I HL (9227)
 3-[4-Iodophenylazo]penta-2,4-dione;

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

 Ca++ gl alc/w 25°C 0.1M U K1=6.62 2004GMc (77895)1691
 Medium: 0.1 mol/L KCl in 3:7 EtOH/H2O mixture

 C11H11N304 HL (9230)
 3-[4-Nitrophenylazo]penta-2,4-dione;

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

 Ca++ gl alc/w 25°C 0.1M U K1=5.77 2004GMc (77955)1692
 Medium: 0.1 mol/L KCl in 3:7 EtOH/H2O mixture

 C11H11O2F HL CAS 38440-21-0 (2906)
 1-(4-Fluorophenyl)-1,3-pentanedione; F.C6H4.CO.CH2.CO.CH3

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

 Ca++ gl diox/w 20°C 75% M T K1=8.49 B2=13.80 1980GMd (77964)1693

C11H12N202 HL Tryptophan CAS 73-22-3 (3)
 2-Amino-3-(3-indolyl)propanoic acid; H2N.CH(CH2.C8H6N)COOH

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

 Ca++ gl KNO3 25°C 0.10M U M K1=2.23 1988MBa (78159)1694

 Ca++ gl KNO3 35°C 0.10M C M K1=2.01 1983KSc (78160)1695
 K(CaHA+L)=2.89

A is adenine.

C11H12N202 HL (9226)
 3-[Diphenylazo]penta-2,4-dione;

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

 Ca++ gl alc/w 25°C 0.1M U K1=6.92 2004GMc (78246)1696
 Medium: 0.1 mol/L KCl in 3:7 EtOH/H2O mixture

 C11H12N205S HL CAS 56475-09-3 (8410)
 3-(4'-Sulfophenylhydrazo)-pentane-2,4-dione;

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

 Ca++ gl KCl 25°C 0.10M U T K1=6.30 2005ACa (78312)1697
 For 35 C K1=6.20; for 45 C K1=6.10

 C11H12N2O6 H2L (3942)
 N-(2-Nitrobenzyl)iminodiethanoic acid; O2N.C6H4.CH2.N(CH2.COOH)2

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

 Ca++ gl KNO3 25°C 0.10M U K1=2.93 1962ANa (78333)1698

 C11H12N2O6 H2L CAS 76268-69-4 (3943)
 N-(4-Nitrobenzyl)iminodiethanoic acid; O2N.C6H4.CH2.N(CH2.COOH)2

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

 Ca++ gl KNO3 25°C 0.10M U K1=2.53 1962ANa (78336)1699

 C11H12N2O7 H3L CAS 76268-70-5 (3360)
 N-(2-Hydroxy-5-nitrobenzyl)iminodiethanoic acid;

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

 Ca++ gl KCl 20°C 0.10M U K1=6.44 1952SAb (78340)1700

 C11H12O2 HL CAS 4023-79-4 (305)
 1-(4-Methylphenyl)butane-1,3-dione; CH3.C6H4.CO.CH2.CO.CH3

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

 Ca++ gl diox/w 20°C 75% M T K1=8.32 B2=13.63 1980GMd (78370)1701

 C11H12O9 H3L CAS 69065-58-3 (2714)
 1,2,4-Trihydroxy-3,4,5-trimethoxycarbonylcyclopentadiene;

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

 Ca++ gl NaClO4 25°C 0.10M C T 1978MSh (78425)1702

DH(Ca+HL)=-11.7 kJ mol-1
 Data obtained from three lgK values at 15, 25 and 35 C.

 C11H13N04 H2L (3364)
 N-2-Tolyliminodiethanoic acid; CH3.C6H4.N(CH2COOH)2

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

 Ca++ gl KCl 30°C 0.10M U K1=1.2 1957TBb (78545)1703

 C11H13N04 H2L CAS 3987-53-9 (966)
 N-Benzyliminodiethanoic acid; C6H5.CH2.N(CH2.COOH)2

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

Ca++ gl oth/un ? ? U K1=3.4 1975DTa (78575)1704

Ca++ gl KCl 30°C 0.10M U K1=3.26 1966SHc (78576)1705

Ca++ gl KCl 25°C 0.10M U K1=3.17 1966SIb (78577)1706

Ca++ gl KNO3 25°C 0.10M U K1=3.13 1962ANa (78578)1707

C11H13NO5 H2L CAS 4596-54-7 (3945)
N-(2'-Methoxyphenyl)iminodiethanoic acid; CH3O.C6H4.N(CH2.COOH)2

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

Ca++ gl KNO3 20°C 0.10M U K1=2.75 1963IFb (78600)1708

C11H13NO5 H3L HBIDA CAS 7372-13-6 (1603)
N-(2-Hydroxybenzyl)iminodiethanoic acid; HO.C6H4.CH2.N(CH2.COOH)2

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

Ca++ gl KCl 20°C 0.10M U K1=6.74 1952SAb (78612)1709

K(Ca+HL)=3.00

C11H13NO6 H4L CAS 1911-59-2 (4852)
2,3-Dihydroxybenzyliminodiethanoic acid; (HO)2.C6H3.CH2.N(CH2.COOH)2

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

Ca++ EMF oth/un ? ? U K(Ca+HL)=6.1 1975DTa (78656)1710

C11H13NO6 H4L CAS 59036-09-8 (2111)
2,5-Dihydroxybenzyliminodiethanoic acid; (HO)2.C6H3.CH2.N(CH2.COOH)2

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

Ca++ gl oth/un 25°C 0.0 U K(Ca+HL)=6.15 1970TTb (78671)1711

C11H13NO6 H4L CAS 31477-66-7 (4853)
2,6-Dihydroxybenzyliminodiethanoic acid; (HO)2.C6H3.CH2.N(CH2.COOH)2

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

Ca++ EMF oth/un ? ? U K(Ca+HL)=4.4 1975DTa (78687)1712

C11H13N3O3 H2L (3363)
Biacetyl oxime salicyloylhydrazone;

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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  alc/w  20°C  50%  U          B2=4.24      1961VLc (78725)1713
Medium: 50% EtOH, 0.1 M KCl
*****
C11H14N2O4          H2L                      (1880)
N-(6-Methyl-2-pyridylmethyl)iminodiethanoic acid; CH3C5H3NCH2N(CH2COOH)2
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  NaNO3  20°C  0.10M C          K1=3.55      1981ANb (78873)1714
*****
C11H14N4O4          L      Tubercidin          CAS 69-33-0 (6412)
7-Deazaadenosine, Tubercidin;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  NaNO3  25°C  0.50M C          K1=-0.07     2002KSb (78950)1715
-----
Ca++      gl  NaNO3  25°C  0.50M M          K1=0.09      1991JCa (78951)1716
*****
C11H15N4O7P          H2L                      CAS 16719-46-3 (6026)
Tubercidin-5'-monophosphoric acid, 7-Deazaadenosine-5-monophosphoric acid;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  NaNO3  25°C  0.10M C          K1=1.43      1988SMb (79065)1717
                      K(Ca+HL)=0.4
*****
C11H16O8S4          H4L                      CAS 51865-18-0 (1138)
(Propanediylidene-tetraethio)tetra-ethanoic acid; ((HOOC.CH.S)2.CH)2.CH2
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  NaClO4 25°C  0.10M U          K1=3.95      1975JBa (79145)1718
                      K(Ca+HL)=3.81
*****
C11H17NO3          H2L      Isoprenaline          CAS 586-06-1 (3950)
3,4-Dihydroxy-1-(1'-hydroxy-2'-(propylamino)ethyl)benzene;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  KCl    25°C  0.10M U T H          K1=4.04      B2= 5.76     1988CVa (79154)1719
Data for 0 and 37 C. DH(K1)=-15.6 kJ mol-1, DS(K1)=25.8 J K-1 mol-1;
DH(K2)=-14.0, DS(K2)=-13.8.
*****
C11H17NO6          H3L                      (3951)
N-(2'-Carboxycyclohexyl)iminodiethanoic acid; HOOC.C6H10.N(CH2.COOH)2
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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	gl	KCl	20°C	0.10M	U		K1=7.66	1966IMa (79163)	1720

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
Ca++	gl	KCl	25°C	0.10M	C		K1=4.30 K(Ca+HL)=4.72 *K(CaHL)=-11.42	1984RFd (79171)	1721

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
Ca++	gl	KNO3	25°C	0.10M	U		K1=10.40	1980KBb (79240)	1722
Ca++	gl	KNO3	20°C	0.10M	U		K1=11.58	1978NLb (79241)	1723
Ca++	vlt	KNO3	25°C	1.00M	U		K1eff=7.64	1977HDa (79242)	1724
Keff at pH 7									

Ca++	dis	none	25°C	0.0	U		K1=10.0	1977MFb (79243)	1725
Measured by liquid chromatography on a chelating resin									
Ca++	gl	KCl	25°C	0.10M	U		K1=11.51	1970AIA (79244)	1726
DL isomer. For D-isomer, K1=11.52									
Ca++	gl	KCl	30°C	0.10M	U		K1=11.47	1963GHa (79245)	1727

C11H18N2O8		H4L					CAS 4408-81-5	(923)	
1,3-Diaminopropane-N,N,N',N'-tetraethanoic acid; ((HOOC.CH2)2N.CH2.)2.CH2									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	gl	R4N.X	25°C	0.50M	M		K1=11.41 K(Ca+HL)=3.98 K(CaL+H)=3.58	1975CSb (79404)	1728
Ca++	cal	KNO3	20°C	0.10M	U	H		1964ANa (79405)	1729
DH(K1)=-7.3 kJ mol ⁻¹ , DS=114 J K ⁻¹ mol ⁻¹									
Ca++	gl	KNO3	20°C	0.10M	U		K1=7.28 K(Ca+HL)=3.16	1964LAa (79406)	1730
Ca++	EMF	KCl	20°C	0.10M	C		K1=7.12	1948SAa (79407)	1731

K(Ca+HL)=3.07

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

Ca++ gl KCl 25°C 0.1M C K1=6.79 2000VGB (79517)1732
Also for I=0.5 M K1=6.05; for I=1.0 M K1=5.92

Ca++ gl KNO3 25°C 0.10M U K1=6.69 1966TKa (79518)1733
K(CaL+H)=6.54

Ca++ oth KNO3 20°C 0.10M U K1=5.5 1965JMb (79519)1734
Method: electrophoresis

Ca++ gl KCl 20°C 0.10M U K1=6.90 1964DSc (79520)1735
By polarography: K1=6.98

Ca++ gl KCl 30°C 0.10M U K1=6.52 1963GHa (79521)1736

Ca++ gl KCl 20°C 0.10M U K1=6.18 1959KRa (79522)1737
K(Ca+HL)=3.20

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

Ca++ gl KNO3 25°C 0.10M U K1=2.94 1974KGa (79588)1738
K(Ca+HL)=2.11

C11H18N5O12P3 H4L CAS 5085-65-4 (4875)

Adenylylmethylenediphosphoric acid;

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

Ca++ ix KCl 25°C 0.10M U K1eff=3.68 1971YBa (79639)1739

pH=7.4. At pH 9.2, K1eff=4.11

C11H20N2O3 HL Pro-Leu CAS 52899-07-7 (258)

Prolyl-leucine; C4H8N.CO.NH.CH(CH2.CH(CH3)2).COOH

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

Ca++ gl KCl 20°C 0.20M U K1=2.22 1982RRc (79704)1740

C11H20N2O5 H2L (5609)

1-Oxa-4,8-diazacyclodecane-N,N'-diethanoic acid;

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

Ca++ cal NaCl04 25°C 0.10M U H K1=3.4 1985EHa (79718)1741
DH(K1)=-3.3 kJ mol⁻¹, DS=53.6 J K⁻¹ mol⁻¹

C11H20N4O6 H2L ICRF 198 CAS 108430-47-3 (8369)
N,N'-(1-Methyl-1,2-ethanediy)bis[N-(2-amino-2-oxoethyl)glycine];

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

Ca++ gl NaCl 37°C 0.15M C K1=6.887 B2= 8.19 1982HMb (79726)1742
B(CaHL)=9.693

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

Ca++ dis none 25°C 0.0 C M 1989TKc (79847)1743
Method: extraction of metal picrate/L from H2O into benzene.
K(Ca+2HA(org))+L(org)=CaA2L(org)+2H)=-1.26. HA is picric acid.

C11H26N3O13P3 H8L (6909)
Diethylenetriamine-N,N,N''-tri(methylenephosphonic)-N',N''-diethanoic acid;

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

Ca++ gl oth/un 25°C 0.10M U 1984ZGa (79963)1744
K(Ca+H2L)=3.60
K(Ca+H3L)=3.13
K(2Ca+H3L)=7.30
K(Ca+H4L)=2.27
K(Ca+H5L)= 1.59; K(2Ca+H2L) = 8.95; K(Ca+H6L)=1.03

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

Ca++ sp non-aq 20°C 100% U K1=5.5 1978JId (80067)1745
Medium: CH2Cl2

Ca++ dis non-aq 25°C 100% U K1=2.0 B2=3.0 1969PKb (80068)1746
Medium: nitrobenzene. K1=1.3(tracer amounts Ca++)

C12H6O12 H6L Mellitic acid (7400)
Benzenehexacarboxylic acid; (C(COOH))6

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	gl	NaCl	25°C	0.0	C			2003CDb (80108)	1747

Kso(Ca3L)=-21.7
Kso(Ca2H2L)=-26.0

Extrapolated from values for 0.1-1.0 M Et4NI or NaCl.

Ca++	ISE	R4N.X	25°C	0	C I		K1=7.50 B(CaHL)=13.69 B(CaH3L)=22.97 B(CaH4L)=25.8 B(Ca2H2L)=21.96	1996RSb (80109)	1748
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B(Ca3L)=16.25. I=0 to 3 M Et4NI etc.

C12H8N2 L Phenanthroline CAS 66-71-7 (144)
1,10-Phenanthroline;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	cal	KCl	25°C	0.25M	U H		K1=1.11	1997MKb (80371)	1749

DH(K1)=-14.0 kJ mol-1; DS=-26 J K-1 mol-1

Ca++	sp	alc/w	25°C	95%	U		K1=2.69	1993GSa (80372)	1750
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Medium: 95% w/w EtOH/H2O, 0.05 M Et4NClO4, by competitive spectrophotometry

Ca++	sp	non-aq	25°C	100%	U I		K1=4.11 K3= 1.94	1992GSa (80373)	1751
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Medium: MeCN. In acetone:K1=3.93, K2=1.57; K3=1.0; in MeOH:K1=2.11, K2=1.21)
By fluorimetry

Ca++	gl	KCl	25°C	0.25M	U T H		K1=1.09	1985CRa (80374)	1752
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K1=1.21(10 C);K1=0.97(40 C).

DH=-13.8 kJ mol-1, DS=-25 J mol-1 K-1

Ca++	gl	KNO3	35°C	0.10M	C		K1=2.20	1979MTb (80375)	1753
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Ca++	gl	NaClO4	25°C	0.10M	C M		K1=1.11 B(CaL(ATP))=5.63	1978MSd (80376)	1754
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Ca++	gl	NaNO3	20°C	0.10M	U		K1=0.7	1963ANg (80377)	1755
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C12H10N2O3 H3L CAS 69323-27-9 (3971)
2,2',4'-Trihydroxyazobenzene; HO.C6H4.N:N.C6H3(OH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	sp	KCl	rt	0.10M	U			1960DEa (80718)	1756

K1eff=1.23 (pH 10)

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

Ca++ gl diox/w 25°C 70% U K1=7.62 B2=14.08 1992DAc (80832)1757

C12H11N09 H5L (3975)
N-(2',5'-Dicarboxy-4'-hydroxyphenyl)iminodiethanoic acid;

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

Ca++ gl KNO3 25°C 0.10M U K(Ca+HL)=5.45 1967UKa (80848)1758

C12H12N06Cl H3L (4004)
(alpha-Carboxy-4'-chlorobenzyl)iminodiethanoic acid;

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

Ca++ gl KCl 20°C 0.10M U K1=6.05 1966IMb (80981)1759

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

Ca++ sp KCl 25°C 0.10M U K1=2.2 1978TSb (81062)1760

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

Ca++ gl NaNO3 25°C 0.50M M K1=0.00 1998KSd (81098)1761

C12H13N05 H2L CAS 90274-75-2 (3979)
N-(2'-Acetylphenyl)iminodiethanoic acid; CH3.CO.C6H4.N(CH2.COOH)2

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

Ca++ gl KNO3 25°C 0.10M U K1=4.11 1965AUa (81230)1762

C12H13N05 H2L CAS 2847-18-9 (3980)
N-(Benzoylmethyl)iminodiethanoic acid; C6H5.CO.CH2.N(CH2.COOH)2

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

Ca++ gl KCl 30°C 0.10M U K1=4.70 1966SHc (81237)1763

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
Ca++	gl	KCl	20°C	0.10M	U			K1=6.17	1966IMb (81241)	1764

C12H13N2O5Br		H2L		(4005)						
(2'-(4''-Bromoanilino)-2'-oxoethyl)iminodiethanoic acid;										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	KCl	30°C	0.10M	U			K1=3.30	1966SHc (81259)	1765

C12H14O14		H6L		CAS 111451-17-3 (5895)						
3,6-Dioxaoctane-1,2,4,5,7,8-hexacarboxylic acid; (CH2(COOH).CH(COOH).O.CH(COOH)-)2										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	KCl	25°C	0.10M	C			K1=6.82	1989MMd (81412)	1766
								K(CaL+H)=5.39		
								K(CaHL+H)=4.37		
								K(CaH2L+H)=2.83		
								K(CaH3L+H)=2.72		

K(CaL+Ca)=3.19

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
Ca++	gl	KCl	20°C	0.10M	U			K1=3.26 B2=5.56	1971KTl (81462)	1767
								K(Ca+HL)=1.55		

C12H15N05		H3L		(4930)						
1-Hydroxy-4-methylphenyl-2-methyleneiminodiethanoic acid;										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	oth/un	25°C	0.0	U			K1=6.13	1970TTb (81492)	1768

C12H15N05		H2L		(3982)						
N-(2'-Phenoxyethyl)iminodiethanoic acid; C6H5O.CH2.CH2.N(CH2.COOH)2										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	KCl	30°C	0.10M	U			K1=3.31	1966SHc (81502)	1769

C12H15N05		H2L		CAS 38782-28-4 (6075)						
N-(2-Hydroxy-2-phenylethyl)iminodiethanoic acid; HO.CH(C6H5)CH2.N(CH2.COOH)2										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	oth/un	25°C	0.10M	C			K1=4.25 B2=7.25	1975MRa	(81505)1770

 C12H15NO5 H3L CAS 56042-30-9 (4929)
 N-(4-Hydroxyphenethylimino)diethanoic acid; HO.C6H4.CH2.CH2.N(CH2.COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	KCl	20°C	0.10M	U				1971KT1	(81507)1771

K(Ca+HL)=3.28
 K(Ca+2HL)=3.68
 K(Ca+H2L)=1.57

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	KCl	25°C	0.10M	U			K1=3.93	1979TSa	(81599)1772

K(Ca+HL)=3.36
 K(Ca+CaL)=3.1

 C12H16O4 L CAS 25887-95-6 (686)
 2,3-Benzo-1,4,7,10-tetraoxacyclododeca-2-ene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	oth	non-aq	25°C	100%	U			K1=2.57 B2=4.46	1989SSc	(81667)1773

Medium: CH3CN. Ca as Ca(NCS)2; for Ca(ClO4)2: K1=2.91; B2=5.8. Method: IR

Ca++	cal	non-aq	25°C	100%	U	H		K1=3.23	1989SSd	(81668)1774
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Medium: CH3CN

Ca++	cal	non-aq	25°C	100%	U	H		K1=3.23 B2=4.78	1988SSc	(81669)1775
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Medium: MeCN

Ca++	cal	alc/w	25°C	100%	U	H		K1=0.4 B2=2.0	1988SVa	(81670)1776
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 C12H17N4O4PS H2L CAS 495-23-8 (895)
 Thiamine orthophosphoric acid, Aneurine monophosphoric acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	NaCl	23°C	0.15M	U			K1=1.50	1989DBb	(81763)1777

Ca++	gl	KN03	45°C	0.10M	U	T		K1=2.61	1981TTa	(81764)1778
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K(CaL+H)=2.03

5 C: K1 = 2.25

C12H18N4O7P2S H3L Cocarboxylase T CAS 136-09-4 (894)
Thiamine pyrophosphoric acid, Aneurine pyrophosphoric acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	NaCl	23°C	0.15M	U			K1=3.60	1989DBb (81931)	1786
Ca++	gl	KNO3	45°C	0.10M	U T			K1=3.32 K(CaL+H)=2.21	1981TTa (81932)	1787
5 C: K1 = 2.53										
Ca++	gl	KNO3	35°C	0.10M	U			K1=3.98 K(Ca+HL)=2.46	1978KBa (81933)	1788

C12H18O8S4 H4L CAS 51865-19-1 (1140)
(Butanediyldenetetraethio)tetraethanoic acid; ((HOOC.CH2.S)2.CH.CH2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	EMF	NaCl04	25°C	0.10M	U			K1=3.59 K(Ca+HL)=3.96	1975JBa (81963)	1789

C12H19N06 H3L (3991)
N-(2'-Carboxycycloheptyl)iminodiethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	KCl	20°C	0.10M	U			K1=8.24	1966IMa (81979)	1790

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
Ca++	gl	KNO3	20°C	0.10M	U			K1=11.75	1969NDa (82016)	1791

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
Ca++	gl	KNO3	20°C	0.10M	U			K1=2.70 K(Ca+HL)=1.0	1973DSc (82049)	1792

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	KNO3	25°C	0.10M	U			K1=2.59 K(Ca+HL)=1.57 K(Ca+CaL)=2.86	1972GBe (82050)	1793

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
Ca++	gl	KNO3	20°C	0.10M	U			K1=10.01	1966MKb	(82120)1794
Ca++	gl	KCl	30°C	0.10M	U			K1=10.74	1963GHa	(82121)1795

 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
Ca++	gl	NaClO4	25°C	0.50M	M	H		K1=5.18 K(CaL+H)=8.67 K(CaHL+H)=7.45	1985CBa	(82199)1796

DH(K1)=1.7 kJ mol⁻¹, DS=105 J K⁻¹ mol⁻¹, DH(CaL+H)=-28.2, DS=71 (by calorim)

Ca++	gl	KNO3	20°C	0.10M	U	H		K(Ca+CaL)=1.42	1964ANa	(82200)1797
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By calorimetry: DH(K1)=-3.8(?) kJ mol⁻¹, DS=124 J K⁻¹ mol⁻¹

Ca++	gl	KNO3	20°C	0.10M	U			K1=5.66 K(Ca+HL)=3.65	1964LAa	(82201)1798
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Ca++	EMF	KCl	20°C	0.10M	C			K1=5.05 K(Ca+HL)=3.45 K(Ca+CaL)=2.0	1948SAa	(82202)1799
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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
Ca++	gl	R4N.X	25°C	0.50M	M			K1=13.08 K(Ca+HL)=4.49 K(CaL+H)=3.71	1975CSb	(82268)1800

Ca++	gl	KCl	25°C	0.10M	U			K1=12.37(DL) K1=12.33(D)	1970AIA	(82269)1801
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Ca++	gl	KCl	20°C	0.10M	U			K1=11.49	1966IPa	(82270)1802
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Ca++	gl	KCl	20°C	0.10M	U			K1=12.34	1963MDa	(82271)1803
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 C12H20N2O8 H4L CAS 63818-08-6 (2584)
 meso-2,3-Diaminobutane-N,N'-di(1,4-butanedioic acid);



Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	KNO3	25°C	0.10M	U			K1=5.13 K(Ca+HL)=1.50 K(Ca+CaL)=2.34	1978SGc (82349)	1804

 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
Ca++	gl	KCl	20°C	0.10M	U			K1=9.60	1966IPa (82369)	1805
Ca++	oth	KNO3	20°C	0.10M	U			K1=11	1965JMb (82370)	1806

Method: electrophoresis

 Ca++ gl KCl 20°C 0.10M U K1=9.67 1963MDa (82371)1807
 K(Ca+HL)=2.76

 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
Ca++	gl	KNO3	20°C	0.10M	U	H		K1=6.21 K(Ca+HL)=3.5	1964ANa (82440)	1808

By calorimetry: DH(K1)=-10.5 kJ mol⁻¹, DS=96.1 J K⁻¹ mol⁻¹

 Ca++ gl KCl 20°C 0.10M U K1=6.21 1964PCa (82441)1809
 K(Ca+HL)=3.49

 C12H20N2O8S2 H4L (3395)
 2,2'-Dithiobisethyleneiminodiethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	KNO3	25°C	0.10M	U			K1=4.93 K(CaL+H)=8.70 K(Ca+HL)=4.07 B(Ca2L)=8.00	1988PGb (82484)	1810

 Ca++ gl KCl 20°C 0.10M U K1=4.32 1964PCa (82485)1811
 K(Ca+HL)=3.41

 C12H20N2O8Se H4L (4007)
 ((2,2'-Selenodiethylene)dinitrilo)tetraethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	oth/un	25°C	0.10M	U			K1=5.12 K(Ca+HL)=3.42	1966KLc (82490)	1812

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
Ca++	cal	KNO3	25°C	0.10M	U	H			1965WHa (82509)	1813
DH(K1)=-26.8 kJ mol-1, DS=100 J K-1 mol-1										

Ca++	gl	KNO3	20°C	0.10M	U	H		K1=10.0 K(Ca+HL)=4.9	1964ANa (82510)	1814
By calorimetry: DH(K1)=-28.6 kJ mol-1, DS=93.6 J K-1 mol-1										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	KCl	20°C	0.10M	U			K1=10.05 K(Ca+HL)=4.87	1964PCa (82511)	1815

C12H20N2O10 H4L CAS 10258-50-1 (3993)										
(2,3-Dihydroxytetramethylenedinitrilo)tetraethanoic acid;										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	KNO3	20°C	0.10M	U			K1=5.73 K(Ca+HL)=4.15 K(CaL+Ca)=3.69	1967DSb (82580)	1816

C12H20N4O6 H2L (7078)										
1,4,7,10-Tetraazacyclododeca-2,9-dione-4,7-diethanoic acid;										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	KCl	25°C	0.10M	C			K1=3.51	1995IOa (82620)	1817
Data also for the -tridecane and -pentadecane analogues and others										

C12H20O8N2 H4L (6908)										
2-Methyl-1,2-diaminopropane-N,N,N'N'-tetraethanoic acid;										
(HOOC.CH2)2N.CH2.C(CH3)2.N(CH2.COOH)2										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	KNO3	20°C	0.10M	C			K1=10.37	1978NLa (82665)	1818

C12H21NO6 H3L (7209)										
1-Carboxy-1-aminoheptane-N,N-diethanoic acid; HOOC.CH(C6H13)N(CH2.COOH)2										

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

Ca++ gl KNO3 20°C 0.10M U K1=6.47 1985LBc (82689)1819

C12H21N3O6 H3L NOTA (5589)
1,4,7-Triazacyclononane-N,N',N''-triethanoic acid;

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

Ca++ gl NaNO3 25°C 0.10M C T H K1=8.92 1987BGc (82723)1820
K(CaL+H)=5.06
DH(K1)=-24.7 kJ mol⁻¹. DH(CaL+H)=-3.3; DS=83.7 J K⁻¹ mol⁻¹

Ca++ EMF NaNO3 25°C 0.10M C K1=8.81 1985MBb (82724)1821

C12H22N2O6 H2L (6394)
1,7-Dioxa-4,10-diazacyclododecan-4,10-diethanoic acid;

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

Ca++ gl R4N.X 25°C 0.10M C K1=8.50 1992ADa (82787)1822
Medium: 0.1 M Me4NNO3

C12H22N2O6 H2L (6641)
7,10-Diaza-1,4-Dioxacyclododecane-7,10-diethanoic acid;

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

Ca++ gl R4N.X 25°C 0.10M C K1=8.12 1992ADa (82801)1823
Medium: 0.1 M Me4NNO3

C12H22N2O6 H3L CAS 73264-08-1 (3390)
N'-n-Butyl-ethylenediamine-N,N,N'-triethanoic acid;

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

Ca++ gl oth/un 24°C ? U K1=1.6 1956BCa (82813)1824

C12H22N4O6 H2L ICRF 243 (5772)
DL-NN'-Dicarboxamidomethyl-NN'-dicarboxymethyl-2,3-diaminobutane;

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

Ca++ gl NaCl 37°C 0.15M U K1=7.256 1985HCa (82831)1825

C12H22N4O6 H2L ICRF 226 CAS 83266-80-2 (8370)
N,N'-(1-Ethyl-1,2-ethanediy)bis[N-(2-amino-2-oxoethyl)glycine];

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

Ca++ gl NaCl 37°C 0.15M C K1=6.683 1982HMb (82840)1826
B(CaH-1L)=-4.483

Ca++ gl R4N.X 25°C 0.10M C K1=8.12 1992ADa (82968)1833
B(CaHL)=13.58

Medium: 0.1 M Me4NNO3

C12H23N3O6 H3L (7085)

2,5,8-Triazanonane-2,5,8-triethanoic acid;
CH3N(CH2COOH)CH2CH2N(CH2COOH)CH2CH2N(CH2COOH)CH3

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

Ca++ gl KCl 25°C 0.10M C K1=7.25 1995PRa (83002)1834

C12H24N2O3 L Cryptand 1,1,1 CAS 37095-49-1 (6636)

4,10,15-Trioxa-1,7-diazabicyclo[5.5.5]heptadecane;

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

Ca++ sp non-aq 20°C 100% U K1=1.3 1992PSa (83017)1835

Medium: DMF, 0.01 M Me4NI

C12H24N2O4 H2L (9225)

5,8-Diaza-4,9-dicarboxydodecane;

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

Ca++ gl KNO3 25°C 0.5M U K1=3.94 2004FCa (83043)1836

K(Ca+HL)=3.53

For 1.0 mol/L KNO3 K1=3.54; K(Ca+HL)=3.19

For 1.5 mol/L KNO3 K1=3.22; K(Ca+HL)=3.06

C12H24N2O12P4 H8L (1351)

1,3-Diaminomethylbenzene-N,N,N'N'-tetra(methylenephosphonic) acid;
C6H4(CH2.N(CH2.PO3H2)2)2

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

Ca++ gl KCl 25°C 0.10M M K1=4.26 1982PBa (83057)1837

K(Ca+HL)=3.87

C12H24N3O6P H3L CAS 176446-04-1 (8684)

1,4,7-Triazacyclononane-N-(methylenemethylphosphinic acid)-N',N''-bis(ethanoic acid);

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

Ca++ gl KCl 25°C 0.10M C T H K1=7.5 1996HSb (83061)1838

At 37 C, K1=7.7.

