SC-Database
Software version = 5.81 Data version = 4.62
Experiment list contains 2162 experiments for
 (no ligands specified)
 Metal : Mg++
 (no references specified)
 (no experimental details specified)

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

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ EMF none 25°C 0.00 U 1973LMa (288) 1
  K(Mg+2e=Mg/Hg)=-65.59(-1.940V)

Mg++ oth none 25°C 0.0 U 1946STa (289) 2
  K(Mg+2e)=-79.75(-2358 mV)

Mg++ oth none 25°C 0.0 U 1945COa (290) 3
  K(Mg+2e)=-80.3(-2375 mV)
****
AsO4--- H3L Arsenate CAS 7778-39-4 (1557)
Arsenate;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ sol oth/un 20°C var U 1956CHd (1127) 4
  Kso(Mg3L2)=-19.68
****
AsW11O39------- H7L (2468)
alpha-Heteromonoarseno-polytungstate;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl NaNO3 25°C 1.00M U K1=0.4 1984COa (1175) 5
****
As2W17H2O61-------- H8L (2469)
alpha-Heteropolydiarseno-polytungstate;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl NaNO3 25°C 1.00M U K1=3.94 1984COa (1186) 6
  K1=1.06 (alpha2 isomer)
****
BO4H4- HL Borate CAS 10043-35-3 (991)
Borate; B(OH)4-

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

---

Mg++ EMF oth/un 25°C 0% M TIH K1=1.487 1995SWa (1296) 7
Method: Pt/H2 electrode. Medium: LiCl/MgCl2/B(OH)3/LiB(OH)4, 0.015-0.15 m.
DH(K1)=10.2 kJ mol-1, DS(K1)=62.6 J K-1 mol-1.

Mg++ gl NaCl 25°C 0.70M U K1=1.13 1988RBa (1297) 8

Mg++ gl none 25°C 0.0 M TIH 1976REa (1298) 9
K(Mg+H2BO3)=1.62
Calculated from data for 0.02-0.16 M MgCl2. Data for 10-50 C.
DH(Mg+H2BO3)=2.0 kJ mol-1, DS=38 J K-1 mol-1.

Mg++ EMF NaCl 25°C 0.68M U K1=0.90 1974BKd (1299) 10

Mg++ oth NaCl 25°C 0.70M U K1=0.73 1972DHa (1300) 11
Method: estimated value

****

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

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

---

Mg++ gl NaClO4 25°C 3.0M U K1=-1.5 1973HHa (1714) 12
Method: also vapor phase osmometry

Mg++ con alc/w 20°C 100% U K1=3.38 1949GOb (1715) 13
Medium: EtOH; I=0 corr.

****

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

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

---

Mg++ cal oth/un 25°C 0.03M C I 1981HWb (2609) 14
DH(Mg + Fe(CN)6)=12.2 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

---

Mg++ EMF NaClO4 25°C 3.0M C HM 1992KSb (3100) 15
Solubility of Eitelite: Ks(NaMg0.5CO3+2H=Na+0.5Mg+CO2+H2O)=14.67.
Pitzer parameters evaluated

Mg++ sol none 25°C 0.0 U K1=3.32 1985LDb (3101) 16
K(Mg+HCO3)=1.23

Mg++ gl NaClO4 25°C 3.00M U T 1977RGb (3102) 17
K(Mg+CO2+H2O=MgCO3+2H)=-15.64

K(Mg+CO2+H2O=MgHCO3+H)=-7.64
K'=-15.00
at 50 C: K(Mg+CO+H2O=MgHCO3+H)=7.46, K(Mg+CO2+H2O)=MgCO3+2H)=-15.23,
K'=-15.37. K': Mg+2CO2+2H2O=Mg(HCO3)2+2H

Mg++ gl none 25°C 0.0 U T H K1=2.984 1977SHb (3103) 18
K(Mg+HL)=1.066
Calculated from data for 0.09-0.33 m MgCl2/KHCO3. Data for 10-90 C.
DH(K)=4.99 kJ mol-1, DS(K)=37.1 J K-1 mol-1. At 90 C, K=1.34

Mg++ gl oth/un 25°C 0.0 M TIH K1=2.98 1977SHc (3104) 19
Calculated from data for 0.04-0.12 m MgCl2/KHCO3. Data for 10-90 C.
DH(K)=8.44 kJ mol-1, DS(K)=85.4 J K-1 mol-1. At 90 C, K1=3.41

Mg++ EMF oth/un 25°C 0.70M U K1=2.05 1974PHc (3105) 20
K(Mg+HL)=0.21
Medium: synthetic seawater

Mg++ EMF oth/un 25°C 0.70M U M 1974PHc (3106) 21
B(MgCaL2)=3.02
Medium: synthetic seawater

Mg++ gl none 25°C 0.0 U T K1=2.88 1974RLa (3107) 22
K1=-21.39+3265/T+0.0446T

Mg++ oth NaCl 25°C 0.70M U K1=1.5 1972DHa (3108) 23
K(Mg+HCO3)=0.02
Method:Estimated data

Mg++ sol none 25°C 0.0 U T M 1971LAa (3109) 24
Kso(MgCaL2)=-17.0
Kso(MgCaL2)=-16.56(0 C),-16.63(5 C),-16.71(10 C),-16.79(15 C),-16.89(20 C)

Mg++ ISE none 25°C 0.0 U I K1=3.24 1971NAa (3110) 25
K(Mg+HL)=1.23
Also data at various ionic strengths

Mg++ sol none 90°C 0.0 U 1970CHa (3111) 26
Kso=-9.1(magnesite)

Mg++ oth none 25°C 0.0 U T 1970CHa (3112) 27
Kso=-8.09
Method: Estimated data. Kso=-7.60(0C),-7.80(10C),-7.99(20C),-8.17(30C),-8.34
(40C), -8.51(50C), -8.69(60C), -8.88(70C), -9.10(80C),-9.29(90C),-9.50(100C)

Mg++ oth none 50°C 0.0 U T 1969HEa (3113) 28
Kso(MgCa(CO3)2)=-17.63
Method: Estimated data. Kso=-17.92(60 C); -19.28(100 C); -21.02(150 C);
-23.26(200 C); -25.83(250 C); -28.46(300 C).(dolomite)

```
Mg++       sol NaClO4 25°C 3.00M U                        1969HOd  (3114)  29
                                        K(Mg+HL)=1.49
K(MgCO3(s)+2H=Mg+CO2(g)+H2O)=9.58(magnesite)
-------------------------------------------------------------------------------
Mg++       sol NaClO4 25°C 3.00M U    M                   1969HOd  (3115)  30
K(CaMg(CO3)2(s)+4H=Mg+Ca+2CO2(g)+2H2O)=18.16(dolomite)
-------------------------------------------------------------------------------
Mg++       EMF NaClO4 25°C 3.00M U        K1=1.79         1969RGa  (3116)  31
                                        K(Mg+HL)=0.15
                                        K(MgHL+HL)=0.47
K1 and K on the basis of Kw=-14.22, K(H+L)=9.57, K(HL+H)=7.80
-------------------------------------------------------------------------------
Mg++       oth oth/un 25°C  0.0  U    M                   1965HAb  (3117)  32
                                        K(CaL(s)+MgL(s))=1.26
-------------------------------------------------------------------------------
Mg++       oth oth/un 18°C  0.0  U    M                   1964HKa  (3118)  33
                                        Kso(MgCaL2)=-17
K(2CaL(s)+Mg=MgCaL2(s)+Ca)=0.54. Method: analysis
-------------------------------------------------------------------------------
Mg++       sol oth/un 180°C  var  U    M                   1964USa  (3119)  34
K(2CaL(s)+Mg=MgCaL2(s)+Ca)=1.28, K(MgCaL2(s)+Mg=2MgL(s)+Ca)=0.37
-------------------------------------------------------------------------------
Mg++       gl  oth/un 22°C  0.0  U                        1963HOd  (3120)  35
                                        K(Mg+HL)=0.86
                                        K(MgL+H)=8.00
-------------------------------------------------------------------------------
Mg++       gl  oth/un 25°C  0.0  U                        1963HOd  (3121)  36
                                        K(Mg+HL)=0.95
-------------------------------------------------------------------------------
Mg++       sol oth/un 25°C  0.0  U    M                   1963SRa  (3122)  37
Medium: 0 corr. K(CaMgL2(s)+2CO2(g)=Mg+Ca+4HL)=-13.19,
K(CaL(s)+MgL(s)=CaMgL2(s))=2.07
-------------------------------------------------------------------------------
Mg++       oth oth/un 25°C  0.0  U   HM                   1963SRa  (3123)  38
K(CaL(s)+MgL(s)=MgCaL2(s))=1.98, DH=-12.3 kJ mol-1
-------------------------------------------------------------------------------
Mg++       gl  none   25°C  0.0  U                        1962GTa  (3124)  39
                                        K(Mg+HL)=1.16
-------------------------------------------------------------------------------
Mg++       gl  none   25°C  0.0  U        K1=3.40         1961GTa  (3125)  40
-------------------------------------------------------------------------------
Mg++       sol none   25°C  0.0  U T                      1961YRb  (3126)  41
                                        Kso(MgCO3(s))=-7.46
                                        Kso(MgCO3(H2O)3(s))=-4.56
I=0 corr. Kso(MgCO3, magnesite)=-7.52(0 C), -7.66(40 C), -7/09(55 C).
Kso(MgCO3(H2O)3, nesquehonite)=-4.70(0 C), -4.49(40 C)
-------------------------------------------------------------------------------
Mg++       sol none   25°C  0.0  U    M                   1960GTa  (3127)  42
                                        Kso(MgCaL2(s))=-19.33
-------------------------------------------------------------------------------
```

```
Mg++       sp  oth/un 20°C 0.10M U        K1=2.18        1960RAa  (3128)  43
-------------------------------------------------------------------------------
Mg++       sol none   25°C  0.0  U T HM                  1959HAb  (3129)  44
                                        K=0.52
K: CaL(s)+MgL(s)=CaMgL2(s). DH(K)=-7.32 kJ mol-1; DS=14.7 J K-1 mol-1
-------------------------------------------------------------------------------
Mg++       sol oth/un 25°C 3.5%  U    M                  1959KRd  (3130)  45
                                        Kso(MgCaL2(s)=Mg+Ca+2L)=-12.35
                                        Ks(MgCaL2+Ca=2CaL(s)+Mg)=-0.15
Medium: 3.5-6.0% sea water. Kso=-11.86, Ks=-0.16(at 4.5% salinity);
Kso=-11.69, Ks=-0.21(at 6.0% salinity). Ks=-16.82(I=0 corr)
-------------------------------------------------------------------------------
Mg++       sol oth/un 25°C 3.5%  U  I M                  1958KRa  (3131)  46
                                        K=1.28
Medium: 3.5-6.0% sea water. K(MgCaL2(s)+Ca=2CaL(s)+Mg)=1.00 at 4.5% salinity
and 0.90(at 6.0% salinity).
-------------------------------------------------------------------------------
Mg++       EMF oth/un 25°C  var  U                      1942NAb  (3132)  47
                                        K(Mg+HL)=3.7
Method: H electrode
-------------------------------------------------------------------------------
Mg++       gl  oth/un 22°C  var  U                      1941GRa  (3133)  48
                                        K(Mg+HL)=0.77
                                        K(MgL+H=MgHL)=-8.50
-------------------------------------------------------------------------------
Mg++       sol none   25°C  0.0  U T H                  1935HRa  (3134)  49
                                        Kso(MgCO3(magnesite))=-7.80
I=0 corr. K=-7.74(38.8 C). By calorimetry, 20 C, 2 M HCl: DH(MgCO3(s)+2H=
Mg+H2O+CO2(g))=-14.6 kJ mol-1
-------------------------------------------------------------------------------
Mg++       sol none   25°C  0.0  U T HM                 1935HRa  (3135)  50
                                        Kso(MgCaL2(s))=-16.50
                                        K'=0.39
                                        K"=-0.58
I=0 corr. Kso=-16.74(38.8 C). K':2CaCO3(s)+Mg=MgCa(CO3)2(s)+Ca) =0.42(38.8C)
K": MgCaL(s)+Mg=2MgL(s)+Ca. K"=-0.61(38.8 C).
-------------------------------------------------------------------------------
Mg++       cal oth/un 20°C  2.0M U   H                  1935HRa  (3136)  51
Medium:HCl. DH(MgCa(CO3)2(s)+4H=Mg+Ca+2CO2(g)+H2O)=-41.8 kJ mol-1.
-------------------------------------------------------------------------------
Mg++       sol none   25°C  0.0  U                      1929KLa  (3137)  52
                                        Kso(MgCO3(s))=-5.0
-------------------------------------------------------------------------------
Mg++       sol none   25°C  0.0  U                      1923MIa  (3138)  53
                                        Ks(MgCO3(s)+H2CO3)=-0.35
I=0 corr. Ks: MgCO3(s)+H2CO3=Mg+2HCO3
-------------------------------------------------------------------------------
Mg++       sol none   22°C  0.0  U T H                  1915JOa  (3139)  54
                                        Kso(MgCO3(s))=-4.01
I=0 corr. Kso=-3.51(3.5 C), -3.73(12 C), -3.94(18 C), -4.23(30 C),
```

-4.49(40 C), -4.68(50 C). DH=-44.4 kJ mol-1

Mg++ sol none 12°C 0.0 U 1900BOa (3140) 55
Kso(MgCO3(s))=-4.59

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	ISE	oth/un	25°C	0.00	U	H	K1=3.77	1975JLa (3553)	56

DH=18.8 kJ mol-1

Mg++ EMF oth/un 25°C 3.0M U K1=3.40 1975LMd (3554) 57
Background salt: LiClO4

Mg++ sp none 25°C 0.0 U I K1=3.81 1957CPa (3555) 58
Also for iso-Pr/H2O mixtures

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	cal	oth/un	25°C	0.10M	U		K1=1.44	1982ARa (3624)	59

Mg++ EMF oth/un 25°C 3.0M U K1=0.79 1975LMd (3625) 60
Background salt: LiClO4

Mg++ sol oth/un 25°C 3.0M U K1=0.04 1967RMd (3626) 61
Medium: LiNO3

Mg++ sol oth/un 25°C 3.0M U H K1=-1.03 1966MRb (3627) 62
Medium: LiCl. By calorimetry: DH(K1)=-14.2 kJ mol-1, DS=-67 J K-1 mol-1

Mg++ con none 25°C 0.0 U K1=2.79 1952GMb (3628) 63

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	ISE	NaNO3	25°C	0	C	TI	K1=0.49	1998RSa (4423)	64

Method: Cl-ISE, extrapolated to I=0

Mg++ oth alc/w 25°C 61% C K1=20.80 1996CHf (4424) 65
Kso(MgCl2.6H2O)=4.55
Method: application of Pitzer theory to literature data.

Mg++ cal none 250°C 0.0 C TIH K1=1.86 1992GOa (4425) 66

Calculated from data for 0.24-1.0 m MgCl2. Data for 250-325 C.
DH(K1)=72.7 kJ mol-1, DS(K1)=175 J K-1 mol-1.

Mg++ sol NaCl 300°C var M TI K1=2.30 1990SSa (4426) 67
300-400 C and 500 bar. Constants at I=0

Mg++ sp NaClO4 25°C 1.00M U K1=<0.77 1983BWa (4427) 68

Mg++ gl KNO3 25°C 3.00M U T H K1=-0.13 1982MSb (4428) 69
K1=-0.14(15 C), K1=-0.08(45 C), K1=-0.02(65 C), K1=0.10(85 C)
DH=2.34 kJ mol-1, DS=5.4 J mol-1 K-1

Mg++ gl KCl 25°C 0.70M U K1=-0.46 1978EWa (4429) 70

Mg++ con none 25°C 0.0 C K1=0.66 1977FFa (4430) 71
P=1 atm. Also data for P=250-2000 atm.

Mg++ sol oth/un 25°C 0.70M C K1=-0.32 1975EWa (4431) 72
Mixed medium of NaCl, KCl, MgCl2, NaClO4, Mg(ClO4)2, Na2SO4.
Method: solubility of gypsum.

Mg++ EMF NaNO3 25°C 0.10M C T H K1=-0.11 1975SCd (4432) 73
Method: Ag,AgCl electrode. Data for 15-60 C.
DH(K1)=-5.42 kJ mol-1, DS(K1)=-20.5 J K-1 mol-1.

Mg++ con non-aq 25°C 100% U K1=2.6 1974KKc (4433) 74
Medium: 50% w/w EtOH/acetone. K1=2.48 to 2.68 (depending upon eqn)

Mg++ oth NaClO4 25°C 3.0M U K1=1.0 1973HHa (4434) 75
Method: vapor phase osmometry

Mg++ sol oth/un 25°C 0.0 U 1967LEa (4435) 76
Ks(KMgCl3(H2O)3,x)=4.00
Ks(MgCl2(H2O)6,y)=4.445
x=carnallite, y=bischofite

Mg++ con alc/w 20°C 100% U T K1=3.79 1960GDa (4436) 77
Medium: EtOH, I=0 corr. K1=3.22(-40 C), 3.40(-20 C), 3.67(0 C)

Mg++ con diox/w 35°C 20% U I K1=1.3 1959DDa (4437) 78
I=0 corr. K1=1.7(30% dioxan)

Mg++ oth NaClO4 0°C sat U I K1=0.62 1959KEb (4438) 79
Method: freezing point, Medium:KClO4 sat. In KClO3 sat K1=0.08.
I=0 corr. K1=0.91

****

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

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

---

Mg++ con mixed 25°C 20% C K1=1.66 2003SIa (6142) 80
Medium: 20% w/w propylene carbonate/ethylene carbonate.

Mg++ con non-aq 25°C 100% C K1=1.54 1992STa (6143) 81
Medium: propylene carbonate.

Mg++ oth non-aq 25°C 100% U T H K1=0.06 1974PKc (6144) 82
Medium: acetone. DH(K1)=5.4 kJ mol-1. K1=-0.40(-90 C), -0.17(-45 C),
-0.07(-25 C), 0.02(0 C), 0.23(45 C). Method: infrared spectra

****

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

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

---

Mg++ ISE none 25°C 0.0 C B2=3.2 2000FGa (6676) 83
Calculated from data for I=0.10 M (TISAB).

Mg++ ISE none 25°C 0.0 C 1993DPd (6677) 84
Kso(MgF2)=-8.12
Method: double membrane F ion selective electrode.

Mg++ ISE NaCl 25°C 1.0M M I K1=1.16 1988CBb (6678) 85
Method: F ion selective electrode and glass electrode. At I=3.0, K1=1.12;
at I=5.0, K1=1.32.

Mg++ ISE alc/w 25°C 100% C B2=11.1 1988TIa (6679) 86

Mg++ gl KNO3 25°C 3.00M U T H K1=1.35 1982MSb (6680) 87
K1=1.31(15 C), K1=1.44(45 C), K1=1.54(65 C), K1=1.64(85 C)
DH=7.32 kJ mol-1, DS=50.6 J mol-1 K-1

Mg++ ISE alc/w 25°C 100% C I K1=4.40 1978BBc (6681) 88
Medium: MeOH, 0.05 M NaClO4. In 0.05 M Et4NClO4 K1=4.56
In H2O, 0.05 M NaClO4 K1=1.80, in 0.05 M Et4NClO4 K1=1.86

Mg++ gl NaClO4 25°C 0.70M U K1=1.36 1978EWa (6682) 89

Mg++ ISE NaClO4 25°C 1.0M U T K1=1.38 1971BHc (6683) 90
K1=1.23(2 C), 1.40(35 C)

Mg++ ISE NaNO3 25°C 1.0M U T H K1=1.32 1971CVa (6684) 91
DH(K1)=6.3 kJ mol-1, DS=46.9 J K-1 mol-1. K1=1.27(15 C), 1.35(35 C)

Mg++ ISE NaClO4 16°C 0.50M U K1=1.26 1970BOa (6685) 92

Mg++ ISE NaCl 25°C 0.10M U I K1=1.46 1970ELd (6686) 93
K1=1.41(I=0.2), 1.34(I=0.4), 1.29(I=0.6), 1.27(I=0.7-1.0)

Mg++ ISE NaClO4 25°C 0.50M U K1=1.32 1969ALa (6687) 94

Mg++ ISE NaNO3 25°C 1.0M U K1=1.31 1969GSa (6688) 95

Mg++ ISE NaClO4 25°C 1.0M U T K1=1.32 1968TWa (6689) 96
K1=1.15(2 C), 1.40(39 C)

Mg++ cal NaClO4 25°C 1.0M U H 1968TWa (6690) 97
By calorimetry: DH(K1)=13.4 J K-1 mol-1, DS(K1)=70.3 J K-1 mol-1

Mg++ ISE NaClO4 25°C 1.0M U H 1968TWa (6691) 98
DH(K1)=11.3 kJ mol-1, DS(K1)=62.8 J K-1 mol-1

Mg++ EMF NaClO4 25°C 0.50M U T H K1=1.30 1954CTa (6692) 99
At 15 C K1=1.20. DH(K1)=17 kJ mol-1, DS=80 J K-1 mol-1. AT I=0 corr, 25 C, K1=1.82

Mg++ con none 27°C 0.0 U T 1923BOa (6693) 100
Kso(MgF2)=-8.19

****

GeW11O39-------- H8L CAS 37369-86-1 (2466)
alpha-Heteromonogermanium-polytungstate;

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

---

Mg++ gl NaNO3 25°C 1.00M U K1=2.96 1984COa (7467) 101

****

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

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

---

Mg++ con alc/w 20°C 100% U K1=3.29 1949GOb (7882) 102
Medium: EtOH, I=0 corr.

****

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

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

---

Mg++ sol none 25°C 0.0 U K1=0.72 1938WDa (8489) 103

Mg++ sol none 25°C 0.0 U K1=0.72 1930DAa (8490) 104

****

MoO4-- H2L Molybdate (443)
Molybdate;

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

---

Mg++ sp oth/un 25°C ? U M 1997STa (8708) 105

K(Mg+H2L=MgL+2H)=-3.1

Ligand: nano-Molibdenomanganate, MnMo9O32------

****

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

Ammonia

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values			Reference	ExptNo
Mg++	vlt	oth/un	0°C	2.40M	U		K1=0.19	B2=0.06		1973SBd (9087)	106
							B3=-0.19				
							B4=-1.0				
							B5=-1.7				

Medium:Na2SO4

Mg++	cal	R4N.X	rt	3.0M	U	H				1952FYa (9088)	107

Medium: NH4NO3. DH(B6?)=-0.42 kJ mol-1; DS(B6?)=-79.5.

Mg++	sol	oth/un	25°C	dil	U		K1=-0.1			1943DVa (9089)	108

Mg++	gl	R4N.X	23°C	2.0M	U		K1=0.23	B2=0.08		1941BJa (9090)	109
							K3=-0.42				
							K4=-0.7				
							K5=-0.95				
							K6=-1.3				

Also by solubility. Medium: NH4NO3.

****

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

Nitrate;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values			Reference	ExptNo
Mg++	sp	oth/un	25°C	5.80M	U		K1=0.061			1980BDa (9562)	110

Mg++	con	non-aq	25°C	100%	U		K1=2.60			1974KKc (9563)	111

Medium:1:1 EtOH/Me2CO

Mg++	ix	mixed	23°C	90%	U		K1=0.20	B2=-0.07		1966WFa (9564)	112

Medium: i-PrOH, 0.5 M HL

****

OH- HL Hydroxide (57)

Hydroxide;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values			Reference	ExptNo
Mg++	EMF	NaCl	25°C	0.0	C	H				1997PWa (10855)	113
							*K1=-11.68				

Method: Pt/H2 electrode. Data for 1-250 C and 0.11-5.0 mol kg-1 NaCl.
DH(*K1)=70.1 kJ mol-1, DS(*K1)=11 J K-1 mol-1. For 1.0 M NaCl, *K1=-11.91.

Mg++	EMF	NaCl	60°C	0.10M	C	TIH				1996BDb (10856)	114

```
                                        K(Mg=Mg(OH)2+2H)=-15.29
Hydrogen electrode. No evi. Mg(OH)+. At I=1.0 M NaCl: K=15.52. Also data at
T=100, 150, 200 C. At I=0.0 M: K=-17.13 (25 C), -15.61 (60 C), DH=112 kJ m-1
--------------------------------------------------------------------------------
Mg++       sol oth/un 350°C  var  U T                    1986WAa (10857) 115
                                        *K1=-5.38
                                        K(Mg(OH)2(s)+H=Mg(OH)+H)=7.22
300-600 C, P=1-3 kbar. Constant at I=0
--------------------------------------------------------------------------------
Mg++       gl  NaNO3  25°C 1.00M U                      1981EIb (10858) 116
                                        *B(2,2)=-21.07
                                        *B(3,4)=-39.16
--------------------------------------------------------------------------------
Mg++       gl  NaClO4 25°C 3.00M U T                    1978BBa (10859) 117
                                        *K1=-12.00
                                        *B(2,1)=-12.30
                                        *B(4,4)=-38.80
--------------------------------------------------------------------------------
Mg++       gl  NaNO3  25°C  1.0M U                      1977EIa (10860) 118
                                        *B(2,2)=-22.07
                                        *B(3,4)=-39.06
--------------------------------------------------------------------------------
Mg++       gl  none   25°C  0.0  U T      K1=2.21       1975MHb (10861) 119
At 10 C: K1=2.18; 90 C: 2.54
--------------------------------------------------------------------------------
Mg++       oth NaCl   25°C 0.70M U        K1=1.6        1972DHa (10862) 120
Method:Estimated data
--------------------------------------------------------------------------------
Mg++       gl  KNO3   37°C 0.15M U                      1970CHc (10863) 121
                                        *K1=-11.5
--------------------------------------------------------------------------------
Mg++       oth none   60°C  0.0  U T      K1=2.8        1969HEa (10864) 122
                                        *Kso=14.84
Method:Literature evaluated data. K1=2.7(50 C). 100 C: K1=3.1, *Kso=13.19.
150 C: K1=3.6,*Kso=11.41. 200 C:K1=4.1,*Kso=10.09.*Kso=9.08(250C),8.53(300C)
--------------------------------------------------------------------------------
Mg++       sol NaClO4 25°C 3.00M U        K1=4.48       1969HOd (10865) 123
                                        *Ks=16.58(brucite)
*Ks(Mg(OH)2+2H=Mg+2H2O)
--------------------------------------------------------------------------------
Mg++       oth none   25°C  0.0  U T                    1968KRa (10866) 124
                                        Kso=-10.50
Method:Estimated data. Kso=-10.71(50 C), -11.45(100 C), -12.48(150 C)
--------------------------------------------------------------------------------
Mg++       sol none   25°C  0.0  U        K1=2.60       1963HOb (10867) 125
                                        Kso=-11.15
--------------------------------------------------------------------------------
Mg++       gl  NaCl   25°C  3.0M U                      1963LEa (10868) 126
*K1=-12.2 or *B(2,1)=-12.3 or *B(4,4)=-39.8. Method: H electrode
--------------------------------------------------------------------------------
```

```
Mg++       EMF KCl    30°C 0.10M C                          1952CCa (10869) 127
                                     *K1=-12.8
-------------------------------------------------------------------------------
Mg++       EMF none    0°C  0.0  C                         1951VIa (10870) 128
                                     Kso(Mg(OH)2)=-9.22
-------------------------------------------------------------------------------
Mg++       con oth/un 20°C  dil  U                          1948KAa (10871) 129
                                     Kso(Mg(OH)2)=-10.85
-------------------------------------------------------------------------------
Mg++       gl  none   25°C  0.0  U        K1=2.58          1948SDa (10872) 130
-------------------------------------------------------------------------------
Mg++       EMF none   25°C  0.0  C                         1941NAa (10873) 131
                                     Kso(Mg(OH)2)=-10.51
Method: H electrode. Also Kso=-10.74
-------------------------------------------------------------------------------
Mg++       sol none   25°C  0.0  U                         1929KLa (10874) 132
                                     Kso(Mg(OH)2)=-11.30
-------------------------------------------------------------------------------
Mg++       EMF oth/un 16°C  var  C                         1925BRa (10875) 133
                                     Kso(Mg(OH)2)=-10.64
Method: H electrode
-------------------------------------------------------------------------------
Mg++       EMF none   18°C  0.0  C        K1=2.1           1925GJa (10876) 134
                                     Kso=-10.93 (stable)
                                     Kso=-9.2 (unstable)
-------------------------------------------------------------------------------
Mg++       con oth/un 20°C  var  U                          1924RKa (10877) 135
                                     Kso(Mg(OH)2)=-9.63
-------------------------------------------------------------------------------
Mg++       sp  oth/un 18°C  var  U        K1=2.4           1923KOa (10878) 136
Medium: MgCl2 var. Method: colorimetry
-------------------------------------------------------------------------------
Mg++       kin oth/un 100°C 0.06M U        K1=2.62         1913KUa (10879) 137
                                     *K1=-9.76
*******************************************************************************
PO4---                H3L    Phosphate        CAS 7664-38-2  (176)
Phosphate;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Mg++       gl  KCl    25°C 0.25M C T                        1996IFa (13057) 138
                                     B(MHL)=13.80
At 37 C: B(MgHL)=13.76
-------------------------------------------------------------------------------
Mg++       gl  NaNO3  25°C 0.10M M                          1996SSa (13058) 139
                                     K(Mg+HL)=1.83
-------------------------------------------------------------------------------
Mg++       gl  NaClO4 25°C  3.0M C  I                       1994CIa (13059) 140
                                     K(Mg+H2L)=0.16
                                     K(Mg+2H2L)=0.64
```

K(Mg+2H2L=MgHL+H3L)=-3.17
K(Mg+3H2L=MgH3L2+H3L)=-2.49
At I=0, SIT extrapolation: K(Mg+H2L)=0.61, K(Mg+2H2L)=1.53, K(Mg+HL)=2.85
K(Mg+HL+H2L)=3.51

Mg++ oth NaCl 25°C 0.15M U T K1=1.9 1993GMa (13060) 141
Method: Coulometric titration. K1=2.9 (37 C)

Mg++ gl NaCl 25°C 0.00 C 1989HFa (13061) 142
K(Mg+HL)=2.70

Mg++ gl KCl 25°C 0.20M U K1=3.13 1985LLa (13062) 143
K(Mg+HL)=1.94
K(Mg+H2L)=1.51

Mg++ sol none 25°C 0.0 U 1984VBa (13063) 144
K(Mg+H2PO4)=1.28
K(Mg+HPO4)=2.85

Mg++ gl R4N.X 37°C 0.10M C I 1982DRc (13064) 145
K(Mg+H2PO4)=1.22
K(Mg+HPO4)=2.16
Additional method: Data for 0.03-0.50 M Et4NI.
At I=0.0 M, K(Mg+H2PO4)=1.66.

Mg++ gl oth/un 20°C ? U 1977KGa (13065) 146
K(Mg+H2PO4)=0.42

Mg++ gl oth/un 25°C 0.68M C K1=3.56 1976ACc (13066) 147
K(Mg+HPO4)=1.47
K(Mg+H2PO4)=0.37
Medium: NaCl/MgCl2 and KCl/MgCl2 mixtures.

Mg++ sol NaClO4 25°C 3.00M C 1976HHc (13067) 148
K(MgHL.3H2O(s)=Mg+HL)=-4.50

Mg++ sp oth/un 30°C 0.30M U I K1=1.20 1975KWa (13068) 149
K1=2.52 using an ISE at I=0.01, 23 C

Mg++ gl NaClO4 25°C 3.00M C 1974HHb (13069) 150
K(Mg+HL)=1.42
K(Mg+H+HL)=6.44

Mg++ gl KNO3 15°C 0.10M U 1972FSa (13070) 151
K(Mg+HL)=1.78

Mg++ gl KNO3 37°C 0.15M U K1=3.4 1970CHc (13071) 152
K(Mg+HL)=1.8
K(Mg+H2L)=0.6
K(MgH2L+HL)=2.5

```
                                        K(2MgHL=(MgHL)2)=1.4
-------------------------------------------------------------------------------
Mg++       oth none   25°C  0.0  U                        1969PGa (13072) 153
                                        K(Mg+HPO4)=2.74
-------------------------------------------------------------------------------
Mg++       gl  oth/un 25°C  0.0  U                        1963TFa (13073) 154
                                        Kso(MgNH4L(H2O)6)=-13.15
                                        Kso(MgKL(H2O)6)=-10.62
                                        Ks(MgHL(H2O)3)=-5.82
                                        K(Mg+HL)=2.91
Also by solubility. Medium:0 corr. Kso(Mg3L2(H2O)n)=-25.20(n=8), -23.1(n=22)
-------------------------------------------------------------------------------
Mg++       sol oth/un 20°C  var  U                        1961CAb (13074) 155
                                        Kso(Mg3L2)=-23.77
-------------------------------------------------------------------------------
Mg++       gl  R4N.X  25°C 0.20M U                        1956SAa (13075) 156
                                        K(Mg+HL)=1.88
Medium: Pr4NCl
-------------------------------------------------------------------------------
Mg++       sol none   38°C  0.0  U                        1954HPa (13076) 157
                                        Kso(Mg3L2)=-27.2
-------------------------------------------------------------------------------
Mg++       sol NaCl   38°C 0.16M U  I                     1943THa (13077) 158
                                        K(Mg+HL)=1.62
                                        Ks(MgHL(s)=Mg+HL)=-4.5
By conductivity, I=0 corr. K(Mg+HL)=2.87
-------------------------------------------------------------------------------
Mg++       gl  none   25°C  0.0  U                        1940GRa (13078) 159
                                        K(Mg+HL)=2.50
-------------------------------------------------------------------------------
Mg++       sol oth/un 25°C  dil  U    M                   1910BUa (13079) 160
                                        Ks(Mg(NH4)L(s)=Mg+NH4+L)=-12.6
*******************************************************************************
PW11O39-------        H7L                        (2467)
alpha-Heteromonophospho-polytungstate;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Mg++       gl  NaNO3  25°C 1.00M U        K1=1.23        1984COa (13399) 161
*******************************************************************************
P2O6----              H4L    Hypophosphate    CAS 9803-60-3  (199)
Hypophosphate;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Mg++       gl  R4N.X  25°C 0.50M U        K1=2.65        1967CMc (13413) 162
Ligand: O3POPHO2---, Medium: Me4NCl
*******************************************************************************
P2O7----              H4L    Pyrophosphate    CAS 2466-09-3  (198)
Diphosphate; from (HO)2PO.O.PO(OH)2
```

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	kin	R4N.X	30°C	0.10M	U		K1=5.69	1978KHa (13550)	163
Mg++	ix	NaClO4	25°C	0.10M	U	I	K1=5.06	1978MOa (13551)	164
Mg++	EMF	R4N.X	25°C	1.00M	U		K(Mg+H2L)=1.33	1973PTa (13552)	165
Medium:Me4NCl									
Mg++	EMF	KNO3	15°C	0.10M	U		K1=5.37 K(Mg+HL)=3.18	1972FSa (13553)	166
Mg++	gl	NaNO3	25°C	0.10M	U		K1=4.7 K(MgL+H)=6.0	1963JWa (13554)	167
Mg++	gl	R4N.X	25°C	1.00M	U	T	K1=5.42 K(MgL+Mg)=2.33 K(Mg+HL)=3.05	1961IRa (13555)	168
Medium: Me4NBr. K(Mg+HL)=4.13(65 C)									
Mg++	gl	none	25°C	0.0	U	T	K1=7.2 B(Mg(OH)L)=9.3	1959WOa (13556)	169
K1=7.1(40 C)									
Mg++	gl	R4N.X	25°C	1.00M	U		K1=5.41 K(MgL+Mg)=2.34 K(Mg+HL)=3.06	1957LWa (13557)	170
Medium: Me4NCl									
Mg++	sp	KNO3	19°C	0.02M	U		K1=5.70	1957VAc (13558)	171
Mg++	cal	oth/un	25°C	var	U	H		1957VAc (13559)	172
DH(K1)=12.1 kJ mol-1, DS=150 J K-1 mol-1									

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P2O8---- H4L CAS 13825-81-5 (2402)

Peroxodiphosphate, also cyclic metaposphates, thiophosphates etc.;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	kin	NaNO3	65°C	1.0M	C		K(Mg+HP2O8)=1.63	1985GGb (13688)	173
Ligand is peroxydisulfate, S2O8----									
Mg++	gl	R4N.X	25°C	1.00M	U		K1=3.33 K(MgL+Mg)=1.32 K(Mg+HL)=1.76	1960CEa (13689)	174
Medium: Me4NCl									

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P2W17O61---------- Polytungstate (2102)
alpha-Heterodiphospho-polytungstate (usually alpha1 isomer)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Mg++	gl	NaNO3	25°C	1.00M	U		K1=4.16		1984COa (13707)	175
							K1=2.16 (alpha2 isomer)			

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Mg++	sp	oth/un	25°C	0.05M	C		K1=5.8		1981BKf (13823)	176
							K(MgL+Mg)=2.04			

Method: by competition with 8-hydroxyquinoline.
Medium: 0.05 M Tris buffer, pH 7.5. K(MgL+Mg) determined by 31P nmr.

Mg++	kin	oth/un	30°C	0.10M	U		K1=5.97		1978KHa (13824)	177
Mg++	gl	KNO3	25°C	0.10M	U T	H	K1=4.93		1973TRa (13825)	178
							K(Mg+HL)=3.33			

At 2 C: K1=6.39, K(Mg+HL)=3.60; 35 C: K1=6.56, K=4.06. DH(K1)=-8.8 kJ mol-1, DH((Mg+HL)=5.9

Mg++	EMF	KNO3	15°C	0.10M	U		K1=5.75		1972FSa (13826)	179
							K(Mg+HL)=4.00			
Mg++	gl	KNO3	45°C	0.10M	U		K1=5.47	B2=6.57	1971TRa (13827)	180
							K(Mg+HL)=3.49			

On the basis of K(HL)=8.13, K(H2L)=5.43, K(MgL+HL)=1.9, K(MgL2+H)=8.9

Mg++	gl	R4N.X	20°C	0.10M	U	H	K1=7.05		1965ANa (13828)	181
							K(Mg+HL)=4.45			
							K(MgL+H)=6.22			

Medium: Me4NNO3. By calorimetry: DH(K1)=18.1 kJ mol-1, DS=196 J K-1 mol-1

Mg++	gl	KCl	25°C	0.10M	U		K1=5.65		1964EMb (13829)	182
							K(Mg+HL)=3.27			
							K(MgL+H)=5.68			
Mg++	gl	NaNO3	25°C	0.10M	U		K1=5.7		1963JWa (13830)	183
							K(MgL+H)=5.8			
Mg++	gl	R4N.X	?	0.10M	U		K1=5.8		1962RKa (13831)	184
							K(Mg+HL)=3.6			

Medium: K,NH4Cl

Mg++	gl	R4N.X	25°C	1.00M	U	T	K1=5.81		1961IRa (13832)	185
							K(MgL+Mg)=2.13			

```
                                        K(Mg+HL)=3.36
Medium: Me4NBr. At 65 C: K1=5.76, K(MgL+Mg)=2.12, K(Mg+HL)=3.40
-------------------------------------------------------------------------------
Mg++       gl  none   25°C  0.0  U T      K1=8.6         1959WOa (13833) 186
                                        B(Mg(OH)L)=11.0
At 40 C: K1=8.3, B(Mg(OH)L)=10.4
-------------------------------------------------------------------------------
Mg++       gl  R4N.X  25°C 1.00M U        K1=5.83        1957LWb (13834) 187
                                        K(MGL+Mg)=2.13
                                        K(Mg+HL)=3.34
Medium: Me4NCl
-------------------------------------------------------------------------------
Mg++       gl  KCl    20°C 0.10M U        K1=5.80        1956MSa (13835) 188
                                        K(Mg+HL)=3.7
*******************************************************************************
P3O9---               H3L                    CAS 13566-25-1  (235)
Cyclotrimetaphosphate;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Mg++       sp  R4N.X    ?  0.10M U        K1=2.74        1962RKa (13941) 189
Medium: NH4Cl
-------------------------------------------------------------------------------
Mg++       con none   25°C  0.0  U        K1=3.31        1949JMa (13942) 190
-------------------------------------------------------------------------------
Mg++       EMF KCl    20°C 0.10M U        K1=1.11        1949ZUa (13943) 191
*******************************************************************************
P4O12----             H4L                    CAS 13598-74-8  (234)
Cyclotetrametaphosphate;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Mg++       sp  R4N.X    ?  0.10M U        K1=4.52        1962RKa (13994) 192
Medium: NH4Cl
-------------------------------------------------------------------------------
Mg++       con none   25°C  0.0  U        K1=5.17        1950JMb (13995) 193
*******************************************************************************
P4O13------           H6L    Tetraphosphate     (1102)
Tetraphosphate;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Mg++       ix  R4N.X  25°C  0.1M U        K1=5.60        1981OMa (14041) 194
For the pentaphosphate: K1=6.03; hexaphosphate: K1=6.22
-------------------------------------------------------------------------------
Mg++       kin oth/un 30°C 0.10M U        K1=6.33        1978KHa (14042) 195
-------------------------------------------------------------------------------
Mg++       gl  R4N.X  25°C  1.0M U        K1=6.04        1968WMc (14043) 196
                                        K(Mg+HL)=3.74
                                        K(Mg+MgL)=2.19
```

Medium: Me4NCl

Mg++ kin oth/un 60°C var U K1=1.75 1967WIc (14044) 197

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P6O12------ H6L CAS 25268-83-1 (6590)

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	sp	R4N.X	25°C	0.10M	C		K1=8.4	1999NWa (14056)	198

Method: competition with EDTA. Medium: 0.10 M Me4NCl, pH 7.

Mg++	sp	KCl	25°C	0.50M	U	I	K1=5.77	1990NTa (14057)	199

Data also at I= 1.0 M KCl: B1=5.16; 1.5 4.95; 2.0 4.82; 2.5 4.49; 3.0 4.26

Mg++	gl	R4N.X	25°C	1.0M	U		K1=3.33 B2=4.65 K(Mg+HL)=1.76	1960CEa (14058)	200

Medium: Me4NCl

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

Thiocyanate;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaClO4	25°C	3.0M	U		K1=-1	1973HHa (14797)	201

Method: also vapor phase osmometry

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

Sulfate;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	sp	oth/un	25°C	0.0	C		K1=2.22	2004BCa (15906)	202

Method: dielectric relaxation spectroscopy. Calculated from data for 0.017-2.24 M MgSO4 solutions. Evidence for Mg2SO4.

Mg++	con	oth/un	25°C	0.0	C	TIH	K1=2.196	2002TBb (15907)	203

Data for 5-35 C and 0.0001 to 2.5 m. Assumes formation of contact plus solvent-separated ion pairs. DH(K1)=6.627 kJ mol-1, DS=64.3 J K-1 mol-1.

Mg++	con	none	20°C	0.0	C	I	K1=2.21	2000TMa (15908)	204

Also data for 0.06-0.69 mole fraction MeOH/H2O.

Mg++	con	none	25°C	0.0	C	I	K1=2.19	1986SDa (15909)	205

Value derived from data for 0.001-0.05 self medium.

Mg++	con	none	25°C	0.0	C		K1=2.17	1985SGd (15910)	206

Mg++	EMF	none	25°C	0.0	C	TI	K1=2.88	1983PGa (15911)	207

Method: Pt/quinhydrone electrode. Data for 5-35 C. At 15 C, K1=2.958.

DH(K1)=-12.9 kJ mol-1. K1 extrap. from data for I=0.015-0.05 M MgSO4/H2SO4

Mg++ oth none 25°C 0.0 C H K1=2.10 1981YYa (15912) 208
Calcd from published osmotic coefficient data. From UV spectrometry (competition with Cu), K1=2.03. From conductivity, K1=2.08, DH=6.78 kJ m-1

Mg++ ISE oth/un 25°C 0.10M C I K1=1.48 1980ELb (15913) 209
Extrapolation to zero concentration: K=2.34.

Mg++ ISE oth/un 25°C 0.10M C I K1=1.48 1980ELc (15914) 210
Medium: MgCl2. At I=0.0 M, K1=2.34. By spectrophotometry (competition with terpyridyl), at I=1.0, K1=0.72; at I=0.0 M, K1=2.29.

Mg++ con none 25°C 0.0 C T K1=2.21 1979FFc (15915) 211
Data for 15-25 C. Also data at 1000 and 2000 atm.
K expressed on molal scale.

Mg++ ISE none 25°C 0.0 M T H K1=2.23 1978EFb (15916) 212
Method: divalent cation electrode in dil NaCl. at 15 C, K1=2.21;
at 35 C, K1=2.26. DH(K1)=4.81 kJ mol-1, DS=59 J K-1 mol-1.

Mg++ gl NaCl 25°C 0.70M U I K1=0.79 1978EWa (15917) 213
In NaClO4: K=0.81

Mg++ gl oth/un 20°C ? U K1=0.40 1977KGa (15918) 214

Mg++ sol oth/un 25°C 0.70M C K1=1.09 1975EWa (15919) 215
Mixed medium of NaCl, KCl, MgCl2, NaClO4, Mg(ClO4)2, Na2SO4.
Method: solubility of gypsum.

Mg++ cal none 25°C 0.0 C H 1975LMe (15920) 216
DH(Mg+SO4)=4.8-5.7 kJ mol-1. Determined from enthalpies of dilution.

Mg++ gl oth/un 25°C 0.50M U T K1=2.47 1975MVa (15921) 217

Mg++ con none 0°C 0.0 U K1=2.2 1975TAa (15922) 218

Mg++ sp none 25°C 0.0 C K1=1.99 1975YYa (15923) 219
By vapour pressure osmometry, K1=2.04

Mg++ cal oth/un 25°C 0.0 U H 1973HPa (15924) 220
DH(K1)=6.5 kJ mol-1

Mg++ con oth/un 0°C 0.0 U T H K1=2.01 1973KAb (15925) 221
K1=2.06(10 C), 2.13(25 C), 2.24(45 C)
DH(K1)=8.54 kJ mol-1, DS=69.5 J K-1 mol-1 (25 C)

Mg++ cal oth/un 25°C 0 U H 1973POa (15926) 222
DH(K1)=5.5 to 5.7 kJ mol-1

Mg++ con none 25°C 0.0 U K1=2.24 1972ISa (15927) 223
Pressure: 100 kg/cm2. K1=2.17(p=200), 2.13(p=400), 2.12(p=600),
2.11(p=800), 2.09(p=1000), 2.06(p=1200)

Mg++ oth none 25°C 0.0 C K1=2.38 B2= 2.20 1972PIa (15928) 224
Calculated from published osmotic coefficient data.

Mg++ con oth/un 25°C 0.0 U K1=2.24 1971HPa (15929) 225

Mg++ con none 25°C 0.0 U K1=2.17 1971ISb (15930) 226
Pressure: 200 kg/cm2. K1=2.13(p=400), 2.13(p=600), 2.11(p=800),
2.09(p=1000), 2.06(p=1200)

Mg++ oth oth/un 0°C 0.0 U K1=2.1 1971ISc (15931) 227
Method: freezing point; K1=1.72 to 2.4(depending upon ion size parameter)

Mg++ ISE oth/un 1.7°C 0.66M U K1=1.18 1970KPa (15932) 228
Medium: synthetic seawater

Mg++ cal none 25°C 0.0 C H 1970LAe (15933) 229
DH(K1)=5.3 kJ mol-1, DS(K1)=61.5 J K-1 mol-1.
Method: heat of dilution measurements.

Mg++ sp oth/un 37°C var U K1=1.3 1970NOa (15934) 230

Mg++ oth none 50°C 0.0 U T K1=2.6 1969HEa (15935) 231
Method: estimated from literature data. K1=2.7 (60 C), 3.2 (100 C),
3.9 (150 C), 4.8 (200 C)

Mg++ cal none 25°C 0.0 U H K1=2.23 1969IEa (15936) 232
DH(K1)=2.1 kJ mol-1, DS=51.2 J K-1 mol-1

Mg++ con mixed 25°C 20% U I K1=2.65 1969SMd (15937) 233
Medium:w/w THF/H2O. 50% THF: K1=3.20; 0%: K1=2.07

Mg++ EMF oth/un 25°C 0.70M U K1=1.01 1968KPa (15938) 234
Medium: synthetic seawater

Mg++ ISE oth/un 35?°C 0.0 U K1=1.97 1968PRd (15939) 235

Mg++ oth oth/un 25°C 0.0 U H K1=2.25 1967HEb (15940) 236
From thermodynamic data. DH(K1)=20.4 kJ mol-1, DS=111.6 J K-1 mol-1

Mg++ sol oth/un 370°C 0.0 U T K1=6.27 1967MAg (15941) 237
K1=2.13(0 C), 2.40(25 C), 2.63(50 C), 2.85(75 C), 3.06(100 C), 3.27(125 C),
3.50(150 C), 3.74(175 C), 4.00(200 C), 4.58(250 C), values for DH1, DS1 etc.

Mg++ oth oth/un 25°C 0.0 U K1=2.22 1966APc (15942) 238
K(Mg(aq)+Laq)=1.70
K(Mg(aq)+L(aq)=MgH2OL)=0.29

K(MgH2OL=MgL)=-0.76
Method:ultrasound absorption. Medium: 0 corr

Mg++ oth oth/un 25°C 0.0 U 1965FIb (15943) 239
K1out=1.4
K(Mg(aq)+Laq=MgH2OL)=0
K(MgH2OL=MgL)=-0.95
Method: sound absorption. Medium:0 corr.

Mg++ con non-aq 25°C 100% U I K1=0.98 1965JTa (15944) 240
Medium: H2NCHO. K1=4.50 in 50% w/w Me2CO in H2NCHO, also other mixtures

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Mg++ con non-aq 25°C 100% U I K1=1.95 1965TJa (15945) 241
Medium: 20% dioxan in H2NCHO. K1=2.33(25%), 2.65(30%), 3.09(35%), 3.58(40%), 4.39(50%), 5.38(60%), 6.42(70%)

Mg++ oth oth/un 20°C var U K1=2.0 1962ETa (15946) 242
K1out/K1in=0.8 and 0
Method:sound absorption. Medium:MgL

Mg++ con oth/un 25°C 0.0 U K1=2.20 1961PFa (15947) 243

Mg++ oth KNO3 -3°C sat U K1=0.36 1960SFb (15948) 244
Method: freezing point

Mg++ oth KNO3 -3°C sat U K1=0.38 B2=1.41 1959RRc (15949) 245
Method: freezing point

Mg++ con alc/w 25°C 50% U I K1=3.86 1958DTa (15950) 246
Medium:50% EtOH. Also K1 for 5-45% EtOH

Mg++ oth KNO3 0°C sat U I K1=0.38 1958KEa (15951) 247
Method: freezing point. K1=1.06(saturated KClO3), 1.56(saturated KClO4) K1=2.19, I=0 corr.