C12H24N4O4 H2L (7343)

1,4,7,10-Tetraazacyclododecane-1,7-bis(ethanoic acid);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	R4N.X	25°C	0.10M	C			K1=7.16	1998CCb (83076)	1839
Ca++	gl	KCl	25°C	0.10M	C			K1=7.8	1997HTa (83077)	1840

C12H24O4S2		L						CAS 296-39-9	(4938)	
1,4,10,13-Tetraoxa-7,16-dithiacyclooctadecane;										
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	cal	non-aq	25°C	100%	C	H		K1=2.70	1992BSc (83130)	1841
Medium: propylene carbonate. DH(K1)=-7.7 kJ mol ⁻¹ , DS(K1)=26 J K ⁻¹ mol ⁻¹ .										

C12H24O6		L						CAS 17455-13-9	(577)	
1,4,7,10,13,16-Hexaoxacyclooctadecane;										
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	EMF	alc/w	25°C	100%	C			K1=4.16	2004ZTa (83211)	1842
Medium: 100% methanol, 0.05 M Bu4NC104. Method: Ag electrode, competition with Ag ⁺ ion.										
Ca++	ISE	alc/w	25°C	100%	C	IH	T	K1=4.0	2003ADa (83212)	1843
IUPAC Tentative. Medium: 0-0.1 M various. DH(K1)=-11.3 kJ mol ⁻¹ In H2O: K1=0.5. In PC: K1=3.75, DH(K1)=-38.5										
Ca++	con	mixed	25°C	20%	C			K1=4.07	2003SIa (83213)	1844
Medium: 20% w/w propylene carbonate/ethylene carbonate.										
Ca++	nmr	non-aq	27°C	100%	U	I		K1=4.14	2000SMd (83214)	1845
Competitive method by ⁷ Li nmr. Medium: acetonitrile (AN). Also data for 50% w/w AN/nitrobenzene (K1=4.21) and 50% w/w AN/nitromethane (K1=4.34).										
Ca++	con	alc/w	25°C	90%	C	TIH	T	K1=2.97	1999SSc (83215)	1846
Medium: 90% w/w MeOH/H2O. Data for 5-40C. DH(K1)=-8.83 kJ mol ⁻¹ , DS(K1)=27.21 J K ⁻¹ mol ⁻¹ .										
Ca++	cal	non-aq	25°C	100%	C	H		K1=2.58	1999WBa (83216)	1847
Medium: N,N-dimethylformamide. DH(K1)=-1.9 kJ mol ⁻¹ .										
Ca++	cal	mixed	25°C	50%	C	IH		K1=2.77	1998BJb (83217)	1848
Medium: 50% (v/v) HCOOH/H2O. DH(K1)=-7.7 kJ mol ⁻¹ For 25% (v/v) HCOOH/H2O, K1=2.50, DH(K1)=-12.5 kJ mol ⁻¹										
Ca++	cal	non-aq	25°C	100%	U	H	T	K1=0.63	1995OKa (83218)	1849
Medium:DMF, 0.1 M NEt4ClO4. DH=-4.6 kJ mol ⁻¹ , DS=-3.3 J K ⁻¹ mol ⁻¹ .										
Ca++	cal	R4N.X	25°C	0.10M	U	H	T	K1=0.45	1995OKa (83219)	1850

Medium: 0.1 M NEt₄Cl. DH=-15.3 kJ mol⁻¹, DS=-43.3 J K⁻¹ mol⁻¹.

Ca++ cal non-aq 25°C 100% U H T K1=5.07 1993BDb (83220)1851
Medium: acetone. DH=-38.9 kJ mol⁻¹; TDS=-10.1 Calorimetric titration

Ca++ dis non-aq 25°C 100% U B(CaPL)=7.16 1993INa (83221)1852

K is the equilibrium constant for extraction of the metal picrate (P) into CH₂Cl₂. For extraction from D₂O, B=7.38.

Ca++ cal non-aq 25°C 100% C H K1=3.68 1992BSc (83222)1853
Medium: propylene carbonate. DH(K1)=-38.5 kJ mol⁻¹, DS(K1)=-59.1 J K⁻¹ mol⁻¹.

Ca++ con oth/un 25°C 0.05M M K1=3.74 1992BUB (83223)1854
K1=3.87 (by calorimetry)

Ca++ con non-aq 25°C 100% C K1=3.81 1992STa (83224)1855
Medium: propylene carbonate.

Ca++ nmr non-aq 30°C 100% U I K1=>5 1991ASc (83225)1856
Medium: nitromethane. In MeCN, K1=3.36.

Ca++ ix none 25°C 0.0 U K1=2.1 1991BMb (83226)1857

Ca++ vlt non-aq 25°C 100% C K1=3.36 1991SSb (83227)1858
Method: competitive complexation with Tl⁺; use of Tl(Hg)/Tl couple.
Medium: acetonitrile, 0.05 M Et₄NClO₄.

Ca++ sp alc/w 25°C 100% U I K1=4.25 1989KSc (83228)1859
In MeOH. In DMF K1=3.03; in DMSO K1=2.49

Ca++ vlt alc/w 25°C 100% C K1=4.40 1987CBd (83229)1860
Medium: methanol, 0.10 M Et₄NI or Bu₄NClO₄. Method: polarography.
Additional method conductivity in methanol: K1=3.96, B(CaL₂)=6.0.

Ca++ cal alc/w 25°C 100% U H 1986BUa (83230)1861
Medium: MeOH. DH(K1)=-11.2 kJ mol⁻¹; DS=36 J K⁻¹ mol⁻¹

Ca++ nmr non-aq 25°C 100% U K1=<1.3 1985BPa (83231)1862
Medium: DMF

Ca++ ISE alc/w 25°C 100% U K1=3.90 1983GGa (83232)1863
Medium: MeOH

Ca++ cal alc/w 25°C 100% U H T K1=3.86 1980LIa (83233)1864
Medium: MeOH. DH=-11.5 kJ mol⁻¹.

Ca++ EMF oth/un 25°C var C T K1=0.48 1979HRa (83234)1865
Method: ISE based on cation exchange membrane. Medium: aqueous,

containing 0.06-0.25 m ligand.

 Ca++ nmr oth/un 25°C 0 U IH K1=1.1 1978SKh (83235)1866
 Method: NMR Ca-43; Ca as Ca(NO3)2; with CaCl2: K1=0.67. Also at I=0 corr

Ca++ cal alc/w 25°C 70% U H K1=2.51 1976ITa (83236)1867
 Medium: 70% w/w MeOH/H2O. DH(K1)=-17.9 kJ mol-1.

Ca++ cal oth/un 25°C 0.10M U T K1=<0.5 1976ITb (83237)1868

 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
Ca++	sp	alc/w	25°C	100%	C			K1=4.05	2002NFa (83784)	1869
Medium: 100% MeOH. Method: electrospray ionization mass spectrometry.										
Ca++	sp	non-aq	25°C	100%	U T H			K1=2.40	1994GSb (83785)	1870
At 35 C: K1=2.31; 45 C: K1=2.24; 55 C: K1=2.10. DH(K1)=-19 kJ mol-1, DS=-18 Medium: DMSO										
Ca++	cal	non-aq	25°C	100%	U H			K1=4.61	1993BDb (83786)	1871
Medium: acetone. DH=-29.8 kJ mol-1; TDS=-3.6										
Ca++	sp	non-aq	20°C	100%	U			K1=3.63	1992PSa (83787)	1872
Medium: DMF, 0.01 M Me4NI										
Ca++	sp	alc/w	25°C	100%	U I			K1=3.89	1989KSc (83788)	1873
In MeOH. In DMF K1=2.70; in DMSO K1=2.35										
Ca++	cal	alc/w	25°C	100%	U H			K1=3.87	1986BUa (83789)	1874
Medium: MeOH. DH(K1)=5.6 kJ mol-1; DS=93 J K-1 mol-1										
Ca++	gl	NaNO3	25°C	0.10M	U			K1=1.74	1986HBc (83790)	1875
Ca++	ISE	alc/w	25°C	100%	U H			K1=3.5	1983CFb (83791)	1876
Medium: MeOH, 0.05 M Et4NClO4										
Ca++	gl	alc/w	25°C	95%	C			K1=4.04	1981ANa (83792)	1877
Medium: 95% MeOH, 0.1 M Me4NCl *****										
C12H26O4S HL SDS CAS 151-21-3 (2522) Dodecyl sulfate; CH3(CH2)11.OSO3H										
Ca++	sol	oth/un	21°C	?	U			B2=5.0 B(Ca2L4)=7.0 B(Ca3L6)=7.7	1979KBb (83977)	1878

C12H26O6 L Pentaglyme CAS 1191-87-3 (2498)
2,5,8,11,14,17-Hexaoxaoctadecane; (CH3.O.CH2.CH2.O.CH2.CH2.O.CH2.)2

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

Ca++ cal non-aq 25°C 100% U H K1=2.51 1993BDb (83987)1879
Medium: acetone. DH=-39.8 kJ mol-1; TDS=-25.5

Ca++ con non-aq 25°C 100% C H K1=4.07 1992BSc (83988)1880
Medium: propylene carbonate. By calorimetry, DH(K1)=-38.0 kJ mol-1,
DS(K1)=-50.0 J K-1 mol-1.

Ca++ con oth/un 25°C 0.05M M K1=2.29 1992BUb (83989)1881

C12H27N3O6P2 H3L CAS 176446-07-4 (8683)
1,4,7-Triazacyclononane-N,N'-bis(methylenemethylphosphinic acid)-N"-ethanoic acid;

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

Ca++ gl KCl 25°C 0.10M C T K1=6.3 1996HSb (84094)1882
At 37 C, K1=6.6.

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

Ca++ gl R4N.X 25°C 0.10M U K1=7.81 1996BJa (84148)1883
K(Ca+HL)=5.27
K(Ca+H2L)=2.18

Medium: 0.1 M Me4NCl

C12H30N3O6P3 H3L (6467)
1,4,7-Tris(methylenemethylphosphinate)-1,4,7-triazacyclononane;

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

Ca++ gl KCl 25°C 0.10M C T K1=4.45 1996HSb (84269)1884
At 37 C, K1=4.40.

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

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

Ca++ gl NaClO4 35°C 0.20M U H K1=2.5 1980KKb (84319)1885
DH=-28.9 kJ mol-1, DS=-50 J K mol-1

C12H32N4O8P4 H4L (7111)

1,4,7,10-Tetraazacyclododecane-1,4,7,10-tetrayltetramethylenetetakis(phosphinic acid);

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

Ca++ gl KNO3 25°C 0.10M C K1=9.458 1995BLa (84385)1886
B(CaHL)=13.4
B(CaH-1L)=-3.6

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

Ca++ gl R4N.X 25°C 0.10M M K1=11.12 1990DSa (84398)1887
B(CaH4L)=45.65
B(Ca2L)=18.67
B(Ca2HL)= 28.32
B(Ca2H2L)=36.03

Medium: Me4NNO3

Ca++ gl KNO3 25°C 1.0M U K1=10.3 1984KMb (84399)1888
K(Ca+HL)=7.7
K(Ca+H2L)=4.7
K(Ca+H3L)=3.1

C13H10N2O6S H2L MordentYellow10 CAS 21542-82-5 (1390)
5-(4'-Sulfophenylazo)salicylic acid; HO3S.C6H4.N:N.C6H3(OH).COOH

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

Ca++ gl KNO3 25°C 0.10M U K1=3.10 1964MTc (84933)1889

C13H10O6 HL CAS 156426-82-3 (8800)
3-Acetoacetyl-7-methyl-2H,5H-pyrano(4,3-b)pyran-2,5-dione;

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

Ca++ sp non-aq 20°C 100% C 1998FLb (85003)1890
K(Ca+HL=CaL+H)=1.97
K(CaL+HL=CaL2+H)=1.26

Method: absorption and fluorescence spectroscopy. Medium: acetonitrile.

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

Ca++ sp KCl 25°C 0.10M U K1=2.4 1978TSb (85215)1891

C13H12O5 HL CAS 17426-76-5 (3401)
O,O-Dimethylpurpurogallin

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

Ca++ gl diox/w 30°C 50% U K1=4.5 B2=8.0 1954BFc (85483)1892

C13H14NO3P H2L CAS 19316-85-7 (1466)
2-Hydroxyphenyl-N-phenylaminomethylphosphinic acid;

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

Ca++ gl NaClO4 20°C 0.10M U K1=4.90 1985SIb (85559)1893

C13H14N3O5P H2L CAS 80767-75-5 (1467)
2-Hydroxy-4-nitrophenyl-N-(2-pyridylmethyl)aminomethylphosphinic acid;

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

Ca++ gl NaClO4 20°C 0.10M U K1=5.60 1985SIb (85636)1894

C13H14N3O5P H2L CAS 80767-76-6 (1468)
2-Hydroxy-4-nitrophenyl-N-(3-pyridylmethyl)aminomethylphosphinic acid;

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

Ca++ gl NaClO4 20°C 0.10M U K1=5.70 1985SIb (85649)1895

C13H14N4 L CAS 13103-75-8 (473)
4-(2-Pyridylazo)-N,N-dimethylaniline; C5H4N.N:N.C6H4.N(CH3)2

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

Ca++ sp NaNO3 25°C 0.15M U K1=0 1953KMa (85675)1896

C13H15NO6 H3L (4999)
2-Benzylnitriilotriethanoic acid;

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

Ca++ oth oth/un 25°C 0.10M U K2=6.29 1962HKa (85731)1897

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

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

Ca++ gl KCl 20°C 0.10M U K1=7.46 1966IMa (85749)1898

C13H15NO6 H3L (4025)

N-(alpha-Carboxy-4'-methylbenzyl)iminodiethanoic acid;

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

Ca++ gl KCl 20°C 0.10M U K1=6.22 1966IMb (85755)1899

C13H15N07 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

Ca++ gl KCl 20°C 0.10M U K1=6.24 1966IMb (85764)1900

C13H15N203P H2L CAS 80767-72-2 (1460)
2-Hydroxyphenyl-(N-2-pyridylmethylamino)methylphosphinic acid;

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

Ca++ gl NaCl04 20°C 0.10M U K1=4.90 1985SIa (85776)1901

C13H15N203P H2L CAS 80767-73-3 (1461)
2-Hydroxyphenyl-(N-3-pyridylmethylamino)methylphosphinic acid;

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

Ca++ gl NaCl04 20°C 0.10M U K1=4.82 1985SIa (85789)1902

C13H15N203P H2L CAS 80767-74-4 (1462)
2-Hydroxyphenyl-(N-4-pyridylmethylamino)methylphosphinic acid;

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

Ca++ gl NaCl04 20°C 0.10M U K1=4.94 1985SIa (85802)1903

C13H15N204P H3L CAS 80767-78-8 (1463)
2-Hydroxyphenyl-(N-2-pyridylmethylamino)methylphosphonic acid;
C6H4(OH)CH(PO3H2).NH.CH2.C5H4N

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

Ca++ gl NaCl04 20°C 0.10M U K1=6.10 1985SIa (85815)1904

C13H15N204P H3L CAS 85946-85-6 (1464)
2-Hydroxyphenyl-(N-3-pyridylmethylamino)methylphosphonic acid;
C6H4(OH)CH(PO3H2).NH.CH2.C5H4N

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

Ca++ gl NaCl04 20°C 0.10M U K1=6.10 1985SIa (85828)1905

C13H15N2O4P H3L CAS 85946-86-7 (1465)
 2-Hydroxyphenyl-(N-4-pyridylmethylamino)methylphosphonic acid;
 C6H4(OH)CH(PO3H2).NH.CH2.C5H4N

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

 Ca++ gl NaClO4 20°C 0.10M U K1=6.15 1985SIa (85841)1906

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

 Ca++ gl KCl 20°C 0.10M U K1=3.39 B2=5.69 1971KT1 (85978)1907
 K(Ca+HL)=1.58

C13H17NO6 H2L CAS 77553-78-7 (6078)
 N-(2-Hydroxy-1-(hydroxybenzyl)-iminodiethanoic acid;
 HO.CH2.CH(CH(OH)(C6H5)).N(CH2.COOH)2

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

 Ca++ gl NaClO4 25°C 1.0M C K1=3.18 1981ASb (85987)1908

 Ca++ gl oth/un 25°C 0.10M C K1=4.07 1975MRa (85988)1909

C13H20N04P H3L (1471)
 2-Hydroxyphenyl-N-(cyclohexylamino)methylphosphonic acid;
 C6H4(OH)CH(PO3H2).NH.C6H11

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

 Ca++ gl NaClO4 20°C 0.10M U K1=6.15 1985SIb (86086)1910

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

 Ca++ gl oth/un 20°C 0.10M U K1=11.08 1960KGa (86105)1911

 Ca++ gl KCl 20°C 0.10M U K1=11.32 1959KRa (86106)1912
 K(Ca+HL)=4.99

 Ca++ oth oth/un 20°C 0.10M U K1=12.2 1957YSb (86107)1913

C13H20O8S4 H4L CAS 51865-20-4 (1139)
 (Pentanediyliidenetetraethio)tetra-ethanoic acid; ((HOOCCCH2S)2CHCH2)2.CH2

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	ISE	KCl	25°C	0.10M	C			K1=1.94	1995BBf (86384)	1921
Method: calcium ion selective electrode. For the beta isomer, K1=1.93.										

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	EMF	KCl	20°C	0.10M	C			K1=9.60 K(Ca+HL)=3.68	1957SSa (86392)	1922
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
Ca++	gl	R4N.X	25°C	0.10M	C			K1=4.93 *K(CaL)=-11.66	1998CCd (86404)	1923
Medium: 0.10 M Me4NNO3.										

Ca++	cal	NaClO4	25°C	0.10M	U	H		K1=3.5	1985EHa (86405)	1924
DH(K1)=-2.5 kJ mol ⁻¹ , DS=57.8 J K ⁻¹ mol ⁻¹										

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
Ca++	con	oth/un	25°C	dil	C			K1=1.26	1999TMa (86491)	1925
Self medium (Ca(NO3)2).										

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
Ca++	gl	R4N.X	25°C	0.10M	M			B(CaH2L)=30.23 B(CaH3L)=38.72 B(CaH4L)=45.26 B(Ca2L)=15.90	1990DSa (86583)	1926

Medium: Me4NNO3. Ca2HL also observed

C14H8N3O8S2F3		HL						(9231)		
1-(2-Thenoyl),4-trifluoro,2-[2-hydroxy-2-sulpho-5-nitrophenylazo]butadi-1,3-one;										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Ca++ gl KCl 25°C 0.1M U K1=7.03 B2=13.28 2004ACa (86606)1927

C14H8O4 H2L Quinizarin CAS 81-64-1 (1060)

1,4-Dihydroxyanthraquinone;

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

Ca++ sp alc/w 20°C 50% U 1982Kmd (86662)1928

K(Ca+HL)=3.2

Medium: 50% v/v EtOH/H2O

C14H8O7S H3L DASA CAS 83-61-4 (950)

1,2-Dihydroxyanthraquinone-3-sulfonic acid, Alizarin Red S;

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

Ca++ gl NaCl 25°C 0.10M C B2=11.7 1992WFb (86707)1929

K(Ca+2HL)=8.04

K(Ca+HL=CaL+H)=-3.72

K(Ca+2HL=CaL2+2H)=10.11

Data from spectrophotometric measurements are also given.

B(p,q,r); pH+qCa+r(HL)=Hp(Ca)q(HL)r: B(-1,1,1)=-3.72; B(-2,1,2)=-10.11.

C14H10N2O6 H4L CAS 15722-48-2 (2938)

3-3'-Azo-bis(6-hydroxybenzoic acid); HOOC.C6H3(OH).N:N.(HO)C6H3.COOH

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

Ca++ sp NaCl 25°C 0.50M U 1990DOa (86906)1930

K(Ca+H2L=CaHL+H)=-8.45

K(Ca+H2L=CaL+2H)=-18.9

C14H11N5O8S2 H5L CAS 1105-53-9 (5084)

1,5-Bis(2-hydroxy-5-sulfohenyl)-3-cyanoformazan;

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

Ca++ gl NaNO3 20°C 0.10M U K1=5.20 1971SEa (87015)1931

C14H12N2O3 H2L CAS 4870-46-6 (3432)

2-Hydroxy-5-methyl-2'-carboxy-azobenzene; HO.C6H3(CH3).N:N.C6H4.COOH

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

Ca++ sp KCl rt 0.10M U 1960DEa (87205)1932

K1eff=1.39 (pH 10)

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
Ca++	gl	KNO3	25°C	0.10M	U			K1=5.75	1973UWb (87667)	1933

C14H15N2O8Cl		H4L						(1903)		
4-Chloro-1,2-diaminobenzene-N,N,N',N'-tetraethanoic acid;										
Ca++	gl	KNO3	25°C	0.50M	C			K1=7.71 K(Ca+HL)=4.82	1997SDa (87738)	1934
Ca++	gl	KCl	25°C	0.10M	U			K1=8.17 B(CaHL)=11.23	1990MDa (87739)	1935

C14H16NO3P		H2L						CAS 25881-35-0	(1469)	
Phenyl-N-(benzylamino)methylphosphonic acid; C6H5.CH(PO3H2).NH.CH2.C6H5										
Ca++	gl	NaClO4	20°C	0.10M	U			K1=6.10	1985SIb (87805)	1936

C14H16NO4P		H3L						CAS 61146-25-6	(1470)	
2-Hydroxyphenyl-N-(benzylamino)methylphosphonic acid; C6H4(OH)CH(PO3H2).NH.CH2.C6H5										
Ca++	gl	NaClO4	20°C	0.10M	U			K1=6.25	1985SIb (87818)	1937

C14H16N2O8		H4L						CAS 40774-59-2	(1901)	
1,2-Diaminobenzene-N,N,N',N'-tetraethanoic acid; C6H4(N(CH2.COOH)2)2										
Ca++	gl	KNO3	25°C	0.50M	C			K1=8.23 K(Ca+HL)=4.82	1997SDa (87932)	1938
Ca++	gl	NaClO4	25°C	1.00M	C	H		K1=8.27	1992NSa (87933)	1939
By calorimetry: DH(K1)=-14.0 kJ mol ⁻¹ , DS=112 J K ⁻¹ mol ⁻¹										
Ca++	gl	KCl	30°C	0.10M	U			K1=9	1963GHa (87934)	1940

C14H16N2O8		H4L						(6108)		
1,3-Phenylenediamine-N,N'-disuccinic acid;										
Ca++	gl	NaCl	25°C	0.50M	C			K1=1.576 B(CaHL)=6.716	1989FRa (87987)	1941

B(CaH2L)=10.901

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

Ca++ gl NaCl 25°C 0.50M C K1=0.87 1984RFe (88008)1942

C14H17N2O4P H3L (1472)
2-Hydroxyphenyl-N-(2-(2'-pyridyl)ethylamino)methylphosphonic
acid;C6H4(OH)CH(PO3H2)NHCH2CH2C5H4N

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

Ca++ gl NaClO4 20°C 0.10M U K1=6.25 1985SIb (88038)1943

C14H18N2O5 HL Aspartame CAS 22839-47-0 (417)
Aspartyl-phenylalanine methyl ester; H2NCH(CH2COOH)CONHCH(CH2Ph)COOCH3

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

Ca++ gl KCl 25°C 0.5M U TIH K1=0.92 1985AAb (88075)1944
B(CaHL)=2.17

DH(K1)=-14.1 kJ mol⁻¹, DS(K1)=-29.6; DH(CaHL)=-12.30, DS(CaHL)=-1.1.

At 35 C, K1=0.84, B(CaHL)=2.10.

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

Ca++ con mixed 25°C 20% C K1=3.79 2003SIa (88218)1945
Medium: 20% w/w propylene carbonate/ethylene carbonate.

Ca++ nmr non-aq 27°C 100% C K1=5.11 2000SMg (88219)1946
Medium: acetonitrile. Method: competitive 7Li nmr technique.

Ca++ cal non-aq 25°C 100% U H K1=4.04 1993BDb (88220)1947
Medium: acetone. DH=-26.3 kJ mol⁻¹; TDS=-3.4

Ca++ vlt non-aq 25°C 100% C K1=3.31 1991SSb (88221)1948
Method: competitive complexation with Tl⁺; use of Tl(Hg)/Tl couple.
Medium: acetonitrile, 0.05 M Et4NC1O4.

Ca++ sp alc/w 25°C 100% U I K1=2.66 1989KSc (88222)1949
In MeOH. In DMF K1=2.32; in DMSO K1=2.12

Ca++ oth non-aq 25°C 100% U K1=3.91 1989SSc (88223)1950
Medium: CH3CN. Ca as Ca(NCS)2; for Ca(ClO4)2: K1=3.64; B2=5.2. Method: IR

Ca++ cal non-aq 25°C 100% U H K1=4.20 1989SSd (88224)1951
Medium: CH3CN

Ca++ cal alc/w 25°C 100% U H K1=1.23 1988SVa (88225)1952

Ca++ ISE R4N.X 25°C 0.10M C K1=2.33 1986XJa (88226)1953

C14H22N2O8 H4L cis-1,2-CDTA CAS 92761-75-6 (2846)
cis-1,2-Diaminocyclohexane-N,N,N',N'-tetraethanoic acid;

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

Ca++ gl KCl 20°C 0.10M U K1=9.45 1959KRa (88427)1954
K(Ca+HL)=2.86

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

Ca++ gl R4N.X 25°C 0.50M M K1=13.68 1975CSb (88537)1955
K(Ca+HL)=4.45
K(CaL+H)=3.85

Ca++ gl alc/w 25°C 99% U K1=9.5 1972Rba (88538)1956
Medium: 0.1(NaClO4), 99% methanol.

Ca++ gl NaClO4 20°C 0.10M U K1=13.15 1970AMa (88539)1957

Ca++ cal KNO3 25°C 0.10M U H K1=13.15 1965WHa (88540)1958
DH(K1)=-25.9 kJ mol⁻¹, DS=146 J K⁻¹ mol⁻¹

Ca++ cal KNO3 20°C 0.10M U T H K1=13.15 1963ANb (88541)1959
DH(K1)=-15.5 kJ mol⁻¹, DS=198.5 J K⁻¹ mol⁻¹

Ca++ cal KNO3 20°C 0.10M U H K1=13.15 1963ANf (88542)1960
DH(K1)=-15.5 kJ mol⁻¹, DS=201 J K⁻¹ mol⁻¹

Ca++ gl KNO3 25°C 0.10M U T H K1=11.34 1960BMb (88543)1961
K1=11.97(0.5 C), 10.84(42.4 C). DH(K1)=-46.0 kJ mol⁻¹, DS=62.8 J K⁻¹ mol⁻¹

Ca++ EMF KNO3 25°C 0.10M U K1=12.3 1960HRa (88544)1962

Ca++ oth oth/un ? ? U K1=12.2 1957YSb (88545)1963

Ca++ vlt oth/un 20°C 0.10M U K1=12.08 1954SGa (88546)1964

Ca++ EMF KCl 20°C 0.10M C K1=12.50 1949SAa (88547)1965
Method: H electrode

 C14H22N2O8 H4L trans-1,3-CDTA CAS 92681-24-8 (2849)
 trans-1,3-Diaminocyclohexane-N,N,N',N'-tetraethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	EMF	KCl	20°C	0.10M	C			K1=4.77 K(Ca+HL)=3.12 K(Ca+CaL)=2.30	1949SAa	(88831)1966

Method: H electrode

 C14H22N2O8 H4L trans-1,4-CDTA CAS 92681-26-0 (2843)
 trans-1,4-Diaminocyclohexane-N,N,N',N'-tetraethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	EMF	KCl	20°C	0.10M	C			K1=4.19 K(Ca+HL)=3.10 K(Ca+CaL)=2.52	1949SAa	(88847)1967

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
Ca++	gl	diox/w	24°C	50%	U			K1=7.0	1979ACa	(88988)1968

 C14H22O8S4 H4L (1160)
 Ethane-tetramercaptopropanoic acid; (CH.(S.CH2.CH2.COOH)2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	NaCl04	25°C	0.10M	U			K1=2.59	1975PJa	(88998)1969

 C14H23N3O10 H5L DTPA CAS 67-43-6 (238)
 Diethylenetriamine-pentaethanoic acid; HOOC.CH2.N(CH2.CH2.N(CH2.COOH)2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	KNO3	25°C	0.1M	C	TI	R	K1=10.7	2005AAa	(89101)1970

IUPAC recommended value. Provisional value, 37 C, 0.15 NaCl: K1=9.8,
 K(CaL+H)=6.00, K(CaHL+H)=4.40, K(CaH2L+H)=3.70

Ca++	gl	NaCl04	25°C	0.10M	C			K1=10.75 K(CaL+H)=6.11	2001CCa	(89102)1971
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Ca++	gl	KCl	25°C	0.10M	C			K1=11.77 K(CaL+H)=6.10	1999SBd	(89103)1972
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Ca++	gl	NaClO4	25°C	0.10M	M			K1=10.58 K(Ca+HL)=5.91	1987ZGa (89104)1973
Ca++	gl	NaCl	37°C	0.15M	C			K1=9.82 B2=11.95 B(CaHL)=15.80 B(CaH2L)=20.23 B(CaH3L)=23.92	1984DMb (89105)1974
Ca++	gl	NaClO4	20°C	0.10M	U			K1=10.84	1970AMa (89106)1975
Ca++	cal	KNO3	27°C	0.10M	U	H		DH(K1)=-23.4 kJ mol ⁻¹ , DS=125.4 J K ⁻¹ mol ⁻¹	1968CLd (89107)1976
Ca++	gl	KNO3	25°C	0.10M	U			K1=10.6	1968WRa (89108)1977
Ca++	cal	KNO3	20°C	0.10M	U	T	H	DH(K1)=-24.9 kJ mol ⁻¹ , DS=123.3 J K ⁻¹ mol ⁻¹	1965ANa (89109)1978
Ca++	cal	KNO3	25°C	0.10M	U	H		DH(K1)=-25.5 kJ mol ⁻¹ , DS=121 J K ⁻¹ mol ⁻¹	1965WHa (89110)1979
Ca++	EMF	KNO3	25°C	0.10M	U			K1=10.7	1960HRa (89111)1980
Ca++	gl	KNO3	25°C	0.10M	C			K1=10.6 K(CaL+H)=6.4	1960WAa (89112)1981
Ca++	EMF	oth/un	20°C	0.10M	U			K1=10.89 K(CaL+Ca)=1.98 K(Ca+HL)=6.42	1959ANd (89113)1982
Ca++	gl	KNO3	25°C	0.10M	U			K1=10.74 B2=12.34	1959CFc (89114)1983
Ca++	gl	oth/un	20°C	0.10M	U			K1=10.63	1958DRa (89115)1984
Ca++	gl	oth/un	25°C	0.10M	U			K1=9.98	1955WAa (89116)1985

		C14H24N2O6			H3L			(3439)	
N-Cyclohexylethylenediamine-N,N',N'-triethanoic acid;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference ExptNo
Ca++	sp	oth/un	24°C	0.16M	U			K1=1.7	1956BCa (89484)1986
By glass electrode K1=1.3									

		C14H24N2O7			H3L			(3440)	
N-(2-Hydroxycyclohexyl)ethylenediamine-N,N',N'-triethanoic acid;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference ExptNo
Ca++	gl	oth/un	25°C	0.10M	U			K1=9.33 B2=11.03	1960SAC (89489)1987

K(Ca+HL)=2.77

Ca++ gl KCl 20°C 0.10M U K1=6.18 1959KRa (89490)1988
K(Ca+HL)=3.29

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

Ca++ gl KNO3 20°C 0.10M U K1=9.02 1969NDc (89500)1989

C14H24N2O8 H4L HMDTA CAS 1633-00-7 (920)
1,6-Diaminohexane-N,N,N',N'-tetraethanoic acid; ((HOOC.CH2)2N.CH2.CH2.CH2)2

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

Ca++ gl KNO3 25°C 0.10M U K1=4.15 1969GKb (89554)1990

K(Ca+HL)=3.28
B(Ca2L)=2.69

Ca++ gl KNO3 20°C 0.10M U K1=4.6 1964ANa (89555)1991

K(Ca+HL)=3.7

Ca++ gl KCl 20°C 0.10M U K1=4.40 1955SAc (89556)1992

C14H24N2O8 H4L CAS 1633-00-7 (5076)
4-Methyl-1,2-diaminopentane-N,N,N',N'-tetraethanoic acid;
(HOOCCH2)2NCH2CH(N(CH2COOH)2)CH2CH(CH3)2

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

Ca++ gl KNO3 20°C 0.10M U K1=11.84 1969NDa (89624)1993

C14H24N2O8S2 H4L (3441)
2,2'-Ethylenebisthio(ethyliminodiethanoic acid);

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

Ca++ gl KCl 20°C 0.10M U K1=4.87 1957SSa (89695)1994

K(Ca+HL)=3.5
K(CaL+Ca)=1.91

C14H24N2O9 H4L CAS 87720-52-3 (1593)
2,2'-Oxybis(propyliminodiethanoic acid)

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

Ca++ gl KCl 20°C 0.10M U K1=5.38 1961ISa (89702)1995

K(Ca+HL)=4.04

Ca++ gl KCl 20°C 0.10M U K1=8.06 1961KGa (89703)1996
K(Ca+HL)=4.66

Ca++ gl oth/un 25°C 0.10M U K1=8.4 1953KPa (89704)1997
K(Ca+HL)=5.2

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

Ca++ gl KCl 20°C 0.10M U K1=5.38 1961ISa (89720)1998
K(Ca+HL)=4.04

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

Ca++ gl KCl 20°C 0.10M C K1=11.118 1985SMg (89797)1999
K(Ca+HL)=5.509

Ca++ gl KNO3 25°C 0.10M U K1=12.8 1982JGa (89798)2000
K(CaL+H)=3.7
K(CaL+2H)=3.2

Ca++ ISE KCl 25°C 0.20M C K1=11.00 1976OWa (89799)2001
Method: Ca ion selective electrode. Medium: 0.20 M KCl, 0.02 M imidazole
buffer, pH 7.25.

Ca++ gl NaCl 25°C 0.70M U K1=10.70 1974JAb (89800)2002
Medium: seawater

Ca++ gl alc/w 25°C 99% U K1=11.1 1972RBa (89801)2003
Medium: 99% MeOH, 0.1 M NaClO4

Ca++ gl KNO3 25°C 0.10M U K1=11.0 1968WRa (89802)2004

Ca++ cal KCl 25°C 0.10M U H 1965BBe (89803)2005
DH(K1)=-33.2 kJ mol⁻¹, DS=97.0 J K⁻¹ mol⁻¹

Ca++ cal KNO3 25°C 0.10M U H 1965WHa (89804)2006
DH(K1)=-33.4 kJ mol⁻¹, DS=96.1 J K⁻¹ mol⁻¹

Ca++ gl KNO3 20°C 0.10M U H K1=10.97 1964ANa (89805)2007
K(Ca+HL)=5.3
By calorimetry: DH(K1)=-35.0 kJ mol⁻¹, DS=90.3 J K⁻¹ mol⁻¹

Ca++ EMF KCl 20°C 0.10M C K1=11.00 1964PCa (89806)2008

K(Ca+HL)=5.33

Method: H electrode

Ca++	EMF	KNO3	25°C	0.10M	U			K1=10.9	1960HRa (89807)2009
Ca++	gl	oth/un	25°C	0.10M	U			K1=10.7	1957SRa (89808)2010

C14H24N2O10			H4L					(2655)	
N,N'-Bis(2-hydroxyethane)-N,N'-ethanediaminedibutanedioic acid;									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference ExptNo
Ca++	gl	KNO3	25°C	0.1M	U			K1=5.75	1985MGb (89974)2011

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
Ca++	gl	alc/w	25°C	90%	U			K1=9.1	1984FWa (90059)2012
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
Ca++	gl	R4N.X	25°C	0.10M	U			K1=12.98	1988ADa (90076)2013

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
Ca++	cal	R4N.X	25°C	0.10M	U	H			1989DSa (90164)2014
DH(CaL)=-15.1 kJ mol ⁻¹ ; DS=117.									
Ca++	gl	R4N.X	25°C	0.10M	C			K1=8.680	1987DDb (90165)2015

								B(Ca2L)=9.9	
Ca++	gl	R4N.X	25°C	0.10M	M			K1=8.74	1986COb (90166)2016

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
Ca++	gl	R4N.X	25°C	0.10M	U			K1=3.9	1990AFa (90218)2017

Ca++ sp non-aq 20°C 100% U K1=3.36 1992PSa (90327)2026
Medium: DMF, 0.01 M Me4NI

Ca++ gl R4N.X 25°C 0.10M C IH K1=2.7 1987CSa (90328)2027
In 10% CH3CN, K=3.5; 20%, K=4.4; 40%, K=5.0; 60%, K=6.3; 70%, K=6.7;
90%, K=7.7; 100%, K=8.5

Ca++ cal alc/w 25°C 100% U H K1=2.53 1986BUa (90329)2028
B(Ca2L2)=5.45
Medium: MeOH. Determined by potentiometry. DH=-2.4 kJ mol⁻¹; DS=96

Ca++ ISE non-aq 25°C 100% U K1=8.65 1984CTc (90330)2029
In propylene carbonate, using competition with Ag and a silver electrode.

Ca++ gl alc/w 25°C 95% C K1=4.5 1981ANa (90331)2030
Medium: 95% MeOH, 0.1 M Me4NCl

Ca++ cal oth/un 25°C 0.10M C 1981LIc (90332)2031
Medium: piperidine/HCl buffer, pH 11.4. DH(K1)=-1.67 kJ mol⁻¹.

Ca++ ISE non-aq 25°C 100% U K1=8.6 1980CRa (90333)2032
Medium: Propylene carbonate

Ca++ EMF non-aq 25°C 100% C K1=2.8 1979BLb (90334)2033
Method: Ag electrode; competition with Ag+. Medium: MeOH, 0.05 M
Me4NClO4.

Ca++ kin oth/un 25°C 0.10M U H K1=2.3 1977LPb (90335)2034
In piperidine buffer, pH 11.5. DH=-1.3 kJ mol⁻¹

Ca++ cal R4N.X 25°C 0.06M C H 1976KLc (90336)2035
Medium: 0.057 M Me4NBr. Method: flow microcalorimetry.
DH(K1)=-0.4 kJ mol⁻¹, DS(K1)=46 J K⁻¹ mol⁻¹.

Ca++ gl R4N.X 25°C 0.05M C I K1=2.50 1975LSc (90337)2036
In 95% MeOH, 0.05 M Me4NBr: K1=4.34

Ca++ kin KCl 25°C 0.10M U H K1=3.20 1975LWb (90338)2037
Using stopped flow. DH=21 kJ mol⁻¹. Also K1=2.80 by potentiometry in
0.04 to 0.08M NMe4Br.

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

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

Ca++ ISE alc/w 25°C 100% U K1=2.80 1983GGa (90514)2038
Medium: MeOH

C14H30N2O4 L CAS 31255-13-7 (2448)
 N,N'-Dimethyl-cyclo-1,10-diaza-4,7,13,16-tetraoxaocadecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	gl	alc/w	25°C	95%	C		K1=4.81	2004KVa (90567)	2039

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

Ca++	gl	oth/un	25°C	?	C		K1=2.06	1991DMa (90568)	2040
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Ca++	ISE	alc/w	25°C	100%	U H		K1=4.2	1983CFb (90569)	2041
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Medium: MeOH, 0.05 M Et4NClO4

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
Ca++	ISE	alc/w	25°C	100%	U		K1=2.5	1988CFa (90606)	2042

Medium: MeOH

Ca++	ISE	alc/w	25°C	100%	U H		K1=1.86	1986BUa (90607)	2043
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Medium: MeOH. DH(K1)=0 kJ mol⁻¹; DS=10 J K⁻¹ 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
Ca++	gl	R4N.X	25°C	0.10M	C		K1=4.86	1995LLa (90622)	2044

Medium: Et4NClO4

C14H30N2O5 L (6929)
 N,N'-Bis(hydroxyethyl)-1,4-diaza-7,10,13-trioxacyclopentadecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	cal	alc/w	25°C	90%	U H		K1=4.13	1994IZa (90637)	2045

Medium: 90% v/v MeOH/H2O. DH(K1)=-16.1 kJ mol⁻¹, DS(K1)=25.2 J K⁻¹ mol⁻¹

C14H30O7 L CAS 1072-40-8 (2499)
 2,5,8,11,14,17,20-Heptaohaxaheneicosane; CH3.O.(CH2.CH2.O)6.CH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	cal	non-aq	25°C	100%	U H		K1=2.43	1993BDb (90682)	2046

Medium: acetone. DH=-44.7 kJ mol⁻¹; TDS=-30.9

Ca++	con	non-aq	25°C	100%	C H		K1=4.24	1992BSc (90683)	2047
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Medium: propylene carbonate. By calorimetry, DH(K1)=-44.0 kJ mol⁻¹,

DS(K1)=-66.8 J K-1 mol-1.

C14H32N2O4 L CAS 102-60-3 (2678)
Tetra(2-hydroxypropyl)-N,N,N',N'-diaminoethane;(-CH2.N(CH2.CH(OH).CH3)2)2

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

Ca++ gl NaNO3 25°C 0.10M U K1=1.63 1986HBc (90734)2048

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

Ca++ gl R4N.X 25°C 0.10M U K1=7.45 1996BJa (90756)2049
K(Ca+HL)=5.45
K(Ca+H2L)=2.15

Medium: 0.1 M Me4NCl

C14H34N4O6P2 H4L CAS 200952-02-9 (7644)
1,4,7,10-Tetraazacyclododecane-1,7-bis(methanephosphonic acid monoethyl ester);

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

Ca++ gl KCl 25°C 0.10M C K1=4.55 1998BRa (90839)2050

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

Ca++ gl R4N.X 25°C 0.10M M 1990DSa (90865)2051
B(CaHL)=19.33
B(CaH2L)=30.18
B(CaH3L)=38.32
B(CaH4L)=45.18

Medium: Me4NNO3

C14H37O12O12P4 H8L (6910)
N'-Hexyl-diethylenetriamine-N,N,N'',N'''-tetra(methylenephosphonic acid);

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

Ca++ gl NaClO4 25°C 0.10M M 1987ZGa (90930)2052
K(Ca+HL)=3.55
K(Ca+H2L)=3.48
K(Ca+H3L)=3.11
K(Ca+H4L)=2.04

K(Ca+H5L)=1.43.

Ca++ gl oth/un 25°C 0.10M U 1984ZGa (90931)2053

K(Ca+HL)=3.55
K(Ca+H2L)=3.48
K(2Ca+H2L)=7.51
K(Ca+H3L)= 3.11

K(Ca+H4L)=2.04; K(2Ca+H3L)=7.20; K(2Ca+HL)=8.27; K(Ca+H5L)=1.43

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

Ca++ gl diox/w 20°C 17% C K1=7.33 B2=13.09 1976JWa (91531)2054

Ca++ gl diox/w 30°C 75% U K1=7.17 B2=13.55 1953UFe (91532)2055

C15H14NOCl HL CAS 268214-29-5 (8398)
4-Chloro-3,5-dimethyl-2-[(phenylimino)methyl]phenol;

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

Ca++ gl diox/w 30°C 75% M K1=4.48 2000ANa (91684)2056
Medium: 75% v/v dioxan/H2O, 0.10 M NaClO4. Data for an extensive series of
4'-substituted phenylimino derivatives.

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

Ca++ gl diox/w 25°C 50% U 1964STa (91724)2057

K(Ca+HL)=4.62
K(Ca+H2L)=2.41

C15H14N2O5S HL (9232)
3-(5-Sulphonylnaphthylazo)penta-2,4-dione;

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

Ca++ gl KCl 25°C 0.1M U H K1=6.55 2004ACb (91731)2058
for 35 C K1=6.44; for 45 C K1=6.32

C15H17N2O8Cl H3L CAS 308124-47-2 (3563)
N,N-Bis(carboxymethyl)-2-(carboxymethoxy)-5-(2-chloro-ethanamido)benzylamine;

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

Ca++ sp KCl 22°C 0.14M C 2000RGa (91970)2059

K1eff=3.91

Medium: KCl/NaCl/HEPES/TRIS at pH 7.2. Method: fluorescence emission.

Also data for the 2-(2-chloroethanamido)-5-(carboxymethoxy)-derivatives

C15H18N2O8 H4L (1934)
1-Methyl-2,5-diaminobenzene-N,N,N',N'-tetraethanoic acid;

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

Ca++ oth oth/un 25°C 0.10M U K1=3.6 1969RMa (92058)2060
K(CaL+H)=4.5

C15H18N2O8 H4L CAS 101455-18-9 (1902)
1-Methyl-3,4-diaminobenzene-N,N,N',N'-tetraethanoic acid;

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

Ca++ gl KNO3 25°C 0.50M C K1=8.61 1997SDa (92079)2061
K(Ca+HL=CaHL)=4.77

C15H18N2O8 H4L (6114)
2,5-Toluenediamine-N,N'-disuccinic acid;

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

Ca++ gl NaCl 25°C 0.50M C K1=0.962 1989FRa (92090)2062

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

Ca++ gl KCl 25°C 0.10M U K1=10.2 1984VOb (92129)2063
For the 4-methoxy derivative: K1=8.1; for the 4-dimethylamino derivative,
K1=8.1.

C15H20N2O6 H3L BEDTA CAS 65311-06-0 (2944)
N-Benzylidiaminoethane-N,N',N'-triethanoic acid;

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

Ca++ gl KCl 25°C 0.10M U K1=7.00 2003SVa (92144)2064
K(Ca+HL)=1.95

Ca++ gl KCl 24°C 0.10M U K1=6.7 1956BCa (92145)2065

C15H22N4O4 H2L (7082)
3,6,9,15-Tetraazabicyclo[9.3.1]pentadeca-1(15),11,13-triene-3,9-diethanoic acid;

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

Ca++ gl KCl 25°C 0.10M C K1=10.0 1995KHa (92244)2066

 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

 Ca++ cal alc/w 25°C 100% U H K1=5.26 1980LIa (92264)2067
 Medium: MeOH. DH=-12.1 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

 Ca++ gl KNO3 25°C 0.10M U K1=10.50 1968MMb (92315)2068
 K(Ca+HL)=8.03
 K(Ca+H2L)=2.9
 B(Ca2L)=2.3

 C15H24O6 HL CAS 57722-03-9 (2353)
 1-Hydroxy-2-(1,4,7,10,13-pentaoxatridecyl)benzene; HO.C6H4.0(CH2CH2O)4CH3

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

 Ca++ sp alc/w 25°C 100% U K1=6.26 1981EMb (92340)2069
 Medium: MeOH

 C15H24O8S4 H4L CAS 53480-91-4 (1161)
 Propane-1,1,3,3-tetramercaptopropanoic acid; CH2(CH(S.CH2.CH2.COOH)2)2

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

 Ca++ gl NaClO4 25°C 0.10M U K1=2.79 1975PJa (92351)2070

 C15H25N3O10 H5L (7436)
 3,6,10-Tri(carboxymethyl)-3,6,10-triazadodecanedioic acid;

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

 Ca++ gl R4N.X 25°C 0.10M C K1=14.45 1998WLa (92363)2071
 B(CaHL)=20.51

Medium: 0.1 M NMe4NO3.

 C15H27N3O6 H3L (6514)
 1,5,9-Triazacyclododecane-N,N',N"-triethanoic acid;

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

 Ca++ gl R4N.X 25°C 0.10M M K1=6.0 1990CBc (92462)2072
 Medium: Me4NCl

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

Ca++ gl R4N.X 25°C 0.10M C K1=9.79 1997CCa (92475)2073
Medium: Me4NNO3

C15H27N3O9 H4L CAS 319016-32-5 (7716)
N'-(2-Hydroxypropyl)-diethylenetriamine-N,N,N",N"-tetraethanoic acid;

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

Ca++ gl R4N.X 25°C 0.10M M K1=8.58 2000Cwa (92483)2074
Medium: 0.1 M NMe4NO3.