Mg++ EMF oth/un 25°C 0.0 U T H K1=2.25 1958NNa (15952) 248
Method: H electrode. K1=1.96(0 C), 2.20(20 C), 2.35(30 C), 2.40(35 C), 2.45 (40 C), 2.49(45 C). DH(K1)=20.3 kJ mol-1, DS=110 J K-1 mol-1(25 C)

Mg++ sp alc/w 25°C 20% U K1=2.61 1957BDb (15953) 249
Medium:20% EtOH

Mg++ oth oth/un 0°C 0.0 U K1=2.19 1956KEb (15954) 250
Method: freezing point

Mg++ oth diox/w 25°C 13% U I K1=2.62 1955BIa (15955) 251
Method ultrasonic data. K1=3.19(25% dioxan)

Mg++ oth oth/un 0°C 0.0 U K1=2.2 1955BPb (15956) 252
Method: freezing point, K1=1.98 to 2.39

Mg++ con oth/un 18°C 0.0 U K1=2.30 1955RSa (15957) 253

Mg++ EMF oth/un 20°C 0.0 U T H K1=2.29 1952JMb (15958) 254
Method: H electrode. K1=2.36(25 C), 2.43(30 C), 2.49(35 C).
DH(K1)=23.8 kJ mol-1, DS=130 J K-1 mol-1(25 C)

Mg++ con oth/un 25°C 0.0 U I K1=2.21 1951DJa (15959) 255
also for dioxan/H2O and glycine/H2O mixtures

Mg++ oth oth/un 20°C 0.0 U K1=2.20 1940MSa (15960) 256
Method: dielectric constant

Mg++ con oth/un 18°C 0.0 U K1=2.11 1938DAa (15961) 257

Mg++ con oth/un 18°C 0.0 U K1=2.21 1927DAb (15962) 258

****

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

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

---

Mg++ cal R4N.X 25°C 0.50M U K1=0.53 1997MKa (16799) 259
DH(K1)=1.70 kJ mol-1

Mg++ cal R4N.X 25°C 0.50M U H K1=0.56 1974ARa (16800) 260
DH=1.67 kJ mol-1.

Mg++ con alc/w 25°C 44% U T K1=3.23 1956BMa (16801) 261
Medium: 44% EtOH. K1=3.31(20 C), 3.36(30 C)

Mg++ sp alc/w 25°C 50% U K1=3.39 1956TMa (16802) 262
Medium: 50% EtOH

Mg++ sp none 25°C 0.0 U K1=1.79 1955GMa (16803) 263

Mg++ sol none 25°C 0.0 U K1=1.84 1951DMb (16804) 264

****

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

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

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Mg++ con oth/un 18°C dil U 1968RVa (17037) 265
Kso=-5.74

Mg++ sol oth/un 20°C 0.0 U 1966LSd (17038) 266
Kso=-5.36

Mg++ sol oth/un 20°C var U 1956CHe (17039) 267

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                                        Kso(MgL)=-4.89
********************************************************************************
SiO3--                H2L    Silicate         CAS 7699-41-4  (747)
Silicate; SiO2(OH)2--
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Mg++       EMF NaClO4 25°C  1.0M U        K1=4.17        1974SSc (17185) 268
                                        K(Mg+HL)=0.64
                                        K(Mg+2HL)=3.82
Method: H electrode
--------------------------------------------------------------------------------
Mg++       oth none    0°C  0.0  U T                     1973CHa (17186) 269
                                        Kso((MgO)2(SiO2)3(H2O)8)=-41.8
Method: Estimated data.(((MgO)2(SiO2)34)9H2O)8,sepiolite). Ks=-41.0(10 C);
-40.4(20 C); -40.1(25 C); -39.8(30 C); -39.2(40 C); -38.7(50 C); -38.2(60 C)
--------------------------------------------------------------------------------
Mg++       oth none   70°C  0.0  U T                     1973CHa (17187) 270
                                        Kso(MgO)2(SiO2)3(H2O)8)=-37.8
Method: Estimated data.(((MgO)2(SiO2)3(H2O)8,sepiolite). Ks=-37.5(80 C);
-37.2(90 C);-36.9(100 C);-36.7(110 C);-36.5(120 C);-36.3(130 C);-36.1(140 C)
--------------------------------------------------------------------------------
Mg++       sol oth/un 51°C  0.0  U T                     1973CHa (17188) 271
                                        Ks((MgO)2(SiO2)3(H2O)8)=-38.8
Ks=-37.5(70 C), -37.2(90 C)(well crystalline);
-38.1(51 C), -37.2(70 C), -37.0(90 C)(poorly cryst)
--------------------------------------------------------------------------------
Mg++       oth none   60°C  0.0  U T                     1969HEa (17189) 272
                                        *Ks(MgSiO3+2H)=9.83
Method: Estimated data.
*Ks=8.48(100 C); 7.14(150 C); 6.16(200C); 5.37(250 C); 4.70(300 C) (MgSiO3)
--------------------------------------------------------------------------------
Mg++       oth none   60°C  0.0  U T                     1969HEa (17190) 273
                                        *Ks(Mg3Si4O10(OH)2+6H)=16.40
Method: Estimated data
*Ks=14.17(100 C); 11.96(150 C); 10.53(200C); 9.42(250 C); 8.45(300 C)
--------------------------------------------------------------------------------
Mg++       oth none   150°C  0.0  U T                     1969HEa (17191) 274
                                        *Ks(MgCa(SiO3)2+4H)=13.01
Method:est.data. *Ks=17.41(60 C),15.23(100 C),11.41(200 C),10.03(250C).
Also *Ks(Ca2Mg5Si8O22(OH)2+14H)=36.42,49.22(60 C),25.27(300 C).Also 100-250C
--------------------------------------------------------------------------------
Mg++       oth none   150°C  0.0  U T                     1969HEa (17192) 275
                                        *Ks(Mg5Al2Si3O10(OH)8+16H)=43
Method:est.data.(chlorite). *Ks=61.90 (60 C),27.34 (300 C); montmorillonite
2.75(60 C),-7.97(300 C). Also data at 60-300 C
--------------------------------------------------------------------------------
Mg++       cal oth/un 25°C  0.0  U T                     1967KBc (17193) 276
                                        K=9.5
K=6.2(100C),-1.5(227 C),-7.7(427 C),-10.9(627 C). K: 2Mg2SiO4(s,forsterite)+
```

3H2O=Mg(OH)2(s,brucite)+Mg3Si2O5(OH)4(chrysotile)

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

alpha-Heterosilicon-polytungstate;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaNO3	25°C	1.00M	U		K1=3.46 K(beta1 isomer)=3.29 K(beta2 isomer)=3.12 K(beta3 isomer)=2.98	1984COa (17233)	277

****

TeO4-- H2L Tellurate (5750)

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	sol	oth/un	20°C	dil	U		Ks(Mg3TeO6)=-16.6	1966KCa (17305)	278

Not corrected for reactions with H+?

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VO4--- H3L CAS 15457-75-7 (1586)

Vanadate; VO2(OH)3-- or polymers

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaClO4	25°C	1.00M	U		K(Mg+H7PV12O36)=3.48	1975KIc (17375)	279

****

CH2O2 HL Formic acid CAS 64-18-6 (37)

Methanoic acid; H.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	ISE	NaCl	25°C	0.03M	U	TIH	K1=0.75	1981EFa (17583)	280
At 35 C, I=0.045: K1=0.85; 45 C, I=0.45: 0.30; 25 C, I=0.45: 1.89 DH=7.2 kJ mol-1, DS=41.8 J K-1 mol-1									
Mg++	sol	NaClO4	25°C	0.80M	U	I	K1=0.28	1977FHc (17584)	281
Mg++	gl	NaNO3	30°C	0.40M	U		K1=0.34	1970BTa (17585)	282
Mg++	gl	oth/un	25°C	0.0	U	T H	K1=1.43	1956NAa (17586)	283
Medium: 0 corr, K(35 C)=1.39, DH(K1)=7.4 kJ mol-1, DS=2.5 J K-1 mol-1									
Mg++	gl	oth/un	25°C	0.0	U		K1=1.43	1948SCa (17587)	284

****

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
Mg++	gl	KCl	25°C	0.10M	C		K1=4.11 K(Mg+HL)=1.61 K(MgL+H)=5.07	1994SCa (17698)	285
Mg++	gl	R4N.X	25°C	0.05M	C		K1=3.59 K(Mg+HL)=1.70	1981FHa (17699)	286

Medium: 0.05 M Et4NClO4.

****

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

Carbamide, Urea; (H2N)2CO

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	sp	NaClO4	22°C	4.00M	U		K1=-0.31 B2=-0.92	1970KLf (17713)	287

****

CH4O3ClP H2L CAS 2565-58-4 (1973)

Chloromethylphosphonic acid; Cl.CH2.PO3H2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	EMF	NaNO3	25°C	0.10M	U		K1=1.62	1970TNa (17927)	288

****

CH4O6Cl2P2 H4L CAS 10596-23-3 (2370)

Dichloromethanediphosphonic acid; Cl2.C(PO3H2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	R4N.X	25°C	0.10M	C	H	K1=6.20 K(Mg+HL)=3.15	1993KLa (17951)	289
Mg++	gl	KCl	25°C	0.10M	U		K1=4.75 K(Mg+HL)=2.92	1976DGe (17952)	290

DH(K1)=12.8 kJ mol-1, DS=162 J K-1 mol-1

****

CH5O3P H2L CAS 13590-71-1 (1752)

Methylphosphonic acid; CH3.PO3H2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaNO3	25°C	0.10M	M		K1=1.86	1992SCa (18119)	291
Mg++	gl	KCl	25°C	0.10M	U		K1=2.22	1986NIa (18120)	292
Mg++	sp	oth/un	30°C	0.30M	U		K1=1.53	1975KWa (18121)	293

****

CH5O4P H2L CAS 2617-47-2 (1977)

Hydroxymethylphosphonic acid; HO.CH2.PO3H2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	R4N.X	25°C	0.10M	U		K1=1.92	1972WFa (18145)	294

Medium: (CH3)4NCl

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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
Mg++	gl	NaNO3	25°C	0.10M	M		K1=1.67	1996SSa (18170)	295
Mg++	sp	oth/un	30°C	0.30M	U		K1=1.34	1975KWa (18171)	296
Mg++	sp	oth/un	20°C	0.10M	U	T	K1=1.57	1965BRb (18172)	297

K1(65 C)=2.09

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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
Mg++	gl	KNO3	25°C	0.10M	C	I R	K1=2.00	2001PRa (18222)	298
							K(Mg+HL)=1.3		

IUPAC Recommended values

Mg++	gl	NaNO3	25°C	0.10M	C		K1=1.94	1994SCa (18223)	299
							K(Mg+HL)=1.22		
							K(MgL+H)=9.36		
Mg++	gl	KNO3	25°C	0.10M	U		K1=2.03	1979WNb (18224)	300
							B(MgHL)=11.38		
Mg++	gl	KNO3	25°C	0.10M	U		K1=2.04	1971WNc (18225)	301
							B(MgHL)=11.35		

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CH6O6P2 H4L Medronic acid CAS 1984-15-2 (2384)

Methanediphosphonic acid; CH2(PO3H2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaCl	37°C	0.15M	C		K1=5.68	1997ZJa (18269)	302
							K(MgL+H)=7.56		
							K(MgL+Mg)=2.68		
Mg++	gl	R4N.X	25°C	0.50M	U		K1=5.78	1968CIa (18270)	303
							K(Mg+HL)=2.92		

Medium: (CH3)4NCl

Mg++	gl	KCl	25°C	0.10M	U		K1=6.38	1967KLa (18271)	304

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                                        K(Mg+HL)=4.02
--------------------------------------------------------------------------------
Mg++       gl  oth/un 25°C 0.10M U       K1=5.51        1963KEa (18272) 305
                                        K(Mg+HL)=2.76
                                        K(Mg+MgL)=2.60
--------------------------------------------------------------------------------
Mg++       gl  R4N.X  25°C  1.0M U T H   K1=4.82        1962IMb (18273) 306
                                        K(Mg+HL)=2.97
Medium: Me4NBr. (50 C):K1=5.07, K=3.33
At I=o corr: K1=6.3, DH(K1)=18.4 kJ mol-1, DS=142 J K-1 mol-1
********************************************************************************
CH6O7P2              H3L                    CAS 56399-35-0  (7664)
Methyldiphosphoric acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Mg++       gl  NaNO3  25°C 0.10M M       K1=3.29        1999SSa (18308) 307
********************************************************************************
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
--------------------------------------------------------------------------------
Mg++       oth NaCl   25°C 0.15M U T     K1=2.18        1993GMa (18757) 308
Method: Coulometric titration. K1=2.39 (37 C)
--------------------------------------------------------------------------------
Mg++       sol oth/un 37°C  dil  C  I     K1=3.604       1989SIb (18758) 309
Medium: 0.001-0.008 M MgCl2 with 0 or 0.15 M NaCl.
--------------------------------------------------------------------------------
Mg++       gl  NaClO4 30°C  1.0M U       K1=2.65        1988GMd (18759) 310
--------------------------------------------------------------------------------
Mg++       gl  KNO3   35°C 0.10M C    M  K1=4.65        1985RRc (18760) 311
                                       B(MgL(cytidine))=8.81
--------------------------------------------------------------------------------
Mg++       gl  KNO3   35°C 0.10M C       K1=4.65        1985RRh (18761) 312
--------------------------------------------------------------------------------
Mg++       gl  oth/un 37°C 0.10M U  I     K1=2.75        1982DMa (18762) 313
Medium: Et4NI; ionic strength range: 0.03-0.5.
--------------------------------------------------------------------------------
Mg++       sol NaClO4 25°C 0.80M U       K1=1.62        1977FHc (18763) 314
--------------------------------------------------------------------------------
Mg++       dis NaClO4 20°C 0.10M U       K1=2.39        1963STc (18764) 315
--------------------------------------------------------------------------------
Mg++       oth KCl    23°C 0.20M U       K1=2.61        1962AMa (18765) 316
Method: interferometer.  Medium: 0.2 KCl,0.1 (HOCH2)3CNH2
--------------------------------------------------------------------------------
Mg++       ISE oth/un 25°C 0.09M U  I     B2=4.24        1959TVa (18766) 317
B2=4.54(I=0.03-0.5)
--------------------------------------------------------------------------------
Mg++       EMF NaNO3  20°C 0.10M U       K1=2.76        1957SAb (18767) 318
```

Mg++ sol oth/un 25°C 0.0 U B2=4.38 1951BAa (18768) 319

Mg++ sol oth/un 37°C 0.62M U K1=2.28 1939PEa (18769) 320
By conductivity, K1=2.28

Mg++ EMF KCl 25°C 0.20M U K1=2.55 1938CKa (18770) 321
Method: H electrode

Mg++ EMF oth/un ? 0.07M U K1=2.65 1928SIa (18771) 322

Mg++ con oth/un 18°C 0.0 U K1=3.43 1927DAb (18772) 323

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C2H3NO4 HL CAS 625-75-2 (2968)
Nitroacetic acid; O2N.CH2.COOH

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

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Mg++ kin oth/un 18°C 0.20M U K1=-0.19 1949PEa (19205) 324
Medium: Ba(NO3)2

****

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

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

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Mg++ gl NaNO3 30°C 0.40M U K1=0.23 1970BTa (19354) 325

****

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

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Mg++ oth none 25°C 0 U T H K1=1.70 1994SHd (19864) 326
Data also at 35, 45 55 C. DH(K1)=3.3 KJ mol-1, DS=43.5 J K-1 mol-1

Mg++ oth NaCl 25°C 0.15M U T K1=0.46 1993GMa (19865) 327
Method: Coulometric titration. K1=0.58 (37 C)

Mg++ sol oth/un 80°C var U K1=1.3 1991FEa (19866) 328
Brucite(Mg(OH)2) solubility measurements Constant at I=0

Mg++ gl alc/w 25°C 100% M K1=4.4 B2=6.6 1988PPa (19867) 329
Medium: MeOH

Mg++ gl R4N.X 25°C 0.16M U I K1=0.55 1985RSa (19868) 330
K1=0.64 (I=0.04); 0.55 (0.25); 0.61 (0.49); 0.71 (1.00)

Mg++ ISE NaCl 25°C 0.03M U TIH K1=0.81 1981EFa (19869) 331
At 35 C, I=0.045: K1=0.85; 45 C, I=0.45: 0.40; 45 C, I=0.45: 1.10

DH=5.1 kJ mol-1, DS=36.8 J K-1 mol-1

Mg++ ISE NaCl 25°C 0.10M C T K1=0.737 1979EFc (19870) 332
Method: divalent ion selective electrode. Data for 15-35 C and for
I=0.025-0.206 M NaCl. At I=0, K1=1.04.

Mg++ sol NaClO4 25°C 0.80M U I K1=0.26 1977FHc (19871) 333

Mg++ gl NaNO3 30°C 0.40M U K1=0.47 1970BTa (19872) 334

Mg++ gl none 25°C 0.0 U K1=1.28 1964AMa (19873) 335

Mg++ gl non-aq 25°C 100% U K2=7.22 1964KLa (19874) 336
Medium: ethanoic acid

Mg++ sp non-aq 25°C 100% U B2=9.92 1961PSa (19875) 337
Medium: ethanoic acid

Mg++ gl none 25°C 0.0 U T H K1=1.25 1956NAa (19876) 338
Medium: 0 corr. K1(35 C)=1.21; DH(K1)=-6.4 kJ mol-1, DS=2.5 J K-1 mol-1

Mg++ sol oth/un 25°C ->0 U K1=0.82 1956NAa (19877) 339

Mg++ EMF KCl 20°C 0.20M U K1=0.51 1938CKa (19878) 340

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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
Mg++	gl	NaClO4	25°C	0.50M	C		K1=1.03	1995PLa (20489)	341

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C2H5NO2 HL Glycine CAS 56-40-6 (85)
2-Aminoethanoic acid; H2N.CH2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaNO3	25°C	0.10M	C	M	K1=3.45	2000KAb (21473)	342
							K(MgA+L)=3.92		
							B(MgAL)=6.42		

H2A=Dipicolinic acid.

Mg++	gl	oth/un	25°C	0.50M	C		K1=1.68	1995CDc (21474)	343
							B(MgHL)=10.05		

Medium: 0.50 M MgCl2.

Mg++	gl	NaNO3	25°C	0.10M	C		K1=3.30	1989GAb (21475)	344

Mg++	gl	NaClO4	37°C	0.15M	C	T	K1=1.979	1987BBd (21476)	345
							B(MgHL)=10.879		

B(MgH2L2)=21.614
B(MgH-1L)=-8.735

Mg++ sp oth/un 25°C 1.0M U K1=1.17 1987HAa (21477) 346

Mg++ gl KNO3 35°C 0.10M C M K1=3.40 1985RRc (21478) 347
K(Mg+HL+cytidine)=8.19
K(MgL(cytidine)+H)=3.59

Mg++ gl KNO3 35°C 0.10M C K1=3.40 1985RRh (21479) 348

Mg++ gl NaCl 20°C 0.15M U M K1=2.33 1983VDb (21480) 349

Mg++ EMF NaClO4 25°C 3.0M C K1=1.53 B2= 2.26 1982BPc (21481) 350
Method: Pt/H2 electrode.

Mg++ gl KCl 25°C 0.50M U M K1=1.34 1969HLa (21482) 351
B(MgLA)=4.77
HA=salicylaldehyde

Mg++ gl KCl 0°C 0.09M U T K1=2.12 1957MMa (21483) 352
K1=2.23(30 C)

Mg++ gl diox/w 30°C 75% U K1=4.8 B2=8.0 1954UFa (21484) 353

Mg++ gl oth/un 25°C ->0 U K1=3.44 1951MOa (21485) 354

Mg++ gl oth/un 25°C 0.01M U K1=3.45 B2=6.46 1949MMa (21486) 355

****

C2H5NO2 HL Acetohydroxamic CAS 546-88-3 (2766)
Acetohydroxamic acid, N-Hydroxyacetamide; CH3.CO.NHOH

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

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Mg++ gl KCl 25°C 0.20M C K1=2.96 1999FEa (21803) 356
B(MgH-1L)=-7.22

****

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

---

Mg++ nmr oth/un 25°C ? U K1=0.95 1991COa (21873) 357

Mg++ gl KNO3 37°C 0.15M M K1=3.90 B2=5.2 1979SPb (21874) 358
K(Mg+HL)=1.84

Mg++ ISE oth/un 23°C 0.01M C K1=2.03 1975KWa (21875) 359

Mg++ kin oth/un 39°C 0.45M U K1=0.91 1971KSa (21876) 360

Ionic strength=0.45-0.75

Mg++ sp KCl 25°C 1.00M U T K1=1.88 1970BSg (21877) 361
4 C: K1=1.48. pH 8 (tris buffer)

Mg++ kin oth/un 39°C 0.60M U K1=0.76 1966OJa (21878) 362

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Mg++	gl	R4N.X	25°C	0.05M	C	H	K1=4.50 K(Mg+HL)=2.60		1981FHa (21888)	363

Medium: 0.05 M Et4NClO4. Data for 0.10-0.25 M.
At I=0.0 M, K1=5.58, DH(K1)=12.6 kJ mol-1, DS(K1)=146 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
Mg++	ISE	non-aq	25°C	100%	M		K1=2.45 B3=4.96 B4=5.13	B2= 3.67	1999NMa (22089)	364

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Mg++	ISE	non-aq	25°C	100%	M		K1=2.65	B2=3.72	1988NHa (22090)	365

Medium: MeCN, 0.01 M Et4NClO4

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Mg++	gl	KNO3	25°C	0.10M	U		K1=2.30		1963TAa (22486)	366

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Mg++	gl	NaNO3	25°C	0.10M	M		K1=1.85		1992SCa (22565)	367

****

C2H7O3P HL CAS 868-85-9 (1756)
Methylphosphonic acid methyl ester; CH3P(O)(OH)(OCH3)

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

Mg++ sp oth/un 30°C 0.30M U K1=0.48 1975KWa (22572) 368

****

C2H7O4P HL CAS 813-78-5 (1754)

Dimethylphosphoric acid; (CH3O)2P(O)OH

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

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Mg++ sp oth/un 30°C 0.30M U K1=0.78 1975KWa (22574) 369

****

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

---

Mg++ gl KNO3 25°C 0.10M U K1=2.00 1979WNb (22611) 370

B(MgHL)=11.54

Mg++ gl KNO3 25°C 0.20M C K1=1.84 1978MAb (22612) 371

K(Mg+HL)=1.27

****

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

---

Mg++ gl KNO3 25°C 0.10M U K1=2.13 1979WNb (22633) 372

B(MgHL)=12.48

Mg++ gl KNO3 25°C 0.20M C K1=2.24 1978MAb (22634) 373

K(Mg+HL)=1.37

****

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

---

Mg++ gl KNO3 25°C 0.20M C K1=1.56 1978MAb (22666) 374

K(Mg+HL)=1.17

Mg++ gl KNO3 25°C 0.20M C K1=1.56 1978MAc (22667) 375

K(Mg+HL)=1.17

K(MgL+H)=9.73

Mg++ gl R4N.X 20°C 0.10M U T K1=2.2 1965HFb (22668) 376

K(Mg+HL)=1.5

Medium: (C3H7)4NI

Mg++ gl KCl 25°C 0.15M U K1=1.70 1962OSa (22669) 377

K(Mg+HL)=1.23

****

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
Mg++	gl	NaCl	25°C	0.0	C		K1=0.38 K(Mg+HL)=-0.15	1999SFc (23124)	378

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	sp	alc/w	25°C	95%	U		K1=1.31	1993GSa (23125)	379

Medium: 95% w/w EtOH/H2O, 0.05 M Et4NClO4, by competitive spectrophotometry

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	diox/w	30°C	75%	U		K1=1.8	1954UFa (23126)	380

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	EMF	KCl	30°C	1.0M	U		K1=0.37	1941BJa (23127)	381

Method: H electrode

****

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
Mg++	gl	R4N.X	25°C	1.0M	U		K1=2.85 K(Mg+HL)=2.67	1962IMb (23259)	382

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
Mg++	gl	R4N.X	25°C	0.50M	U		K1=6.26 K(Mg+HL)=2.99	1968CIa (23265)	383

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
Mg++	cal	none	25°C	0	U	H	K(Mg+L+OH)=10.85	1998KKa (23345)	384

DH(Mg+L+OH)= -65.5 kJ/mol

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaCl	37°C	0.15M	C		K1=6.03 K(MgL+H)=7.48 k(MgL+OH)=3.24 K(MgL+Mg)=3.67	1997ZJa (23346)	385