C15H28N2O8 H2L (7126)
1,4,10,13-Tetraoxa-7,16-diazacyclooctadecane-7-malonic acid;

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

Ca++ gl NaCl 25°C 0.15M U K1=6.58 1995BGa (92492)2075

C15H30N2O3 L CAS 72640-82-5 (6040)
4,7,13-Trioxa-1,10-diazabicyclo[8.5.5]eicosane;

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

Ca++ gl R4N.X 25°C 0.10M C I K1=2.3 1991DLA (92513)2076
In 95% v/v MeOH/H2O: K1=3.6

C15H32N4O4 H2L (8283)
2,12-Dimethyl-5,9-di(methylcarboxy)-2,5,9,12-tetraazatridecane

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

Ca++ gl KNO3 25°C 0.10M C K1=1.98 1989HAa (92555)2077

C15H36N3O9P3 H3L (6749)
1,4,7-Triazacyclononane-N,N'N''-tris(methylenephosphonatemonoethylester)

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

Ca++ gl R4N.X 25°C 0.10M C K1=5.1 1992LRa (92608)2078

C16H9N2OBr3 HL CAS 84317-74-8 (5169)
1-(2,4,6-Tribromophenylazo)-2-hydroxynaphthalene;

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

Ca++ gl mixed 25°C 75% U K1=5.33 1972MCb (92643)2079
Medium: 75% acetone, 0.1 M KNO3

C16H11N2OBr HL CAS 7150-24-5 (5172)
1-(4-Bromophenylazo)-2-hydroxynaphthalene;

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

Ca++ gl mixed 25°C 75% U K1=6.44 1972MCb (92693)2080
Medium: 75% acetone, 0.1 M KNO3

C16H11N2OCl HL CAS 24390-65-6 (5170)
1-(2-Chlorophenylazo)-2-hydroxynaphthalene;

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

Ca++ gl mixed 25°C 75% U K1=5.84 1972MCb (92708)2081
Medium: 75% acetone, 0.1 M KNO3

C16H11N2OCl HL CAS 10149-93-6 (5171)
1-(4-Chlorophenylazo)-2-hydroxynaphthalene;

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

Ca++ gl mixed 25°C 75% U K1=6.37 1972MCb (92723)2082
Medium: 75% acetone, 0.1 M KNO3

C16H11N2OI HL CAS 25023-35-2 (5173)
1-(4-Iodophenylazo)-2-hydroxynaphthalene;

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

Ca++ gl mixed 25°C 75% U K1=6.53 1972MCb (92738)2083
Medium: 75% acetone, 0.1 M KNO3

C16H11N2O2Cl H2L CAS 3566-94-7 (3474)
1-(5-Chloro-2-hydroxyphenylazo)-2-hydroxynaphthalene;

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

Ca++ gl diox/w 30°C 75% U K1=8.35 1957SFb (92755)2084
K(Ca+H2L=CaL+2H)=-15.4

C16H11N2O9ClS2 H4L Plasmocorinth CAS 1058-92-0 (5203)
3-(5-Chloro-2-hydroxyphenylazo)chromotropic acid (Eriochrome Blue SE)

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

Ca++ sp oth/un 25°C 0.10M U K1=5.05 1961BRa (92784)2085

Medium: NaOH

C16H11N3O3 HL CAS 6410-09-9 (5151)
1-(2-Nitrophenylazo)-2-hydroxynaphthalene;

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

Ca++ gl mixed 25°C 75% U K1=2.99 1972MCb (92792)2086
Medium: 75% acetone, 0.1 M KNO3

C16H11N3O3 HL CAS 6410-46-1 (5152)
1-(4-Nitrophenylazo)-2-hydroxynaphthalene;

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

Ca++ gl mixed 25°C 75% U K1=3.72 1972MCb (92807)2087
Medium: 75% acetone, 0.1 M KNO3

C16H11N3O4 H2L CAS 14847-54-2 (3461)
1-(2-Hydroxy-5-nitrophenylazo)-2-hydroxynaphthalene;

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

Ca++ gl diox/w 30°C 75% U K1=8.36 1957SFb (92842)2088
K(Ca+H2L=CaL+2H)=-13.2

C16H12N2O HL CAS 842-07-9 (5156)
1-Phenylazo-2-hydroxynaphthalene;

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

Ca++ gl mixed 25°C 75% U K1=7.02 1972MCb (92913)2089
Medium: 75% acetone, 0.1 M KNO3

C16H12N2O2 H2L CAS 9486-98-2 (3462)
1-(2-Hydroxyphenylazo)-2-hydroxynaphthalene;

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

Ca++ gl mixed 25°C 75% U K(Ca+HL)=6.98 1972MCb (92941)2090

Medium: 75% acetone, 0.1 M KNO3

Ca++ sp KCl rt 0.10M U K1eff=2.26 (pH 10) 1960DEa (92942)2091

Ca++ gl diox/w 30°C 75% U K1=8.61 1957SFb (92943)2092
K(Ca+H2L=CaL+2H)=-16.1

C16H12N2O2 H2L CAS 14934-27-1 (5157)

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	mixed	25°C	75%	U			K(Ca+HL)=6.76	1972Mcb (92965)	2093

Medium: 75% acetone, 0.1 M KNO3

C16H12N2O4S H2L CAS 13964-82-4 (3475)

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	mixed	25°C	75%	U			K1=3.29	1972Mcb (92991)	2094

Medium: 75% acetone, 0.1 M KNO3

C16H12N2O5S H3L SolochromeVio R CAS 94205-83-1 (4093)

1-(2'-Hydroxy-5'-sulfophenylazo)-2-naphthol;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	sp	oth/un	25°C	0.0	U			K1=6.6 B2=9.60	1962CRa (93018)	2095

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
Ca++	gl	KNO3	25°C	0.10M	U			K(Ca+HL)=2.70	1971KMb (93054)	2096

Ca++	gl	KNO3	25°C	0.10M	U			K(Ca+HL)=2.70	1968NMB (93055)	2097
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C16H12N2O9S2 H5L CAS 26197-92-2 (4094)

2-(2'-Hydroxyphenylazo)chromotropic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	KNO3	25°C	0.10M	U			K(Ca+HL)=5.01	1968NMB (93073)	2098

C16H12N2O11S3 H5L (4095)

2-(2'-Sulphophenylazo)chromotropic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	KNO3	25°C	0.10M	U			K(Ca+HL)=2.91	1968NMB (93080)	2099

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

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

Ca++ gl KNO3 25°C 0.10M U K1=4.17 1971KTc (93178)2100

Ca++ gl oth/un 30°C ? U K1=5.5 1964PCa (93179)2101

C16H13N2O10AsS2 H5L (5204)

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

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

Ca++ gl KNO3 25°C 0.10M U K1=3.50 1971KTc (93223)2102

C16H13N2O10PS2 H5L (5205)

1-(2-Phosphonophenylazo)-2-hydroxynaphthalene-3,6-disulfonic acid;

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

Ca++ gl KNO3 25°C 0.10M U K1=3.80 1971KMa (93228)2103

K(Ca+HL)=2.98

K(CaL+H)=10.28

C16H13N2O11AsS2 H6L Arsenazo I CAS 520-10-5 (277)

2-(2'-Arsonophenylazo)chromotropic acid;

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

Ca++ gl KNO3 25°C 0.10M U K1=5.20 1971KTc (93242)2104

Ca++ gl KNO3 25°C 0.10M U 1968NMb (93243)2105

K(Ca+HL)=5.09

C16H13N3O8S2 H4L CAS 56973-75-2 (4108)

8-Amino-1-hydroxy-2-(2'-hydroxyphenylazo)-naphthalene-3,6-disulfonic acid;

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

Ca++ sp KCl ? 0.10M U K1=2.50 1960DEa (93289)2106

C16H13N3O8S2 H4L (4109)

8-Amino-1-hydroxy-2-(2'-hydroxyphenylazo)-naphthalene-5,7-disulfonic aic

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

Ca++ sp KCl rt 0.10M U 1960DEa (93292)2107

K1eff=3.08 (pH 10)

1,2-Dimethylbenzene-tetrathioethanoic acid; C₆H₄(CH(S.CH₂.COOH)₂)₂

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	NaCl04	25°C	0.10M	U			K1=3.5	1974JBa (93883)	2114

C16H19N2O9Cl		H5L		(3483)						
5-Chloro-2-hydroxy-1,3-phenylenebis(methylamine-N,N-diethanoic acid);										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	EMF	KCl	20°C	0.10M	C			K1=8.5 K(Ca+HL)=7.09 K(Ca+H2L)=2.8	1952SAb (93917)	2115

Method: H electrode

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	KNO3	20°C	0.10M	U			K1=11.25	1989SLa (94020)	2116
Ca++	gl	KNO3	20°C	0.10M	U			K1=11.25	1969NDb (94021)	2117
Ca++	gl	KCl	25°C	0.10M	U			K1=10.90	19670Tb (94022)	2118

C16H20N2O10		H6L		(704)						
1,2-Dihydroxy-3,6-di-(methyleneiminodiethanoic acid)-benzene;										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	KNO3	25°C	0.10M	C			K1=8.00 K(Ca+H2L)=5.14 K(Ca+HL)=7.18 K(CaHL+H)=9.09 K(CaL+H)=11.05	1988ZHa (94060)	2119

B(Ca2L)=14.35

C16H20N2O10		H6L		CAS 28021-27-4 (5166)						
1,4-Dihydroxyphenyl-2,5-bis(methyleneimino)-N,N,N',N'-tetraethanoic acid;										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	oth/un	25°C	0.0	U			K(Ca+HL)=7.0 K(Ca+H2L)=5.3 K(Ca+H3L)=2.2 K(2Ca+HL)=15.3	1970TTb (94073)	2120

C16H20N2O12S H6L (3484)
2-Hydroxy-5-sulfo-1,3-phenylenebis(methylamine-N,N-diethanoic acid);

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

Ca++ EMF KCl 20°C 0.10M C K1=9.2 1952SAb (94081)2121
K(Ca+HL)=7.88
K(Ca+H2L)=2.8

Method: H electrode

C16H22N2O4P2 H2L (7262)
1,2-Diaminoethane-N,N'-bis(methylenephosphinic acid); (CH2NHCH2PO(OH)C6H5)2

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

Ca++ gl R4N.X 25°C 0.10M M K1=2.92 1996BCa (94125)2122
Medium: 0.1 M Me4NNO3.

C16H22O6 L (6733)
4'-Acetyl-2,3-benzo-1,4,7,10,13-pentaoxacyclopentadeca-2-ene;

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

Ca++ cal alc/w 25°C 100% U H K1=0.5 1988SVa (94246)2123

C16H23NO8 L CAS 53408-96-1 (1765)
2,3-(4'-Nitrobenzo)-1,4,7,10,13,16-hexaoxacyclooctadeca-2-ene;
4'-Nitrobenzo-18-crown-6

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

Ca++ ISE R4N.X 25°C 0.10M C K1=3.55 1986XJa (94263)2124

C16H24N2O8 H4L CAS 38557-30-1 (1256)
Ethylene-bis(N,N'-(2,6-dicarboxy)piperidine); ((HOOC)2.C5H8N.CH2.)2

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

Ca++ gl NaNO3 25°C 0.10M U K1=7.28 1979PBa (94315)2125

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

Ca++ oth alc/w 35°C 3.0% C K1=1.64 1999MTd (94373)2126
Method: capillary zone electrophoresis. Medium: 3% v/v EtOH/H2O, 0.005 M
acetate buffer, pH 5.5.

Ca++ cal non-aq 25°C 100% C H K1=2.50 1999WBa (94374)2127

Medium: N,N-dimethylformamide. DH(K1)=-15.7 kJ mol⁻¹.

Ca++ cal non-aq 25°C 100% U H K1=6.05 1993BDb (94375)2128
Medium: acetone. DH=-40.7 kJ mol⁻¹; TDS=-14.2 Calorimetric titration

Ca++ cal non-aq 25°C 100% C H K1=2.28 1986ICa (94376)2129
Medium: MeOH. DH(K1)=-8.62 kJ mol⁻¹, DS(K1)=14.7 J K⁻¹ mol⁻¹.

Ca++ sp alc/w 25°C 100% U K1=3.50 1981EMb (94377)2130
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

Ca++ gl R4N.X 25°C 0.10M M K1=4.3 1991FGb (94487)2131
B(CaHL)=8.5

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

Ca++ sp non-aq RT 100% C K1=4.84 2001AVa (94509)2132
Method: spectrophotometric titration. Medium: acetonitrile.

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

Ca++ ISE alc/w 25°C 100% U K1=3.8 1988CFa (94554)2133
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

Ca++ gl R4N.X 25°C 0.10M C K1=5.34 2002DCb (94561)2134
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

Ca++ gl R4N.X 25°C 0.10M U K1=6.6 1990AFa (94584)2135

B(CaHL)=15.2

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

Ca++ gl R4N.X 25°C 0.10M U K1=9.0 1990AFa (94598)2136
B(CaHL)=16.7

C16H26O8S4 H4L CAS 53480-92-5 (1162)
Butane-1,1,4,4-tetramercaptopropanoic acid; (CH2.CH(S.CH2.CH2.COOH)2)2

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

Ca++ gl NaClO4 25°C 0.10M U K1=2.55 1975PJa (94637)2137

C16H26O12 H3L CAS 172911-85-2 (7641)
Methyl-2,3,4-tris-0-(2-carboxyethyl)-alpha-D-glucopyranoside;

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

Ca++ ISE KCl 25°C 0.10M C K1=2.07 1995BBf (94641)2138
Method: calcium ion selective electrode. For the beta isomer, K1=2.05

C16H27N5O8 H3L (6621)
1,4,7-Tris(carboxymethyl)-1,4,7,10,13-pentaazacyclopentadecan-9,14-dione;

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

Ca++ gl KCl 25°C 0.10M C K1=5.65 1995IOa (94661)2139

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

Ca++ gl KNO3 20°C 0.10M U K1=6.05 1969NDc (94703)2140

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

Ca++ gl KNO3 20°C 0.10M U K1=9.24 1969NDc (94728)2141

C16H28N2O8 H4L (5138)
1,2-Diaminooctane-N,N,N',N'-tetraethanoic acid;
(HOOCCH2)2N.CH2.CH(C6H13)N(CH2COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Ca++	gl	KNO3	20°C	0.10M	U		K1=11.70	1979MBd (94754)	2142

C16H28N2O8			H4L				(2850)		
1,8-Diaminooctane-N,N,N',N'-tetraethanoic acid; ((H00CCH2)2N(CH2)4)2									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Ca++	gl	KNO3	20°C	0.10M	U		K1=4.6 K(Ca+HL)=3.7	1964ANa (94785)	2143
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Ca++	gl	KCl	20°C	0.10M	U		K1=4.51 K(Ca+HL)=3.68 K(Ca+CaL)=3.03	1955SAb (94786)	2144
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C16H28N4O8			H4L	DOTA			CAS 60239-18-1	(1017)	
1,4,7,10-Tetraazacyclododecane-1,4,7,10-tetraethanoic acid;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Ca++	gl	R4N.X	25°C	0.10M	C		K1=17.219 K(CaL+H)=3.80 K(CaL+2H)=7.57	2000BCa (94853)	2145
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Medium: 0.10 M NMe4Cl.

Ca++	gl	R4N.X	25°C	0.10M	M		K1=16.70	1996CHc (94854)	2146
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Medium: 0.1 M Me4NCl.

Ca++	gl	KCl	25°C	0.10M	C		K1=16.37 K(CaL+H)=3.60	1991CMb (94855)	2147
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Ca++	cal	R4N.X	25°C	0.10M	C	H		1984DFa (94856)	2148
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Medium: 0.10 M Me4NNO3. DH(K1)=-48.9 kJ mol⁻¹, DS(K1)=167 J K⁻¹ mol⁻¹.

Ca++	gl	R4N.X	25°C	0.10M	C		K1=17.226 K(Ca+HL)=8.68 K(Ca+H2L)=3.11	1982DSa (94857)	2149
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Ca++	EMF	KCl	20°C	0.10M	C		K1=15.9	1981SFa (94858)	2150
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Method: Pt/H2 electrode.

Ca++	gl	KCl	20°C	0.10M	U		K1=15.85	1976SFb (94859)	2151

C16H29N3O7			H3L				(7395)		
4,8,12-Tris(carboxymethyl)-1-oxa-4,8,12-triazacyclotetradecane;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Ca++	gl	R4N.X	25°C	0.10M	C		K1=4.85	1997CCa (94949)	2152
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K(Ca(OH)L+H)=9.91

Medium: Me4NNO3

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

Ca++ gl R4N.X 25°C 0.10M C K1=8.51 2000CDd (94958)2153

Medium: 0.10 M (Me4N)NO3.

C16H29N3O9 H4L TTDA-HP (7932)

N'-(2-Hydroxypropyl)di(carboxymethyl)triazadodecanedioic acid;

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

Ca++ gl R4N.X 25°C 0.10M M K1=12.02 2001Cwa (94981)2154

K(Ca+HL)=6.29

Medium: 0.10 M Me4NNO3. Method: by competition with EDTA

C16H29N5O8 H3L (6505)

Diethylenetriaminepentaethanoic acid N,N'-bismethylamide;

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

Ca++ gl NaClO4 25°C 0.10M C H 1993RCa (94994)2155

K(Ca+HL)=2.20

DH(K1)=-25.9, DH(Ca+HL)=-5.3 kJ mol⁻¹. DS(K1)=50, DS(Ca+HL)=24 J K⁻¹ mol⁻¹

Ca++ gl NaCl 25°C 0.10M U K1=7.17 1990CQa (94995)2156

K(CaL+H)=4.45

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

Ca++ gl R4N.X 25°C 0.10M C H K1=8.707 1989DSa (95019)2157

By calorimetry: DH(CaL)=-34.7 kJ mol⁻¹; DS=46.

Ca++ gl NaNO3 25°C 0.10M U K1=8.57 1988HSb (95020)2158

Ca++ gl R4N.X 25°C 0.10M U K1=8.39 1983CRb (95021)2159

C16H30N4O6 H2L (6295)

1,2-Diaminoethane-N,N'-bis(2-propylethanoamide)-N,N'-diethanoic acid;(Me2CHNHCOCH2N(CH2COOH)CH2)2

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

Ca++ gl KCl 25°C 0.10M U K1=6.51 B2=12.66 1999WwA (95068)2160
 K(CaL+H)=3.43
 *K(CaL)=-10.93

 C16H30N4O8 H4L (3473)
 N,N'-Dimethyl-2,2'-ethylenedi-iminobis(ethylenediethanoic acid);

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

Ca++ gl KCl 20°C 0.10M U K1=9.45 1964PCa (95079)2161
 K(Ca+HL)=4.39

 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

Ca++ gl alc/w 25°C 95% M K1=4.01 1990LNa (95115)2162
 Medium: 95% MeOH, 0.05 M Bu4NBr. For the 9,13-dihydroxy- analogue: K1=4.55

 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

Ca++ ISE non-aq 25°C 100% C H K1=5.81 1999WBa (95153)2163
 Medium: N,N-dimethylformamide. Method: competitive titration against
 Ag+, using Ag+ ISE. By calorimetry: DH(K1)=-38.5 kJ mol-1.

 Ca++ gl R4N.X 25°C 0.05M C H K1=7.7 1996BCh (95154)2164
 Medium: 0.05 M Et4NClO4. By calorimetry: DH(K1)=-5.3 kJ mol-1.

 Ca++ kin non-aq 25°C 100% U T K1=3.85 1996GSa (95155)2165
 Medium: DMSO. Also K1=3.72 (T=35 C), 3.60 (T=45 C) and 3.48 (T=55 C).

 Ca++ EMF non-aq 25°C 100% C H K1=3.47 1995CDb (95156)2166
 Medium: DMSO, 0.1 M Et4NClO4. DH=-25.6 kJ mol-1, DS=-19.4 J K-1 mol-1.

 Ca++ sp non-aq 25°C 100% U T H K1=3.67 1994GSb (95157)2167
 At 35 C: K1=3.55; 45 C: K1=3.44; 55 C: K1=3.33. DH(K1)=-21 kJ mol-1, DS=1
 Medium: DMSO

 Ca++ sp non-aq 20°C 100% U K1=6.6 1992PSa (95158)2168
 Medium: DMF, 0.01 M Me4NI

 Ca++ cal alc/w 25°C 100% U H B(Ca2L2) >5 1986BUa (95159)2169
 Medium: MeOH. DH=-32.5 kJ mol-1; DS=80

 Ca++ sp non-aq 25°C 100% U K1=3.29 1983PSc (95160)2170

Medium: DMSO

Ca++ ISE non-aq 25°C 100% U K1=6.67 1981CRa (95161)2171

Medium: DMF

Ca++ ISE non-aq 25°C 100% U K1=11.4 1980CRa (95162)2172

Medium: Propylene carbonate

Ca++ kin oth/un 25°C 0.10M U H K1=6.86 1977LPb (95163)2173

In piperidine buffer, pH 11.5. DH=-5.4 kJ mol⁻¹

Ca++ cal R4N.X 25°C 0.06M C H 1976KLc (95164)2174

Medium: 0.057 M Me4NBr. Method: flow microcalorimetry.

DH(K1)=-12.1 kJ mol⁻¹, DS(K1)=92 J K⁻¹ mol⁻¹.

Ca++ gl R4N.X 25°C 0.05M C I K1=6.95 1975LSc (95165)2175

In 95% MeOH: K1=9.61

Ca++ kin KCl 25°C 0.10M U H K1=6.79 1975LWb (95166)2176

Using stopped-flow. DH=-29.7 kJ mol⁻¹. Also K1=6.95 by potentiometry in 0.04 to 0.08M NMe4Br; DH=-11.3

C16H32N4O4 L (6794)

4,10-Bis(N,N-dimethylethanamido)-1,7-dioxo-4,10-diazacyclododecane;

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

Ca++ cal alc/w 25°C 100% U H K1=>5.5 1990KMb (95317)2177

Medium: MeOH. DH=-46.6 kJ mol⁻¹

C16H32N4O6 H2L (7344)

4,10-Bis(2-hydroxyethyl)-1,4,7,10-Tetraazacyclododecane-1,7-bis(ethanoic acid);

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

Ca++ gl KCl 25°C 0.10M C K1=10.1 1997HTa (95325)2178

C16H32N4O6 L CAS 98608-90-3 (1322)

N,N'-Bis(carbamoylmethyl)-1,7,10,16-tetraoxa-4,13-diazacyclooctadecane;

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

Ca++ gl NaClO4 25°C 0.50M U K1=5.65 1981KMb (95331)2179

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

Ca++ gl NaNO3 25°C 0.10M C K1=7.54 1995MHa (95372)2180

 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

 Ca++ gl R4N.X 25°C 0.10M C K1=2.8 1995LLa (95408)2181
 Medium: Et4NClO4

 C16H34N2O5 L DHPK-21 CAS 106288-71-5 (8327)
 N,N'-Bis(2-hydroxypropyl)-1,4,10-trioxa-7,13-diazacyclopentadecane;

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

 Ca++ gl NaNO3 25°C 0.10M C K1=3.86 1986HBe (95425)2182

 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

 Ca++ gl R4N.X 25°C 0.10M C K1=4.08 1995LLa (95440)2183
 Medium: Et4NClO4

 Ca++ gl NaClO4 25°C 0.50M U K1=4.08 1981KMb (95441)2184

C16H34N4O2 L CAS 60598-04-1 (1530)
 4,7-Dimethyl-1,4,7,10-tetraaza-13,18-dioxabicyclo[8,5,5]eicosane;

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

 Ca++ gl R4N.X 25°C 0.10M U K1=2.2 1978LMa (95466)2185

C16H36N4O4 L (6703)
 1,4,7,10-Tetrakis(2-hydroxyethyl)-1,4,7,10-tetraazacyclododecane;

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

 Ca++ gl R4N.X 25°C 0.10M C K1=7.41 2000DFb (95565)2186
 Medium: 0.10 M Et4NClO4.

 C16H38N4O6P2 H2L CAS 583879-34-9 (9251)
 4,10-Dimethyl-1,4,7,10-tetraazacyclododecane-1,7-bis(methanephosphonic acid
 monoethyl ester);

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

 Ca++ gl R4N.X 25°C 0.10M C K1=3.45 2003BGa (95593)2187
 K(CaL+OH)=3.6
 K(CaL+2OH)=7.2

Medium: 0.10 M Me4NCl.

C16H41N3O12P4 H8L (6911)
N'-Octyl-diethylenetriamine-N,N,N'',N''-tetra(methylenephosphonic acid);

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

Ca++ gl NaClO4 25°C 0.10M M 1987ZGa (95665)2188
K(Ca+HL)=3.63
K(Ca+H2L)=3.43
K(Ca+H3L)=3.22
K(Ca+H4L)2.30

K(Ca+H5L)=0.91.

Ca++ gl oth/un 25°C 0.10M U 1984ZGa (95666)2189

K(Ca+HL)=3.63
K(Ca+H2L)=3.43
K(2Ca+H2L)=7.54
K(Ca+H3L)= 3.22

K(Ca+H4L)=2.30; K(2Ca+H3L)=7.16; K(2Ca+HL)=8.02; K(Ca+H5L)=0.91

C17H12N2O10S2 H5L CAS 3440-76-4 (4119)
2-(2'-Carboxyphenylazo)chromotropic acid;

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

Ca++ gl KNO3 25°C 0.10M U 1971KMb (95715)2190
K(Ca+HL)=3.37

Ca++ gl KNO3 25°C 0.10M U 1968NMb (95716)2191
K(Ca+HL)=3.40

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

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

Ca++ gl mixed 25°C 75% U K1=6.96 1972MCb (95790)2192
Medium: 75% acetone, 0.1 M KNO3

C17H14N2O HL CAS 6756-41-8 (5215)
1-(4-Methylphenylazo)-2-hydroxynaphthalene;

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

Ca++ gl mixed 25°C 75% U K1=7.58 1972MCb (95805)2193
Medium: 75% acetone, 0.1 M KNO3

C17H14N2O2 HL CAS 1229-55-6 (5216)
1-(2-Methoxyphenylazo)-2-hydroxynaphthalene;

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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  mixed  25°C  75%  U          K1=7.66      1972MCb (95824)2194
Medium: 75% acetone, 0.1 M KNO3
*****
C17H14N2O2      HL          CAS 13441-91-1 (5217)
1-(4-Methoxyphenylazo)-2-hydroxynaphthalene;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  mixed  25°C  75%  U          K1=7.39      1972MCb (95839)2195
Medium: 75% acetone, 0.1 M KNO3
*****
C17H14N2O8S2    H4L          CAS 15475-90-8 (2605)
2-(2-Tolylazo)-chromotropic acid;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  KNO3   25°C  0.10M U          K(Ca+HL)=2.56
*****
C17H14N2O9S2    H4L          (5228)
2-(2-Methoxyphenylazo)chromotropic acid;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  KNO3   25°C  0.10M U          K(Ca+HL)=3.25
*****
C17H16O4         H2L          CAS 4372-32-1 (486)
Dibenzylpropanedioic acid; HOOC.C(CH2.C6H5)2.CO0H
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      sp  none   25°C  0.0  U          K1=2.56      1976K0a (96174)2198
*****
C17H18N3O3F     HL  Ciprofloxacin CAS 189257-90-7 (7142)
1-Cyclopropyl-6-fluoro-1,4-dihydro-4-oxo-7[1-piperazinyl]-3-quinoline carboxylic
acid;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  KCl    25°C  0.20M C          K1=3.17      1996TBc (96221)2199
B(CaHL)=11.29
*****
C17H20N4O6      HL  Riboflavin      CAS 83-88-5 (1438)
7,8-Dimethyl-10(D-1'-ribityl)isoalloxazine, Vitamin B2, Vitamin H
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
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Ca++ sol mixed 25°C 95% U K1=2.1 1983LRb (96327)2200
Medium: acetone, 1 M LiClO4.3H2O. Also data in MeCN

Ca++ sol oth/un 22°C U K1=0.23 1980Lda (96328)2201
Medium: variable Ca(ClO4)2 content 0.1-0.9 M
The same constant measured spectrophotometrically: K1=-0.65

C17H21N4O9P H3L CAS 130-40-5 (3495)
Flavin mononucleotide, Riboflavin-5'-phosphoric acid;

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

Ca++ ix NaCl 23°C 0.10M U K1=2.06 1958WAa (96383)2202

C17H22N2O9 H5L CAS 85929-35-7 (3493)
2-Hydroxy-5-methyl-1,3-phenylenebis(methyliminodiethanoic acid);

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

Ca++ EMF KCl 20°C 0.10M C K1=8.4 1952SAb (96402)2203
K(Ca+HL)=6.67
K(Ca+H2L)=2.8

Method: H electrode

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

Ca++ gl R4N.X 25°C 0.10M C K1=12.379 1997DQa (96445)2204
K(CaL+H)=3.66

Medium:Me4NNO3

Ca++ EMF KCl 20°C 0.10M C K1=8.3 1981SFa (96446)2205
Method: Pt/H2 electrode.

C17H26N4O4 H2L CAS 205595-08-0 (8972)
3,11-Bis(carboxymethyl)-3,7,11,17-tetraazabicyclo[11.3.1]heptadeca-1(17),13,15-triene;

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

Ca++ gl R4N.X 25°C 0.10M C K1=3.32 1998CDa (96501)2206
Medium: 0.10 M Me4NNO3.

C17H27N05 L CAS 98269-22-8 (8844)
13-(2-Methoxyphenyl)-1,4,7,10-tetraoxa-13-azacyclopentadecane;

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

Ca++ sp alc/w RT 50% C I K1=1.7 2002GNe (96542)2207
Medium: 50% v/v MeOH/H2O, pH 7.4 (0.01 M Tris buffer), 0.1 M Me4NCl.
In 10% MeOH/H2O, K1=1.2.

C17H28O8S4 H4L (1163)
Pentane-1,1,5,5-tetramercaptopropionic acid; CH2(CH2.CH(S.CH2.CH2.COOH)2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Ca++	gl	NaClO4	25°C	0.10M	U			K1=3.11	1975PJa (96562)2208	
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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
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Ca++	gl	KCl	25°C	0.10M	C			K1=16.37 K(CaL+H)=3.60	1991CMb (96623)2209	
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Ca++	cal	KNO3	25°C	0.10M	C	H			1984DFa (96624)2210	
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DH(K1)=-25.5 kJ mol⁻¹, DS(K1)=146 J K⁻¹ mol⁻¹.

Ca++	gl	KNO3	25°C	0.10M	C			K1=12.085 K(Ca+HL)=5.451	1982DSa (96625)2211	
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Ca++	EMF	KCl	20°C	0.10M	C			K1=10.4	1981SFa (96626)2212	
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Method: Pt/H2 electrode.

Ca++	gl	KCl	20°C	0.10M	U			K1=8.06	1976SFb (96627)2213	
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C17H30O6 H2L CAS 159029-04-6 (7605)
15-(Methoxymethoxy)-9,11-dioxo-pentadecanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Ca++	sp	alc/w	RT	80%	C			K1=2.23	1994HWc (96669)2214	
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Medium: 80%MeOH/H2O. Also data for many analogues.

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
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Ca++	gl	R4N.X	25°C	0.10M	C			K1=7.23 *K(CaL)=-9.7	2000CDd (96677)2215	
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Medium: 0.10 M (Me4N)NO3.

C17H32N4O6 H3L (6696)
1,4,7,10-Tetraazacyclododecane-1,4,7-tri(2-methyl)ethanoic acid;

C8H17N4(CH(CH3)COOH)3

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

Ca++ gl R4N.X 25°C 0.10M C K1=13.82 1995Kta (96688)2216
K(CaL+H)=5.76
K(Ca+HL)=6.2

Medium: Me4NCl

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

Ca++ gl R4N.X 25°C 0.10M M K1=10.65 1996CHc (96692)2217
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

Ca++ gl R4N.X 25°C 0.10M C K1=14.06 2000BCa (96707)2218
K(CaL+H)=5.38

Ca++ gl R4N.X 25°C 0.10M M K1=14.18 1996CHc (96708)2219
Medium: 0.1 M Me4NCl.

Ca++ gl R4N.X 25°C 0.10M C K1=14.83 1995Kta (96709)2220
Medium: 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

Ca++ gl R4N.X 25°C 0.10M M K1=13.96 1996CHc (96723)2221
Medium: 0.1 M Me4NCl

C17H32N4O9 H3L CAS 124628-01-9 (2013)
1,4,7,10-Tetraazacyclododecane-1,4,7-tri(2-hydroxymethylethanoic acid);

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

Ca++ gl R4N.X 25°C 0.10M C K1=8.84 2000BCa (96730)2222
K(CaL+H)=5.80
K(CaL+2H)=11.34
K(CaL+OH)=5.94

Medium: 0.10 M NMe4Cl.

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

Ca++ gl alc/w 25°C 95% C K1=2.24 2004KVa (96754)2223
Medium: 95% MeOH/H2O, 0.01 M Et4NC1O4.

C17H36N4O4 H2L (8282)
2,12-Dimethyl-5,9-di(2-carboxyethyl)-2,5,9,12-tetraazatridecane;

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

Ca++ gl KNO3 25°C 0.10M C K1=1.9 1989HAa (96777)2224

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

Ca++ gl NaNO3 25°C 0.10M U K1=4.60 1988HSb (96783)2225

C18H12N2O11S2 H5L (5251)
2-(2'-Oxalophenylazo)chromotropic acid;

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

Ca++ gl KNO3 25°C 0.10M U 1971KMb (96866)2226

K(Ca+HL)=3.41

C18H14N2O3 H3L (4127)
2-(2',4'-Dihydroxyphenylazo)-4-phenylphenol;

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

Ca++ sp KCl rt 0.10M U 1960DEa (96915)2227

K1eff=1.68 (pH 10)

C18H14N2O9S2 H4L (5252)
2-(2'-Methyl-benzoylazo)chromotropic acid;

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

Ca++ gl KNO3 25°C 0.10M U 1971KMb (96933)2228

K(Ca+HL)=2.95

C18H14N2O10S2 H5L (5253)
2-(2-Phenylethanoic acidazo)chromotropic acid;

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

Ca++ gl KNO3 25°C 0.10M U K1=7.2 1958FFa (97383)2236
K(Ca+HL)=4.8
K(Ca+H2L)=1.7

C18H20N4O4 H2L (7083)
2,11-Diaza[3.3](2,6)pyridinophane-N,N'-diethanoic acid;

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

Ca++ gl KCl 25°C 0.10M C K1=10.0 1995KHa (97469)2237

C18H22N2O8 H4L (5244)
(trans-1,2,3,4-Tetrahydronaphthalene-2,3-dinitrilo)tetraethanoic acid;

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

Ca++ gl KNO3 25°C 0.10M U K1=11.63 1970YKa (97525)2238

C18H22N4O4 H2L CAS 2444-14-6 (3502)
N,N'-Bis(2-pyridylmethyl)diaminoethane-N,N'-diethanoic acid;

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

Ca++ gl oth/un 25°C 0.10M U K1=7.9 1965LCa (97535)2239

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

Ca++ gl diox/w 24°C 50% U K1=6.3 1979ACa (97556)2240

C18H24N2O2 H2L CAS 58015-12-6 (5245)
N,N'-Bis(2-hydroxy-5-methylphenylmethylene)ethylenediamine;

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

Ca++ EMF oth/un ? ? U K1=9.5 1975DTa (97583)2241
K(Ca+H2L)=2.2

C18H26N4O8 H4L CAS 319016-30-3 (7715)
N'-(2-Pyridylmethyl)-diethylenetriamine-N,N,N'',N''-tetraethanoic acid;

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

Ca++ gl R4N.X 25°C 0.10M M K1=8.35 2000Cwa (97690)2242
Medium: 0.1 M NMe4NO3.

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

Ca++ gl KCl 25°C 0.10M M K1=4.4 1996MBb (97706)2243

Ca++ gl KCl 25°C 0.20M C K1=4.4 1992RMa (97707)2244

C18H26O8N2P2 H6L CAS 53431-87-1 (2325)
N,N'-Bis(2-hydroxybenzyl)ethylenediamine-N,N'-bis(methylenephosphonic)

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

Ca++ gl KNO3 25°C 0.10M C K1=8.36 1975MMc (97738)2245
K(Ca+H2L)=3.61
K(CaL+H)=10.72
K(CaHL+H)=9.59

C18H27N2O3F L CAS 173417-90-8 (6571)
23-Fluoro-4,7,20-trioxa-1,10-diazatricyclo[8.7.5.1,12,16]tricoso-12,14,16(23)triene
;

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

Ca++ EMF non-aq 25°C 100% C H K1=2.21 1999BHa (97745)2246
Medium: MeOH, 0.05 M Et4NClO4. By calorimetry DH(K1)=-0.4 kJ mol⁻¹.
Method: by competition with Ag+, using Ag/Ag+ electrode.

C18H27N3O12 H6L (3503)
1,3,5-Triaminocyclohexane-N,N,N',N',N'',N''-hexaethanoic acid;

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

Ca++ gl KCl 30°C 0.10M U K1=5.5 1963GHa (97752)2247
K(CaL+Ca)=3.6
K(Ca+HL)=4.7
K(Ca+H2L)=2.9

C18H28N4O4 H2L (7378)
7-Methyl-3,7,11,17-tetraazabicyclo[11.3.1]heptadeca-1(17),13,15-triene-3,11-diethan
oic acid;

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

Ca++ gl R4N.X 25°C 0.10M C K1=3.74 1997CDb (97780)2248
Medium: NMe4NO3

C18H28N4O10 H3L Ac-DVDA CAS 93620-52-1 (5414)
N-Acetyl-aspartyl-valyl-aspartyl-alanine;

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

Ca++ gl KCl 25°C 0.50M U K1=3.60 1984ABc (97789)2249
B(CaHL)=3.11

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

Ca++ EMF non-aq 25°C 100% U K1=6.05 1982MRb (97799)2250
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

Ca++ gl diox/w 24°C 50% U K1=7.4 1979ACa (97826)2251

C18H28O10 H2L (OEOAcAcOE)2 CAS 62950-36-1 (2254)
1,4,10,13,16,22-Hexaoxacyclotetracosane-6,8,18,20-tetraone;

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

Ca++ gl diox/w 24°C 50% U K1=7.8 1979ACa (97864)2252

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

Ca++ gl R4N.X 25°C 0.10M C K1=5.36 2002DCb (97902)2253
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

Ca++ gl NaCl 25°C 0.15M U K1=7.55 1995BGa (97923)2254

C18H30N4O12 H6L CAS 869-52-3 (3504)
2,2',2''-Nitrilotris(ethyliminodiethanoic acid); N(CH2.CH2.N(CH2.COOH)2)3

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

Ca++ EMF KCl 20°C 0.10M C K1=9.4 1964PCa (97939)2255
K(Ca+HL)=7.65

Method: H electrode

C18H30N4O12 H6L TTHA CAS 869-52-3 (694)
 Triethylenetetraaminehexaethanoic acid;((HOOC.CH2)2N.CH2.CH2.N(CH2.COOH).CH2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	KNO3	20°C	0.10M	U			K1=10.52 K(CaHL+H)=4.75 K(CaL+H)=8.56 K(Ca+CaL)=4.3	1969ALb (97987)	2256
Ca++	gl	KNO3	25°C	0.10M	U			K(CaHL+H)=4.87 K(CaL+H)=8.53 B(Ca2L)=14.2	1967BMd (97988)	2257
Ca++	gl	KNO3	25°C	0.10M	U			K1=9.89 K(Ca+H2L)=3.76 K(Ca+HL)=8.23 K(CaL+Ca)=4.32 K(Ca2L+Ca)=3.01	1965BMf (97989)	2258
Ca++	gl	KCl	30°C	0.10M	U			K1=10.06 K(Ca+H2L)=2.4 K(Ca+HL)=8.07 K(CaL+Ca)=4.10	1963GHa (97990)	2259

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
Ca++	gl	KCl	25°C	0.10M	C			K1=8.53 K(CaL+H)=6.99	1991CMb (98168)	2260
Ca++	cal	KNO3	25°C	0.10M	C	H			1984DFa (98169)	2261
DH(K1)=-8.8 kJ mol ⁻¹ , DS(K1)=130 J K ⁻¹ mol ⁻¹ .										
Ca++	gl	KNO3	25°C	0.10M	C			K1=8.322 K(Ca+HL)=5.09	1982DSa (98170)	2262

Ca++ EMF KCl 20°C 0.10M C K1=9.5 1981SFa (98171)2263
 Method: Pt/H2 electrode.

Ca++ gl KCl 20°C 0.10M U K1=9.48 1976SFb (98172)2264

 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

Ca++ EMF KCl 20°C 0.10M C K1=11.9 1981SFa (98241)2265
Method: Pt/H2 electrode. For the 3-ethyl- derivative, K1=8.3;
for the 3,3-dimethyl- derivative, K1=4.3

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

Ca++ gl R4N.X 25°C 0.10M C K1=10.14 1999CDb (98252)2266
K(CaL+Ca)=3.04

Medium: 0.10 M NMe4NO3.

C18H33N09 HL 4NH18-C6A CAS 83572-66-1 (5404)
2-Carboxy-3-N-butylformamide-1,4,7,10,13,16-hexaoxacyclooctadecane;

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

Ca++ gl alc/w 25°C 90% U K1=5.8 B2=9.9 1984FWa (98285)2267
Medium: 90% v/v MeOH/H2O, 0.05 M R4NX

C18H34N2O8 H2L CAS 68670-15-5 (5851)
1,4,10,13-Tetraoxa-7,16-diazacyclooctadecane-7,16-di-(3-propanoic acid);

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

Ca++ gl KCl 25°C 0.15M U K1=7.10 1995BGa (98330)2268

C18H34N4O6 H2L (6845)
1,2-Diaminoethane-N,N'-bis(t-butylethanoamide)-N,N'-diethanoic
acid;Me3CNHCOCH2N(CH2COOH)CH2)2

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

Ca++ gl KCl 25°C 0.10M U K1=6.65 B2=13.42 1999WWa (98363)2269
K(CaL+H)=3.46
*K(CaL)=-11.09

C18H34N4O8 H3L (7256)
1,4,7,10-Tetraazacyclododecane-1-(2-hydroxy-3-methoxypropyl)-4,7,10-triethanoic
acid;

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

Ca++ gl R4N.X 25°C 0.10M M K1=13.72 1996CHc (98366)2270
Medium: 0.1 M Me4NCl

C18H34N4O9 H3L DO3A-B (7301)
10-[2,3-Dihydroxy-(1-hydroxymethyl)-propyl]-1,4,7,10-tetraazacyclododecane-1,4,7-triethanoic ac.;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	NaCl	25°C	0.10M	C	I		K1=12.1	1996TKa (98373)	2271
In 0.1 M KCl K=13.3; In 0.1 M Me4NCl K=14.3 *****										
C18H36N2O5		L				Cryptand 1,2,2H		(6605)		
1,10-Diaza-4,7,14,20,23-Pentaoxabicyclo[8.8.7]pentacosane;										
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	alc/w	25°C	95%	M			K1=5.20	1990LNa (98403)	2272
Medium: 95% MeOH, 0.05 M Bu4NBr. For the 12,16-dihydroxy- analogue: K1=5.92 *****										
C18H36N2O5		L				Cryptand 2,2,1H		CAS 119017-37-7 (6588)		
5,8,15,18,23-Pentaoxa-1,12-diazabicyclo[10.8.5]pentacosane;										
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	alc/w	25°C	95%	M			K1=4.36	1990LNa (98411)	2273
Medium: 95% MeOH, 0.05 M Bu4NBr. For the 9,16-dihydroxy- analogue: K1=5.63 *****										
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
Ca++	cal	non-aq	25°C	100%	C	H		K1=3.16	1999WBa (98479)	2274
Medium: N,N-dimethylformamide. DH(K1)=-17.0 kJ mol ⁻¹ .										
Ca++	gl	R4N.X	25°C	0.05M	C	H		K1=5.9	1996BCh (98480)	2275
Medium: 0.05 M Et4NClO4. By calorimetry: DH(K1)=-2.3 kJ mol ⁻¹ .										
Ca++	sp	non-aq	25°C	100%		U		K1=2.03	1994GSb (98481)	2276
Medium: DMSO										
Ca++	gl	non-aq	25°C	100%		U	H	K1=12.9	1993BDb (98482)	2277
Medium: acetone. DH=-73.5 kJ mol ⁻¹ ; TDS=-0.2										
Ca++	cal	non-aq	25°C	100%	C	H			1992BSc (98483)	2278
Medium: propylene carbonate. DH(K1)=-63.8 kJ mol ⁻¹ , DS(K1)=-9.1 J K ⁻¹ mol ⁻¹ .										
Ca++	ISE	oth/un	25°C	0.05M		M		K1=8.14	1992BUb (98484)	2279
K1=8.16 (by calorimetric competitive titration)										
Ca++	sp	non-aq	20°C	100%		U		K1=3.98	1992PSa (98485)	2280
Medium: DMF, 0.01 M Me4NI										
Ca++	EMF	R4N.X	25°C	0.10M	C	IH		K1=4.91	1987CSa (98486)	2281

In 0.1M Et4NClO4. In 5% CH3CN, K=5.43; 10%, K=5.77; 20%, K=6.11; 30%, K=6.67
 40%, K=7.01; 50%, K=7.60, 60%, K=8.12; 100%, K=10.5

 Ca++ cal alc/w 25°C 100% U H 1986BUa (98487)2282
 B(Ca2L2)=8.16

Medium: MeOH. DH=-22.0 kJ mol-1; DS=82

 Ca++ con none 25°C 0.0 C K1=4.26 1986KHe (98488)2283
 Method: conductance stopped-flow. Medium pH 11.3.

 Ca++ ISE non-aq 25°C 100% U K1=10.76 1984CTc (98489)2284
 In propylene carbonate

 Ca++ sp non-aq 25°C 100% U K1=1.91 1983PSc (98490)2285
 Medium: DMSO

 Ca++ gl alc/w 25°C 95% C K1=7.5 1981ANa (98491)2286
 Medium: 95% MeOH, 0.1 M Me4NCl

 Ca++ ISE non-aq 25°C 100% U K1=3.84 1981CRa (98492)2287
 Medium: DMF

 Ca++ ISE non-aq 25°C 100% U K1=10.7 1980CRa (98493)2288
 Medium: Propylene carbonate

 Ca++ kin oth/un 25°C 0.10M U H K1=4.45 1977LPb (98494)2289
 In piperidine buffer, pH 11.5. DH=-2.1 kJ mol-1.

 Ca++ cal R4N.X 25°C 0.06M C IH 1976KLc (98495)2290
 Medium: 0.057 M Me4NBr. Method: flow microcalorimetry. DH(K1)=-0.8 kJ
 mol-1, DS(K1)=82 J K-1 mol-1. In 95% (v/v) MeOH/H2O, DH(K1)=-27.6, DS=53.

 Ca++ gl R4N.X 25°C 0.10M C H K1=4.57 1975ANa (98496)2291
 Medium: Me4NCl. DH(K1)=-0.8 kJ mol-1, DS=84.1

 Ca++ gl R4N.X 25°C 0.05M C I K1=4.4 1975LSc (98497)2292
 In 95% MeOH: K1=7.60

 Ca++ kin KCl 25°C 0.10M U H K1=4.40 1975LWb (98498)2293
 Using stopped-flow. DH=-2.9 kJ mol-1. By potentiometry K1=4.40 in 0.04-0.08
 NMe4Br.

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

 Ca++ cal alc/w 25°C 100% U H K1=4.10 1990KMb (98779)2294
 Medium: MeOH. DH=-45.9 kJ mol-1

C18H36N4O6 H2L (7345)
4,10-Bis(2-hydroxypropyl)-1,4,7,10-Tetraazacyclododecane-1,7-bis(ethanoic acid);

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

Ca++ gl KCl 25°C 0.10M C K1=11.0 1997HTa (98787)2295

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

Ca++ gl R4N.X 25°C 0.10M C K1=2.4 1995LLa (98831)2296
Medium: Et4NC1O4

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

Ca++ gl NaNO3 25°C 0.10M U K1=3.59 1986HBc (98849)2297

C18H38N4O8P2 H6L CAS 187240-55-7 (7347)
1,4,7,10-Tetraazacyclododecane-1,7-bis(ethanoic acid)-4,10-bis(methylene-ethylphosphonic acid);

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

Ca++ gl KCl 25°C 0.10M C K1=9.7 1997HTa (98865)2298

C18H38N4O10P2 H6L CAS 187240-54-6 (7346)
1,4,7,10-Tetraazacyclododecane-1,7-bis(ethanoic acid)-4,10-bis(ethylmethylenephosphonic acid);

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

Ca++ gl KCl 25°C 0.10M C K1=9.4 1997HTa (98869)2299

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

Ca++ gl R4N.X 25°C 0.10M U K1=5.43 1996BJa (98886)2300
Medium: 0.1 M Me4NC1

C19H17N3O4S2 HL Cephaloridine CAS 50-59-9 (8404)
7-[a-(2-Thienyl)acetamido]-3-(1-pyridylmethyl)-3-cephem-4-carboxylic acid betaine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	gl	KNO3	25°C	0.10M	C		K1=3.75	2000GFb (99188)	2301

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
Ca++	gl	diox/w	30°C	75%	U		K1=6.5	1965SMh (99245)	2302

C19H19N07			H2L				(7003)		
3-Methoxy-5-(N,N-dicarboxymethyl)aminomethyl-4-hydroxybenzophenone;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	gl	KCl	20°C	0.10M	U		K1=6.7 K(Ca+HL)=3.0	1981SYa (99256)	2303

C19H20N2O2			L	Butazolidine			CAS 50-33-9	(4143)	
4-Butyl-1,2-diphenylpyrazolidine-3,5-dione;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	gl	alc/w	20°C	50%	U		K1=1.35	1957WSa (99293)	2304
Medium: 50% EtOH, 0.1 M KCl									

C19H22N2O6			H4L				CAS 102165-09-3	(9199)	
Propylenediamine-N,N'-bis(2-hydroxyphenylethanoic acid);									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	gl	NaCl	25°C	0.10M	C		K1=6.17 B(CaHL)=16.43 B(CaH2L)=25.86	2004SGb (99325)	2305

Additional method: UV-visible spectrometry

C19H23O6P			L				(5731)		
1,2:8,9-Dibenzo-5-methylphosphinyl-3,7,10,13,16-pentaoxacyclohexadeca-1,8-diene;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	oth	non-aq	25°C	100%	U		K1=2.44 B2=4.79	1989SSc (99343)	2306
Medium: CH3CN. Ca as Ca(NCS)2; for Ca(ClO4)2: K1=3.02; B2=5.74. Method: IR									
With 5-adamantyl analogue: K1=3.6, B2=6.1									

C19H28N4O6			H3L				CAS 106967-44-6	(8973)	
3,7,11-Tris(carboxymethyl)-3,7,11,17-tetraazabicyclo[11.3.1]heptadeca-1(17),13,15-triene;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	gl	R4N.X	25°C	0.10M	C		K1=5.85	1998CDa (99404)	2307
Medium: 0.10 M Me4NNO3. *****									
C19H28N4O8		H4L		TTDA-PY			(7933)		
N'-(2-Pyridylmethyl)di(carboxymethyl)triazadodecanedioic acid;									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	gl	R4N.X	25°C	0.10M	M		K1=12.02 K(Ca+HL)=7.96	2001CWa (99415)	2308
Medium: 0.10 M Me4NNO3. Method: by competition with EDTA *****									
C19H30O14		H4L					CAS 172606-64-3	(7668)	
Methyl-1,3,4,5-tetrakis-0-(2-carboxyethyl)-beta-D-fructopyranoside;									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	ISE	KCl	25°C	0.10M	C		K1=2.25	1995BBf (99440)	2309
Method: calcium ion selective electrode. *****									
C19H30O14		H4L					CAS 172606-65-4	(7683)	
Methyl-1,3,4,6-tetrakis-0-(2-carboxyethyl)-alpha-D-fructofuranoside;									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	ISE	KCl	25°C	0.10M	C		K1=2.13	1995BBf (99441)	2310
Method: calcium ion selective electrode. *****									
C19H30O14		H4L					CAS 172911-87-4	(7642)	
Methyl-2,3,4,6-tetrakis-0-(2-carboxyethyl)-alpha-D-glucopyranoside;									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	ISE	KCl	25°C	0.10M	C		K1=2.28	1995BBf (99443)	2311
Method: calcium ion selective electrode. For the beta isomer, K1=2.18 *****									
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
Ca++	gl	R4N.X	25°C	0.10M	C		K1=3.29 K(Ca+HL)=2.74	1988DDa (99462)	2312
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
Ca++	gl	R4N.X	25°C	0.10M	U		K1=4.6	1978LMa (99485)	2313

C20H13N3O7S		H3L		Eriochrome B1 T			CAS 1787-61-7	(997)	
1-(1-Hydroxy-2-naphthylazo)-6-nitro-2-naphthol-4-sulfonic acid;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	sp	oth/un	18°C	0.02M	U		K1=5.4	1948SBa (99554)	2314

C20H13N3O7S		H3L		EriochromeBla A			CAS 16279-54-2	(5299)	
3-Hydroxy-4-(2-hydroxy-1-alpha-naphthylazo)-7-nitronaphthalene-1-sulfonic acid;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	sp	oth/un	18°C	0.02M	U		K1=5.25	1948SBa (99582)	2315

C20H14N2O		HL					(5291)		
1-(1-Naphthylazo)-2-hydroxynaphthalene;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	gl	mixed	25°C	75%	U		K1=6.03	1972MCb (99594)	2316
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
Ca++	gl	mixed	25°C	75%	U		K1=6.77	1972MCb (99609)	2317
Medium: 75% acetone, 0.1 M KNO3									

C20H14N2O2		H2L					CAS 13082-06-9	(3506)	
1,1'-Azo-(2-hydroxynaphthalene);									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	gl	diox/w	30°C	75%	U			1957SFb (99624)	2318
K(Ca+H2L=CaL+2H)=-15.0									

C20H14N2O5S		H3L		Solochrome 6B			CAS 3564-14-5	(3507)	
1-(1-Hydroxy-2-naphthylazo)-2-naphthol-4-sulfonic acid, Mordant Black3, Eriochrome blue-black B;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	sp	oth/un	18°C	0.02M	U		K1=5.7	1948SBa (99641)	2319

C20H14N2O5S H3L EriochrBluBlk R CAS 2538-85-4 (3508)
3-Hydroxy-4-(2-hydroxy-1-naphthylazo)naphthalene-1-sulfonic acid;

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

Ca++ sp oth/un 25°C 0.10M U K1=5.58 1957HRa (99682)2320

Ca++ sp oth/un 18°C 0.02M U K1=5.25 1948SBa (99683)2321

C20H14N2O8S2 H4L PalatineFB GGNA CAS 89276-70-0 (3509)
3-Hydroxy-4-(1-hydroxy-8-sulfo-2-naphthylazo)naphthalene-1-sulfonic acid;

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

Ca++ gl oth/un ? ? U K1=7.5 1959RSb (99703)2322

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

Ca++ sp none 25°C 0.0 U K(Ca+HL=CaL+H)=7.79
1980WNa (99721)2323

Data for similar ligands also included

Ca++ sp none 25°C 0.0 U K1eff=2.82
1978BRb (99722)2324

Keff at pH 10

C20H16N2O HL CAS 36458-50-1 (5293)
2-(Naphthylaminomethyl)-8-hydroxyquinoline;

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

Ca++ gl diox/w 25°C 50% U K1=3.5 1972HUb (99760)2325
Medium: 50% v/v dioxan, 0.1 M KCl

C20H16N2O2 H2L CAS 3946-91-6 (2733)
N,N'-Bis(2'-hydroxybenzylidene)-1,2-diaminobenzene; (HOC6H4CH:N)2.C6H4

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

Ca++ gl mixed 25°C 80% C K1=4.28 1997HMc (99769)2326
B(CaHL)=13.49

Medium: 80% w/w DMSO/H2O, 0.5 M NaClO4.