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	cal	oth/un	25°C	0.04M	U	T	K1=7.7	1986VKa (23347)	386

```
                                        B(Mg2L)=11.3
DH1=13.5 kJ mol-1, DS1=192 J K-1 mol-1; DH(M+ML)=23.5, DS(M+ML)=148
--------------------------------------------------------------------------------
Mg++       cal R4N.X  25°C 0.50M U   H    K1=6.40        1986VKb (23348) 387
Medium: Et4N.Cl  DH1=5.1 kJ mol-1, DS1=140 J K-1 mol-1
--------------------------------------------------------------------------------
Mg++       gl  NaCl   25°C 0.02M U        K1=7.95        1986VZa (23349) 388
                                        K(Mg+HL)=4.10
                                        B(Mg2L)=10.96
--------------------------------------------------------------------------------
Mg++       cal KCl    25°C 0.02M U T                     1984VKd (23350) 389
                                        K(Mg+HL)=3.42
DH=14.48 kJ mol-1;  DS=114 J mol-1 K-1.
--------------------------------------------------------------------------------
Mg++       gl  KNO3   25°C 0.10M U        K1=4.49        1980ZRc (23351) 390
                                        K(Mg+HL)=3.31
                                        K(Mg+H2L)=1.39
--------------------------------------------------------------------------------
Mg++       gl  KCl    25°C 0.10M U        K1=6.17        1976DGe (23352) 391
                                        K(Mg+HL)=3.03
--------------------------------------------------------------------------------
Mg++       gl  R4N.X  25°C 0.10M U        K1=7.28        1972WFa (23353) 392
                                        K(Mg+HL)=3.70
                                        B(2Mg+L)=10.7
Medium: (CH3)4NCl
--------------------------------------------------------------------------------
Mg++       gl  R4N.X  25°C 0.50M U        K1=6.39        1968CIa (23354) 393
                                        K(Mg+HL)=3.32
Medium: (CH3)4NCl
--------------------------------------------------------------------------------
Mg++       gl  KCl    25°C 0.10M U        K1=6.55        1967KLa (23355) 394
                                        K(2Mg+H-1L))=14.95
                                        K(2Mg+L)=10.50
********************************************************************************
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
--------------------------------------------------------------------------------
Mg++       gl  KCl    25°C 0.20M C        K1=3.47        1999MKa (23449) 395
                                        B(MgHL)=12.70
                                        B(MgH2L)=17.08
                                        B(MgH-1L)=-8.29
--------------------------------------------------------------------------------
Mg++       gl  KNO3   25°C  0.1M C        K1=4.25        1985MMa (23450) 396
                                        B(MgHL)=13.50
                                        B(MgH2L)=18.74
                                        K(Mg(OH)L+H)=7.1
********************************************************************************
C3H4N2                   L    Imidazole        CAS 288-32-4  (90)
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1,3-Diazole, imidazole; C3H4N2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaNO3	25°C	0.50M	M		K1=0.16	1998KSa (23857)	397
Mg++	gl	oth/un	25°C	0.15M	C	I	K1=0.10	1989DDb (23858)	398

Medium: MgCl2. Also data for I=0.3-1.0 M.

Mg++	sp	non-aq	21°C	100%	U	M		1983LKa (23859)	399
							K(MgA+L)=4.98		
							K(MgA+2L)=5.19		

Medium: C2H4Cl2. A=tetraphenylporphin

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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
Mg++	gl	NaClO4	30°C	1.0M	U	M	K1=2.05	1988GMd (24043)	400
							K(Mg(ox)+L)=3.40		
							K(Mg(cit)+L)=2.50		

****

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
Mg++	ix	KNO3	25°C	0.10M	U		K1=2.045	1995RKc (24371)	401

At I=0.15 M K1=1.970; at 0.20 M K1=1.918

Mg++	gl	NaCl	25°C	1.00M	C		K1=1.73	1988BSa (24372)	402
Mg++	sp	none	25°C	0.0	U	T	K1=2.86	1976KOa (24373)	403

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

Mg++	gl	NaClO4	25°C	0.10M	U		K1=2.11	1968OVa (24374)	404
							K(Mg+HL)=0.96		
Mg++	gl	NaClO4	20°C	0.10M	U		K1=1.95	1963CAa (24375)	405
							K(Mg+HL)=0.83		
Mg++	EMF	oth/un	25°C	->0	U		K1=2.84	1952EMa (24376)	406

Method: H electrode. d(logK1)/dT=0.008

Mg++	EMF	oth/un	25°C	0.04M	U		K1=2.85	1949SDa (24377)	407
Mg++	EMF	KCl	25°C	0.20M	U		K1=1.91	1938CKa (24378)	408
							K(Mg+HL)=0.47		

```
Mg++       con oth/un 25°C  ->0  U        K1=2.43        1932MDa (24379) 409
--------------------------------------------------------------------------------
Mg++       gl  oth/un   ?  0.07M U        K1=2.06        1928SIa (24380) 410
********************************************************************************
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
--------------------------------------------------------------------------------
Mg++       gl  NaClO4 20°C 0.10M U        K1=2.17        1963CAa (24614) 411
                                         K(Mg+HL)=1.23
********************************************************************************
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
--------------------------------------------------------------------------------
Mg++       oth none   25°C    0  U T H    K1=2.36        1994SHd (24976) 412
Data also at 35, 45 55 C. DH(K1)=1.9 KJ mol-1, DS=51.5 J K-1 mol-1
--------------------------------------------------------------------------------
Mg++       ISE NaCl   25°C 0.03M U TIH    K1=1.01        1981EFa (24977) 413
At 35 C, I=0.045: K1=1.10; 45 C, I=0.45: 0.48; 25 C, I=0.45: 1.12
DH=4.3 kJ mol-1, DS=36.8 J K-1 mol-1
--------------------------------------------------------------------------------
Mg++       sol NaClO4 25°C 0.80M U  I     K1=0.12        1977FHc (24978) 414
--------------------------------------------------------------------------------
Mg++       EMF KCl    20°C 0.20M U        K1=0.54        1938CKa (24979) 415
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
--------------------------------------------------------------------------------
Mg++       gl  NaClO4 25°C  0.5M C        K1=0.93        1995PLa (25384) 416
--------------------------------------------------------------------------------
Mg++       oth NaCl   25°C 0.15M U T      K1=0.61        1993GMa (25385) 417
Method: Coulometric titration. K1=0.64 (37 C)
--------------------------------------------------------------------------------
Mg++       gl  NaClO4 37°C 0.15M C        K1=1.235       1987BBd (25386) 418
--------------------------------------------------------------------------------
Mg++       EMF oth/un 25°C  1.0M U        K1=0.73   B2=1.30   1965VTa (25387) 419
Method: quinhydrone electrode.
--------------------------------------------------------------------------------
Mg++       EMF oth/un 25°C  ->0  U        K1=1.37        1954DMb (25388) 420
Method: H electrode
--------------------------------------------------------------------------------
Mg++       EMF KCl    20°C 0.20M U        K1=0.93        1938CKa (25389) 421
Method: H electrode
********************************************************************************
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C3H6O4 HL Glyceric acid CAS 473-81-4 (2520)
2,3-Dihydroxypropanoic acid; HO.CH2.CH(OH).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Mg++	EMF	KCl	20°C	0.20M	U		K1=0.86		1938CKa (25629)	422

Method: H electrode

****

C3H7NO L DMF CAS 68-12-2 (598)
N,N-Dimethylformamide; HCO.N(CH3)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Mg++	ISE non-aq		25°C	100%	M		K1=2.21 B3=3.57 B4=3.72	B2= 3.29	1999NMa (25653)	423

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Mg++	ISE non-aq		25°C	100%	M		K1=2.32	B2=3.34	1988NHa (25654)	424

Medium: MeCN, 0.01 M Et4NClO4

****

C3H7NO2 HL Alanine CAS 56-41-7 (86)
2-Aminopropanoic acid; H2N.CH(CH3).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Mg++	gl	oth/un	25°C	->0	U	T	K1=1.96		1951MOa (26136)	425

****

C3H7NO2 HL B-Alanine CAS 107-95-9 (575)
3-Aminopropanoic acid; H2N.CH2.CH2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Mg++	gl	KNO3	25°C	0.50M	C		K1=1.38		2003FCa (26445)	426

for 1.0 M KNO3 K1=1.53; for 1.5 M KNO3 K1=1.65;

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C3H7NO2 HL DL-Alanine CAS 302-72-7 (189)
DL-2-Aminopropanoic acid; H2N.CH(CH3).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Mg++	gl	NaCl	20°C	0.15M	U	M	K1=1.96		1983VDb (26539)	427

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Mg++	gl	KCl	25°C	0.20M	C		K1=2.63	B2= 3.90	2000FEc (26619)	428

****

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
Mg++	gl	KNO3	25°C	0.10M	U	I	K1=3.37	1990RAb (27111)	429

Data also for 10% w/w EtOH/H2O (K1= 3.63) and 25% (K1=3.88)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaCl	25°C	3.00M	M		K1=1.03	1988BFa (27112)	430
Mg++	gl	NaCl	25°C	3.00M	C		K1=1.03	1985PBb (27113)	431

D-, L- and DL-serine studied.

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C3H7NO3 HL iso-Serine CAS 632-12-2 (351)
DL-3-Amino-2-hydroxypropanoic acid; H2N.CH2.CH(OH).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaCl	20°C	0.15M	U	M	K1=1.47	1983VDb (27231)	432

****

C3H7O4P H2L CAS 6913-02-6 (1755)
Prop-2-onephosphonic acid; CH3.CO.CH2.PO3H2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	sp	oth/un	30°C	0.30M	U	I	K1=1.30	1975KWa (27293)	433

K1=2.54 using an ISE at I=0.01, 23 C

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C3H7O5P H3L CAS 5926-41-4 (3549)
2-Phosphonopropanoic acid; CH3.CH(PO3H2).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	sp	oth/un	37°C	0.07M	U		K1=2.3	1970NOa (27300)	434

Medium: tris buffer

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	R4N.X	25°C	0.25M	U		K1=2.26	1957WBa (27301)	435

Medium: 0.1-0.4 M (C3H7)4NI

****

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
Mg++	gl	R4N.X	25°C	0.05M	C		K1=2.28 K(Mg+HL)=1.70	1981FHa (27310)	436

Medium: 0.05 M Et4NClO4.

****

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
Mg++	gl	NaNO3	25°C	0.10M	U		K1=1.57	1992LCb (27321)	437

****

C3H7O7P H3L CAS 28474-06-8 (3552)
D-2,3-Dihydroxypropanoic acid 2-phosphate (D-2-phosphoglyceric acid)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	R4N.X	25°C	0.25M	U		K1=2.45	1957WBa (27330)	438

Medium: 0.1-0.4 M (C3H7)4NI

****

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
Mg++	gl	KNO3	25°C	0.20M	C		K1=2.59	1978MAb (27349)	439
							K(Mg+HL)=1.00		

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KCl	25°C	0.10M	C	I R	K1=3.3	2001PRa (27397)	440
							B(MgHL)=12.1		
IUPAC Recommended value									
Mg++	gl	NaCl	25°C	0.5M	C		K1=2.52	1996AMa (27398)	441
							B(MgHL)=11.15		
							B(MgH2L)=15.73		
							B(Mg2L)=3.49		
Mg++	gl	KNO3	25°C	0.1M	C		K1=3.31 B2=5.47	1985MMa (27399)	442
							B(MgHL)=12.12		
Mg++	gl	KNO3	25°C	0.10M	M		K1=3.25	1978LCa (27400)	443
							K(MgL+OH)=2.8		

****

C3H8NO6P H3L Phosphoserine CAS 17885-08-4 (1865)
Serine dihydrogenphosphate, O-Phosphoserine; NH2.CH(CH2.OPO3H2).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	25°C	0.20M	C		K1=2.00	1978MAb (27457)	444
							K(Mg+HL)=1.30		

```
Mg++       gl  KNO3   25°C 0.20M C        K1=2.00        1978MAc (27458) 445
                                          K(Mg+HL)=1.30
                                          K(MgL+H)=9.02
--------------------------------------------------------------------------------
Mg++       gl  KNO3   37°C 0.15M U  I     K1=2.55        1971CHb (27459) 446
                                          K(Mg+HL)=1.82
                                          K(Mg+H2L)=1.35
                                          K(MgH2L+HL)=2.0
                                          K(2MgHL=Mg2H2L2)=2.2
Also in Et4NBr
--------------------------------------------------------------------------------
Mg++       gl  R4N.X  20°C 0.10M U        K1=3.3         1965HFa (27460) 447
                                          K(Mg+HL)=2.5
Medium: (C3H7)4NI
--------------------------------------------------------------------------------
Mg++       gl  KCl    25°C 0.15M U        K1=2.4         1959OSa (27461) 448
                                          K(Mg+HL)=1.60
--------------------------------------------------------------------------------
Mg++       gl  oth/un 25°C 0.15M U        K1=2.4         1957OSa (27462) 449
********************************************************************************
C3H9O4P                H2L                          (6694)
(Phosphonylmethoxy)ethane; H2O3P.CH2.O.CH2.CH3
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Mg++       gl  NaNO3  25°C 0.10M M        K1=1.95        1992SCa (28019) 450
********************************************************************************
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
--------------------------------------------------------------------------------
Mg++       gl  NaNO3  25°C 0.10M U        K1=1.63        1992LCb (28044) 451
--------------------------------------------------------------------------------
Mg++       gl  KCl    20°C 0.10M U        K1=1.80        1957SAa (28045) 452
********************************************************************************
C3H10NO3P              H2L                          (1986)
1,1-Dimethyl-1-aminomethylphosphonic acid; H2N.C(CH3)2.PO3H2
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Mg++       gl  KNO3   25°C 0.10M U        K1=2.01        1979WNb (28072) 453
                                          B(MgHL)=11.62
********************************************************************************
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
--------------------------------------------------------------------------------
Mg++       gl  KNO3   25°C 0.10M U        K1=2.01        1979WNb (28087) 454
```

B(MgHL)=12.57

****

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
Mg++	gl	KNO3	25°C	0.10M	C		K1=2.0	1993SKc (28099)	455

****

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
Mg++	gl	KCl	20°C	0.10M	U		K1=3.04	1951SRa (28386)	456
							K(Mg+HL)=2.08		

****

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
Mg++	gl	oth/un	25°C	0.10M	U		K1=2.8	1962IMb (28392)	457
Mg++	gl	KCl	20°C	0.10M	U		K1=2.84	1951SRa (28393)	458
							K(Mg+HL)=2.08		

****

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
Mg++	gl	R4N.X	25°C	0.50M	U		K1=6.83	1968CIa (28398)	459
							K(Mg+HL)=3.33		

Medium: Me4NCl

****

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
Mg++	gl	KCl	25°C	0.20M	C		K1=4.74	1999MKa (28442)	460
							B(MgHL)=14.16		
							B(MgH2L)=18.72		
							B(MgH-1L)=-7.42		
Mg++	gl	KNO3	25°C	0.10M	C		K1=5.13	1993SKc (28443)	461
							K(MgL+H)=9.72		
							K(MgHL+H)=5.0		

Mg++ gl NaClO4 25°C 0.10M U K1=5.00 1988LDa (28444) 462

****

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
Mg++	gl	NaCl	37°C	0.15M	C		K(Mg+H+L)=16.81 K(Mg2L+H)=9.28 K(2Mg+L)=10.85 K(MgHL+H)=6.86	1999ZJa (28458)	463

****

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
Mg++	gl	KNO3	25°C	0.10M	C	H	K1=7.54 K(MgL+H)=9.42 K(MgHL+H)=6.10	1993SMa (28547)	464

DH(K1)=25.8, DH(MgHL)=-48.6, DH(MgH2L)=8.8 kJ mol-1.

Mg++	gl	KNO3	25°C	0.10M	C		K1=7.52 K(MgL+H)=9.42 K(MgHL+H)=6.10 K(MgH2L+H)=4.8	1987SAa (28548)	465

Mg++	cal	none	25°C	0.0	U	TIH		1987VOa (28549)	466

DH(K1)=-39.7 kJ mol-1, DH(Mg+HL)=-30.2

Mg++	gl	KNO3	25°C	1.0M	U		K1=6.49 K(Mg+HL)=3.24 K(Mg+H2L)=2.7 K(Mg+H3L)=1.9	1967CCb (28550)	467

****

C3H12NO10P3 H6L CAS 15834-10-3 (3559)

Nitrilotri(methylphosphonic acid) N-oxide; O-N(CH2.PO3H2)3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	25°C	1.0M	U		K1=8.3 K(Mg+HL)=3.6 K(Mg+H2L)=2.1 K(Mg+H3L)=1.05	1967CCc (28604)	468

****

C3H12O10P4 H6L (7924)

Tris(dihydroxy-phosphonylmethyl)phosphineoxide;

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

---

Mg++	gl	R4N.X	20°C	0.10M	C	K1=7.52 K(MgL+Mg)=3.8 K(MgHL+H)=6.12 K(MgL+H)=7.96 K(Mg+H2L)=3.56	1977ANb (28610) 469

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference ExptNo
Mg++	gl	diox/w	30°C	50%	U		K1=2.63	1973CSb (28718) 470

Medium: 50% dioxan, 0.1 M NaClO4

****

C4H3N3O4 H3L Oxonic acid CAS 937-13-3 (1296)
4,6-Dihydroxy-1,3,5-triazine-2-carboxylic acid; C3N3(OH)2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference ExptNo
Mg++	sp	NaClO4	20°C	0.20M	U		K1=3.10	1981LDa (28758) 471

****

C4H4N2O2 HL Uracil CAS 66-22-8 (412)
2,4-Dihydroxypyrimidone, 2,4-Pyrimidinedione;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference ExptNo
Mg++	gl	KNO3	45°C	0.10M	U		K1=2.6	1974KKa (28856) 472

****

C4H4N2S HL CAS 1450-85-7 (1521)
2-Mercapto-1,3-diazine, 2-Mercaptopyrimidine; C4H3N2.SH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference ExptNo
Mg++	gl	KNO3	45°C	0.10M	C		K1=2.76	1986KZa (28936) 473

****

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
Mg++	gl	KNO3	30°C	0.10M	U		K1=5.1	1983SKa (28952) 474
Mg++	gl	KNO3	45°C	0.10M	U		K1=3.9	1973TKa (28953) 475

****

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

Mg++ sp none 25°C 0.0 U T K1=2.30 1976KOa (29045) 476
Also data at 15,30,35 C. Determined colourimetrically
****
C4H4O4F2 H2L CAS 665-31-6 (515)
2,2-Difluorosuccinic acid; HOOC.CF2.CH2.COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ con none 25°C 0.0 U K1=2.31 1984TWa (29234) 477
****
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
---
Mg++ kin oth/un 25°C 0.27M U K1=6.0 1987TLa (29259) 478
Result given for enol form. For ligand hydrate, K1=5.4

Mg++ kin KCl 25°C 0.50M U I K1=0.81 1982BLb (29260) 479
K(2Mg+L=Mg2H-1L+H)=-6.4
K(MgL=MgH-1L+H)=-8.6
K(MgL(keto)=MgL(enol))=-0.5
Also in 50% dioxan/H2O

Mg++ gl KCl 25°C 0.10M U K1=6.27 B2=11.09 1964TGa (29261) 480
K(Mg+HL)=1.96
k=keto form, e=enol. K(Mg+HL(k))=1.91, K(Mg+HL(e))=2.20, K(MgHL(e)=MgHL(k))=
0.49 by spectrophotometry
****
C4H5N2Cl L CAS 872-49-1 (7589)
5-Chloro-1-methylimidazole;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl NaNO3 25°C 0.50M M K1=0.13 1998KSa (29334) 481
****
C4H5N3O HL Cytosine CAS 71-30-7 (1096)
2-Oxy-6-aminopyrimidine;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl KNO3 35°C 0.10M U M 1986RRe (29406) 482
K(Mg+HL+HA)=8.29
K(Mg(HL)A+H)=3.30
K(Mg+HL+D)=8.07
K(Mg+HL+HC)=6.91
HA is glycine; H2D is oxalic acid; C is histamine.
K(Mg(HL)C+H)=3.06

Mg++ gl KNO3 35°C 0.10M U T H 1983KSa (29407) 483

K(Mg+HL)=1.76
K(Mg+2HL)=3.24

Mg++ gl KNO3 30°C 0.10M U K1=2.2 1983SKa (29408) 484

Mg++ gl KNO3 45°C 0.10M U K1=2.7 1974KKa (29409) 485
K(Mg+HL)=2.4

****

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
Mg++	gl	NaNO3	25°C	0.50M	M		K1=0.12	1998KSa (29574)	486

****

C4H6N4O L CAS 56-06-4 (5994)
2,4-Diamino-6-hydroxypyrimidine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	45°C	0.10M	C		K1=2.7	1986KZa (29671)	487

****

C4H6N4O L CAS 1672-50-0 (5993)
4,5-Diamino-6-hydroxypyrimidine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	45°C	0.10M	C		K1=3.14	1986KZa (29682)	488

****

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
Mg++	gl	R4N.X	25°C	0.10M	C	TIH	K1=1.47	1984DDa (29924)	489
							B(MgHL)=5.95		

Medium: Et4NI. Data for 0.05-1.0 M and 15-45 C.DH(K1)=8.0 kJ mol-1, DS(K1)
=54 J K-1 mol-1; DH(MgHL)=7.1, DS=138. At I=0, K1=2.18, B(MgHL)=6.64.

Mg++ EMF KCl 25°C 0.20M U K1=1.20 1938CKa (29925) 490
K(Mg+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
Mg++	gl	NaNO3	30°C	0.40M	U		K1=0.31	1970BTa (30086)	491

****

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
Mg++	gl	NaClO4	25°C	0.10M	U		K1=1.73	1968OVa (30113)	492

****

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
Mg++	cal	NaNO3	25°C	1.00M	U	H	K1=1.42	1980ARa (30575)	493

DH(K1)=4.1 kJ mol-1

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaClO4	20°C	0.10M	U			1963CAa (30576)	494
							K(Mg+H2L)=0.90		
							K(Mg+HL)=1.70		
Mg++	EMF	KCl	25°C	0.20M	U		K1=1.55	1938CKa (30577)	495
							K(Mg+HL)=0.77		

****

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
Mg++	gl	oth/un	25°C	0.0	C	I	K1=2.51	1999DGa (30845)	496
							B(MgHL)=5.12		

Medium: artificial seawater. Extrapolated from data for 5-45% salinity.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	oth/un	25°C	0.25M	C	TIH	K1=1.70	1987DDe (30846)	497
							K(Mg+HL)=0.62		

Medium: Mg(NO3)2. At I=0 M, K1=2.51; at 1.0 M, K1=1.82. Data for
12.5-48 C. At 25 C, I=0.25 M: DH(K1)=19.2 kJ mol-1, DS(K1)=97 J K-1 mol-1.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KCl	25°C	0.10M	C		K1=1.61	1984MMg (30847)	498
							K(MgL+H)=2.0		
Mg++	gl	KNO3	25°C	0.10M	C		K1=2.15	1975FCc (30848)	499
							B(MgHL)=5.88		
Mg++	gl	KNO3	25°C	0.10M	U		K1=2.06	1974MSa (30849)	500
Mg++	gl	KCl	30°C	0.10M	U		K1=1.7	1957TBb (30850)	501

****

C4H6O6 H2L DL-Tartaric acd CAS 133-37-9 (94)
DL-Tartaric acid,DL-2,3-Dihydroxybutanedioic acid; HOOC.CH(OH).CH(OH).COOH

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

```
Mg++       gl  NaClO4 25°C 1.00M M    M                  1988MOa (31007) 502
                                        K(Mg+H2L+(ascorbate))=3.77
-------------------------------------------------------------------------------
Mg++       oth oth/un 25°C  dil  C        K1=2.349       1982HKa (31008) 503
Method: isotachophoresis. Medium: 0.006-0.019 M tartrate buffer, pH 5.1.
*******************************************************************************
C4H6O6               H2L    L-Tartaric acid  CAS 87-69-4  (92)
L-Tartaric acid, L-2,3-Dihydroxybutanedioic acid; HOOC.CH(OH).CH(OH).COOH
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Mg++       nmr KNO3   25°C 1.50M U                        1994PRa (31179) 504
Keff(Mg+BO4(H-1L)2=MgBO4(H-1L)2)<1.04, Keff(MgL+BO4(H-1L)2=MgBO4(H-1L)2+L)<0
At pH 11.5
-------------------------------------------------------------------------------
Mg++       ix  oth/un 30°C  dil  C T      K1=1.18        1992LHb (31180) 505
Medium: 0.2-5.0 mM tartaric acid eluent. At 40 C, K1=1.39
-------------------------------------------------------------------------------
Mg++       gl  NaClO4 37°C 0.20M U        K1=1.91        1967TTb (31181) 506
-------------------------------------------------------------------------------
Mg++       dis NaClO4 20°C 0.10M U        K1=<2          1963STc (31182) 507
-------------------------------------------------------------------------------
Mg++       gl  diox/w 30°C  75%  U        K1=7.9    B2=13.2   1954UFa (31183) 508
-------------------------------------------------------------------------------
Mg++       EMF KCl    25°C 0.20M U        K1=1.36        1938CKa (31184) 509
                                        K(Mg+HL)=0.92
*******************************************************************************
C4H7NO2S              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
-------------------------------------------------------------------------------
Mg++       gl  NaCl   37°C 0.15M C        K1=1.683       1981HMa (31472) 510
*******************************************************************************
C4H7NO3               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
-------------------------------------------------------------------------------
Mg++       gl  NaClO4 30°C 0.40M U        K1=0.32        1970BTa (31498) 511
*******************************************************************************
C4H7NO4              H2L    Aspartic acid    CAS 56-84-8  (21)
Aminobutanedioic acid; H2N.CH(CH2.COOH).COOH
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Mg++       gl  NaNO3  25°C 0.10M C    M   K1=4.35        2000KAb (31806) 512
                                        K(MgA+L)=4.59
                                        B(MgAL)=7.09
H2A=Dipicolinic acid
```

Mg++ gl NaClO4 37°C 0.15M C K1=2.040 B2=4.426 1987BBd (31807) 513
B(MgH2L)=14.074
B(MgHL)=10.501
B(MgH-1L)=-8.666

Mg++ gl KNO3 25°C 0.10M M K1=2.82 1981GVa (31808) 514

Mg++ gl KCl 25°C 0.10M U K1=2.43 1953LMa (31809) 515

****

C4H7NO4 H2L IDA CAS 142-73-4 (118)
Iminodiethanoic acid; HN(CH2.COOH)2

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

---

Mg++ gl alc/w 25°C 78% C K1=5.61 1995LBb (32190) 516
Medium: 78% EtOH/H2O, 0.01 M LiNO3. (Kw=-14.76.K(CdL+MgL)=3.43).
Methods: glass electrode and Cd specific ion electrode

Mg++ dis R4N.X ? 0.10M U K1=3.2 1969ASb (32191) 517
Method: chromatography. Medium: NH4Cl

Mg++ gl KNO3 20°C 0.10M U H K1=2.94 1964ANa (32192) 518
By calorimetry: DH(K1)=12.3 kJ mol-1, DS=98.2 J K-1 mol-1

Mg++ EMF KCl 20°C 0.10M U K1=2.94 1964PCa (32193) 519
Method: H electrode

Mg++ EMF oth/un 20°C ->0 U K1=3.66 1945SKa (32194) 520
Method: H electrode

****

C4H8N2O3 HL Asparagine CAS 70-47-3 (17)
2-Aminobutanedioic acid 4-amide; H2N.CH(CH2.CO.NH2).COOH

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

---

Mg++ gl NaCl 25°C 1.00M C K1=1.33 1996BFb (32679) 521

Mg++ gl oth/un 20°C 0.01M U B2=4.0 1950ALa (32680) 522

****

C4H8N2O3 HL Gly-Gly CAS 556-50-3 (54)
Glycyl-glycine; H2N.CH2.CO.NH.CH2.COOH

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

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Mg++ gl oth/un 25°C 0.15M U K1=1.34 1958LCa (33015) 523

Mg++ gl oth/un 25°C ->0 U K1=1.06 1951MOa (33016) 524

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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
Mg++	gl	KCl	30°C	0.10M	U		K1=1.9	1957TBb (33080)	525

****

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
Mg++	oth	none	25°C	0	U	T H	K1=2.37	1994SHd (33324)	526

Data also at 35, 45 55 C. DH(K1)=2.0 KJ mol-1, DS=52.0 J K-1 mol-1

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	ISE	NaCl	25°C	0.03M	U	TIH	K1=1.01	1981EFa (33325)	527

At 35 C, I=0.045: K1=1.11; 45 C, I=0.45: 0.36; 25 C, I=0.45: 1.12
DH=5.2 kJ mol-1, DS=39.7 J K-1 mol-1

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	sol	NaClO4	25°C	0.80M	U	I	K1=-0.02	1977FHc (33326)	528
Mg++	EMF	KCl	25°C	0.20M	U		K1=0.53	1938CKa (33327)	529

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
Mg++	gl	NaClO4	25°C	0.50M	C		K1=0.98	1995PLa (33442)	530
Mg++	EMF	NaClO4	25°C	1.0M	U		K1=0.81 B2=1.47	1965VTa (33443)	531

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
Mg++	EMF	KCl	25°C	0.20M	U		K1=0.60	1938CKa (33619)	532

Method: H electrode

****

C4H9NO2 HL Dimethylglycine CAS 1118-68-9 (88)
N,N-Dimethyl-2-aminoethanoic acid; (CH3)2N.CH2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	oth	none	25°C	0.0	U	H		1956MAa (34030)	533

DG(K1)=-9.6 kJ mol-1, DH=0, DS=67

****

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
Mg++	gl	NaCl	37°C	0.15M	U		B2=3.31 B3=5.36	1986XHa (34286)	534

****

C4H10NO6P H2L CAS 6401-59-8 (2399)
O-Phospho-2-methylserine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	25°C	0.20M	C		K1=2.36 K(Mg+HL)=1.60 K(MgL+H)=9.31	1978MAc (34475)	535

****

C4H10NO6P H2L CAS 1114-81-4 (2400)
O-Phospho-threonine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	25°C	0.20M	C		K1=2.27 K(Mg+HL)=1.60 K(MgL+H)=9.0	1978MAc (34483)	536

****

C4H10N2O4S 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
Mg++	gl	KNO3	25°C	0.10M	C	M	K1=3.72	2001AAa (34622)	537

Also data for ternary complexes with 5'-GMP, 5'-IMP and 5'-CMP.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	25°C	0.10M	C		K1=3.55	2000ADa (34623)	538
Mg++	gl	NaClO4	37°C	0.10M	U	T	K1=0.3	1992GHa (34624)	539

Method: coulometric titration. At 25 C, K1=0.4.