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

Ca++ gl diox/w 30°C 75% U 1957SFb (99791)2327
K(Ca+H2L=CaL+2H)=-14.5

C20H19N08 L (2558)
4-Dedimethylamino-tetracycline;

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

Ca++ gl NaCl 37°C 0.15M C K1=4.061 B2=5.913 1988LVa (99852)2328

C20H21N3O8S2 H4L (2841)
2-(2-Hydroxy-3,6-disulfo-1-naphthylazo)-5-(N,N-diethylamino)phenol;

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

Ca++ sp none 25°C 0.0 U K1=6.5 1984WNa (99912)2329

C20H22O9 H2L (5624)
1,7-bis(2-Carboxymethoxyphenyl)-1,4,7-trioxaheptane;

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

Ca++ gl alc/w 25°C 90% M K1=6.07 1998KLa (99936)2330

Medium: 90% v/v MeOH/H2O, 0.1 M Me4NCl

C20H24N2O6 H4L CAS 115538-91-5 (9198)
Butylenediamine-N,N'-bis(2-hydroxyphenylethanoic acid);

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

Ca++ gl NaCl 25°C 0.10M C K1=7.16 20045Gb (99958)2331

B(CaHL)=16.31
B(CaH2L)=25.47
Additional method: UV-visible spectrometry

C20H24N2O6 H4L HBED CAS 3625-89-6 (2208)

N,N'-Di-(2-hydroxybenzyl)-diaminoethane-N,N'-diethanoic acid;

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

Ca++ gl KNO3 25°C 0.10M U K1=9.29 1967LMd (99982)2332

K(Ca+HL)=5.52
K(Ca+H2L)=2.02

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

Ca++ EMF alc/w 25°C 100% C K1=3.34 2004ZTa (100069)2333
Medium: 100% methanol, 0.05 M Bu4NClO4. Method: Ag electrode,
competition with Ag+ ion.

Ca++ con mixed 25°C 20% C K1=3.78 2003SIa (100070)2334
Medium: 20% w/w propylene carbonate/ethylene carbonate.

Ca++ vlt non-aq 25°C 100% C K1=3.23 1991SSb (100071)2335
Method: competitive complexation with Tl+; use of Tl(Hg)/Tl couple.
Medium: acetonitrile, 0.05 M Et4NClO4.

Ca++ dis non-aq 25°C 100% U K1=3.8 1989DMa (100072)2336
Medium: CHCl3

Ca++ oth non-aq 25°C 100% U K1=4.2 1989SSc (100073)2337
Medium: CH3CN. Ca as Ca(NCS)2; for Ca(ClO4)2: K1=4.6. Method: IR-spec.

Ca++ vlt alc/w 25°C 100% C K1=3.52 1987CBd (100074)2338
B(Ca2L)=5.98
Medium: methanol, 0.10 M Et4NI or Bu4NClO4. Method: polarography.

Ca++ sol none 25°C 0.0 U I K1=0.0 1975SNa (100075)2339

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

Ca++ EMF non-aq 25°C 100% C H K1=4.36 1999BHa (100437)2340
Medium: MeOH, 0.05 M Et4NClO4. By calorimetry DH(K1)=-2.2 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

Ca++ EMF non-aq 25°C 100% C H K1=2.15 1999BHa (100454)2341
Medium: MeOH, 0.05 M Et4NClO4. By calorimetry DH(K1)=3.7 kJ mol-1.
Method: by competition with Ag+, using Ag/Ag+ electrode.

C20H34O5 HL ProstaglandinE1 CAS 745-65-3 (6330)
Prostaglandin E1, [11a,13E,15S]-11,15-Dihydroxy-9-oxoprost-13-enoic acid

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

Ca++ dis NaNO3 20°C 0.15M C K1=1.57 1973APa (100523)2342
Method: ion exchange using 45Ca isotope. With prostaglandin F1(beta): K1=0.9

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

Ca++ EMF KCl 20°C 0.10M C K1=3.1 1981SFa (100571)2343
Method: Pt/H2 electrode. For the 3,3,10,10-tetramethyl- homologue, K1=3.0

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

Ca++ EMF alc/w 25°C 100% C K1=3.94 2004ZTa (100613)2344
Medium: 100% methanol, 0.05 M Bu4NClO4. Method: Ag electrode,
competition with Ag+ ion.

Ca++ con mixed 25°C 20% C K1=3.81 2003SIa (100614)2345
Medium: 20% w/w propylene carbonate/ethylene carbonate.

Ca++ vlt non-aq 25°C 100% C K1=3.96 1991SSb (100615)2346
Method: competitive complexation with Tl+; use of Tl(Hg)/Tl couple.
Medium: acetonitrile, 0.05 M Et4NClO4.

C20H37N5O8 H3L (7381)
Diethylenetriamine-N,N,N',N'',N''-pentaethanoic acid bis(isopropylamide);

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

Ca++ gl KCl 25°C 0.10M C K1=7.39 1997WCa (100728)2347

C20H38N4O10 H3L CAS 214461-75-3 (1659)
10-(2-Hydroxypropyl)-1,4,7,10-tetraazacyclododecane-1,4,7-tris(2-hydroxymethylethanoic acid);

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

Ca++ gl R4N.X 25°C 0.10M C K1=11.09 2000BCa (100747)2348
K(CaL+Ca)=3.70
Medium: 0.10 M NMe4Cl.

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

Ca++ gl alc/w 25°C 95% M K1=3.75 1990LNa (100781)2349
Medium: 95% MeOH, 0.05 M Bu4NBr. For the 12,19-dihydroxy- analogue: K1=6.64

C20H40N2O6 L Cryptand 3,2,1H (6589)

1,7-Diaza-4,11,14,17,23,26-hexaoxabicyclo[13.8.5]octacosane;

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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  alc/w  25°C  95%  M      K1=3.72      1990LNa (100790)2350
Medium: 95% MeOH, 0.05 M Bu4NBr. For the 9,19-dihydroxy- analogue: K1=6.81
*****
C20H40N2O7      L      Cryptand 3,2,2      CAS 31255-22-8 (1763)
Cryptand 3,2,2
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  alc/w  25°C  90%  M      K1=4.74      1977LSc (100803)2351
Medium: 90% (w/w) MeOH/H2O, 0.1 M Et4NBr.
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Ca++      cal R4N.X  25°C  0.06M C  H      1976KLc (100804)2352
Medium: 0.057 M Me4NBr. Method: flow microcalorimetry.
DH(K1)=-0.7 kJ mol-1, DS(K1)=40 J K-1 mol-1.
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Ca++      gl  R4N.X  25°C  0.05M C  I      K1=2.0      1975LSc (100805)2353
In 95% MeOH: K1=4.47
*****
C20H40N8O4      L      CAS 219143-29-0 (1185)
1,4,7,10-Tetrakis(methylcarbamoylemethyl)-1,4,7,10-tetraazacyclododecane;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  R4N.X  25°C  0.10M C      K1=9.47      2000BCa (100844)2354
K(CaL+H)=3.9
Medium: 0.10 M NMe4Cl.
*****
C20H42N2O6      L      (6402)
7,16-Bis(1,1-dimethyl-2-hydroxyethyl)-1,4,10,13-tetraoxa-7,16-diazacyclooctadecane;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  NaNO3  25°C  0.10M C      K1=2.97      1991DHa (100859)2355
*****
C20H42N2O8      L      (6935)
N,N'-Bis(1-hydroxy-2-ethoxyethyl)-1,4-diaza-7,10,13,16-tetraoxacyclooctadecane;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      cal alc/w  25°C  90%  U  H      K1=4.38      1994IZa (100870)2356
L=N,N'-Bis(1-Hydroxy-2-ethoxyethyl)-1,4-diaza-7,10,13,16-tetraoxacycloocta-
decane. Medium: 90% v/v MeOH/H2O. DH(K1)=-13.8 kJ mol-1.
*****
C20H42N4O4      L      CAS 39678-14-3 (1543)
4,7-Dimethyl-1,4,7,10-tetraaza-13,16,21,24-tetraoxa-bicyclohexacosane;
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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	gl	R4N.X	25°C	0.10M	U		K1=4.3 K(Ca+HL)=1.6	1978LMa (100880)	2357

 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
Ca++	gl	NaNO3	25°C	0.10M	U		K1=5.68	1988HSb (100922)	2358

 C20H44N4O4 L (6730)
 1,4,7,10-Tetra-(2-methoxyethyl)-1,4,7,10-tetraazacyclododecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	gl	R4N.X	25°C	0.10M	C		K1=5.47	1993SFb (100935)	2359

Medium: 0.1 M Et4NClO4.

 C20H48N4O8P4 H4L (6569)
 1,4,7,10-Tetraazacyclododecane-1,4,7,10-tetrakis(methyleneethylphosphinic acid);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	gl	KCl	25°C	0.10M	C		K1=9.39	1997HTa (100988)	2360

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	gl	KNO3	25°C	0.10M	C		K1=9.39	1991LSc (100989)	2361

 C21H14N2O7S H4L CAS 3737-95-9 (5313)
 3-Hydroxy-4-(2-hydroxy-4-sulfo-1-naphthylazo)-2-naphthalenecarboxylic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	sp	alc/w	20°C	25%	U		K1=6.26	1971KBc (101027)	2362

Medium: 25% MeOH, 0.1 M KCl

 C21H18N2O2 H2L (7319)
 N,N'-3,4-Toluenebis(salicylideneimine); CH3.C6H3(N:CH.C6H4OH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	gl	mixed	25°C	80%	C		K1=4.31 B(CaHL)=14.32	1997HMa (101112)	2363

In 80 % (wt/wt) DMSO-H2O, I= 0.5 M NaClO4

 C21H21N2O8Cl H2L Demeclocycline CAS 64-73-3 (5759)
 7-Chloro-6-demethyltetracycline;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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 Ca++ gl NaCl 37°C 0.15M U K1=4.569 1985LBb (101175)2364
 B(Ca2L)=8.343
 B(CaH2L2)=24.269
 B(CaHL2)=16.355

Ca++ gl KNO3 25°C 0.10M C K1=5.52 1979DDd (101176)2365
 K(Ca+HL)=3.29

Also data for other tetracycline analogues.

 C21H26N4O4Br2 H2L CAS 354154-84-0 (8978)
 N,N'-Bis-(2-(N"-2-hydroxy-5-bromobenzyl)aminoethyl)malondiamide;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	diox/w	25°C	13%	C			K1=4.12 B(CaHL)=13.90 B(CaH-2L)=-16.59	2001CLa (101282)	2366

Medium: 13% v/v dioxane/H2O, 0.10 M KNO3.

 C21H27O7P H2L (6338)
 1,2:8,9-Dibenzo-5-phospha-5-oxo-5-methyl-19-crown-7;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	oth	non-aq	25°C	100%	U			K1=1.66 B2=3.87	1989SSc (101298)	2367

Medium: CH3CN. Ca as Ca(NCS)2; for Ca(ClO4)2 K1=2.07; B2=4.4. Method: IR
 Data also for 5-adamantyl, 5-phenyl and 5-phenoxy analogues

 C21H30N4O8 H3L Tyr-Val-Asp-Ala (6015)
 Tyrosyl-valyl-aspartyl-alanine

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	nmr	KCl	25°C	0.50M	U			K1=3.04 K(Ca+HL)=2.44 (definition ?)	1987ZAa (101365)	2368

 C21H30N7O17P3 H4L NADPH CAS 2646-71-1 (7185)
 Nicotinamide adenine dinucleotide phosphate reduced;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	nmr	none	RT	0	U			K1eff=2.61	1995MMF (101372)	2369

Medium: D2O, pH 8.5-9.5. Coordination site is the adenine phosphate. For the ribose phosphate site, K1eff=2.49; for nicotinamide phosphate, K1=2.02

 C21H31N3O9 H4L TTDA-H1P (7934)
 N'-(2-Hydroxy-1-phenylethyl)di(carboxymethyl)triazadodecanedioic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	gl	R4N.X	25°C	0.10M	M		K1=12.86 K(Ca+HL)=5.30	2001Cwa	(101397)2370

Medium: 0.10 M Me4NNO3. Method: by competition with EDTA

 C21H31N3O9 H4L TTDA-H2P (7935)
 N'-(2-Hydroxy-2-phenylethyl)di(carboxymethyl)triazadodecanedioic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	gl	R4N.X	25°C	0.10M	M		K1=12.74 K(Ca+HL)=4.45	2001Cwa	(101402)2371

Medium: 0.10 M Me4NNO3. Method: by competition with EDTA

 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
Ca++	gl	R4N.X	25°C	0.10M	M		K1=11.26	1996CHc	(101405)2372

Medium: 0.1 M Me4NCl.

 C21H31N5O8 H4L (8194)
 3,6,9,12,18-Pentaazabicyclo[12.3.1]heptadeca-1(18),14,16-triene-3,6,9,12-tetraethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	EMF	KCl	20°C	0.10M	C		K1=5.5	1981SFa	(101412)2373

Method: Pt/H2 electrode.

 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
Ca++	gl	alc/w	25°C	95%	C		K1=2.44	2004KVa	(101459)2374

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

 C22H16N2O2 H2L (4153)
 2'-Hydroxy-1-(5'-phenyl-phenylazo)-2-hydroxynaphthalene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	sp	KCl	rt	0.10M	U		K1eff=1.75 (pH 10)	1960DEa	(101526)2375

 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

Ca++ sp KNO3 25°C 0.20M U 1967BMc (101575)2376
B(CaH8L2)=94.0

C22H19N07S H3L CAS 450358-61-9 (8842)
N-[2-(Carboxymethoxy)-4-(5-phenyl-2-thienyl)phenyl]-N-(carboxymethyl)glycine;

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

Ca++ gl KCl 37°C 0.10M C 2002CSa (101682)2377
K1eff=4.02 (pH 7.01)
K1eff=4.44 (pH 7.40)

Method: fluorimetry. Medium pH 7.01-7.40

C22H22N2O8 L Methacycline CAS 3963-95-9 (6020)
Methacycline;

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

Ca++ gl NaCl 37°C 0.15M C K1=5.306 1988LBa (101722)2378
B(CaH2L2)=24.860

C22H23N2O8Cl H2L Aureomycin CAS 56235-18-8 (3515)
Chlorotetracycline;

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

Ca++ gl NaCl 37°C 0.15M U 1985LBb (101753)2379
B(CaH2L2)=25.230
B(CaH2L)=17.984

C22H24N2O8 H2L Tetracycline CAS 60-54-8 (2201)
Tetracycline;

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

Ca++ gl NaCl04 25°C 0.10M C 1996SJa (101792)2380
B(CaHL)=7.50

Ca++ cal oth/un 25°C ? U T H 19950Ca (101793)2381
Keff(Ca+L)=-2.94
Medium: 20mM Tris(hydroxymethyl)aminomethane, pH 9.5. DH=-41.8 kJ mol⁻¹,
DS=-44.4 J K⁻¹ mol⁻¹

Ca++ gl NaNO3 25°C 0.10M C M K1=7.90 1989GAb (101794)2382
K(CaL+Gly)=4.10

Ca++ gl NaCl 37°C 0.15M C B2=8.731 1981BBc (101795)2383

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	sol	non-aq	25°C	100%	U		K1=3.86	1987TCa (101921)	2390
Medium: CH2Cl2, 2% MeCN. Metal as picrate									

C22H26N4O10		H4L		BAPTA			(7230)		
1,2-Bis(o-aminophenoxy)ethane-N,N,N',N'-tetraethanoic acid; ((HOOCCH2)2NCH(OC6H4NH2)2									
Ca++	gl	R4N.X	25°C	0.10M	C		K1=6.78	1993YTa (101969)	2391

C22H26O10		H2L					(5628)		
1,10-bis(2-Carboxymethoxy-phenyl)-1,4,7,10-tetraoxadecane;									
Ca++	gl	alc/w	25°C	90%	M		K1=6.04	1998KLa (102006)	2392
Medium: 90% v/v MeOH/H2O, 0.1 M Me4NCl									

C22H29N5O6		H3L					(6506)		
N,N''-2-Bis(2-pyridylmethyl)diethylenetriamine-N,N',N''-triethanoic acid;									
Ca++	gl	NaCl	25°C	0.10M	U		K1=7.97 K(Ca+H)=5.30	1990CQa (102095)	2393

C22H31N3O10		H5L					CAS 445269-58-9 (8992)		
(4S)-4-Benzyl-3,6,10-tris(carboxymethyl)-3,6,10-triazadodecanedioic acid;									
Ca++	gl	R4N.X	25°C	0.10M	M		K1=15.95	2002CLb (102180)	2394
Medium: 0.1 M Me4NNO3.									

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;									
Ca++	gl	R4N.X	25°C	0.05M	U	H	K1=3.9	1998DBa (102263)	2395
Medium: 0.05 M Et4NClO4. By calorimetry: DH(K1)=-2.8 kJ mol-1,									
Ca++	EMF	alc/w	25°C	100%	U	H	K1=7.04	1987BUB (102264)	2396
In MeOH, 0.05M Et4NClO4. DH=-17.7 kJ mol-1									
Ca++	ISE	NaClO4	25°C	0.10M	U	I	K1=4.05	1984CTc (102265)	2397

In propylene carbonate K1=10.10

C22H41N5O8 H3L CAS 189687-33-0 (7103)
Diethylenetriamine-N,N',N''-triethanoic acid-N,N''-bis(butylamide);

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

Ca++ gl KCl 25°C 0.10M C K1=7.45 1997WCa (102386)2398

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

Ca++ gl NaNO3 25°C 0.10M C K1=3.07 1991DHa (102400)2399

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

Ca++ gl alc/w 25°C 95% M K1=4.12 1990LNa (102411)2400
Medium: 95% MeOH, 0.05 M Bu4NBr. For the 12,22-dihydroxy- analogue: K1=8.73

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

Ca++ gl R4N.X 25°C 0.05M C K1=2 1975LSc (102424)2401

C22H44N6O5S2 L CAS 503465-08-5 (9241)
9,20,23,28,31-Pentaoxa-1,4,6,12,14,17-hexaazabicyclo[15.8.8]tritiacontane-5,13-dithione;

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

Ca++ gl alc/w 25°C 95% C K1=2.48 2004KVa (102434)2402
Medium: 95% MeOH/H2O, 0.01 M Et4NClO4.

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

Ca++ gl R4N.X 25°C 0.10M U K1=1.5 1978LMa (102481)2403

C23H23N5O5 L CAS 218619-58-0 (7808)
Dibenzo-pyridino-18-crown-6;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	EMF	alc/w	25°C	100%	C		K1=3.04	2004ZTa (102651)	2404
Medium: 100% methanol, 0.05 M Bu4NClO4. Method: Ag electrode, competition with Ag+ ion.									

C23H25N05S		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
Ca++	sp	non-aq	20°C	100%	C		K1=5.6 B2=10.30	2003FFa (102688)	2405
Medium: CH3CN.									

C23H26N207		H2L					(2559)		
6-Desoxy-6-dimethyl-tetracycline;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	gl	NaCl	37°C	0.15M	C		K1=5.159 B2=9.942 B(CaHL)=12.718 B(CaL2)=19.550 B(CaH2L2)=26.376	1988LVa (102706)	2406

C23H27N208I		H2L					CAS 6602-90-0	(361)	
4-Methyltetracycline Iodide;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	gl	KNO3	25°C	0.10M	U		K1=4.0	1979HFa (102717)	2407

C23H27N307		L					Minocycline CAS 13614-98-7	(2203)	
Minocycline, 6-Dimethyl-6-deoxy-7-dimethylaminotetracycline;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	gl	NaCl	37°C	0.15M	C		K1=5.981 B(CaHL)=14.183 B(CaH2L2)=27.228	1981BBc (102725)	2408

C23H30N204		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
Ca++	sp	non-aq	RT	100%	C		K1=4.71	2001AVa (102746)	2409
Method: spectrophotometric titration. Medium: acetonitrile.									

C23H30N404Br2		H2L					CAS 354154-85-1	(8979)	
N,N'-Bis-(3-N"-2-hydroxy-5-bromobenzyl)aminopropyl malondiamide;									

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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  diox/w 25°C 13% C          K1=4.26      2001CLa (102762)2410
          B(CaHL)=14.69
          B(CaH-2L)=-16.47

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Medium: 13% v/v dioxane/H2O, 0.10 M KNO3.

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C23H30N4O7          L          CAS 356535-57-4 (8845)
13-[2-Methoxy-4-[(4-nitrophenyl)azo]phenyl]-1,4,7,10-tetraoxa-13-azacyclopentadecan
e;

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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      sp  alc/w  RT   50% C          K1=ca.0.3    2002GNe (102767)2411

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Medium: 50% v/v MeOH/H2O, pH 7.4 (0.1M Tris buffer), 0.1 M Me4NCl.

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C23H33N3O11        H5L          CAS 158599-72-5 (7657)
S-2-(4-Ethoxybenzyl)-1,4,7-triazaheptane-N,N,N',N'',N'''-pentaethanoic acid;

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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  KCl    25°C 0.10M C          K1=11.74     1999SBd (102817)2412
          K(CaL+H)=5.75
          K(CaLH+H)=4.16
          K(CaL+Ca)=2.18

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C23H42N2O9          HL          CAS 111216-12-7 (5568)
2-Carboxy-3-monopiperidine-18-crown-6 derivative;

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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      nmr alc/w 25°C 90% U          K1=5.1       1987DDa (102839)2413
          K(Ca+HL)=5.0

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Medium: 90% MeOH/H2O

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C24H20B-          HL          CAS 4358-26-3 (2489)
Tetraphenylborate;

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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      dis non-aq 25°C 100% U I      K1=2.15     1969PKb (102883)2414

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Medium: 0.01-0.10 nitrobenzene. K1(0.01)=2.20, K1(0.05)=2.30

(tracer amounts Ca++)

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C24H20N4O14Cl2P2S2 H8L          (4165)
2,7-Bis(4'-chloro-5'-methyl-2'-phosphonophenylazo)chromotropic acid;

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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
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Ca++ sp KNO3 25°C 0.20M U 1967BMc (102913)2415
B(CaH8I2)=95.9

C24H24N2O6 H4L CAS 385439-50-9 (9197)
p-Xylylenediamine-N,N'-bis(o-hydroxyphenyl)ethanoic acid;

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

Ca++ gl NaCl 25°C 0.10M C K1=6.05 2004SGb (102943)2416
B(CaHL)=16.55
B(CaH2L)=25.07

Additional method: UV-visible spectrometry

C24H24N2O8 H4L CAS 89593-26-0 (8632)
N,N'-[1,2-Ethylenediylbis(2,1-phenylenemethylene)]bis[N-(carboxymethyl)]glycine;

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

Ca++ gl KCl 20°C 0.10M U K1=4.8 1984VSc (102947)2417

C24H25O7P L (2067)
Phenylphosphonyldibenzo-17-crown-6

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

Ca++ sol non-aq 25°C 100% U K1=3.75 1987TCa (102962)2418
Medium: CH2Cl2 2% MeCN. Metal as picrate

C24H26N2O8 H4L CAS 89561-09-1 (8633)
N,N'-[1,2-Ethylenediylbis(2,1-phenylenemethylene)]bis[N-(carboxymethyl)]glycine;

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

Ca++ gl KCl 20°C 0.10M U K1=4.5 1984VSc (102972)2419

C24H26N2O8 H4L CAS 89561-11-5 (8635)
N,N'-[1,2-Ethylenediylbis(4,1-phenylenemethylene)]bis[N-(carboxymethyl)]glycine;

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

Ca++ gl KCl 20°C 0.10M U K1=3.2 1984VSc (102977)2420

C24H28N2O2 L CAS 101821-61-8 (9065)
4-{2-[10-(2-Morpholinoethyl)-9-anthryl]methyl}morpholine;

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

Ca++ sp diox/w 25°C 40% C K1=2.62 2003GHb (103002)2421
Method: fluorescence spectroscopy. Medium: 40% w/w dioxane/H2O, 0.05 M
Et4NC104.

 C24H28N2O8 H4L CAS 89561-10-4 (8634)
 N,N'-[1,2-Ethanediy]bis(2,1-phenylenemethylene)]bis[N-(carboxymethyl)]glycine;

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

 Ca++ gl KCl 20°C 0.10M U K1=4.0 1984VSc (103005)2422

C24H30O7 HL (6603)
 2-[(7,8,16,17-Tetrahydro-6H,15H-dibenzo[1,4,8,11]tetraoxacyclotetradeca-7-yl)oxy]-hexanoic acid;

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

 Ca++ dis oth/un 25°C ? U K1=0.79 B2=4.23 1991BUa (103031)2423

C24H31N3O8 H3L CAS 35369-55-2 (6972)
 N,N''-Bis(2-hydroxybenzyl)-2,5,8-triazanonane-N,N',N''-triethanoic acid;

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

 Ca++ gl NaNO3 25°C 0.50M C K1=7.94 1994HCb (103050)2424
 K(CaL+H)=10.68
 K(CaHL+H)=8.84

 Ca++ gl KCl 25°C 0.10M C K1=8.47 1994MMF (103051)2425
 K(CaL+H)=10.85
 K(CaHL+H)=9.20
 K(CaH2L+H)=7.58
 K(CaH3L+H)=6.8

 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

 Ca++ con mixed 25°C 20% C K1=4.01 2003SIa (103101)2426
 Medium: 20% w/w propylene carbonate/ethylene carbonate.

 Ca++ vlt alc/w 25°C 100% C K1=2.53 1987CBd (103102)2427
 Medium: methanol, 0.10 M Et4NI or Bu4NClO4. Method: polarography.
 Additional method conductivity in methanol: K1=2.40.