****

C4H10N3O5P H3L Phosphocreatine (3594)
Phosphocreatine, N-(Imino(phosphonoamino)methyl)-N-methylglycine;
H2O3P.HN.C(:NH)N(CH3)CH2COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	nmr	R4N.X	37°C	0.25M	C		K(Mg+HL)=1.43	2002CFb (34636)	540

Method: 31P nmr. Medium: 20% v/v D2O/H2O, 0.25 M Me4NCl, pH 7.0.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	sp	oth/un	30°C	0.10M	U		K1=1.6	1964OPa (34637)	541

Medium: buffer=N-ethylmorpholine

****
C4H10O2S L CAS 111-48-8 (4275)
3-Thiapentan-1,5-diol; HO.CH2.CH2.S.CH2.CH2.OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	sp	NaClO4	25°C	1.0M	C		K1=-0.28	1979SRa (34682)	542

****
C4H10O6Cl2P2 CAS 134757-52-1 (5246)
Clodronic acid monoisopropyl ester; H3L

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	R4N.X	25°C	1.0M	C		K1=3.65	1995RLa (34716)	543

Medium: 1.0 M Me4NCl.
****
C4H11NO3 L Tris buffer CAS 77-86-1 (550)
2-Amino-2-(hydroxymethyl)-propan-1,3-diol; (HO.CH2)3C.NH2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	R4N.X	25°C	1.00M	C	I	K1=0.30	1982SSf (35052)	544

In 90 % (v/v) DMSO/water mixture: K1=0.50 (I=0.25 M)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	25°C	0.10M	C	M	K1=<0.7	1979FHa (35053)	545
							K(Mg(ATP)+L) < 0.7		

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	25°C	0.10M	C		K1=6.95	2000SDa (35102)	546
							K(MgL+H)=8.07		
							K(MgHL+H)=5.22		
							K(MgH2L+H)=4.0		
Mg++	ix	NaNO3	RT	0.10M	U		K1=6.0	1985PMc (35103)	547

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaNO3	25°C	0.10M	C		K1=1.69	1988MSa (35285)	548

****
C4H12NO3P 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

```
--------------------------------------------------------------------------------
Mg++       gl  KNO3   24°C 0.10M U        K1=3.68        1989YKa (35308) 549
--------------------------------------------------------------------------------
Mg++       gl  KNO3   25°C 0.10M U        K1=2.15        1979WNb (35309) 550
                                          B(MgHL)=11.73
********************************************************************************
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
--------------------------------------------------------------------------------
Mg++       gl  oth/un 25°C 0.10M U        K1=2.7         1962IMb (35575) 551
--------------------------------------------------------------------------------
Mg++       gl  KCl    20°C 0.10M U        K1=2.77        1951SRa (35576) 552
                                          K(Mg+HL)=2.05
********************************************************************************
C4H12O7P2             H3L                    CAS 52811-47-9  (7665)
N-Butyldiphosphoric acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Mg++       gl  NaNO3  25°C 0.10M M        K1=3.41        1999SSa (35584) 553
********************************************************************************
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
--------------------------------------------------------------------------------
Mg++       gl  KCl    25°C 0.20M C        K1=4.25        1999MKa (35605) 554
                                          B(MgHL)=14.73
                                          B(MgH2L)=19.73
--------------------------------------------------------------------------------
Mg++       gl  KNO3   25°C  1.0M U        K1=4.42        1967CCb (35606) 555
                                          K(Mg+HL)=2.33
                                          K(Mg+H2L)=1.9
********************************************************************************
C4H13N3                 L    Dien          CAS 111-40-0  (584)
1,4,7-Triazaheptane, 2,2'Iminobis(ethylamine), diethylenetriamine;
NH2.(CH2)2.NH.(CH2)2.NH2
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Mg++       gl  NaCl   25°C  0.0  C        K1=0.95        1999SFc (35764) 556
                                          K(Mg+HL)=0.25
                                          K(Mg+H2L)=-0.21
Extrapolated from data for 0.03-0.96 M NaCl using the Pitzer equation.
--------------------------------------------------------------------------------
Mg++       gl  KCl    25°C  0.0  C        K1=1.22        1992DDa (35765) 557
                                          K(Mg+HL)=0.21
********************************************************************************
```

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
Mg++	gl	KCl	25°C	0.10M	U		K1=<2	1965DKb (35867)	558

****

C5H2O4F6 H2L CAS 376-73-8 (516)
Hexafluoropentanedioic acid; HOOC.CF2.CF2.CF2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	con	none	25°C	0.0	U		K1=2.44	1984TWa (35930)	559

****

C5H3N4Cl L 6-Chloropurine CAS 87-42-3 (3032)
6-Chloropurine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	45°C	0.10M	U		K1=5.9	1971TKc (35988)	560

****

C5H4NBr L CAS 1120-87-2 (8780)
4-Bromopyridine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaNO3	25°C	0.50M	C		K1=0.07	2002KSb (36002)	561

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaNO3	25°C	0.50M	C		K1=0.02	2002KSb (36022)	562

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaCl	20°C	0.15M	U		K1=3.35	1979DZe (36074)	563
							K(Mg+HL)=2.22		

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaClO4	25°C	0.50M	U	I		1983MDa (36106)	564
							K(Mg+H2L)=2.41		

```
                                        K(Mg+HL)=3.89
                                        K(Mg+H2L)=2.58 (0.1 NaClO4)
-------------------------------------------------------------------------
Mg++       gl  NaCl   20°C 0.15M U    M   K1=2.35        1983VDb (36107) 565
-------------------------------------------------------------------------
Mg++       gl  NaCl   20°C 0.15M U        K1=3.89        1979DZe (36108) 566
                                        K(Mg+HL)=2.35
*************************************************************************
C5H4N4O                HL    Hypoxanthine     CAS 68-94-0  (1174)
6-Hydroxypurine;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Mg++       gl  KNO3   25°C 0.10M U T H                    1983KSa (36188) 567
                                        K(Mg+HL)=2.25
                                        K(Mg+2HL)=4.12
-------------------------------------------------------------------------
Mg++       gl  KNO3   45°C 0.10M U        K1=6.65        1971TKc (36189) 568
*************************************************************************
C5H4N4S                HL    6-Purinethiol    CAS 6112-76-1  (115)
6-Mercaptopurine,  6-Thiohypoxanthine;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Mg++       gl  KNO3   45°C 0.10M U        K1=6.0         1971TKc (36225) 569
*************************************************************************
C5H4O2S                HL    2-Thenoic acid   CAS 527-72-0  (2312)
Thiophene-2-carboxylic acid; C4H3S.COOH
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Mg++       gl  NaClO4 30°C 0.20M U T H    K1=1.95        1976SSd (36253) 570
*************************************************************************
C5H5N                   L    Pyridine         CAS 110-86-1  (31)
Pyridine, Azine;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Mg++       gl  NaNO3  25°C 0.50M C        K1=0.03        2002KSb (36590) 571
-------------------------------------------------------------------------
Mg++       gl  KCl    25°C 1.00M U  I     K1=-0.42       1986CCd (36591) 572
K=-0.19 if values calculated by including MgL+ and H(py)Cl species.
-------------------------------------------------------------------------
Mg++       sp  non-aq 21°C 100%  U    M                  1983LKa (36592) 573
                                        K(MgA+L)=3.63
                                        K(MgA+2L)=2.90
Medium: C2H4Cl2. A=tetraphenylporphin
-------------------------------------------------------------------------
Mg++       gl  NaClO4 35°C 0.20M U        K1=2.08        1971SBb (36593) 574
*************************************************************************
```

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
Mg++	gl	KCl	25°C	0.20M	C		K1=3.08	B2= 5.73	2000FEc (36750)	575

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
Mg++	gl	KNO3	37°C	0.15M	C		K1=3.44	B2=5.89	1980SHb (36778)	576

C5H5NO2 HL CAS 1121-23-9 (2315)
3-Hydroxypyridin-4(1H)-one;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Mg++	gl	KNO3	37°C	0.15M	C		K1=4.33	B2=7.48	1980SHb (36825)	577

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
Mg++	gl	NaNO3	25°C	0.50M	C		K1=-0.08		2002KSb (36858)	578

C5H5N5 L Adenine CAS 73-24-5 (237)
6-Aminopurine; H2N.C5H3N4

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Mg++	gl	KNO3	35°C	0.10M	U T	H	K(Mg+HL)=2.71 K(Mg+2HL)=2.83		1983KSa (36965)	579
Mg++	gl	KNO3	30°C	0.10M	U		K1=6.7		1983SKa (36966)	580
Mg++	gl	KNO3	45°C	0.10M	U		K1=3.05		1971TKc (36967)	581

C5H5N5S H3L 6-Thioguanine CAS 3647-48-1 (4307)
2-Amino-6-mercaptopurine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Mg++	gl	KNO3	45°C	0.10M	U		K1=2.8 K(Mg+H2L)=3.3		1973TKa (37011)	582

C5H5N5S H3L CAS 154-42-7 (4308)

2-Mercapto-6-aminopurine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	45°C	0.10M	U			1973TKa (37019)	583
							K(Mg+H2L)=2.9		
							K(MgH2L=MgHL+H)=3.0		

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
Mg++	gl	NaNO3	25°C	0.50M	C		K1=-0.07	2002KSb (37122)	584
Mg++	sp	alc/w	25°C	95%	U		K1=1.12	1993GSa (37123)	585

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
Mg++	sp	NaClO4	25°C	0.50M	U			1963SBd (37202)	586
							K(Mg+HL)=-0.06		

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
Mg++	gl	KNO3	35°C	0.10M	U		K1=3.06	1982TSa (37273)	587
Mg++	gl	KNO3	45°C	0.10M	U		K1=2.8	1974KKa (37274)	588

C5H6N6 HL Diaminopurine CAS 1904-98-9 (4290)
2,6-Diaminopurine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	45°C	0.10M	U		K1=2.5	1973TKa (37337)	589

C5H6O7 H3L (8107)
Carboxymethyltartronic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KCl	25°C	0.10M	C		K1=2.77	1984MMg (37488)	590
							K(MgL+H)=3.07		

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
Mg++	gl	NaCl	25°C	0.1M	U		K1=3.27 B2= 5.85	1998AVa (37900)	591

For 1.5 M NaCl K1=2.53; B2=5.71; for 1.0 M NaCl K1=2.72; B2=5.72
for 0.5 M NaCl K1=2.89, B2=5.73; for 0.2 M NaCl K1=3.15, B2=5.74

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	diox/w	28°C	70%	U		K1=7.32 B2=13.43	1992ZHa (37901)	592

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	dis	NaClO4	25°C	0.10M	C		K1=3.5	1986SNa (37902)	593

Method: rate of distribution of volatile ligand between aqueous phase and
inert gas phase. K(H+L)=9.17 assumed.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	oth	NaClO4	25°C	0.10M	C	I R	K1=3.34 B2=5.86	1982SLc (37903)	594

IUPAC evaluation. I=0 corr.: K1=3.65, B2=6.28

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	diox/w	24°C	50%	U		K1=4.5	1979ACa (37904)	595

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	cal	oth/un	25°C	0.05M	U		K1=3.30 B2= 5.75 DH(K1)=-4.31 kJ/mol DH(B2)=-18.1	1979PKc (37905)	596

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	diox/w	20°C	17%	C		K1=7.18 B2=13.54	1976JWa (37906)	597

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	oth/un	20°C	0.0	U	T H	K1=3.67 B2=6.38	1954IHa (37907)	598

DH(K1)=-7.5 kJ mol-1, DS=46; DH(K2)=-18, DS=-10. 0 C: K1=3.75, K2=2.75;
30 C: K1=3.363, K2=2.54; 40 C: K1=3.65, 2.44

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	diox/w	30°C	75%	U		K1=7.49 B2=13.58	1953UFb (37908)	599

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C5H8O4 H2L CAS 595-46-0 (1144)
Dimethylmalonic acid; HOOC.C(CH3)2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaClO4	25°C	0.10M	U		K1=1.55	1968OVa (38207)	600

****

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
Mg++	sp	none	25°C	0.0	U	T	K1=2.63	1976KOa (38234)	601

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaClO4	25°C	0.10M	U		K1=1.62	1968OVa (38235)	602

****

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
Mg++	EMF	KCl	25°C	0.20M	U		K1=1.08 K(Mg+HL)=0.52	1938CKa (38307)	603

****

C5H9NO2 HL Proline CAS 147-85-3 (44)

Pyrrolidine-2-carboxylic acid; C4H8N.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	oth/un	20°C	0.03M	U		B2=4	1950ALa (38600)	604

****

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
Mg++	gl	oth/un	25°C	0.10M	U		K1=2.6	1975IMa (38815)	605

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
Mg++	gl	NaNO3	25°C	0.10M	C	M	K1=3.20 K(MgA+L)=3.32 B(MgAL)=5.82	2000KAb (39053)	606

H2A=Dipicolinic acid.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaCl	25°C	1.00M	C		K1=1.33	1988BSa (39054)	607
Mg++	gl	NaClO4	37°C	0.15M	C		K1=2.196 B(MgH2L)=14.876 B(MgHL)=11.081 B(MgH-1L2)=-6.125	1987BBd (39055)	608
Mg++	gl	KNO3	25°C	0.10M	M		K1=2.79	1981GVa (39056)	609
Mg++	gl	KCl	25°C	0.10M	U		K1=1.9	1953LMa (39057)	610

****

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
Mg++	gl	KNO3	25°C	0.10M	U		K1=3.44	1977TIa (39231)	611

```
Mg++       vlt NaClO4 25°C 0.10M U        K1=3.5         1969VPa (39232) 612
--------------------------------------------------------------------------------
Mg++       gl  KCl    25°C 0.10M U   H    K1=3.48   B2=5.83   1968NPb (39233) 613
By calorimetry:DH(K1)=11.9 kJ mol-1, DS=110.8 J K-1 mol-1, DH(K2)=-2.0,DS=33
--------------------------------------------------------------------------------
Mg++       cal KNO3   20°C 0.10M U   H                   1965ANa (39234) 614
DH(K1)=13.0 kJ mol-1, DS=110.4 J K-1 mol-1
--------------------------------------------------------------------------------
Mg++       EMF oth/un 25°C  ->0  U   H                   1956MAa (39235) 615
Method: H electrode. DG(K1)=-23.8 kJ mol-1, DH=-8.4, DS=104.6
--------------------------------------------------------------------------------
Mg++       gl  KCl    20°C 0.10M U        K1=3.44        1955SAa (39236) 616
--------------------------------------------------------------------------------
Mg++       EMF oth/un 20°C  ->0  U        K1=4.41        1945SKa (39237) 617
Method: H electrode
********************************************************************************
C5H9NO4S              H2L                        (1736)
3-(Carboxymethyl)thio-L-alanine; HOOC.CH2.S.CH2.CH(NH2)COOH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Mg++       gl  NaClO4 25°C  1.0M U        K1=2.58        1979GSc (39311) 618
********************************************************************************
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
--------------------------------------------------------------------------------
Mg++       gl  NaNO3  25°C 0.10M U        K1=5.15   B2= 9.50  1993GAa (39529) 619
--------------------------------------------------------------------------------
Mg++       gl  KNO3   35°C 0.10M C    M                   1985RRc (39530) 620
                                        K(Mg+HL)=2.44
                                        K(MgL(cytidine)+H)=2.96
                                        K(Mg+HL+cytidine)=8.48
********************************************************************************
C5H9N3O4S             H2L                      CAS 16907-58-7  (2106)
Thiosemicarbazone-diethanoic acid; H2N.CS.NH.N(CH2.COOH)2
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Mg++       gl  KCl    30°C 0.10M U        K1=0.7         1967GNb (39564) 621
                                        K(Mg+HL)=0
--------------------------------------------------------------------------------
Mg++       cal KNO3   30°C 0.10M U   H                   1967GNc (39565) 622
DH(K1)=-5.9(?) kJ mol-1, DS=-4(?) J K-1 mol-1
********************************************************************************
C5H9N3O5              H2L                      CAS 4438-86-2  (3622)
Semicarbazone-1,1-diethanoic acid; H2N.CO.NH.N(CH2.COOH)2
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
```

```
--------------------------------------------------------------------------------
Mg++       gl  KCl    30°C 0.10M U        K1=1.4         1967GNb (39594) 623
                                          K(Mg+HL)=0
--------------------------------------------------------------------------------
Mg++       cal KNO3   30°C 0.10M U   H                   1967GNc (39595) 624
DH(K1)=40.9 kJ mol-1, DS=163 J K-1 mol-1
********************************************************************************
C5H10NO7P             H4L    PMIDA            CAS 5994-61-6  (2433)
N-(Phosphonomethyl)iminodiethanoic acid; H2O3P.CH2.N(CH2.COOH)2
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Mg++       gl  KNO3   25°C 0.10M C        K1=6.41        2000SDa (39661) 625
                                          K(MgL+H)=6.63
                                          K(MgHL+H)=4.2
--------------------------------------------------------------------------------
Mg++       ix  NaNO3   RT  0.10M U        K1=6.4         1985PMc (39662) 626
--------------------------------------------------------------------------------
Mg++       oth KNO3    RT  0.10M C                       1980MVa (39663) 627
                                          K(Mg+HL)=2.1
Method: paper electrophesis.
--------------------------------------------------------------------------------
Mg++       gl  KCl    30°C 0.10M U        K1=6.0         1958OMb (39664) 628
--------------------------------------------------------------------------------
Mg++       EMF KCl    20°C 0.10M U        K1=6.28        1949SAa (39665) 629
                                          K(Mg+HL)=1.96
Method: H electrode
********************************************************************************
C5H10O2S              HL                   CAS 7244-82-8  (3042)
3-Ethylthiopropanoic acid; CH3.CH2.S.CH2.CH2.COOH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Mg++       gl  diox/w 30°C  50%  U        K1=3.0    B2=6.0    1956IFa (40242) 630
********************************************************************************
C5H11NO2              HL    Nor-Valine     CAS 760-78-1  (689)
2-Aminopentanoic acid; CH3.CH2.CH2.CH(NH2).COOH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Mg++       gl  NaNO3  25°C 0.10M C    M   K1=3.35        2000KAb (40833) 631
                                          K(MgA+L)=3.85
                                          B(MgAL)=6.35
H2A=Dipicolinic acid.
--------------------------------------------------------------------------------
Mg++       gl  NaCl   20°C 0.15M U    M   K1=1.56        1983VDb (40834) 632
********************************************************************************
C5H11NO2              HL    DL-Valine      CAS 516-06-3  (186)
DL-2-Amino-3-methylbutanoic acid; H2N.CH(CH(CH3)2).COOH
--------------------------------------------------------------------------------
```

```
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Mg++       gl  NaCl   20°C 0.15M U    M   K1=1.56        1983VDb (40893) 633
*************************************************************************
C5H11N2O7P            H3L                        (3635)
Glycyl-O-phosphoryl-D,L-serine;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Mg++       gl  KCl    25°C 0.15M U        K1=1.86        1962OSa (41377) 634
                                         K(Mg+HL)=1.64
                                         K(Mg+MgL)=1.4
*************************************************************************
C5H11N2O7P            H3L                     CAS 6665-42-5  (3636)
O-Phosphorylserylglycine;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Mg++       gl  KCl    25°C 0.15M U        K1=1.94        1962OSa (41382) 635
                                         K(Mg+HL)=1.40
                                         K(Mg+MgL)=1.25
*************************************************************************
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
-------------------------------------------------------------------------
Mg++       gl  NaNO3  25°C 0.10M C        K1=1.58        1988MSa (41418) 636
-------------------------------------------------------------------------
Mg++       gl  KNO3   15°C 0.10M U        K1=1.70        1972FSa (41419) 637
*************************************************************************
C5H12NO4P              HL                     CAS 51276-47-2  (5704)
2-Amino-4-(methylhydroxyphosphoryl)butanoic acid;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Mg++       gl  NaClO4 23°C 0.10M U        K1=3.23        1990YTa (41443) 638
*************************************************************************
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
-------------------------------------------------------------------------
Mg++       gl  KNO3   25°C 0.10M U  I                    1970CMc (41571) 639
                                         K(Mg+HL)=1.54
I=1.0 M, K(Mg+HL)=1.71
*************************************************************************
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
-------------------------------------------------------------------------
Mg++       gl  KCl    25°C 0.20M C                          2002MKc (41751) 640
                                     B(MgH2L)=23.20
                                     B(MgHL)=17.60
                                     B(MgH2L2)=32.73
                                     B(MgHL2)=21.18
*************************************************************************
C5H13NO7P2            H4L                    CAS 75006-88-1  (640)
1-Acetylaminopropylidene-1,1-diphosphoric acid;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Mg++       gl  KNO3   30°C 0.15M U        K1=7.69   B2=13.15  1983LSa (41753) 641
                                     K(Mg+HL)=3.31
*************************************************************************
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
-------------------------------------------------------------------------
Mg++       gl  KNO3   30°C 0.15M U        K1=8.34   B2=14.08  1983LSa (41757) 642
                                     K(Mg+HL)=3.33
*************************************************************************
C5H13O14P3            H5L    PRPP            CAS 108321-05-7  (2385)
5-Phosphorylribose-1-pyrophosphate;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Mg++       gl  KCl    25°C 0.20M U        K1=3.2          1978TLa (41812) 643
                                     B(Mg2L)=4.8
                                     B(MgHL)=9.4
                                     B(MgH2L)=11.0
*************************************************************************
C5H13O14P3            H4L                    CAS 62746-84-3  (8234)
Ribose 5'-triphosphate;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Mg++       sp  oth/un 25°C 0.05M C        K1=4.77         1981BKf (41813) 644
                                     K(MgL+Mg)=1.60
Method: by competition with 8-hydroxyquinoline.
Medium: 0.05 M Tris buffer, pH 7.5. K(MgL+Mg) determined by 31P nmr.
*************************************************************************
C5H14NO3P             H2L                    CAS 13138-37-9  (1985)
1-Aminopentylphosphonic acid; CH3.(CH2)3.CH(NH2).PO3H2
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Mg++       gl  KNO3   25°C 0.10M U        K1=2.03         1979WNb (41823) 645
```

B(MgHL)=11.59

****

C5H14NO3P H2L CAS 72696-97-0 (1990)
Diethylaminomethylphosphonic acid; (C2H5)2N.CH2.PO3H2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	25°C	1.0M	U		K1=2	1967CCa (41832)	646
							K(Mg+HL)=1.3		

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaClO4	25°C	0.1M	U		K1=3.82	1975SLa (41836)	647
							K(Mg+HL)=2.86		

****

C5H15NO6P2 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
Mg++	gl	KCl	25°C	0.20M	C		K1=6.12	2002MKc (41942)	648
							B(MgH2L)=22.61		
							B(MgHL)=17.23		
							B(MgH2L2)=32.22		

****

C5H15NO7P2 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
Mg++	sol	KCl	22°C	0.10M	U			1985KSa (41954)	649
							K(Mg+HL)=3.30		
Mg++	gl	KCl	25°C	0.10M	U		K1=6.57	1979KBa (41955)	650
							K(Mg+HL)=6.32		

****

C5H17NO13P4 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
Mg++	gl	KNO3	25°C	1.0M	U		K1=7.40	1982SBa (42019)	651
							K(Mg+HL)=6.85		
							K(Mg+H2L)=4.54		
							K(Mg+H3L)=3.17		
							K(Mg+H4L)=2.67		

****

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
Mg++	con	alc/w	30°C	100%	U	I M	K2=2.85	1979PSa (42088)	652

Medium: iso-PrOH. In H2O: K2=1.49

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	sp	oth/un	25°C	->0	U		K1=2.8	1960KAb (42089)	653
Mg++	sp	oth/un	21°C	0.40M	U		B2=2.43	1955BKa (42090)	654

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
Mg++	sp	oth/un	21°C	0.40M	U		B2=2.38	1955BKa (42222)	655

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
Mg++	gl	KCl	25°C	0.10M	M		K1=4.53 B2=7.71 B(CuH-1L)=-5.8	1987HAb (42262)	656

****

C6H4N4O HL CAS 900-47-0 (3083)
4-Hydroxypteridine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	oth/un	20°C	0.01M	U		K1=<1	1953ALa (42277)	657

****

C6H4O4 H2L CAS 615-94-1 (1280)
2,5-Dihydroxy-1,4-benzoquinone;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KCl	30°C	25%	M	TIH	K1=3.35	1991GDe (42303)	658

Medium: 35% Dioxan/H2O, 0.1 M NaClO4. Other solvents and backgrounf concs.

****

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

```
Mg++       gl  NaNO3  20°C 0.10M U        K1=2.20        1960ANb (42491) 659
--------------------------------------------------------------------------
Mg++       gl  oth/un 25°C  0.0  U        K1=2.58   B2=3.95   1957LUa (42492) 660
--------------------------------------------------------------------------
Mg++       gl  NaNO3  25°C 0.10M U        K1=2.5         1957SYb (42493) 661
**************************************************************************
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
--------------------------------------------------------------------------
Mg++       gl  KCl    25°C 0.10M M        K1=5.72   B2=9.77   1986HAc (42854) 662
**************************************************************************
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
--------------------------------------------------------------------------
Mg++       gl  KCl    25°C 0.10M M        K1=5.21   B2=8.85   1985HAa (42910) 663
**************************************************************************
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
--------------------------------------------------------------------------
Mg++       kin KCl    39°C 1.00M C        K1=6.2         1987HJb (42982) 664
**************************************************************************
C6H6NBr                L                      (8782)
5-Bromo-2-methylpyridine;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Mg++       gl  NaNO3  25°C 0.50M C        K1=-0.07       2002KSb (43193) 665
**************************************************************************
C6H6NCl                L                      CAS 10445-91-7  (8781)
4-(Chloromethyl)pyridine;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Mg++       gl  NaNO3  25°C 0.50M C        K1=0.06        2002KSb (43209) 666
**************************************************************************
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
--------------------------------------------------------------------------
Mg++       gl  NaNO3  25°C 0.10M C        K1=1.29        1988MSa (43244) 667
--------------------------------------------------------------------------
Mg++       kin KCl    39°C 1.00M C        K1=14.8        1987HJb (43245) 668
**************************************************************************
```

C6H6N2O2 HL (8281)
3-Hydroxy-2-amidocarboxypyridine, Hydroxypicolinamide;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	25°C	0.10M	C		K1=2.64	1990ARa (43372)	669

****

C6H6N2O4 HL Methylorotic CAS 706-36-2 (2611)
3N-Methyl-2,4-dihydroxypyrimidine-6-caboxylic acid, methylorotic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	sp	oth/un	20°C	var	C		K1=4.11	1981LGc (43470)	670
Medium: phosphate (0.1 M) or borax (0.01 M) buffers.									
Mg++	gl	NaCl	20°C	0.15M	U		K1=3.98	1979DZc (43471)	671
							K(Mg+HL)=2.15		

****

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
Mg++	sp	alc/w	25°C	95%	U		K1=1.98	1993GSa (43712)	672
Medium: 95% w/w EtOH/H2O, 0.05 M Et4NClO4, by competitive spectrophotometry									
Mg++	gl	KNO3	35°C	0.10M	C		K1=4.12	1985RRh (43713)	673
Mg++	gl	NaClO4	30°C	0.10M	U		K1=5.24	1966APb (43714)	674

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	nmr	oth/un	25°C	0.0	U		K1=0.75	1992AVa (43895)	675
Medium: pH 7.4 buffer									

****

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
Mg++	sp	KCl	25°C	0.50M	U		K1=2.59	1974TAa (44191)	676
Mg++	gl	KNO3	25°C	0.10M	U		K1=2.92 B2=5.11	1962MUa (44192)	677
Mg++	EMF	KCl	21°C	0.10M	U		K1=3.0	1959OKb (44193)	678
Method: H electrode									

****

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
Mg++	gl	KNO3	30°C	0.10M	U		K1=6.27 B2=10.41	1963MNc (44279)	679

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KCl	20°C	0.10M	U		K1=6.86 K(Mg+HL)=1.98	1964PCa (44396)	680

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KCl	25°C	0.10M	C		K1=3.43 K(MgL+H)=3.33	1984MMg (44535)	681

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaNO3	25°C	0.50M	C		K1=-0.02	2002KSb (44600)	682
Mg++	gl	NaClO4	35°C	0.20M	U		K1=2.59	1971SBb (44601)	683

****

C6H7N L beta-Picoline CAS 108-99-6 (324)
3-Methylpyridine; C5H4N.CH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaNO3	25°C	0.50M	C		K1=0.04	2002KSb (44689)	684
Mg++	gl	NaClO4	35°C	0.20M	U		K1=2.44	1971SBb (44690)	685

****

C6H7N L gamma-Picoline CAS 108-89-4 (325)
4-Methylpyridine; C5H4N.CH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaClO4	35°C	0.20M	U		K1=2.80	1971SBb (44812)	686

****

C6H7NO2 HL CAS 19365-01-6 (2311)
3-Hydroxy-1-methylpyridin-4(1H)-one;

```
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Mg++       gl  KNO3   37°C 0.15M C        K1=3.44   B2=5.89   1980SHb (45042) 687
*******************************************************************************
C6H7O3P              H2L                     CAS 1571-33-1  (521)
Phenylphosphonic acid; C6H5.PO3H2
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Mg++       sp  oth/un 30°C 0.30M U        K1=1.72        1975KWa (45199) 688
*******************************************************************************
C6H7O4P              H2L                     CAS 701-64-4  (5866)
Phenyl phosphoric acid; C6H5O.PO(OH)2
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Mg++       gl  NaNO3  25°C 0.10M C        K1=1.53        1988MSa (45229) 689
*******************************************************************************
C6H8NO4P             H2L                       (3713)
2-Pyridylmethanephosphoric acid (1'-picolyl phosphate)
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Mg++       gl  KNO3   25°C 0.10M U        K1=1.7         1968MTd (45246) 690
*******************************************************************************
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
-------------------------------------------------------------------------------
Mg++       sp  alc/w  25°C  95%  U        K1=1.73        1993GSa (45270) 691
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
-------------------------------------------------------------------------------
Mg++       gl  KCl    20°C 0.10M U        K1=1.86        1955SAa (45415) 692
*******************************************************************************
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
-------------------------------------------------------------------------------
Mg++       gl  NaClO4 25°C 0.10M U        K1=2.1         1966OCb (45504) 693
                                        K(Mg+HL)=0.95
*******************************************************************************
C6H8O5                HL                      (5458)
```

4-Ethyl-oxaloethanoic acid HOOC.CO.CH2.C(O)O.CH2.CH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	kin	KCl	25°C	0.50M	U		K1=1.06 K(Mg+H-1L=MgH-1L)=3.7	1982BLb (45530)	694

****

C6H8O6 H3L Tricarballylic CAS 99-14-9 (1620)
1,2,3-Propanetricarboxylic acid; HOOC.CH2.CH(COOH).CH2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	oth/un	25°C	0.0	C	I	K1=3.256 B(MgHL)=8.605 B(MgH2L)=12.392 B(Mg2L)=4.21	1994DFc (45558)	695
							Values at I=0 calculated from data for 0.013-0.33 M MgCl2.		
Mg++	gl	NaClO4	20°C	0.10M	U		K1=2.06 K(Mg+HL)=1.20 K(Mg+H2L)=0.77	1964COb (45559)	696
Mg++	gl	oth/un	25°C	0.15M	U		K1=2.00 K(Mg+HL)=0.91	1964PCa (45560)	697

****

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
Mg++	gl	NaClO4	25°C	1.00M	M	M	K(Mg+H2L+(ascorbate))=3.77	1988MOa (45621)	698
Mg++	gl	NaClO4	20°C	1.00M	M		K(Mg+HL)=0.98 K(Mg+2HL)=1.85	1983MOa (45622)	699

****

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
Mg++	gl	NaClO4	25°C	1.0M	U		K(Mg+H-1L)=3.81 K(Mg+H-1L+H)=14.13 K(Mg+H-1L+2H)=18.19 K(Mg+H-1L-H)=-8.57	1976PCb (45729)	700
							Data are for DL isomeric mixture.		
Mg++	gl	R4N.X	25°C	0.10M	U		K1=1.43 B2=2.72	1970GTa (45730)	701

****

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
Mg++	gl	oth/un	25°C	0.0	C	I	K1=4.71 K(Mg+H+L)=8.84 K(Mg+2H+L)=12.2	1999DGa (45991)	702

Medium: artificial seawater. Extrapolated from data for 5-45% salinity.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaClO4	25°C	0.50M	C		K1=2.71 B(MgHL)=6.55	1995PLa (45992)	703

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	oth	NaCl	25°C	0.15M	U	T	K1=3.27	1993GMa (45993)	704

Method: Coulometric titration. K1=3.24 (37 C)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaClO4	30°C	1.0M	U		K1=3.62	1988GMd (45994)	705

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaClO4	37°C	0.15M	C		K1=3.333 B2=5.126 B(MgH2L)=11.008 B(MgHL)=7.483 B(MgHL2)=10.411 B(Mg2H-2L2)=-12.638	1987BBd (45995)	706

B(MgH-2L)= -18.468

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	37°C	0.10M	U	I	K1=3.451 B(MgHL)=7.23	1982ADa (45996)	707

Ionic strength range: 0.03-0.3.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	oth/un	25°C	0.00	U	H	K1=4.71 K(Mg+HL)=2.42	1982ADa (45997)	708

DH1=-22.00 kJ mol-1, DS1=164 J mol-1 K-1.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	oth	oth/un	25°C	dil	C		K1=4.917 K(Mg+HL)=1.672	1982HKa (45998)	709

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KCl	25°C	0.10M	M	I	K1=3.63 K(Mg+HL)=1.76 K(Mg+H2L)=0.54	1980PEa (45999)	710

Extrapolated to I=0.0 M: K1=4.85; K(MgHL)=2.67; K(MgH2L)=1.0.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	25°C	0.10M	C		K1=3.38 B(MgHL)=7.66	1975FCc (46000)	711

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaCl	37°C	0.15M	C		K1=3.34 K(Mg+HL)=1.62	1974MEa (46001)	712

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	R4N.X	25°C	0.10M	U		K1=1.92 B2=3.85	1970GTa (46002)	713

```
--------------------------------------------------------------------------------
Mg++       gl  oth/un 32°C 0.10M U        K1=3.6         1965PPb (46003) 714
--------------------------------------------------------------------------------
Mg++       gl  R4N.X  25°C 0.10M U        K1=3.73        1965TGa (46004) 715
                                          K(Mg+HL)=1.85
Medium: Me4NCl
--------------------------------------------------------------------------------
Mg++       gl  NaClO4 20°C 0.10M U        K1=3.40        1964COb (46005) 716
                                          K(Mg+HL)=1.84
                                          K(Mg+H2L)=0.84
--------------------------------------------------------------------------------
Mg++       ix  R4N.X  25°C 0.10M U        K1=3.16        1964TMb (46006) 717
Medium: NH4Cl
--------------------------------------------------------------------------------
Mg++       ix  oth/un 25°C  0.0  U        K1=3.96        1964TMb (46007) 718
--------------------------------------------------------------------------------
Mg++       sp  R4N.X  25°C 0.10M C        K1=3.55        1961WAa (46008) 719
Medium: 0.16 M Me4NCl.
--------------------------------------------------------------------------------
Mg++       vlt oth/un 25°C 0.15M U        K1=3.29        1959LLa (46009) 720
                                          K(Mg+HL)=1.60
Same values at I=0.09
--------------------------------------------------------------------------------
Mg++       oth oth/un 25°C 0.16M U        K1=3.2         1934HMa (46010) 721
Method: frog heart contraction
********************************************************************************
C6H8O7P2              H3L                     CAS 101378-64-7  (7666)
Phenyldiphosphoric acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Mg++       gl  NaNO3  25°C 0.10M M        K1=3.24        1999SSa (46344) 722
********************************************************************************
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
--------------------------------------------------------------------------------
Mg++       gl  NaCl   25°C 1.00M C        K1=0.92        1988BSa (46357) 723
********************************************************************************
C6H9NO6               H3L                     CAS 41035-84-1  (4367)
N-Carboxymethyl-L-aspartic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Mg++       gl  KNO3   25°C 0.10M U        K1=4.57        1975GNb (46373) 724
********************************************************************************
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
--------------------------------------------------------------------------
Mg++       gl  KNO3   20°C 0.10M C TIH  R K1=5.43        1982ANa (46677) 725
IUPAC evaluation
--------------------------------------------------------------------------
Mg++       dis R4N.X    ?  0.10M U        K1=6.4         1969ASb (46678) 726
Method: chromatography. Medium: NH4Cl
--------------------------------------------------------------------------
Mg++       gl  KCl    20°C 0.10M U      T K1=5.46        1966IMb (46679) 727
--------------------------------------------------------------------------
Mg++       gl  KNO3   25°C 0.10M U T H  T K1=5.36        1960BMb (46680) 728
K1=5.33(0.5 C), 5.37(42.5 C). DH(K1)=12.6 kJ mol-1, DS=142 J K-1 mol-1
--------------------------------------------------------------------------
Mg++       EMF oth/un 30°C  0.0  U T H    K1=6.61        1956HMa (46681) 729
Method: H electrode. K1=6.31(0 C), 6.39(10 C), 6.50(20 C).
DH(K1)=20.3 kJ mol-1, DS=192 J K-1 mol-1
--------------------------------------------------------------------------
Mg++       EMF oth/un 25°C  0.0  U   H                   1956MAa (46682) 730
Method: H electrode. DG(K1)=-37.24 kJ mol-1, DH=16.7, DS=184 J K-1 mol-1
--------------------------------------------------------------------------
Mg++       gl  KCl    20°C 0.10M U      T K1=5.41        1955SAa (46683) 731
--------------------------------------------------------------------------
Mg++       gl  KCl    20°C 0.10M U        K1=7.0    B2=10.2   1948SBa (46684) 732
--------------------------------------------------------------------------
Mg++       EMF oth/un 20°C  0.0  U        K1=7.00        1945SKb (46685) 733
Method: H electrode
**************************************************************************
C6H9NO7               H3L                      CAS 3055-17-2  (3694)
Nitrilotriethanoic acid N-oxide; O-N(CH2.COOH)3
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Mg++       gl  KNO3   25°C 0.10M U        K1=2.83        1967CCc (47134) 734
**************************************************************************
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
--------------------------------------------------------------------------
Mg++       gl  KNO3   35°C 0.10M C    M                   1985RRc (47525) 735
                                       K(Mg+HL)=3.35
                                       K(MgL(cytidine)+H)=2.58
                                       K(Mg+HL+cytidine)=8.43
--------------------------------------------------------------------------
Mg++       gl  KNO3   35°C 0.10M C                        1985RRh (47526) 736
                                       K(Mg+HL)=3.35
--------------------------------------------------------------------------
Mg++       gl  KNO3   35°C 0.10M C    M   K1=2.80        1983KSc (47527) 737
                                       K(Mg+HA+L)=3.35
                                       K(Mg+HB+L)=2.81
```

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
Mg++	gl	KCl	22°C	0.10M	U		K1=3.2	1964PCa	(47735) 738

****

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
Mg++	gl	KCl	22°C	0.10M	U		K1=5.8	1964PCa	(47747) 739

****

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
Mg++	gl	KNO3	25°C	0.10M	C		K1=2.51	1983LRc	(47837) 740
Mg++	gl	KNO3	25°C	0.10M	C		K1=2.51	1979NAb	(47838) 741
Mg++	gl	KCl	20°C	0.10M	U		K1=2.47	1955SAa	(47839) 742

****

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
Mg++	gl	KNO3	25°C	0.10M	U		K1=6.80 K(Mg+HL)=5.98 K(Mg+H2L)=4.16	1990GKa	(47871) 743

****

C6H10N4OS L (2622)
4,5-Dimethyl-2,4,6,8-tetraazabicyclo[3,3,O]-octane-3-one-7-thione;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	25°C	0.10M	U		K1=4.18	1986KKa	(47890) 744

****

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
Mg++	sp	none	25°C	0.0	U	T	K1=2.95	1976KOa	(48023) 745

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

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	25°C	0.10M	U		K1=1.9	1974MSa	(48329) 746
Mg++	gl	oth/un	25°C	0.10M	U		K1=2.78	1961KEa	(48330) 747

****

C6H10O7 HL Glucuronic acid CAS 6556-12-3 (599)
D-Glucuronic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	R4N.X	25°C	0	M	I	K1=1.03	1996GMb	(48416) 748

At I=0.16 M: K1=0.65

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KCl	20°C	0.10M	U		K1=4.32	1955SAa	(48609) 749
							K(Mg+HL)=2.50		

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	dis	R4N.X	?	0.10M	U		K1=4.8	1969ASb	(48682) 750

Method: chromatography. Medium: NH4Cl

Mg++	vlt	NaClO4	25°C	0.10M	U		K1=3.5	1969VPa	(48683) 751
Mg++	gl	KCl	20°C	0.10M	U		K1=3.44	1955SAa	(48684) 752
Mg++	gl	KCl	30°C	0.10M	U		K1=3.54	1952CCa	(48685) 753

****

C6H11NO7S H3L CAS 39716-94-4 (3125)
N-2-Sulfoethyliminodiethanoic acid (taurine-NN-diacetic acid)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	EMF	KCl	20°C	0.10M	U		K1=3.48	1949SAa	(48845) 754

Method: H electrode

****

C6H11N3O4 HL Gly-Gly-Gly CAS 556-33-2 (415)
Glycyl-glycyl-glycine; H2N.CH2.CO.NH.CH2.CO.NH.CH2.COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl KCl 30°C 0.09M U T H K1=1.95 1957MMa (48972) 755
K1=1.60(0.35 C), 2.08(48.8 C). DH(K1)=8.4 kJ mol-1, DS=59 J K-1 mol-1
****
C6H12NO7P H4L CAS 55339-27-0 (3127)
N-2-Phosphoethyliminodiethanoic acid; H2O3P.CH2.CH2.N(CH2.COOH)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ EMF KCl 20°C 0.10M U K1=6.33 1949SAa (49033) 756
K(Mg+HL)=2.14
Method: H electrode
****
C6H12N2O4 H2L EDDA CAS 5657-17-0 (119)
1,2-Diaminoethane-N,N'-diethanoic acid; HOOC.CH2.NH.CH2.CH2.NH.CH2.COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ cal NaClO4 25°C 0.10M U H K1=4.3 1983EHa (49222) 757
DH1=12.3 kJ mol-1, DS1=124 J K-1 mol-1

Mg++ gl KCl 30°C 0.10M U K1=3.9 1952CMc (49223) 758
****
C6H12N2O4 H2L N,N-EDDA CAS 5835-29-0 (2333)
1,2-Diaminoethane-N,N-diethanoic acid; H2N.CH2.CH2.N(CH2.COOH)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl KCl 20°C 0.10M U K1=4.53 1955SAa (49298) 759
****
C6H12N2O4 H2L CAS 4726-83-4 (5911)
N,N-Dihydroxyhexanediamide; HN(OH).CO.(CH2)4.CO.NH(OH)

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl NaNO3 25°C 0.10M C K1=3.33 1989EHa (49331) 760
B(MgHL)=12.43
****
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
---
Mg++ ISE none 25°C 0.0 C K1=-0.22 1975AHa (49626) 761
****
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
Mg++	EMF	KCl	20°C	0.20M	U		K1=0.70	1938CKa (49694)	762

Method: H electrode

****

C6H13NO2 HL Isoleucine CAS 73-32-5 (424)

2-Amino-3-methylpentanoic acid; CH3.CH2.CH(CH3).CH(NH2).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaCl	20°C	0.15M	U	M	K1=1.85	1983VDb (49897)	763

****

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
Mg++	gl	KNO3	25°C	0.10M	U	I	K1=3.69	1990RAb (50056)	764

Data also for 10% w/w EtOH/H2O (K1=3.94) and 25% (4.21)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaCl	20°C	0.15M	U	M	K1=1.89	1983VDb (50057)	765

****

C6H13NO2 HL Norleucine CAS 616-06-8 (602)

2-Aminohexanoic acid (2-Aminocaproic acid) CH3.(CH2)3.CH(NH2).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaCl	20°C	0.15M	U	M	K1=1.90	1983VDb (50168)	766
Mg++	gl	oth/un	20°C	0.01M	U		B2=<4	1950ALa (50169)	767

****

C6H13NO4 HL Bicine CAS 150-25-4 (2124)

N,N-Bis(2-hydroxyethyl)glycine; (HO.CH2.CH2)2N.CH2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	25°C	0.10M	C		K1=1.80	1991KNa (50338)	768
Mg++	gl	KCl	30°C	0.10M	U		K1=1.15	1953CCa (50339)	769

****

C6H13NO4S HL MES CAS 4432-31-9 (7807)

4-Morpholineethanesulfonic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaClO4	37°C	0.10M	U	T	K1=0.5	1992GHa (50429)	770

Method: coulometric titration. At 25 C, K1=0.6.

****

C6H13N3O3 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
Mg++	gl	KNO3	25°C	0.10M	U		K1=1.66 B2=1.86	1970CMc (50571)	771

****

C6H13O9P H2L CAS 26177-86-6 (7139)
Fructose-6-phosphoric acid; C6H11O5.H2PO4

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaClO4	25°C	0.10M	C		K1=3.32	1996GCa (50606)	772
Mg++	gl	KCl	20°C	0.10M	U		K1=1.59	1957SAa (50607)	773

****

C6H13O9P 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
Mg++	nmr	oth/un	25°C	?	U		K1=1.18	1991COa (50619)	774

****

C6H13O9P H2L CAS 56-73-5 (3703)
d-Glucose-6-phosphoric acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	nmr	oth/un	25°C	?	U		K1=0.90	1991COa (50624)	775

****

C6H14NO2P HL (6465)
Piperidinemethylphosphinic acid; C5H10N.CH2.PO2H2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaClO4	25°C	0.10M	C		K1=3.46	1992LBa (50635)	776

****

C6H14N4O2 L (1529)
1,8-Diamino-3,6-diaza-2,7-octanedione; (H2N.CH2.CO.NH.CH2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KCl	25°C	1.0M	U		K1=0.54	1953CGa (50928)	777

****

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
Mg++	gl	KNO3	25°C	0.10M	U		K1=2.21	1970CMc (50999)	778
Mg++	gl	oth/un	25°C	?	U		K1=1.30	1960PEd (51000)	779

****
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
---
Mg++ cal non-aq 25°C 100% C H 1992BSc (51046) 780
Medium: propylene carbonate. DH(K1)=-3.6 kJ mol-1.