 Ca++ ISE alc/w 25°C 100% U K1=2.66 1983GGa (103103)2428
 Medium: MeOH

 C24H36N2O4Fe L CAS 145519-34-2 (6831)
 1,1'-(1,4,10,13-Tetraoxa-7,16-diazacyclooctadeca-7,16-diyl)dimethylferrocene;

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

Ca++ nmr non-aq 25°C 100% U K1=7.16 1992MGa (103254)2429
Method:NMR. Medium: MeCN, 0.1 M Bu4NPF6. Data also for other ferrocene[2.2]
cryptands

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
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Ca++ gl KNO3 25°C 0.10M C K1=3.63 1986DSa (103262)2430

C24H36N4S2 CAS 638211-87-7 (9252)
Eicosahydro-7,10:19,22-diepthiodibenzo[1,4,11,14]tetraazacycloeicosine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Ca++ gl KCl 25°C 0.10M C K1=21.65 2003GMb (103277)2431

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
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Ca++ gl R4N.X 25°C 0.10M M K1=5.6 1991FGb (103304)2432
B(CaHL)=9.6

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
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Ca++ gl NaClO4 25°C 0.20M C K1=7.93 1985KFa (103364)2433
K(Ca+HL)=7.93

Ca++ EMF KCl 20°C 0.10M C K1=7.6 1981SFa (103365)2434
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
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Ca++ con mixed 25°C 20% C K1=3.88 2003SIa (103423)2435
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

Ca++ gl NaNO3 25°C 0.10M C K1=4.72 1991DCa (103451)2436

C24H48N2O9 L Cryptand 3,3,3 CAS 132162-61-9 (1761)
Cryptand 3,3,3

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

Ca++ gl R4N.X 25°C 0.05M C K1=<2 1975LSc (103461)2437

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

Ca++ gl R4N.X 25°C 0.10M U K1=4.1 1981GLa (103477)2438

C24H48N6O6S2 L CAS 503465-10-9 (9242)
9,12,23,26,31,34-Hexaoxa-1,4,6,15,17,20-hexaazabicyclo[18.8.8]hexatricacontane-5,16-d
ithione;

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

Ca++ gl alc/w 25°C 95% C K1=2.61 2004KVa (103501)2439
Medium: 95% MeOH/H2O, 0.01 M Et4NClO4.

C24H48N8O4 L (6789)
1,4,7,10-Tetrakis(N,N-dimethylethanamido)-1,4,7,10-tetraazacyclododecane;

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

Ca++ gl R4N.X 25°C 0.10M M K1=6.80 1990K Mb (103515)2440
Medium: 0.10 M Me4NNO3

C24H72O12Si12 L CAS 18919-94-3 (1287)
Tetracosamethyl-cyclododecasiloxane; ((CH3)2SiO)12

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

Ca++ con alc/w 25°C 100% U K1=0.61 19800Pa (103589)2441
Medium: MeOH, 0.1 M Me4NBr

C25H27N9O8S2 H2L CAS 62893-19-0 (8405)
Cefoperazone;

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

Ca++ gl KNO3 25°C 0.10M C K1=4.27 2000GFb (103657)2442

Pentaoxa-4,10,16,22,27-tetraaza-1,7,13,19-tricyclo-tetratriacontane;

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

Ca++ gl R4N.X 25°C 0.10M U K1=2.4 1981GLa (103832)2449

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

Ca++ gl alc/w 25°C 95% C K1=3.88 2004KVa (103840)2450
Medium: 95% MeOH/H2O, 0.01 M Et4NClO4.

C26H18N4O9S2 H5L Alizarin black CAS 3258-74-0 (4168)
1-(3'-(2"-Hydroxy-1"-naphthylazo)-21-hydroxy-5'-sulfophenylazo)-2-hydroxy-naphthalen
e-6-HSO4;

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

Ca++ sp oth/un 25°C 0.10M U 1962RAa (103852)2451
K(2Ca+HL=Ca2L+H)=-1.1
K(2Ca+2HL=Ca2L2+2H)=-4.5
K(Ca+HL)=6-7
K(Ca2L2+2Ca)=2.3

C26H25N09S 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

Ca++ sp KNO3 25°C 0.10M U K1=6.53 1974Y0a (103938)2452
B(CaHL)=13.69

C26H27N3O10 H4L (7231)
2-((2-Amino-5-methylphenoxy)-methyl)-6-methoxy-8-aminoquinoline-N,N,N',N'-tetraetha
noic acid;

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

Ca++ gl R4N.X 25°C 0.10M C K1=7.28 1993YTa (103955)2453

C26H28O4 H2L B(CH2AcAcCH2)2B (2253)
3,5,16,18-Tetraoxo[7.7]metacyclophane ;Cyclo-(-C6H4.(CH2)2.CO.CH2.CO.(CH2)2-)2

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

Ca++ gl diox/w 24°C 50% U K1=4.1 1979ACa (104016)2454

C26H31N08S2 L CAS 136195-71-6 (6832)
Crown Ether Styryl Dye;

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

Ca++ sp non-aq 25°C 100% U K1=6 K2=<4 1992BFa (104032)2455
Medium: CH3CN

C26H32N2O2 L CAS 588691-41-2 (9066)
4-{2-[10-(2-Morpholinoethyl)-9-anthryl]ethyl}morpholine;

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

Ca++ sp diox/w 25°C 40% C K1=4.52 2003GHb (104036)2456
K(CaL+Ca)=2.78

Method: fluorescence spectroscopy. Medium: 40% w/w dioxane/H2O, 0.05 M Et4NClO4.

C26H32N2O10 H4L CAS 149746-36-1 (7027)
1,2-Bis(2-amino-5-methylphenoxy)ethane-N-(2-methyl-2-propanoic)-N,N',N'-triethanoic acid;

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

Ca++ sp KCl 37°C 0.10M U K1=8.10 1993CMA (104041)2457
Also data for aryl, alkyl & fluoro substituted analogues

C26H32N2S2 L CAS 677034-81-0 (9064)
4-(2-{10-[2-(1,4-Thiazinan-4-yl)ethyl]-9-anthryl}ethyl)thiomorpholine;

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

Ca++ sp non-aq 25°C 100% C K1=4.36 2003GHa (104042)2458
K(CaL+Ca)=2.90

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

Ca++ sp non-aq 25°C 100% C K1=6.51 2003GHa (104071)2459
K(CaL+Ca)=4.12

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

C26H34N6O8 H4L CAS 132709-65-0 (8941)
3,6,14,17,23,24-Hexaazatricyclohexacos-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

Ca++ gl KCl 25°C 0.10M M K1=13.6 1996MBb (104089)2460
K(CaL+H)=5.1
K(CaHL+H)=2.8

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

Ca++ gl alc/w 25°C 90% M K1=7.86 1998KLa (104104)2461
Medium: 90% v/v MeOH/H2O, 0.1 M Me4NCl

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

Ca++ gl R4N.X 25°C 0.05M U H 1998DBa (104123)2462
Medium: 0.05 M Et4NClO4. By calorimetry: DH(K1)=-0.6 kJ mol⁻¹,

Ca++ EMF alc/w 25°C 100% U H K1=5.96 1987BUB (104124)2463
In MeOH, 0.05M Et4NClO4. DH=-6.4 kJ mol⁻¹

Ca++ ISE NaClO4 25°C 0.10M U I K1=3.45 1984CTc (104125)2464
In propylene carbonate, K1=9.74

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

Ca++ cal non-aq 25°C 100% C H 1995ZBa (104153)2465
K(Ca+H2L)=4.48
Medium: methanol. DH(K)=-3.3 kJ mol⁻¹, DS(K)=74.8 J K⁻¹ mol⁻¹.

C26H38N6 L CAS 180684-75-7 (7295)
1,8,14,17,24,31-Hexaazatricyclo[25.3.1.1.0.0]dotriaconta-10,12,14,26,28,

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

Ca++ gl KNO3 25°C 0.20M C K1=4.2 1996FJa (104202)2466

C26H43NO6 HL Glycocholic ac. CAS 475-31-0 (5821)
N-Cholyglycine, N-3,7,12-Trihydroxy-24-oxocholan-24-yl-glycine;

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

Ca++ nmr oth/un 25°C ? U 1986KBb (104270)2467

K1eff=2.02

At pH 5.0

C26H45N07S HL Taurocholic ac. CAS 145-42-6 (5822)
Cholyltaurine; 5-Cholan-24-oic acid N-(2-sulfoethyl)amide-3,7,12-triol;

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

Ca++ nmr oth/un 25°C ? U 1986KBb (104275)2468

K1eff=1.23

At pH 5.0

C26H48N206 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

Ca++ EMF a/c/w 25°C 100% U K1=5.12 1987BUB (104292)2469

C26H50N207 L (6931)
N,N'-Bis(1-tetrahydrofuryl-2-ethoxyethyl)-1,4-diaza-7,10,13-trioxacyclopentadecane;

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

Ca++ cal a/c/w 25°C 90% U H K1=3.2 1994IZa (104318)2470
L=N,N'-Bis(1-tetrahydrofuryl-2-ethoxyethyl)-1,4-diaza-7,10,13-trioxacyclopentadecane. Medium: 90% v/v MeOH/H2O. DH(K1)=-9.9 kJ mol⁻¹.

C26H52N405 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

Ca++ gl R4N.X 25°C 0.10M U K1=<2 1981GLa (104325)2471

C26H52N607S2 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

Ca++ gl a/c/w 25°C 95% C K1=3.44 2004KVa (104335)2472
Medium: 95% MeOH/H2O, 0.01 M Et4NC104.

C26H52N607S2 L CAS 503465-12-1 (9243)
9,12,15,26,29,34,37-Heptaoxa-1,4,6,18,20,23-hexaazabicyclo[21.8.8]nonatricontane-5,19-dithione;

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

Ca++ gl alc/w 25°C 95% C K1=2.55 2004KV a (104345)2473
Medium: 95% MeOH/H2O, 0.01 M Et4NClO4.

C27H29N010 H2L Daunorubicine CAS 23541-50-6 (5660)
Daunomycin;

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

Ca++ sp oth/un 20°C 0.15M U K(Ca+HL)=3.3 1982KMd (104437)2474

C27H32N05S+ 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

Ca++ sp non-aq 25°C 100% C K1=5.14 2002GVc (104513)2475
Medium: acetonitrile, 0.01 M Et4NClO4.

C27H33N07 L FLC CAS 223390-37-2 (8805)
2-[4-Dimethylaminophenyl]-6-methyl-3-(1,4,7,10-tetraoxacyclododec-2-ylmethoxy)-4H-1-Benzopyran-4;

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

Ca++ sp non-aq ns 100% C K1=5.52 2000LXa (104523)2476
Medium: acetonitrile. By fluorescence, K1=5.48.

C27H33N709 HL CAS 159356-07-7 (8682)
N,N'N'-(Nitrilotri-2,1-ethanediyl)tris[1,2-dihydro-3-hydroxy-1-methyl-2-oxo]4-pyridinecarboxamide

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

Ca++ gl KCl 25°C 0.10M U K1=7.6 1995XFa (104541)2477
B(CaHL)=13.7
B(CaH2L)=18.9

C27H33N9015P2 H2L FAD CAS 146-14-5 (3521)
Flavin adenine dinucleotide;

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

Ca++ ix NaCl 23°C 0.1M U K1=2.02 1958WAa (104543)2478

C27H36N1009 H3L TrenHOPY (7967)
Tris[(2,3-dimethyl-5-hydroxy-6-carboxamido-4-pyrimidinone)ethyl]amine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	KCl	25°C	0.10M	U			K1=7.51 B(CaH2L)=19.67	2001SBb (104577)	2479

 C27H38N6O12 H4L DGYVDA (6016)
 Aspartyl-glycyl-tyrosyl-valyl-aspartyl-alanine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	nmr	KCl	25°C	0.50M	U			K(Ca+HL)=3.07 ? K(Ca+H2L)=1.93 ?	1987ZAa (104583)	2480

 C27H44O L Vitamin D3 CAS 67-97-0 (6103)
 7-Dehydrocholesterol, Cholecalciferol

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	alc/w	37°C	70%	U			K1=3.37 B2=7.33	1989QYa (104607)	2481

Medium: 70% (v/v) EtOH/H2O, 0.1 M KNO3

 C27H47N3O6 L (8029)
 Tripodal ionophore 3;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	sp	non-aq	25°C	100%	C			K(CaP+L=LiPL)=4.19	2001Lfa (104621)	2482

Method: Analyses by spectrophotometry. Medium: chloroform. P is picrate.

 C28H24O16S4 H8L CAS 206559-10-6 (7767)
 25,26,27,28-Tetrahydroxycalix[4]arene-5,11,17,23-tetrasulfonic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	cal	oth/un	25°C	0.10M	C	H		K(Ca+H4L)=3.32	2001BIa (104691)	2483

Medium: 0.10 m Na4H4L, pH=2. DH(Ca+H4L)=3.0 kJ mol⁻¹.

 C28H34N2O6 HL CAS 83874-22-0 (6920)
 Cezomycin;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	alc/w	25°C	100%	C			K1=5.4 B2=12.8	1994ABc (104754)	2484

Medium: MeOH; 0.1 M (C4H9)4NCF3SO3H

 C28H35N3O6 L CAS 114880-42-1 (7377)
 3-(p-13-Aza-1,4,7,10-tetroxacyclopentadecan-13ylstyryl)-7-dimethylamino-1,4-benzoxa

zin-2-one;

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

Ca++ sp non-aq RT 100% C K1=4.28 1998ABc (104758)2485
Medium: acetonitrile. Method: fluorescence spectroscopy.

C28H3507P L CAS 90275-27-7 (2068)
Adamantylphosphonyldibenzo-17-crown-6

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

Ca++ sol non-aq 25°C 100% U K1=4.69 1987TCa (104765)2486
Medium: CH2Cl2, 2% MeCN. Metal as picrate

C28H36N202 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

Ca++ sp diox/w 25°C 40% C K1=5.07 2003GHb (104774)2487
K(CaL+Ca)=4.05
Method: fluorescence spectroscopy. Medium: 40% w/w dioxane/H2O, 0.05 M
Et4NClO4.

C28H36N207S2 HL CAS 150196-54-6 (7735)
3-(3-Sulfopropyl)-2-[4-[N-(1,4,7,10,13-pentaoxa-16-azacyclooctadeca)]]styryl-benzot
hiazolium;

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

Ca++ sp non-aq 18°C 100% C K1=1.7 1997LHa (104780)2488
Medium: acetonitrile.

C28H37N508 H3L (7382)
Diethylenetriamine-N,N,N',N'',N''-pentaethanoic acid bis(benzylamide);

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

Ca++ gl KCl 25°C 0.10M C K1=7.13 1997WCa (104799)2489

C28H3809 H2L (3355)
1,7-Bis(2-carboxybutoxyphenyl)-1,4,7-trioxahseptane; (HOOCCH(C4H9)O(C6H4)OCH2CH2)2O

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

Ca++ gl alc/w 25°C 90% M K1=6.80 1998KLa (104808)2490
Medium: 90% v/v MeOH/H2O, 0.1 M Me4NCl

C28H38010 H2L CAS 100113-54-0 (3391)

1,10-Bis(2-carboxybutoxyphenyl)-1,4,7,10-tetraoxadecane;
 (HOOC(C₄H₉)O(C₆H₄)OCH₂CH₂OCH₂)₂

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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  alc/w  25°C  90%  M          K1=6.00      1998KLa (104812)2491
Medium: 90% v/v MeOH/H2O, 0.1 M Me4NC1
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 C₂₈H₄₀O₆ L CAS 29471-17-8 (1262)
 2,3:11,12-Bis(4'-tert-butylbenzo)-1,4,7,10,13,16-hexaoxacyclooctadecane;

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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      EMF non-aq 25°C 100% U          K1=6.86      1982MRb (104832)2492
Medium: anhydrous propylene carbonate, 0.1M Et4NC1O4
```

 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;

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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      vlt non-aq 25°C 100% C          K1=4.12      1991SSb (104866)2493
Method: competitive complexation with Tl+; use of Tl(Hg)/Tl couple.
Medium: acetonitrile, 0.05 M Et4NC1O4.
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Ca++      sp  alc/w  25°C 100% U I          K1=4.25      1987GKb (104867)2494
Medium: MeOH. In DMF K1=3.28, in DMSO K1=2.92
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-----
Ca++      EMF non-aq 25°C 100% U          K1=5.23      1982MRb (104868)2495
Medium: anhydrous propylene carbonate, 0.1M Et4NC1O4
```

 C₂₈H₅₂N₄O₁₀ H5L CAS 137203-80-6 (8096)
 1-N-Dodecyltriethylenetetramine-N,N',N'', N''',N''''-pentaethanoic acid;

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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      gl  alc/w  25°C  50%  C          K1=11.3      2001SYb (104987)2496
                                K(CaL+Ca)=5.5
                                K(CaL+H)=10.7
                                K(CaHL+H)=4.6
```

Medium: 50% EtOH/H₂O, 0.10 M KNO₃.

 C₂₈H₅₄N₂O₈ L (6936)
 N,N'-Bis(1-furanyl-2-ethoxyethyl)-1,4-diaza-7,10,13,16-tetraoxacyclooctadecane;

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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Ca++      cal alc/w  25°C  90%  U  H          K1=4.25      1994IZa (105025)2497
L=N,N'-Bis(1-furanyl-2-ethoxyethyl)-1,4-diaza-7,10,13,16-tetraoxacycloocta-
decane. Medium: 90% v/v MeOH/H2O. DH(K1)=-15.3 kJ mol-1.
```

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

Ca++ gl alc/w 25°C 95% C K1=3.10 2004KVa (105036)2498
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]dotetradecane-5,22-dithio

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

Ca++ gl alc/w 25°C 95% C K1=2.67 2004KVa (105046)2499
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

Ca++ sp mixed 25°C 90% C 1997KKa (105096)2500
K(Ca(SCN)2+L)=2.93

Method: fluorescence emission. Medium: MeOH/CHCl3 (9:1 v/v).

C30H18N6O21S6 H9L Calcichrome (4173)
Cyclo-tris-7-(1-azo-8-hydroxynaphthalene-3,6-disulfonic acid);

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

Ca++ sp NaNO3 20°C 0.20M U 1965BBb (105178)2501
B(CaH2L)=26.45

C30H30N20O10 L CAS 259886-49-2 (8959)
Cucurbit[5]uril;

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

Ca++ sol none 25°C dil C K1=1.73 2001BCf (105213)2502
Method: dissolution of ligand in a 0.002-0.02 M CaX2 solution; spectro
photometric measurement. For decamethylcucurbit[5]uril, K1=1.61

C30H36N8O3 Furan-cryptand CAS 121954-37-8 (7451)
39,40,41-Trioxa-1,4,11,14,17,24,29,36-octaazapentacyclo[12.12.12.1.1.1]henLetetraco
ntadodecane;

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

Ca++ sp non-aq 25°C 100% U H K1=6.64 1996AAb (105247)2503
Medium: MeCN

tacyclo[12.12.12.1(6,9).1(19,22).1(31,34)]hentetetraconta-4,6,8....dodecaene

C30H41N5O10 H3L (7506)
1,4,7,10,13-Tetraaza-1,13-(2-methoxybenzyl)-tridecane-2,12-dione-4,7,10-triethanoic
acid;

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

Ca++ gl KCl 25°C 0.10M U K1=7.74 1998Wlb (105294)2504
K(CaL+H)=5.22

C30H49N3O8 H4L (5361)
Dodecylbenzenediethylenetriaminetetraethanoic acid;

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

Ca++ EMF KNO3 20°C 0.10M U 1968CHa (105348)2505
K(Ca+2H3L)=16.92
K(2Ca+2H2L)=15.28
K(3Ca+2HL)=14.62

C30H57N08 HL 18NH15-C5A CAS 79145-86-1 (5405)
2-Carboxy-3-N-octadecanylformamide-1,4,7,10,13-pentaoxycyclopentadecane;

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

Ca++ gl alc/w 25°C 90% U K1=3.5 B2=7.1 1984FWa (105380)2506
Medium: 90% v/v MeOH/H2O, 0.05 M R4NX

C30H62N2O3 L (2956)
1,10-Di(decylaza)-4,7,13-trioxacyclopentadecane;

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

Ca++ cal alc/w 25°C 100% U H K1=2.51 1986BUa (105386)2507
Medium: MeOH. DH(K1)=-11.7 kJ mol⁻¹; DS=9 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''-sulf
onic acid;

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

Ca++ gl KNO3 25°C 0.10M C M K1=8.64 1998GBa (105439)2508
K(CaL+H)=10.10
K(CaL+Ca)=4.69
K(Ca2L+H)=8.47

Ca++ sp KNO3 25°C 0.10M U K1=8.65 1974Y0a (105440)2509
K(Ca+HL)=6.82
K(Ca+H2L)=2.97
K(Ca+CaL)=6.02
K(Ca+CaHL)=2.5

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

Ca++ gl KCl 25°C 0.10M U K1=4.2 1982LVa (105586)2510

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

Ca++ gl KCl 25°C 0.10M U K1=5.5 1982LVa (105591)2511

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

Ca++ gl oth/un 25°C 0.10M U K1=7.91 1981GMd (105603)2512
B(CaHL)=19.11
B(Ca2L)=12.76

Ca++ gl KCl 20°C 0.1M U K1=7.8 1954AGb (105604)2513
K(Ca+HL)=6.9
K(Ca+H2L)=3.2
K(Ca+CaL)=5.0
K(Ca+H3L)=2.3

K(Ca+CaHL)=1

C32H33N3O12F2 L CAS 149696-88-8 (7035)
2,3:14,15-Difluorobenzo-8,9-(4-dicarboxymethyliminobenzo)-4,13-diaza-4,13-dicarboxy
methylcyclooc-

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

Ca++ sp R4N.X 30°C 0.10M U K1eff=5.70 1993SKf (105616)2514

Medium: Me4NCl. K1eff at pH 7.2

C32H37N09S H4L SemiMeThymolBlu (427)

3-(N,N-Di(carboxymethyl)-aminomethyl)thymolsulfonephthalein;

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

Ca++ sp KNO3 25°C 0.10M U K1=6.52 1974Y0a (105660)2515
B(CaHL)=14.34

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

Ca++ cal non-aq 25°C 100% C H K(Ca+HL)=4.71
1995ZBa (105676)2516

Medium: methanol. DH(K)=-25.2 kJ mol⁻¹, DS(K)=5.7 J K⁻¹ mol⁻¹.

C32H38N4O6Cl2 H2L (7214)
7,16-Bis((5-chloro-8-hydroxy-7-quinolinyl)methyl)-1,4,10,13-tetraoxa-7,16-diazacycl
oocadecane;

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

Ca++ cal alc/w 25°C 100% U H K(Ca+H2L)=5.31
1996BBf (105686)2517

Medium: MeOH; 0.1 M Me4NCl. DH(K)=-3.5 kJ mol⁻¹. Data also for similar
ariat ligands with substituted oxine side chains

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

Ca++ sp non-aq 18°C 100% C K1=4.2 1997LHa (105753)2518

Medium: acetonitrile.

C32H43O9P H2L CAS 120885-36-1 (6339)
1,2:12,13-Dibenzo-7-phospha-7-oxo-7-adamantyl-24-crown-9

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

Ca++ oth non-aq 25°C 100% U K1=2.32 B2=4.24 1989SSc (105760)2519
In CH3CN; Ca++ is used as Ca(NCS)2; For Ca(ClO4)2 K1=3.24; B2=5.31;

Method: IR-spectroscopy

C32H45N5O10 H3L (7507)
1,4,7,10,13-Pentaaza-1,13-di(2-ethyl-(2-methoxyphenyl))tridecane-2,12-dione-4,7,10-
triethanoic a;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	KCl	25°C	0.10M	U			K1=7.54 K(CaL+H)=5.37	1998WLB (105783)	2520

 C32H48N2O3 L CAS 170801-55-5 (8952)
 1,5-Bis[2,2'-azo-4,4'-(1,1,3,3-tetramethylbutyl)phenoxy]-3-oxapentane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	sp	alc/w	RT	100%	C			K1=1.35	2000GDa (105794)	2521

Medium: MeOH.

 C32H48N2O4 L CAS 170801-51-1 (8953)
 6,7,9,10-Tetrahydro-2,14-bis(1,1,3,3-tetramethylbutyl)dibenzotrioxadiazacyclotridecine 16-oxide;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	sp	alc/w	RT	100%	C			K1=1.15	2000GDa (105798)	2522

Medium: MeOH.

 C32H58N2O12 H2L CAS 88454-81-3 (5409)
 2,11-Bis(carboxy)-3,12-bis(octanylformamide)-18-crown-6 (anti);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	alc/w	25°C	90%	U			K1=10.1	1984FWa (105835)	2523

Medium: 90% v/v MeOH/H2O, 0.05 M R4NX

 C32H58N2O12 H2L CAS 88454-82-4 (5408)
 3,11-Bis-carboxy-2,12-bis(octanylformamide)-18-crown-6 (syn);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	alc/w	25°C	90%	U			K1=8.9 B(CaHL)=12.7	1984FWa (105841)	2524

Medium: 90% v/v MeOH/H2O, 0.05 M R4NX

 C32H64N4O10 L CAS 42133-16-4 (8579)
 4,10,13,19,25,28,33,36,41,44-Decaoxa-1,7,16,22-tetraazatricyclo[20.8.8.87,16]hexate tracontane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	alc/w	25°C	90%	M			K1=4.0	1977LSc (105847)	2525

Medium: 90% (w/w) MeOH/H2O, 0.1 M Et4NBr.

 C33H39N11 L Pyr-cryptand CAS 141258-00-6 (7452)
 1,4,12,15,18,26,31,39,42,43,44-Undecaazapentacyclo[13.13.13.1.1.1]tetratetraconta

pentadecane;

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

Ca++ sp non-aq 25°C 100% U H K1=6.26 1996AAb (105912)2526
Medium: CH3CN
.13.1(6,10).1(20,24).1(33,37)]tetratetraconta-4-6-8-10(44),11...pentadecaene

C33H41N3O6 L (8027)
Tripodal ionophore ;

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

Ca++ sp non-aq 25°C 100% C 2001Lfa (105920)2527
K(CaP+L=LiPL)=5.16
Method: Analyses by spectrophotometry. Medium: chloroform. P is picrate.

C33H44N3O14P H6L CAS 193901-91-6 (7981)
(4,4-Diphenylcyclohexyl)(methylene-2-dien pentaethanoic acid) phosphoric acid;

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

Ca++ gl NaClO4 25°C 0.10M C K1=10.45 2001CCa (105935)2528
K(CaL+H)=5.66

C34H38N2O14 H2L (7072)
7,16-Bis(3-carboxy-6-methoxy-2-oxo-2H-1-benzopyran-7-yl)-1,4,10,13-tetraoxa-diazacy
cloctadecane;

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

Ca++ sp none RT 0 U K1=2.22 1994CGa (106026)2529
Method: fluorimetry

C34H53N5O8 H3L (7508)
1,4,7,10,13-Pentaaza-1,13-bis(adamantanyl)tridecane-2,12-dione-4,7,10-triethanoic
acid;

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

Ca++ gl KCl 25°C 0.10M U K1=7.49 1998Wlb (106091)2530
K(CaL+H)=5.27

C34H53O8Br H2L CAS 38784-08-6 (2336)
5-Bromolasalocid;

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

Ca++ gl alc/w 25°C 100% M 1988JTa (106094)2531
K(Ca+HL)=4.81

K(Ca+2HL)=7.4

Medium: MeOH

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

Lasalocid acid;

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

Ca++ nmr non-aq 20°C 100% C 1998MLa (106110)2532

K(Ca+HL)=0.0

Medium: CD3OD. Method: 13C nmr.