Mg++ con non-aq 25°C 100% C K1=2.6 1992MSe (51047) 781
Medium: 100% MeOH. Anion: picrate. Also data for nitrophenolate anions.
****
C6H14O8P2 H4L CAS 36011-96-8 (4391)
trans-1,2-Cyclohexanediol diphosphate; C6H10(OPO3H2)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl R4N.X 20°C 0.10M U K1=3.72 1969HRa (51116) 782
K(Mg+HL)=2.28
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
---
Mg++ gl NaClO4 25°C 0.10M C K1=3.75 1996GCa (51123) 783

Mg++ gl oth/un 25°C 0.08M U K1=2.7 1965MCb (51124) 784
K(Mg+HL)=2.12
****
C6H14O12P2 H4L CAS 84364-89-6 (7140)
Fructose-2,6-diphosphoric acid; C6H10O4.(H2PO4)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl NaClO4 25°C 0.10M C K1=3.90 1996GCa (51129) 785
****
C6H15NO3 Triethanolamine CAS 102-71-6 (447)
Tris-(2-hydroxyethyl)amine; L

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl R4N.X 25°C 1.00M C I K1=0.24 1982SSf (51282) 786
In 90 % (v/v) DMSO/water mixture: K1=0.51 (I=0.25 M)
****
C6H15NO7P2 H4L CAS 126104-92-5 (8889)
N-2-Methylenetetrahydrofuryloaminomethane-1,1-diphosphonic acid;

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

```
------------------------------------------------------------------------------
Mg++       gl  KCl    25°C 0.20M C        K1=7.28   B2=10.46  2002MKc (51342) 787
                                          B(MgH2L)=22.48
                                          B(MgHL)=17.10
                                          B(MgH-1L)=-4.79
                                          B(MgH2L2)=31.84
B(MgHL2)=21.59.
******************************************************************************
C6H15N4O5P            H2L                     CAS 1189-11-3  (3715)
Phosphoarginine; H2N.CH(CH2.CH2.CH2.NH.C(:NH).NH2).CO.OPO3H2
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Mg++       sp  oth/un 30°C 0.10M U        K1=2.0         1964OPa (51456) 788
Medium: 0.1 M N-ethylmorpholine buffer
******************************************************************************
C6H15O15P3            H6L    Ins(1,2,6)P3     CAS 28841-62-5  (6479)
D-myo-Inositol 1,2,6-trisphosphoric acid;
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Mg++       gl  KCl    37°C 0.20M U  I     K1=3.91        1990BJb (51532) 789
                                          B(MgHL)=13.50
In But4NBr 0.1 M: K1=5.61, B(MgHL)=13.50, B(MgH2L)=19.41, B(Mg3L)=11.28
******************************************************************************
C6H16NO4P             H2L                       (8073)
1-Amino-2-hydroxy-4-methylpentane-2-phosphonic acid;
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Mg++       gl  NaClO4 25°C  0.1M U        K1=3.84        1975SLa (51561) 790
                                          K(Mg+HL)=2.87
******************************************************************************
C6H16NO4P              HL                     CAS 387383-55-3  (8776)
N,N,N-Trimethyl-2-(phosphonomethoxy)ethylamine;
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Mg++       gl  NaNO3  25°C 0.10M M        K1=1.40        2002FGb (51572) 791
******************************************************************************
C6H16N2O4P2           H2L                       (6466)
Piperazine-1,4-diylbis(methylene)bis(phosphinic acid); H2O2P.CH2.C4H8N2.CH2.PO2H2
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Mg++       gl  NaClO4 25°C 0.10M C        K1=0.6         1992LBa (51709) 792
******************************************************************************
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
Mg++	gl	KCl	25°C	0.10M	U		K1=<3	1967KLa	(51790) 793

****

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
Mg++	gl	KCl	25°C	0.20M	C		K1=6.41 B(MgH2L)=23.20 B(MgHL)=17.55 B(MgH2L2)=32.37 B(Mg3H2L2)=40.62	2002MKc	(51802) 794

****

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
Mg++	gl	KCl	25°C	0.20M	C		K1=6.43 B(MgH2L)=22.98 B(MgHL)=17.41 B(MgH2L2)=32.23 B(Mg3H2L2)=39.67	2002MKc	(51806) 795

****

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
Mg++	gl	KNO3	25°C	0.10M	C		K1=7.83 K(MgL+H)=8.91 K(MgHL+H)=8.07 K(MgH2L+H)=5.74 K(MgH3L+H)=4.3	1999DOa	(51824) 796

****

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
Mg++	gl	R4N.X	25°C	0.10M	M		K1=3.96	1996BCa	(51929) 797

Medium: 0.1 M Me4NNO3.

****

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

```
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Mg++       gl  KNO3   25°C 0.10M C        K1=5.67        1999DOa (51948) 798
                                          K(MgL+H)=8.80
                                          K(MgHL+H)=6.9
*************************************************************************
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
-------------------------------------------------------------------------
Mg++       gl  KNO3   25°C 0.10M C        K1=5.36        1999DOa (51968) 799
                                          K(MgL+H)=9.99
                                          K(MgHL+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
-------------------------------------------------------------------------
Mg++       ISE non-aq 25°C 100%  M        K1=3.96   B2= 5.05  1999NMa (51977) 800
                                          B3=6.36
                                          B4=7.60
Method: ISE based on benzo-12-crown-4 coupled to polyacrylamide.
Medium: propylenecarbonate, 0.01 M Et4NClO4.
*************************************************************************
C6H18N4                 L    Trien-tetramine  CAS 112-24-3  (11)
1,4,7,10-Tetraazadecane; H2N.CH2.CH2.NH.CH2.CH2.NH.CH2.CH2.NH2
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Mg++       gl  NaCl   25°C  0.0  C        K1=1.39        1999SFc (52090) 801
                                          K(Mg+HL)=1.05
                                          K(Mg+H2L)=0.25
                                          K(Mg+H3L)=-0.33
Extrapolated from data for 0.03-0.96 M NaCl using the Pitzer equation.
*************************************************************************
C6H20N2O8P4           H4L                        CAS 938-16-3  (4402)
Ethylenediaminetetra(methylenephosphonous acid);
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Mg++       gl  KNO3   25°C 0.10M U        K1=1.94        1971MMh (52247) 802
*************************************************************************
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
-------------------------------------------------------------------------
```

```
Mg++       gl  KCl    25°C 0.10M C  I   R                2001PRa (52313) 803
                                        K(Mg+HL)=5.40
                                        K(MgL+H)=10.00
                                        K(MgHL+H)=8.76
                                        K(MgH2L+H)=6.91
IUPAC Recommended values. MgH3L+H)=5.2
-------------------------------------------------------------------------------
Mg++       gl  NaCl   37°C 0.15M C       K1=5.49        1995JWa (52314) 804
                                        K(MgL+H)=9.21
                                        K(MgL+OH)=2.34
                                        K(MgHL+H)=8.63
                                        K(MgH2L+H)=7.06
-------------------------------------------------------------------------------
Mg++       gl  KNO3   25°C 0.10M C   H    K1=8.35        1993SMa (52315) 805
                                        K(MgL+H)=10.07
                                        K(MgHL+H)=8.73
                                        K(MgH2L+H)=6.86
                                        K(MgH3L+H)=5.35
DH(K1)=16.5, DH(MgHL)=-25.7, DH(MgH2L)=-20.7, DH(MgH3L)=0.3, DH(MgH4L)=0.6
kJ mol-1.
-------------------------------------------------------------------------------
Mg++       gl  KCl    25°C 0.10M U       K1=5.69        1980RZa (52316) 806
                                        K(MgL+H)=10.60
                                        K(MgH2L+H)=8.23
                                        K(MgHL+H)=9.10
                                        K(MgH3L+H)=7.07
-------------------------------------------------------------------------------
Mg++       gl  KNO3   25°C 0.10M U       K1=4.78        1979RZa (52317) 807
                                        K(Mg+HL)=4.03
                                        K(Mg+H2L)=3.45
                                        K(Mg+H3L)=3.06
-------------------------------------------------------------------------------
Mg++       gl  KNO3   25°C 0.10M C       K1=8.43        1976MMa (52318) 808
                                        K(MgL+H)=9.95
                                        K(MgHL+H)=8.79
                                        K(MgH2L+H)=6.96
                                        K(MgH3L+H)=4.97
-------------------------------------------------------------------------------
Mg++       gl  KCl    25°C 0.10M U       K1=8.63        1967KDa (52319) 809
                                        K(Mg+HL)=6.58
                                        K(Mg+H2L)=5.00
                                        K(Mg+H3L)=4.07
                                        K(Mg+H4L)=2.45
*******************************************************************************
C7H4NO4Cl             H2L                    CAS 4722-94-5  (3780)
4-Chloropyridine-2,6-dicarboxylic acid; Cl.C5H2N(COOH)2
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Mg++       gl  NaClO4 22°C 0.10M U       K1=2.38        1964BBe (52383) 810
```

****

C7H4N2O7 H2L CAS 609-99-4 (400)
3,5-Dinitrosalicylic acid; (O2N)2.C6H2(OH).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	sp	KCl	25°C	0.50M	U		K1=2.16	1974TAa (52459)	811
Mg++	gl	KNO3	25°C	0.10M	U	T	K1=2.30	1969DDc (52460)	812

K1(30 C)=2.43, K1(35 C)=2.65

****

C7H4N4O4 L CAS 50365-37-2 (7762)
5,6-Dinitrobenzimidazole;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaNO3	25°C	0.50M	M		K1=-0.11 K(Mg+H-1L)=0.62 *K(MgL)=-8.19	1999KSa (52516)	813

****

C7H5NOS HL CAS 7405-23-4 (3177)
4-Hydroxybenzothiazole;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	diox/w	25°C	50%	U		K1=4.54 B2=8.54	1960FFa (52590)	814

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	25°C	0.10M	U		K1=2.3	1958YYa (52619)	815

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	25°C	0.10M	U		K1=2.4	1958YYa (52648)	816

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaNO3	25°C	0.10M	C		K1=2.50	2000KAb (52745)	817
Mg++	gl	NaCl	30°C	0.10M	M		K1=1.94	1985RAa (52746)	818

```
Mg++       gl  oth/un 25°C 0.10M U        K1=2.32        1966BSe (52747) 819
By ion exchange: K2=0.7
-------------------------------------------------------------------------------
Mg++       gl  NaNO3  20°C 0.10M U        K1=2.30        1960ANb (52748) 820
-------------------------------------------------------------------------------
Mg++       gl  KNO3   25°C 0.10M U        K1=2.7         1957SYb (52749) 821
-------------------------------------------------------------------------------
Mg++       gl  KCl    30°C 0.10M U        K1=2.4         1957TBb (52750) 822
*******************************************************************************
C7H5NO4                HL                      CAS 97-51-8  (1887)
5-Nitrosalicylaldehyde; O2N.C6H3(OH).CHO
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Mg++       gl  diox/w 25°C  50%  U T      K1=3.18   B2=5.81   1973CGc (52935) 823
Medium: 50% dioxan, 0.3 M NaClO4.  Temperature range 15-50 C
K1(15 C)=3.06, K1(50 C)=2.31, K2(15 C)=2.58, K2(50 C)=2.23
*******************************************************************************
C7H5NO5               H3L                      CAS 499-51-4  (3150)
4-Hydroxypyridine-2,6-dicarboxylic acid; HO.C5H2N(COOH)2
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Mg++       gl  NaClO4 22°C 0.10M U        K1=3.68        1964BBa (53071) 824
-------------------------------------------------------------------------------
Mg++       gl  oth/un 20°C 0.10M U        K1=3.7         1963ANd (53072) 825
                                         K(MgL+H)=8.09
*******************************************************************************
C7H5N3O2                L                      CAS 94-52-0  (7761)
5-Nitrobenzimidazole;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Mg++       gl  NaNO3  25°C 0.50M M        K1=-0.09       1999KSa (53100) 826
                                         K(Mg+H-1L)=0.41
                                         *K(MgL)=-10.08
*******************************************************************************
C7H5O2Br               HL                      CAS 4584-68-3  (2691)
3-Bromotropolone;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Mg++       gl  diox/w 30°C  50%  U        K1=4.9    B2=8.8    1954BFd (53112) 827
*******************************************************************************
C7H5O2Br               HL                      CAS 586-76-5  (1367)
4-Brombenzoic acid; Br.C6H4.COOH
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Mg++       ISE NaCl   25°C  0.0  C TIH    K1=1.65        1991EAa (53117) 828
```

Method: Mg ISE. Data for 0.02-0.05 M NaCl, 15-45 C. DH(K1)=2.31 kJ mol-1,
DS(K1)=38.8 J K-1 mol-1. Also data for 2-bromo- and 3-bromobenzoic acid.

****

C7H5O2Br HL CAS 1761-61-1 (1886)
5-Bromosalicylaldehyde; Br.C6H3(OH).CHO

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Mg++	gl	diox/w	25°C	50%	U	T	K1=3.18	B2=5.86	1973CGc (53130)	829

Medium: 50% dioxan, 0.3 M NaClO4. Temperature range 15-50 C
K1(15 C)=3.36, K1(50 C)=3.18, K2(15 C)=2.82, K2(50 C)=2.53

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	EMF	diox/w	20°C	50%	U		K1=2	1963CCa (53131)	830

Medium: 50% dioxan, 0.3 M NaClO4

****

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
Mg++	ISE	NaCl	25°C	0.0	C	TIH	K1=1.62	1991EAa (53143)	831

Method: Mg ISE. Data for 0.02-0.05 M NaCl, 15-45 C. DH(K1)=2.31 kJ mol-1,
DS(K1)=38.8 J K-1 mol-1. Also data for 3-chloro- and 4-chlorobenzoic acid.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	ISE	NaCl	25°C	0.03M	U	TIH	K1=0.681	1982EFa (53144)	832

At 35 C, I=0.045 M: K1=0.715; 45 C, I=0.45 M: 0.340. Further data available

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	EMF	diox/w	20°C	50%	U		K1=2	1963CCa (53157)	833

Medium: 50% dioxan, 0.3 M NaClO4

****

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
Mg++	EMF	diox/w	20°C	50%	U		K1=3	1963CCa (53207)	834

Medium: 50% dioxan, 0.3 M NaClO4

****

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
Mg++	gl	diox/w	25°C	50%	U	T	K1=3.30	B2=6.04	1973CGc (53222)	835

Medium: 50% dioxan, 0.3 M NaClO4. Temperature range 15-50 C

K1(15 C)=3.39, K1(50 C)=3.07, K2(15 C)=2.87, K2(50 C)=2.58

****

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
Mg++	gl	KNO3	20°C	0.10M	U		K1=2.91		1965ABa (53503)	836
Mg++	gl	NaClO4	22°C	0.10M	U		K1=2.88		1964BBa (53504)	837

****

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
Mg++	gl	KCl	25°C	0.50M	U		K1=1.72		1969HLa (53615)	838
Mg++	gl	diox/w	30°C	75%	U		K1=3.88		1964JVa (53616)	839
Medium: 75% dioxan, 0.1 M NaClO4										
Mg++	EMF	diox/w	20°C	50%	U		K1=2		1963CCa (53617)	840
Medium: 50% dioxan, 0.3 M NaClO4										
Mg++	gl	diox/w	25°C	75%	U		K1=6.25	B2=10.55	1954UFa (53618)	841
Mg++	gl	diox/w	25°C	50%	U		K1=3.69	B2=6.80	1949MMa (53619)	842

****

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
Mg++	sp	NaClO4	25°C	0.10M	U		K1=3.82		1970HOa (53663)	843
Mg++	gl	diox/w	30°C	50%	U		K1=5.5	B2=9.9	1953BFa (53664)	844

****

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
Mg++	gl	alc/w	25°C	100%	M		K1=4.7	B2=7.1	1988PPa (53818)	845
Medium: MeOH										
Mg++	ISE	NaCl	25°C	0.03M	U	TIH	K1=0.981		1982EFa (53819)	846
At 35 C, I=0.045 M: K1=0.97; at 45 C, I=0.45: K1=0.380										
Mg++	gl	KNO3	30°C	0.40M	U		K1=0.1		1970BTa (53820)	847

****

C7H6O3 H2L CAS 1194-98-5 (4408)
2,5-Dihydroxybenzaldehyde; (OH)2.C6H3.CHO

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	diox/w	30°C	50%	U		K(Mg+HL)=3.20 K(MgHL+HL)=2.50	1969VMa (53948)	848

Medium: 50% dioxan, 0.1 M NaClO4

****

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
Mg++	cal	R4N.X	25°C	0	U	IH	K1=1.59	1997MAa (54131)	849

Medium: Me4NCl. I=0.025 K1=1.43, DH(K1)=2.7 kJ mol-1; I=0.050: K1=1.33, DH(K1)=3.1. I=0.075 M: K1=1.24, DH(K1)=3.9. I->0: DH(K1)=2.2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	sp	NaCl	25°C	0.50M	U	T	K(Mg+HL=MgL+H)=-8.48	1990DOa (54132)	850
Mg++	gl	alc/w	25°C	100%	M		K(Mg+HL)=4.2 K(Mg+2HL)=6.6	1988JTa (54133)	851

Medium: MeOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	cal	alc/w	25°C	100%	U	H		1988PPa (54134)	852

Medium: MeOH. DH(MgL)=27.4 kJ mol-1; DS=172. DH(MgL2)=38.7; DS=264

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	ISE	NaCl	25°C	0.03M	U	TIH	T K(Mg+HL)=1.35	1982EFa (54135)	853

At 35 C, I=0.045 M: K1=1.39; at 45 C, I=0.045 M: K1=1.35

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaClO4	37°C	0.15M	C	T	K1=5.156	1978AKa (54136)	854
Mg++	gl	diox/w	30°C	75%	U		K1=3.30	1964JVa (54137)	855

Medium: 75% dioxan, 0.1 M NaClO4

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	diox/w	30°C	75%	U		K1=4.7	1954UFa (54138)	856

****

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
Mg++	EMF	NaCl	25°C	0.0	C	T H	K(Mg+HL)=1.148	1984EFa (54374)	857

Method: Mg selective electrode. Extrapolated from data for 0.15-0.30 M NaCl. DH(K)=4.51 kJ mol-1, DS(K)=37.2 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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaClO4	30°C	0.10M	U		K1=6.30	1966APb (54655)	858
Mg++	gl	KNO3	30°C	0.10M	U		K1=5.67 B2=9.84	1963MNc (54656)	859

****

C7H6O4 H3L CAS 99-10-5 (4409)
3,5-Dihydroxybenzoic acid; C6H3(OH)2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	EMF	NaCl	25°C	0.0	C	T H	K(Mg+H2L)=0.965	1984EFa (54714)	860

Method: Mg selective electrode. Extrapolated from data for 0.15-0.30 M NaCl. DH(K)=6.48 kJ mol-1, DS(K)=40.4 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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	EMF	KNO3	25°C	0.10M	U		B(Mg2L)=10.7	1985SCd (54746)	861

Method: divalent cation liquid ion exchange electrode

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	EMF	R4N.X	25°C	0.0	C	T H	K(Mg+H3L)=1.476	1984EFa (54747)	862

Method: Mg selective electrode. Extrapolated from data for 0.15-0.30 M Et4NCl. DH(K)=2.68 kJ mol-1, DS(K)=37.3 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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaNO3	25°C	0.10M	C		K1=4.70	1982HNa (54929)	863

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	oth/un	25°C	->0	U		K1=0.72	1958LUa (55208)	864

****

C7H7NO2 H2L Salicylaldoxime CAS 94-67-7 (1486)
2-Hydroxybenzaldehyde oxime; HO.C6H4.CH:N.OH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl oth/un 25°C ->0 U 1958LUa (55305) 865
K(Mg+HL)=0.64
K(Mg+2HL)=4.10
****
C7H7NO2 HL Salicylamide CAS 65-45-2 (3155)
2-Hydroxybenzamide; HO.C6H4.CO.NH2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl diox/w 30°C 75% U K1=2.79 1964JVa (55325) 866
Medium: 75% dioxan, 0.1 M NaClO4
****
C7H7NO2 HL CAS 3222-47-7 (3154)
6-Methylpyridine-2-carboxylic acid; CH3.C5H3N.COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl NaNO3 20°C 0.10M U K1=2.00 1960ANb (55426) 867
****
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
---
Mg++ gl KCl 25°C 0.20M C K1=2.67 B2= 4.61 2000FEc (55493) 868
B(MgH-1L)=-8.48
****
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
---
Mg++ gl NaNO3 25°C 0.10M C K1=3.39 2000KHa (55586) 869
****
C7H8N2O2 HL Salicylic hydra CAS 936-02-7 (2646)
2-Hydroxybenzoic acid hydrazide; HO.C6H4.CO.NH.NH2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl diox/w 25°C 25% U K1=2.66 1975GSb (55871) 870
****
C7H8N2O2 L CAS 15513-52-7 (5516)
3-Nitro-2,6-dimethylpyridine;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl NaNO3 25°C 0.50M U K1=0.3 1983BEb (55897) 871

****
C7H8N4 L (1928)
Bis(imidazol-2-yl)methane; C3H3N2.CH2.C3H3N2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	35°C	0.20M	U		K1=1.63	1989RVa (55995)	872

****
C7H8O2 HL Salicyl alcohol CAS 90-01-7 (3727)
2-Hydroxybenzyl alcohol; HO.C6H5.CH2.OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	diox/w	30°C	75%	U		K1=4.95	1964JVa (56091)	873

Medium: 75% dioxan, 0.1 M NaClO4
****
C7H8O8P2 H4L (6892)
1,2-((Phenylenedioxo)methylene)diphosphonic acid); C6H4O2C(PO3H2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	R4N.X	25°C	0.50M	U		K1=5.67 K(Mg+HL)=3.03	1985GMb (56165)	874

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
Mg++	gl	NaNO3	25°C	0.50M	C		K1=0.04	2002KSb (56284)	875

****
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
Mg++	gl	KNO3	25°C	0.1M	U		K1=5.15	1976NGb (56466)	876

****
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
Mg++	gl	KNO3	25°C	0.10M	U		K1=4.03	1988KMa (56471)	877

****
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

```
------------------------------------------------------------------------------
Mg++       ISE NaNO3  20°C 0.04M U        K1=6.95        1988BLa (56530) 878
                                          K(Mg+HL)=4.2
******************************************************************************
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
------------------------------------------------------------------------------
Mg++       gl  KNO3   25°C 0.10M U        K1=6.5         1990GKa (56555) 879
                                          K(Mg+HL)=4.0
******************************************************************************
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
------------------------------------------------------------------------------
Mg++       gl  KCl    25°C 0.20M C        K1=5.88   B2= 9.05  2002MKc (56702) 880
                                          B(MgH2L)=20.68
                                          B(MgHL)=14.55
                                          B(MgH-1L)=-4.88
                                          B(MgH2L2)=26.84
B(MgHL2)=18.51.
******************************************************************************
C7H11NO5              H2L                          (3164)
1-Amino-2-propanone-N,N-diethanoic acid; CH3.CO.CH2.N(CH2.COOH)2
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Mg++       gl  KNO3   25°C 0.10M U        K1=2.7         1963ANa (56829) 881
******************************************************************************
C7H11NO6              H3L                          (2926)
2-Aminobutanoic-N-propane-1,3-dioic acid; HOOC.CH(C2H5)NH.CH(COOH)2
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Mg++       gl  KNO3   25°C 0.10M U        K1=3.10        1982KKa (56838) 882
******************************************************************************
C7H11NO6              H3L                      CAS 40199-58-4  (3165)
N-(2'-Carboxyethyl)iminodiethanoic acid; HOOC.CH2.CH2.N(CH2.COOH)2
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Mg++       gl  KCl    30°C 0.10M U        K1=5.2         1953CMa (56875) 883
------------------------------------------------------------------------------
Mg++       EMF KCl    20°C 0.10M U        K1=5.28        1949SAa (56876) 884
Method: H electrode
******************************************************************************
C7H11NO6              H3L    MNTA          (1026)
Nitrilo(2-propanoic)-diethanoic acid; HOOC.CH(CH3).N(CH2.COOH)2
```

```
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Mg++       gl  KNO3   20°C 0.10M U        K1=5.83        1974RMf (56902) 885
--------------------------------------------------------------------------------
Mg++       gl  KCl    20°C 0.10M U        K1=5.84        1966IMa (56903) 886
********************************************************************************
C7H11NO6P2            H4L    DPHP               (226)
2,6-bis(Dioxyphosphorylmethyl)pyridine; C5H3N.(CH2.PO3H2)2
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Mg++       gl  KCl    25°C 0.10M U        K1=3.61        1988KPa (56929) 887
                                         K(Mg+HL)=2.75
********************************************************************************
C7H11NO6P2            H4L                    CAS 4712-06-5  (4470)
Amino(phenyl)methylenediphosphonic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Mg++       gl  KCl    25°C 0.10M U        K1=7.39        1969DMd (56937) 888
                                         K(Mg+HL)=5.46
********************************************************************************
C7H12N2O5             H2L    Gly-Glu         CAS 7412-78-4  (280)
Glycyl-glutamic acid; H2N.CH2.CO.NH.CH(CH2.CH2.COOH).COOH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Mg++       gl  KNO3   20°C 0.10M U        K1=3.78        1980BBc (57173) 889
********************************************************************************
C7H12N2O6P2           H4L                    CAS 70010-76-3  (8892)
N-(3-Methyl-2-pyridyl)aminomethane-1,1-diphosphonic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Mg++       gl  KCl    25°C 0.20M C        K1=6.12   B2= 8.65  2002MKc (57188) 890
                                         B(MgH2L)=21.34
                                         B(MgHL)=15.33
                                         B(MgH-1L)=-5.89
                                         B(MgH2L2)=27.83
********************************************************************************
C7H12N3O5P            H2L    PMEC            CAS 117087-39-5  (8366)
1-[2-(Phosphonomethoxy)ethyl]cytosine;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Mg++       gl  NaNO3  25°C 0.10M M        K1=1.88        1999BHb (57199) 891
                                         K(Mg+HL)=0.5
                                         K(MgL+H)=5.6
********************************************************************************
```

C7H12O2 HL CAS 7424-54-6 (4421)
Heptane-3,5-dione; CH3.CH2.CO.CH2.CO.CH2.CH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	diox/w	25°C	50%	U		K1=4.52 B2=8.32	1973AHb (57241)	892

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	diox/w	24°C	50%	U		K1=4.5	1979ACa (57288)	893

****
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
Mg++	sp	none	25°C	0.0	U	T	K1=2.51	1976KOa (57333)	894

Also data at 15,30,35 C. Determined colourimetrically
****
C7H12O4 H2L CAS 510-20-3 (482)
Diethylpropanedioic acid (Diethylmalonic acid); HOOC.C(C2H5)2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	sp	none	25°C	0.0	U	T	K1=2.63	1976KOa (57356)	895

Also data at 15,30,35 C. Determined colourimetrically
****
C7H13NO4S H2L (3184)
N-(2-Methylthioethyl)iminodiethanoic acid; CH3.S.CH2.CH2.N(CH2.COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KCl	20°C	0.10M	U		K1=3.02	1955SAa (57544)	896

****
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
Mg++	gl	KCl	20°C	0.10M	U		K1=3.31	1955SAa (57572)	897

****
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
Mg++	gl	KCl	30°C	0.10M	U		K1=3.3	1954CMa (57588)	898

****

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
Mg++	EMF	KNO3	20°C	0.10M	U		K1=3.52	1968MRb (57596)	899

****

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
Mg++	gl	KNO3	20°C	0.10M	U		K1=3.02	1980MRc (57607)	900

****

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
Mg++	cal	NaClO4	25°C	0.10M	U	H	K1=3.4	1983EHa (57815)	901

DH(K1)=10.5 kJ mol-1, DS=99 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
Mg++	gl	KCl	25°C	0.15M	U		K1=1.79	1962OSa (57832)	902
							K(Mg+HL)=1.46		
							K(MgL+Mg)=0.9		

****

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
Mg++	gl	NaNO3	25°C	0.10M	M		K1=1.43	2003FHa (57841)	903

****

C7H15NO4S HL MOPS CAS 1132-61-2 (2792)
3-(N-Morpholino)propanesulfonic acid; C4H8ON-CH2.CH2.CH2.SO3H

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	25°C	0.10M	C		K1=3.51	2001AOa (57962)	904

****

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