Ca++ dis non-aq 25°C 100% U 1993LPa (106111)2533

K(Ca+2HL=CaL2+2H)=-9.7

Method: extraction into CHCl3. K is for Ca(aq)+2HL(org)=CaL2(org)+2H(aq).

Ca++ gl alc/w 25°C 100% M 1988JTa (106112)2534

K(Ca+HL)=5.00

K(Ca+2HL)=7.5

Medium: MeOH

Ca++ cal alc/w 25°C 100% U H 1988PPa (106113)2535

Medium: MeOH. DH(CaL)=20.7 kJ mol⁻¹; DS=165. DH(CaL2)=31.4; DS=256

Ca++ gl alc/w 25°C 100% U 1982BDc (106114)2536

K(Ca+4HL)=4.88

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

Ca++ gl alc/w 25°C 90% U 1984FWa (106176)2537

K1=9.4
B(CaHL)=13.8

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

Ca++ gl R4N.X 25°C 0.10M U 2001BBa (106199)2538

K1=8.54
K(CaL+H)=8.44

K(CaHL+H)=7.79

K(CaH2L+H)=5.46

Medium: 0.10 M NMe4NO3.

C36H33N7O15S3 H6L O-TRENSEX CAS 169209-69-2 (7370)

Tris-N-(2-aminoethyl-(8-hydroxyquinoline-5-sulphonato-7-carboxamido))amine;

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

Ca++ gl NaCl04 25°C 0.10M C K1=14.98 2002BBd (106238)2539
B(CaH2L)=26.76

C36H36N24O12 L Cucurbituril CAS 283175-97-3 (6744)
Cucurbit[6]uril;

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

Ca++ sol none 25°C dil C K1=3.61 2001BCf (106248)2540
Method: dissolution of ligand in a 0.002-0.02 M CaX2 solution;
spectrophotometric measurement.

Ca++ cal mixed 25°C 50% C H K1=2.80 1998BJb (106249)2541
Medium: 50% (v/v) HCOOH/H2O. DH(K1)=-6.5 kJ mol⁻¹

Ca++ sol none 25°C 0.0 U K1=9.13 1992BCa (106250)2542

C36H42N8 L Xylyl-cryptand CAS 172881-87-7 (7456)
1,4,12,15,18,26,31,39-Octaazapentacyclo[13.13.13.1.1.1]tetratatetracontadecane;

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

Ca++ sp non-aq 25°C 100% U K1=4.5 1996AAAd (106314)2543
B(Ca2L)=6.29

Medium: CH3CN

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

Ca++ cal non-aq 25°C 100% U K1=2.65 B2=3.50 1991SGa (106329)2544
Medium: CH3CN; Ca as Ca(NCS)2

Ca++ cal alc/w 25°C 100% U H K1=2.85 B2=3.55 1989SGc (106330)2545
Medium: EtOH. K=2.82 for polyethylene glycol analogue with 45 -(OCH2CH2)-
units

C36H47N3O6 L (8028)
Tripodal ionophore 2;

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

Ca++ sp non-aq 25°C 100% C 2001LFA (106371)2546
K(CaP+L=LiPL)=4.63

Method: Analyses by spectrophotometry. Medium: chloroform. P is picrate.

C36H52N8O6S2 L CAS 86701-12-4 (4454)
Ascidicyclamide;

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

Ca++ nmr mixed 25°C 95% C K1=2.9 2000CGa (106394)2547
Medium: 95% acetonitrile/H2O. Method: 1H nmr

C36H56N8O8S2 L L-Allothreonine CAS 108312-45-4 (4586)
Cyclo(-L-allothreonyl-2-[(1R)-1-amino-2-methylpropyl]-4-thiazolecarbonyl-L-isoleucyl-2);

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

Ca++ sp non-aq 25°C 100% C K1=4.0 B2= 4.50 2000CGa (106433)2548
Medium: acetonitrile. Method: circular dichroism.

C36H58N10O10S4 H5L CAS 136685-24-0 (6875)
(1-Cys-,1'-Cys,4-Cys-,4'-Cys)-dithiobis(Ac-1-Cys-Pro-D-Val-4-Cys-NH2);

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

Ca++ gl non-aq 20°C 100% U K1=3.21 B2=6.86 1993EAa (106439)2549
Method: circular dichroism. Medium: MeCN, ClO4-

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

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

Ca++ ISE alc/w 25°C 100% M K1=4.45 1984CTa (106485)2550
Medium: MeOH. In EtOH K1=6.78

Ca++ ISE non-aq 25°C 100% M K1=6.02 1984CTa (106486)2551
Medium: N,N-dimethylformamide. In DMSO K1=5.60

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

Ca++ sp KNO3 25°C 0.10M U K1=8.25 1974Y0a (106574)2552
B(CaHL)=19.15
B(CaH2L)=26.50
K(Ca+CaL=Ca2L)=5.38
K(Ca+CaHL=Ca2HL)=2.1

C38H32O4P2 L (1320)

1,4-Di(2-diphenylphosphinylphenyl)-1,4-dioxabutane;
Ph2PO.C6H4.O.CH2.CH2.O.C6H4.P(O)Ph2

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

Ca++ cal alc/w 25°C 100% U H K1=1.35 B2=3.46 1989SGc (106646)2553
Medium: C2H5OH

C38H42N4O24S4 H9L (5477)
1,5,10,14-Tetrakis(2,3-dihydroxy-5-sulfobenzoyl)-1,5,10,14-tetraazatetradecane;

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

Ca++ gl KNO3 25°C 0.10M C 1982KRb (106667)2554

B(CaH4L)=48.89
B(CaH3L)=39.86
B(CaH2L)=30.12
B(Ca2L)=16.2

C38H44N2O12 H4L Thymolphthalexo CAS 1913-93-5 (1963)
Thymolphthalexon, Thymolphthalein-3',3''-bis(methyliminodiethanoic acid)

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

Ca++ sp NaNO3 20°C 0.20M U 1965BBb (106673)2555

B(Ca2L2)=42.74

C38H48N8O6S2 H4L CAS 81098-23-9 (1789)
Patellamide B;

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

Ca++ nmr mixed 25°C 95% C K1=2.8 2000CGa (106678)2556
Data for Patellamide D. Medium: 95% acetonitrile/H2O. Method: 1H nmr

C38H68N8O10 L CAS 269398-65-4 (4484)
Cyclo[-2-aminobutanoyl-isoleucyl-threonyl-D-valyl-2-aminobutanoyl-isoleucyl-threonyl-D-valyl-];

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

Ca++ sp non-aq 25°C 100% C K1=5.5 2000CGa (106703)2557
Medium: acetonitrile. Method: circular dichroism

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

Ca++ EMF non-aq 25°C 100% C K1=9.96 1997PKc (106728)2558

Medium: nitrobenzene

C40H36O5P2 L CAS 86341-96-0 (5724)
1,7-Di(2-diphenylphosphinyl)phenyl-1,4,7-trioxahепtane;Ph2PO.C6H4.O.C2H4.O.C2H4.O.C
6H4.POPh2

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

Ca++ EMF non-aq 25°C 100% C K1=12.39 1997PKc (106737)2559

Medium: nitrobenzene

Ca++ EMF non-aq 25°C 100% C K1=16.50 1997PKc (106738)2560

Medium: nitrobenzene

Ca++ cal alc/w 25°C 100% U H K1=1.44 B2=2.51 1989SGc (106739)2561

Medium: EtOH. Also for 1,4,7,10-tetraoxadecane analogue, 1,4,7,10,13-
analogue and for 1,4,7,10,13,16- analogue

C40H38N2O16 H6L FluoRhod-1 (7028)
FluoRhod-1;

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

Ca++ sp oth/un 37°C ? U K1=5.12 1993SMc (106752)2562

Method: spectrofluorimetry. Also data for analogous alkyl substituted
ligands, including FluoRhod-2 (K1=5.97).

C40H50N2O10 L CAS 143902-45-8 (8935)
Decamethylcucurbit[5]uril;

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

Ca++ cal mixed 25°C 50% C H K1=2.40 2000ZKb (106802)2563

Medium: 50% v/v formic acid/H2O. Method: competitive calorimetric
titration with SrCl2. DH(K1)=17.1 kJ mol-1, DS(K1)=103 J K-1 mol-1.

C42H40O5P2 L CAS 163172-12-6 (2080)
Bis((2-diphenylphosphinylmethyl)phenyl)diethyleneglycol ether;

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

Ca++ EMF non-aq 25°C 100% C K1=10.14 1997PKc (106920)2564

Medium: nitrobenzene

C42H52N4O6 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

Ca++ sp R4N.X 25°C 0.10M C 2004COa (106960)2565
K(Ca+H2L=CaL+2H)=13.57

Medium: buffered 0.1 M Et4NCl, pH 8.5. By fluorescence emission spectroscopy, K=13.57.

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

Ca++ EMF non-aq 25°C 100% C K1=8.36 1997PKc (107124)2566
Medium: nitrobenzene

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

Ca++ gl non-aq 25°C 100% C K1=9.9 2000ABb (107139)2567
B(CaHL)=16.7
B(Ca2L)=13.58
B(Ca2HL2)=31.69

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]arene;

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

Ca++ sp non-aq 25°C 100% C K1=5.9 B2= 9.70 1999USa (107154)2568
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

Ca++ gl alc/w 25°C 90% M K1=3.6 1977LSc (107191)2569
Medium: 90% (w/w) MeOH/H2O, 0.1 M Et4NBr.

C45H48N3O3P3 L CAS 90179-28-5 (5682)
N,N',N''-tris(Diphenylphosphinylmethyl)-1,4,7-triazacyclononane;

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

Ca++ con non-aq 25°C 100% U I M 1984YSb (107221)2570
K(CaI+L)=3.2

Medium: tetrahydrofuran:CHCl3 1:1. In CH3CN:CHCl3 1:1 K=2.4

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

Ca++ sp mixed 25°C 90% C 1997KKa (107245)2571
K(Ca(SCN)2+L)=2.16

Method: fluorescence emission. Medium: MeOH/CHCl3 (9:1 v/v).

C46H46N2O16 H4L (7071)
7,16-Bis[2-(2,4-dicarboxyphenyl)-5-methoxy-1-benzofuran-6-yl]-tetraoxa-7,16-diazacyclooctadecane;

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

Ca++ sp none RT 0 U K1=1.82 1994CGa (107254)2572

Method: fluorimetry

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

Ca++ EMF non-aq 25°C 100% C K1=13.11 1997PKc (107274)2573

Medium: nitrobenzene

C46H56N4O10 HL Vincristine CAS 2068-78-2 (5998)
Vincristine;

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

Ca++ vlt oth/un 25°C 0.15M U 1986BVa (107289)2574
K(Ca+H2L)=3.27

Medium: 0.15 M Na acetate, pH 5.5

C46H58N4O9 HL Vinblastine CAS 143-67-9 (6046)
Vinblastine;

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

Ca++ ISE KCl 25°C 1.00M U K1=3.2 1989Vsa (107291)2575

C46H58O6 HL (6716)
Calix[4]arene-0(1)-ethanoic acid;

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

Ca++ gl alc/w 25°C 100% C K1=7.9 1993ABb (107293)2576

B(CaHL)=20.3
B(CaH2L)=32.42
B(CaH3L)=42.3

Medium: MeOH, 0.01 M Et4NClO4. Data also for tert-butyl and ethyl esters

C47H75NO17 H2L Nystatin CAS 1400-61-9 (5799)
Nystatin, Mycostatin;

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

Ca++ sol mixed 25°C 1% U K1=3.54 B2=6.93 1985B0a (107336)2577
Medium: 1 % v/v DMF/water; 3 M NaClO4

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

Ca++ EMF non-aq 25°C 100% C K1=11.54 1997PKc (107368)2578
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

Ca++ EMF non-aq 25°C 100% C K1=13.64 1997PKc (107372)2579
Medium: nitrobenzene

C48H54N6O8 L CAS 449738-94-7 (8791)
1,7-Dioxa-4,10-diazacyclododecane-4,10-bis[methylene-8-(1,3,3-trimethyl-6-nitro-spirobenzopyran)]

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

Ca++ sp alc/w 25°C 100% C K1=7.80 2002NFa (107382)2580
Medium: 100% MeOH. Method: electrospray ionization mass spectrometry.

C48H60O8 H2L R-Bu-Calixarene CAS 147513-53-9 (6705)
4-tert-Butylcalix[4]arenedicarboxylic acid;

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

Ca++ gl alc/w 25°C 100% C K1=9.0 1993ABb (107397)2581
B(Ca2L)=11.8

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
Ca++	sp	non-aq	25°C	100%	C		K1=3.29	2004BCb (107418)	2582
Medium: acetonitrile, 0.01 M Et4NClO4.									

C48H96N2O4		L					CAS 72469-41-1	(5351)	
N,N-Dioctadecyl-N',N'-dipropyl-3,6-dioxaoctanediamide;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	ISE	oth/un	21°C	100%	C		K1=14.9	1999CPa (107443)	2583
Medium: PVC/DOS ion selective electrode membrane (DOS: bis(2-ethylhexyl)-sebacate). Data for structurally related ionophores.									

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
Ca++	EMF	non-aq	25°C	100%	C		K1=12.66	1997PKc (107453)	2584
Medium: nitrobenzene									

C52H62N6O10		; L					CAS 190781-91-0	(8792)	
1,4,10,13-Tetraoxa-7,16-diazacyclododecane-7,16-bis[methylene-8-(trimethyl-6-nitro-spirobenzopyra									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	sp	alc/w	25°C	100%	C		K1=8.38	2002NFa (107478)	2585
Medium: 100% MeOH. Method: electrospray ionization mass spectrometry.									

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
Ca++	gl	alc/w	25°C	100%	C		K1=22.44 B(CaHL)=30.24 B(CaH2L)=36.39 B(CaH3L)=40.25	1993ABb (107485)	2586
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
Ca++	EMF	non-aq	25°C	100%	C	H	K1=>9	1999USa (107495)	2587
Medium: MeOH, 0.10 M Et4NCl. Method: by competition with Ag+.									

DH(K1)=-29 kJ mol⁻¹

C52H68N4O8 L (4823)
25,27-Bis(N,N-diethylaminocarbonylmethoxy)-26,28-bis(N-butylaminocarbonylmethoxy)calix[4]arene;

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

Ca++ sp non-aq 25°C 100% C K1=<1 1999USa (107503)2588
Medium: MeOH, 0.10 M Et4NCl

C52H72O6 L (9263)
5,11,17,23-Tetra(t-butyl)-25,27-dimethoxy-26,28-dimethoxyethoxycalix[4]arene;

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

Ca++ sp non-aq 25°C 100% C K1=3.22 2004BCb (107524)2589
Medium: acetonitrile, 0.01 M Et4NClO4.

C56H80O8 L (9259)
5,11,17,23-Tetra(t-butyl)-25,26,27,28-tetramethoxyethoxycalix[4]arene;

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

Ca++ sp non-aq 25°C 100% C K1=3.91 2004BCb (107610)2590
Medium: acetonitrile, 0.01 M Et4NClO4.

C58H78O11 HL CAS 465527-74-6 (9287)
7,13,19,25-Tetra-t-butyl-28-methoxy-27,29,30-triethylacetate-2,3-dihomo-3-oxacalix[4]arene;

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

Ca++ sp alc/w 25°C 100% C K1=3.1 2001MAa (107618)2591
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;

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

Ca++ sp non-aq 25°C 100% C K1=4.63 B2= 8.07 2004BCb (107627)2592
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

Ca++ gl non-aq 25°C 100% C K1=9.96 2000ABb (107662)2593
B(CaHL)=16.85
B(Ca2L)=15.43
B(Ca2HL2)=31.6

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

Ca++ sp alc/w 25°C 100% U H K1=5.1 2000ABa (107671)2594
Medium: 100% MeOH, DH(K1)=-6.4 kJ mol⁻¹ by colorimetry
K value for Mg++ less than 1

C60H84N4O8 L CAS 246035-32-5 (2735)
25,27-Bis(N,N-diethylaminocarbonylmethoxy)-26,28-bis(aminocarbonylmethoxy)-t-butylc
alix[4]arene;

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

Ca++ sp non-aq 25°C 100% C K1=6.0 1999USa (107675)2595
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

Ca++ sp non-aq 25°C 100% C K1=>6 1991ACc (107689)2596
Medium: acetonitrile, 0.01 M Et4NClO4.

C62H111N11O12 L CAS 59865-13-3 (9048)
Cyclosporin A;

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

Ca++ nmr non-aq 25°C 100% C K1=4.4 2003CGa (107715)2597
Method: ¹H nmr. Medium: d3-acetonitrile, 0.1 M C(ClO4)₂. By competition
with patellamide, K1=5.1.

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

Ca++ sp non-aq 25°C 100% C K1=3.00 2004BCb (107759)2598

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

Ca++ sp non-aq 25°C 100% C K1=3.78 2004BCb (107774)2599

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

Ca++ sp non-aq 25°C 100% C K1=>6 1999USa (107800)2600

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

Ca++ cal alc/w 25°C 100% U H 1995ABc (107809)2601

Medium: 100% Methanol. DH(K1)=-25.0 kJ mol-1, DS(K1)>88 J K-1 mol-1.

C69H102N4O9 L CAS 116352-85-3 (9286)
para-t-Butyldihomooxalix[4]arene tetra(diethyl)amide;

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

Ca++ EMF alc/w 25°C 100% C K1=5.0 2004MFa (107827)2602

Method: competitive potentiometry with Ag+. Medium: MeOH, 0.01 M Et4NCl.

C77H82O9 L CAS 253317-20-3 (9288)
p-Tert-butyldihomooxalix[4]arene tetraphenylketone;

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

Ca++ sp alc/w 25°C 100% C K1=4.0 1999MAb (107889)2603

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

Ca++ dis non-aq 25°C 100% U 1995FDa (107960)2604

K=5.48

Medium: CDCl3. Method: by H2O/CDCl3 extraction of picrate salt.

K: MA(org)+L(org)=MLA(org) where A=picrate.

C102H174N6O73 L CAS 571203-64-0 (9253)
4,13-Bis(2-(6-deoxy-b-cyclodextrin-6-yl)aminoethylamidomethyl)-4,13-diazatrioxacycl
opentadecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	R4N.X	25°C	0.10M	C			K1=5.35 K(Ca+HL)=4.59 K(Ca+H2L)=3.47	2003WWa (107971)	2605

Medium: 0.10 M Et4NClO4.

C112H120N4O16P4 L CAS 195455-62-0 (9276)
1,21,23,25-Tetrapentyl-7,11,15,28-tetra[(diphenylphosphinyl)acetamidomethylene]
cavitand;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	ISE	NaCl	rt	0.01M	C			K1=14.0	2003MGa (107987)	2606

Method: segmented sandwich membrane ISE.

Phosphonic acid diethyl ester derivative: K1=16.9

C114H198N6O73 L CAS 571203-66-2 (9254)
4,13-Bis(8-(6-deoxy-beta-cyclodextrin-6-yl)aminoethylamidomethyl)-4,13-diazatrioxac
yclopentadecan

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	gl	R4N.X	25°C	0.10M	C			K1=5.15 K(Ca+HL)=4.89 K(Ca+H2L)=4.49	2003WWa (107997)	2607

Medium: 0.10 M Et4NClO4.

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ca++	dis	non-aq	25°C	100%	U			K=5.57	1995FDa (108003)	2608

K=5.57

Medium: CDCl3. Method: by H2O/CDCl3 extraction of picrate salt.

K: MA(org)+L(org)=MLA(org) where A=picrate.

C120H200N8O16 L CAS 169888-21-5 (7490)
C-Undecylcalix[4]resorcinarene octa-alpha-(N,N-diethyl acetamide);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Ca++ dis non-aq 25°C 100% U 1995FDa (108014)2609
K=7.74

Medium: CDC13. Method: by H2O/CDC13 extraction of picrate salt.
K: MA(org)+L(org)=MLA(org) where A=picrate.

Polymer (1877)
4-Bis(carboxymethyl)-iminomethylene-oligostyrene; (C13H15NO4)n

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

Ca++ gl KNO3 25°C 0.10M U K1=4.56 1980YTb (108043)2610
(H2L)n: (.CH2.CH.C6H4.CH2.N(CH2.COOH)2)n where n=6-8

Polymer (5383)
4-Polyvinyl-N-benzyliminodiethanoic acid;

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

Ca++ EMF oth/un ? ? U K1=2.91 1966HEa (108049)2611

Polymer Albumin (3526)
Albumin;

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

Ca++ sol oth/un 38°C 0.16M U 1936WHa (108064)2612
K1'=2.20

Polymer H2L X-14885A (4547)
Antibiotic X14885A, calcium ionophore

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

Ca++ gl alc/w 25°C 100% U K1=7.9 1989ABb (108072)2613
Medium: MeOH, I=0 M. When I=0.1 M, K=6.0

Polymer H2L (8999)
Bacteriorhodopsin;

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

Ca++ ISE oth/un 22°C dil C 1995YAA (108080)2614
K1eff=5.11
K2eff=4.34

Method: Ca ion selective electrode. Medium pH 3.9.

Polymer HL Bleomycin (2324)
Bleomycin A2, B2 etc.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	gl	oth/un	25°C	?	U		K1=3.92	1980LPb (108083)	2615

Polymer					Calmodulin		CAS 73298-54-1	(2957)	
Calmodulin									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo	
Ca++	ISE	KCl	25°C	0.11M	C	H	K1=6.79 K3=5.39 K4=5.02	B2=13.03	1989HGa (108104)	2616
In PIPES buffer, pH 7.0. DH(B4)=22.5 kJ mol ⁻¹ ; DS(B4)=523.7.										

Polymer					Casein		(3527)			
Casein;										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	oth	NaCl	38°C	0.16M	U		K11=3.43, K12=3.11, K13=2.90 K14=2.74, K15=2.61, K16=2.49 K17=2.38, K18=2.28, K19=2.18 K1,10=2.08, K1,11=1.97	1946KLa (108115)	2617
K1,12=1.85, K1,13=1.72, K1,14=1.56, K1,15=1.36, K1,16=1.04. See reference for definitions. Calculated from Weir & Hastings, J.Biol.Chem., 1936, 114, 397									

Ca++	oth	oth/un	5°C	0.20M	U		K'=2.73	1942CLa (108116)	2618
Method: ultracentrifuge. Medium: 0.2 NaOH +40g casein/l. See reference for definition									

Ca++	sol	oth/un	?	?	U		K1=2.23	1936WHa (108117)	2619

Polymer					Cephalin		(4184)		
Cephalin									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	oth	NaCl	25°C	0.16M	U		K'=3.10, Frog heart	1943DZa (108118)	2620
See reference for definition									

Polymer					DNA		(4185)		
Deoxyribonucleic acid;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ca++	oth	NaCl	25°C	0.20M	U	I	K'=1.92(calf thymus)	1957WNa (108132)	2621

Method:dialysis. By ion exchange: K'=2.21. See reference for definitions

Polymer (5379)
 Dextran derivative of N-propyliminodiethanoic acid;

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

 Ca++ gl oth/un 20°C 0.10M U K1=3.64 1968VGa (108159)2622

Polymer Globulin (3528)
 Globulin;

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

 Ca++ oth NaCl 25°C 0.16M U 1939DGa (108198)2623

K'=3.0(pseudoglobulin)
 K'=2.9(euglobulin P1)
 K'=2.0(euglobulin P2)
 K'=3.1(euglobulin P3)

From frog heart(horse serum). See reference for definitions

 Ca++ sol oth/un ? ? U K1=2.32 1936WHa (108199)2624

Polymer Humic acid (1524)
 Humic acid;

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

 Ca++ gl KCl 24°C 0.10M C 19990Wa (108229)2625

K1eff=3.6
 Keff(2Ca+L)=6.7

 Ca++ dis NaCl04 25°C 0.10M U 1981CSa (108230)2626
 K(Ca+HnL)=ca.2.5 at pH 3.9

Polymer (4181)
 Phosphatidic acid;

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

 Ca++ gl oth/un 24°C 0.10M U K1=4.2 1966AKa (108267)2627

 Ca++ oth oth/un 24°C 0.03M U K1=4.14 1965AKa (108268)2628
 Method: light scattering. Medium: 0.03 M NaCl, 0.05 M tris buffer

Polymer (4183)
 Phosphatidylserine;

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

Ca++ gl R4N.X 20°C 0.10M U K1=4.1 1965HFb (108275)2629
K(Ca+HL)=4.0

Medium: Pr4NI

Polymer (4192)
Polyacrylic acid and 7.5% divinylbenzene copolymer

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

Ca++ gl NaNO3 25°C 1.0M U H 1968GLc (108303)2630
K'=-8.03(n'=0.1)

K'=-8.71(n'=0.2), -9.39(n'=0.3), DH=27.6(n'=0.1), 39.7(n'=0.2) kJ mol⁻¹

DS=-59(n'=0.1), -33(n'=0.2) J K⁻¹ mol⁻¹. See ref. for definition

Polymer HL (3531)
Polyacrylic acid;

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

Ca++ gl KCl 25°C 1.0M U 1955GLb (108319)2631
K'=2.0

See reference for definitions. K'=2.6 (Co), 1.8(Mg), 3.36(Mn), 3.32(Zn)

Polymer Elastase CAS 39445-21-1 (7314)
Porcine pancreatic elastase;

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

Ca++ oth oth/un 25°C 0.15M U 1980JMb (108385)2632
K1eff=5.32

Medium: 0.1 M KCl, 0.05 M MOPS, pH 6.85. Method: enhancement of Tb lumin-
escence

Polymer RNA (4205)
Ribonucleic acid;

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

Ca++ oth NaCl 25°C 0.15M U 1957WNa (108412)2633
K'=2.32(calf liver)

Method: dialysis. See reference for definition

Polymer (4182)
Triphosphoinositide;

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

Ca++ gl R4N.X 20°C 0.10M U K1=5.0 1965HFb (108418)2634
K(Ca+HL)=3.8

Medium: Pr4NI. Ligand assumed as H2L

Polymer L (8039)
alpha-Amylase;

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

Ca++ cal oth/un 27°C 0.01M C H 2000SKa (108420)2635
K1eff=0.26

Medium: tris buffer, pH 7.3. DH(K1eff)=-16 kJ mol⁻¹.
Additional method: dialysis.

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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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