```
--------------------------------------------------------------------------------
Mg++       gl  R4N.X  25°C  1.0M C        K1=2.02        1995RLa (58091) 905
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
--------------------------------------------------------------------------------
Mg++       gl  KNO3   25°C 0.10M C        K1=3.42        2000ADa (58135) 906
********************************************************************************
C7H17NO7P2             HL                     CAS 220491-02-1  (7714)
N-2-Methyltetrahydrofuryliminodi(methylenephosphonic acid);
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Mg++       gl  KCl    25°C 0.20M C        K1=5.06   B2= 7.99  1999MKa (58151) 907
                                          B(MgHL)=14.08
                                          B(MgH2L)=19.15
                                          B(MgHL2)=18.41
                                          B(MgH2L2)=27.16
********************************************************************************
C7H17NO7S              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
--------------------------------------------------------------------------------
Mg++       gl  KNO3   25°C 0.10M C    M   K1=3.77        2001AAa (58175) 908
Also data for ternary complexes with 5'-GMP, 5'-IMP and 5'-CMP.
--------------------------------------------------------------------------------
Mg++       gl  KNO3   25°C 0.10M C        K1=3.37        2000ADa (58176) 909
********************************************************************************
C7H19NO6P2             H4L                    (7464)
N-(3-Methylbutyl)imino-bis(methylenephosphonic acid);
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Mg++       gl  KCl    25°C 0.20M C        K1=4.36        1999MKa (58271) 910
                                          B(MgHL)=15.09
                                          B(MgH2L)=20.31
********************************************************************************
C7H20N2O4P2            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
--------------------------------------------------------------------------------
Mg++       gl  R4N.X  25°C 0.10M M                         1996BCa (58329) 911
                                          K(Mg+OH+L)=12.8
Medium: 0.1 M Me4NNO3.
```

****

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
Mg++	ISE	KNO3	25°C	0.1M	U		K1=7.49		1985SNd (58384)	912
							B(MgHL)=17.64			
							B(MgH3L)=35.14			
							B(MgH2L)=27.11			
							B(MgH4L)=41.60			
							B(MgH5L)=45.99			
							B(Mg2L)=6.97			

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Mg++	sp	alc/w	25°C	95%	U		K1=4.68		1993GSa (58485)	913
Medium: 95% w/w EtOH/H2O, 0.05 M Et4NClO4										
Mg++	sp	alc/w	25°C	100%	U	I	K1=3.85		1988KGa (58486)	914
Medium: MeOH. Also in DMF (K1=3.57) and DMSO (3.22).										
Mg++	sp	oth/un	?	0.10M	U				1949SGa (58487)	915
							K(Mg+H2L)=1(?), 2.2(?)			

****

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
Mg++	gl	diox/w	20°C	17%	C		K1=6.16	B2=11.11	1976JWa (58597)	916

****

C8H6N2O HL CAS 17056-99-4 (3220)
5-Hydroxyquinoxaline;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Mg++	gl	diox/w	20°C	50%	U		K1=3.44	B2=6.39	1954IRa (58745)	917
Medium: 50% dioxan, 0.3 M NaClO4										

****

C8H6N2O HL (6290)
8-Hydroxycinnoline, (2-Hydroxybenzo)pyrimidine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Mg++	gl	diox/w	20°C	50%	U		K1=3.02	B2=5.20	1954IRa (58766)	918

Medium: 50% dioxan, 0.3 M NaClO4

****

C8H6N2O HL 8-Quinazolinol CAS 7757-02-2 (3221)
8-Hydroxyquinazoline;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	diox/w	20°C	50%	U		K1=3.89 B2=6.80	1954IRa (58776)	919

Medium: 50% dioxan, 0.3 M NaClO4

****

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
Mg++	gl	NaCl	25°C	0.10M	U		K1=2.53	1989SKa (58940)	920
Mg++	con	none	25°C	0.0	U		K1=2.49	1984TWa (58941)	921
Mg++	gl	oth/un	25°C	.493M	U	T	K1=2.51	1975PAb (58942)	922

15 C: K1=2.52; 20 C: 2.50; 30-35 C: 2.51

****

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
Mg++	con	none	25°C	0.0	U		K1=1.82	1984TWa (59071)	923

****

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
Mg++	gl	NaClO4	22°C	0.10M	U		K1=3.09	1964BBa (59351)	924

****

C8H8O2 HL 2-Acetylphenol CAS 118-93-4 (1888)
2-Hydroxyacetophenone; HO.C6H4.CO.CH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	diox/w	30°C	75%	U		K1=7.22	1970KDa (59455)	925

Medium: 75% dioxan, 0.1 M NaClO4

****

C8H8O2 HL o-Toluic acid CAS 118-90-1 (7862)
2-Methylbenzoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	ISE	NaCl	25°C	0.0	C	TIH	K1=1.63	1991EAa (59475)	926

Method: Mg ISE. Data for 0.02-0.05 M NaCl, 15-45 C. DH(K1)=2.72 kJ mol-1, DS(K1)=40.3 J K-1 mol-1. Also data for 3-methyl- and 4-methylbenzoic acid.

****

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
Mg++	ISE	NaCl	25°C	0.03M	U	TIH	K1=0.936		1982EFa (59499)	927

At 35 C, I=0.045 M: K1=0.87; at 45 C, I=0.45: K1=0.340

****

C8H8O2 HL CAS 1004-72-4 (3190)
alpha-Methyltropolone;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Mg++	gl	diox/w	30°C	50%	U		K1=6.0 B3=13.2	B2=10.6	1954BFb (59580)	928

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Mg++	gl	diox/w	30°C	50%	U		K1=6.0 B3=13.7	B2=10.6	1954BFb (59591)	929

****

C8H8O3 HL CAS 673-22-3 (3194)
4-Methoxysalicylaldehyde; CH3O.C6H3(OH).CHO

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	diox/w	30°C	75%	U		K1=3.29	1967KBb (59978)	930

Medium: 75% dioxan, 0.1 M NaClO4

****

C8H8O3 HL Phenoxyacetic CAS 122-59-8 (1153)
Phenoxyethanoic acid; C6H5.O.CH2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	none	25°C	0.0	C	TIH	K1=1.00	1985CDb (60036)	931

Calculated from protonation data for I=0.04-0.9 M MgCl2. Data for 10-45 C. DH(K1)=-0.9 kJ mol-1, DS(K1)=16 J K-1 mol-1.

****

C8H8O4 H3L CAS 102-32-9 (1826)
3,4-Dihydroxyphenylethanoic acid; C6H3(OH)2.CH2COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaClO4	30°C	0.10M	U		K1=4.94	1966APb (60068)	932

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Mg++	gl	diox/w	35°C	50%	U		K1=2.88	B2=4.92	1971MAa (60081)	933

Medium: 50% dioxan, 0.1 M NaClO4

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Mg++	gl	mixed	24°C	50%	U		K1=3.10	B2=5.71	1993ZMa (60105)	934

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
Mg++	gl	NaCl	37°C	0.15M	U		K1=2.73	1988HYa (60123)	935
							B(MgHL)=7.17		
							B(MgHL2)=10.01		

****

C8H9NO2 HL CAS 17194-82-0 (1382)
2-Hydroxyacetophenone oxime; HO.C6H4.C(CH3):NOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Mg++	gl	diox/w	30°C	75%	U		K1=5.23	B2=10.20	1958KVa (60214)	936

Medium: 75% dioxan, 0.1 M NaClO4

****

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
Mg++	gl	KCl	25°C	0.20M	C		K1=2.39	B2= 4.05	2000FEc (60280)	937

****

C8H9NO4 H2L (4520)
Dehydroethanoic acid oxime;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Mg++	gl	diox/w	35°C	50%	U				1971MAa (60487)	938
							K(Mg+HL)=2.48			
							K(Mg+2HL)=4.84			

Medium: 50% dioxan, 0.1 M NaClO4

```
**************************************************************************
C8H9N3OS              H2L                     CAS 5351-90-6  (2103)
Salicylidenethiosemicarbazone; HO.C6H4.CH:N.NH.CS.NH2
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Mg++       gl  alc/w  20°C  50%  U        K1=<3.5        1959HOa (60557) 939
**************************************************************************
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
--------------------------------------------------------------------------
Mg++       cal KNO3   25°C  0.1M C   H                   1981CSb (60614) 940
DH(K1)=+3.8 kJ mol-1, DS=163 K J mol-1
--------------------------------------------------------------------------
Mg++       gl  KNO3   25°C 0.10M U T      K1=8.09        1977SVa (60615) 941
--------------------------------------------------------------------------
Mg++       cal R4N.X  20°C  0.1M C                       1976ANb (60616) 942
                                        DH1= 2.34 kJ/mol
in Me4NCl
--------------------------------------------------------------------------
Mg++       gl  R4N.X  25°C 0.10M C        K1=8.35        1975JTa (60617) 943
--------------------------------------------------------------------------
Mg++       gl  KNO3   20°C 0.10M U        K1=8.19   B2=11.81  1963IFb (60618) 944
--------------------------------------------------------------------------
Mg++       ISE oth/un 20°C  0.0  U        K1=8.85   B2=11.95  1946SKa (60619) 945
**************************************************************************
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
--------------------------------------------------------------------------
Mg++       gl  KNO3   25°C 0.12M U        K1=1.96        1979RZb (60671) 946
**************************************************************************
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
--------------------------------------------------------------------------
Mg++       gl  KNO3   37°C 0.15M C        K1=4.38   B2=7.31   1980SHb (60756) 947
                                        B(MgHL)=11.46
                                        B(MgHL2)=15.00
                                        B(MgH2L2)=21.9
                                        B(Mg2L)=5.6
**************************************************************************
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
```

```
------------------------------------------------------------------------------
Mg++       gl  KNO3   37°C 0.15M C        K1=4.50   B2=7.56   1980SHb (60762) 948
                                          B(MgHL)=12.47
                                          B(MgHL2)=16.21
                                          B(MgH2L2)=23.8
                                          B(Mg2L)=6.3
B(Mg2L2)=10.2
******************************************************************************
C8H10O9              H4L                      CAS 137172-86-2  (6612)
SS-Oxydisuccinic acid; O(CH(COOH)CH2.COOH)2
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Mg++       gl  KCl    25°C 0.10M C        K1=4.44        1992MMa (60901) 949
                                          K(MgL+H)=4.18
                                          K(MgHL+H)=4.11
                                          K(MgH2L+H)=2.77
                                          K(Mg+HL)=2.67
K(Mg+H2L)=1.97, K(Mg+H3L)=1.34
******************************************************************************
C8H10O9              H4L                      CAS 84852-72-2  (6611)
meso-Oxydisuccinic acid; O(CH(COOH)CH2.COOH)2
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Mg++       gl  KCl    25°C 0.10M C        K1=5.09        1992MMa (60913) 950
                                          K(MgL+H)=4.05
                                          K(MgHL+H)=3.44
                                          K(MgH2L+H)=3.30
                                          K(Mg+HL)=3.17
K(Mg+H2L)=1.75, K(Mg+H3L)=1.08
******************************************************************************
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
------------------------------------------------------------------------------
Mg++       gl  KCl    25°C 0.10M C        K1=3.91        1989MMd (60925) 951
                                          K(MgL+H)=4.27
******************************************************************************
C8H11NO                L                     CAS 20819-02-5  (5524)
4-Methoxy-2,6-dimethylpyridine;
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Mg++       gl  NaNO3  25°C 0.50M U        K1=1.1         1983BEb (61033) 952
******************************************************************************
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
---
Mg++ gl NaClO4 25°C 1.0M C 1997GCa (61072) 953
K(Mg+H2L=MgHL+H)=-7.79
K(Mg+H2L=MgL+2H)=-16.04
K(Mg+H2L=MgH-1L+3H)=-26.61
K(Mg+2H2L=MgL2+4H)=-34.36
Ligand defined as H2L. K(Mg+2H2L=MgH-2L2+6H)=-55.78, K(MgL=MgH-1L+H)=-10.57,
K(MgH2L=MgHL+H)=-8.25, K(Mg+2H2L=MgH-1L2+5H)=-45.2 etc.

Mg++ gl KCl 25°C 0.10M U T H 1986CVb (61073) 954
K(Mg+HL)=4.68
K(Mg+2HL)=6.78
Data for 0-37 C. At 37 C, K(Mg+HL)=4.30, K(Mg+2HL)=6.10.
DH(Mg+HL)=-19.9 kJ mol-1, DS=-23.4 J K-1 mol-1; DH(Mg+2HL)=-15.6, DS=11.8

Mg++ nmr oth/un 27°C ? U M 1977GFa (61074) 955
Keff(Mg(ATP)+L)=1.08
In D2O. pD=6.8
****
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
---
Mg++ gl KCl 25°C 0.10M U T H K1=5.16 B2= 7.30 1982CVa (61159) 956
Data for 0 and 37 C. DH(K1)=-21.8 kJ mol-1, DS(K1)=20 J K-1 mol-1;
DH(K2)=-11.2, DS(K2)=8.4.
****
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
---
Mg++ gl NaCl 25°C 1.00M C K1=1.15 1988BSa (61179) 957
****
C8H11NO8 H4L CAS 24868-49-3 (2572)
2-Amino(N,N-diethanoic)-1,4-butanedioic acid;HOOCCH(N(CH2COOH)2)CH2COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl KNO3 25°C 0.10M U K1=5.92 1975NGa (61184) 958
****
C8H11NO8 H4L CAS 7408-20-0 (2608)
Amino-di(butanedioic acid);HN(CH(COOH)CH2.COOH)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl KNO3 25°C 0.1M C K1=5.52 1999VZb (61199) 959

```
---------------------------------------------------------------------------
Mg++       gl  KNO3   25°C  0.1M U        K1=5.50        1978MNa (61200) 960
***************************************************************************
C8H11NO8P2            H5L                          (6894)
N-(4-Carboxyphenyl)aminomethylenedi(phosphonic acid); HOOC.C6H4.NH.CH(PO3H2)2
---------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
---------------------------------------------------------------------------
Mg++       gl  KNO3   25°C 0.10M U        K1=7.57        1990GKa (61228) 961
                                         K(Mg+HL)=3.40
***************************************************************************
C8H12N2O8             H4L                      CAS 35039-85-1  (4537)
1,2-Diaminoethane-N,N'-dimalonic acid; (HOOC)2.CH.NH.CH2.CH2.NH.CH(COOH)2
---------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
---------------------------------------------------------------------------
Mg++       gl  KNO3   20°C 0.10M U        K1=4.86        1973DSc (61490) 962
                                         K(Mg+HL)=2.0
---------------------------------------------------------------------------
Mg++       gl  KNO3   25°C 0.10M U        K1=4.93        1973MAb (61491) 963
                                         K(Mg+HL)=1.80
---------------------------------------------------------------------------
Mg++       gl  KNO3   25°C 0.10M U        K1=4.51        1972GBd (61492) 964
                                         K(Mg+HL)=2.34
                                         K(Mg+MgL)=2.49
***************************************************************************
C8H12N5O4P            H2L                      CAS 106941-25-7  (6693)
9-(2-(Phosphonylmethoxy)ethyl)adenine; H2O3P.CH2.O.CH2.CH2.adenine
---------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
---------------------------------------------------------------------------
Mg++       gl  NaNO3  25°C 0.10M M    M   K1=1.22        2000KLb (61649) 965
                                         K(PtLA+Mg)=1.22
A=diethylenetriamine
---------------------------------------------------------------------------
Mg++       gl  NaNO3  25°C 0.10M M        K1=1.87        1992SCa (61650) 966
***************************************************************************
C8H13NO6              H3L                          (3835)
2-Amino-2-carboxypropane-N,N-diethanoic acid; HOOCC(CH3)2N(CH2COOH)2
---------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
---------------------------------------------------------------------------
Mg++       gl  KNO3   20°C 0.10M U        K1=4.24        1974RMf (61756) 967
---------------------------------------------------------------------------
Mg++       gl  KCl    20°C 0.10M U        K1=6.30        1966IMa (61757) 968
***************************************************************************
C8H13NO6              H3L                          (5681)
2-Aminobutanoic-N,N-diethanoic acid; CH3CH2CH(COOH)N(CH2COOH)2
---------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
```

Mg++ gl KNO3 20°C 0.10M U K1=5.31 1974RMf (61782) 969
****
C8H13NO6 H3L (3232)
N-(Carboxymethyl)iminodipropanoic acid; HOOC.CH2.N(CH2.CH2.COOH)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl NaClO4 25°C 0.50M C K1=2.94 1995CDa (61808) 970

Mg++ gl KCl 30°C 0.10M U K1=3.6 1953CMa (61809) 971
****
C8H13NO6S H3L (5675)
2-Mercapto-1-aminoethane-N,N,S-triethanoic acid; HOOC.CH2.S.CH2.CH2.N(CH2COOH)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl NaClO4 25°C 0.10M U K1=3.49 1975POa (61817) 972
K(Mg+HL)=1.6
****
C8H13N6O4P H2L (7462)
9-[2-(Phosphonomethoxy)ethyl]-2,6-diaminopurine;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl NaNO3 25°C 0.10M M K1=1.89 1999BSa (61874) 973
K(Mg+HL)=0.5
****
C8H14N2O4 H2L CAS 124099-98-5 (5607)
1,4-Piperazine-N,N'-diethanoic acid; HOOC.CH2.C4H8N2.CH2.COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ cal NaClO4 25°C 0.10M U H K1=2.4 1985EHa (61943) 974
DH(K1)=1.4 kJ mol-1, DS=50.9 J K-1 mol-1

Mg++ EMF KCl 20°C 0.10M U K1=1.5 1963IPb (61944) 975
Method: H electrode
****
C8H14N2O6P2 HL (7465)
N-(3-Pyridylmethyl)imino-bis(methylphosphonic acid);

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl KCl 25°C 0.20M C K1=4.25 1999MKa (61967) 976
B(MgHL)=13.29
B(MgH2L)=18.78
B(MgH3L)=23.19
B(MgH-1L)=-7.60
****

C8H14N4O5 HL Tetraglycine CAS 637-84-3 (1849)
Glycyl-Glycyl-Glycyl-Glycine; H2N.CH2.CO.NH.CH2.CO.NH.CH2.CO.NH.CH2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	25°C	0.15M	U		K1=1.32	1958LCa (62021)	977

****

C8H14O4 H2L Suberic acid CAS 505-48-6 (517)
Octanedioic acid; HOOC.(CH2)6.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	con	none	25°C	0.0	U		K1=2.10	1984TWa (62094)	978

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	25°C	0.10M	U		K1=1.8	1974MSa (62146)	979

****

C8H15NO6 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
Mg++	gl	NaClO4	25°C	1.0M	C		K1=1.96	1981ASb (62216)	980

****

C8H15N2O9P H4L (3847)
O-Phosphoryl-L-seryl-L-glutamic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KCl	25°C	0.15M	U		K1=2.09 K(Mg+HL)=1.63 K(Mg+MgL)=1.81 K(Mg+MgHL)=1.51 K(Mg2L+H)=7.49	1962OSa (62235)	981

K(Mg+H2L)=1.00

****

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
Mg++	cal	NaClO4	25°C	0.10M	U	H	K1=3.2	1983EHa (62468)	982

DH1=23.3 kJ mol-1, DS1=139.9 J K-1 mol-1

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	20°C	0.10M	U		K1=2.82	1966MKb (62469)	983

Mg++ gl KCl 20°C 0.10M U K1=2.8 1958ISa (62470) 984
****
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
---
Mg++ gl KCl 20°C 0.10M U K1=2.8 1958ISa (62499) 985

Mg++ gl KCl 30°C 0.10M U K1=1.6 1953CCb (62500) 986
****
C8H16N2O4 H2L (266)
N,N'-Dimethylethylenediamine-N,N'-diethanoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl KNO3 25°C 0.10M C K1=5.36 1993WLa (62524) 987
K(Mg+HL)=1.3

Mg++ cal NaClO4 25°C 0.10M U H K1=5.2 1983EHa (62525) 988
DH1=8.5 kJ mol-1, DS1=128.0 J K-1 mol-1

Mg++ EMF oth/un 25°C 0.0 U H 1956MAa (62526) 989
Method: H electrode. DG(K1)=-32.6 kJ mol-1, DH=4, DS=130 J K-1 mol-1
****
C8H16N2O4 H2L CAS 38937-66-5 (5912)
N,N-Dihydroxyoctanediamide; HN(OH).CO.(CH2)6.CO.NH(OH)

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl NaNO3 25°C 0.10M C K1=3.73 1989EHa (62537) 990
B(MgHL)=12.53
****
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
---
Mg++ EMF oth/un 20°C 0.10M U K1=3.20 1972DKa (62582) 991

Mg++ gl KNO3 20°C 0.10M U K1=3.2 1970DKa (62583) 992
****
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
---
Mg++ nmr non-aq 27°C 100% C K1=4.14 2000SMg (62657) 993
Medium: acetonitrile. Method: competitive 7Li nmr technique.

Mg++ EMF non-aq 25°C 100% U T K1=2.61 B2=6.2 1982MRb (62658) 994
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
---
Mg++ gl KNO3 25°C 0.10M C K1=3.84 2000ADa (62775) 995
****
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
---
Mg++ gl NaCl 25°C 0.15M C K1=2.62 1990JKa (62808) 996
****
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
---
Mg++ gl NaCl 25°C 0.10M C K1=2.12 1999HLb (62857) 997
****
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
---
Mg++ gl KCl 25°C 0.10M U K1=8.11 1965DKb (62895) 998
****
C8H18N2O10P2 H6L CAS 2310-83-0 (5667)
1,2-Diaminoethane-N,N-diethanoic-N',N'-dimethylphosphonic acid;
(HOOC.CH2)2NCH2CH2N(CH2.PO3H2)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl KNO3 25°C 0.10M U 1976TIa (62917) 999
K(Mg+H2L)=3.7
****
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
---
Mg++ cal non-aq 25°C 100% C H 1992BSc (62980)1000
Medium: propylene carbonate. DH(K1)=-6.9 kJ mol-1.

Mg++ con non-aq 25°C 100% C K1=3.1 1992MSe (62981)1001

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-ethanediyloxy))-bis-ethanol; O(CH2.CH2.O.CH2.CH2.OH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	con	non-aq	25°C	100%	C		K1=2.8	1992MSe (63001)	1002

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
Mg++	gl	mixed	25°C	90%	C	I	K1=0.91	1982SSf (63052)	1003

Medium: 90% DMSO/H2O

Mg++	gl	KNO3	25°C	1.0M	C		K1=0.34	1980SAb (63053)	1004
							K(Mg(ATP)+L)=0.59		

****
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
Mg++	gl	KCl	25°C	0.20M	C		K1=4.04	1999MKa (63083)	1005
							B(MgHL)=15.43		
							B(MgH2L)=20.39		

****
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
Mg++	gl	KNO3	25°C	0.50M	C		K1=2.25	1988RPb (63284)	1006

****
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
Mg++	gl	KCl	25°C	0.10M	U		K1=<2	1965DKb (63333)	1007

****
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
Mg++	gl	NaCl	25°C	0.0	C		K1=1.67	1999SFc (63466)	1008

K(Mg+HL)=1.05
K(Mg+H2L)=0.55
K(Mg+H3L)=0.0
K(Mg+H4L)=-0.5
Extrapolated from data for 0.03-0.96 M NaCl using the Pitzer equation.
K(Mg+MgL)=-0.1

****

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
Mg++	gl	NaNO3	25°C	0.50M	M		K1=0.00	1998KSa (63504)	1009

****

C9H5NOBr2 HL CAS 521-74-4 (3279)
5,7-Dibromo-8-hydroxyquinoline;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	dis	R4N.X	20°C	1.0M	U		K1=4.76 B2=9.65	1969SRb (63516)	1010

Medium: 1 M NH4Cl, 17-20 C

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	diox/w	35°C	75%	U		K1=3.20 B2=6.15	1971MAb (63556)	1011

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

****

C9H6NOCl HL CAS 130-16-5 (1268)
5-Chloro-8-hydroxyquinoline;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	diox/w	25°C	60%	U		K1=5.38 B2=10.43	1973SCd (63657)	1012

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
Mg++	gl	oth/un	20°C	0.03M	U		K1=3.68	1977KCb (63773)	1013

K1=3.08 by solubility

Mg++	gl	KNO3	28°C	0.10M	U		K1=3.25 B2=7.20	1971LSb (63774)	1014
Mg++	gl	oth/un	25°C	0.0	U		K1=3.80 B2=6.20	1952NEa (63775)	1015

****

C9H6N2O3 HL CAS 5437-99-0 (3865)
5-Nitro-8-hydroxyquinoline;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	diox/w	25°C	60%	U		K1=4.27 B2=8.17	1973SCd (63859)	1016

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
Mg++	gl	oth/un	25°C	0.0	U		K1=3.28 B2=4.70	1955NUa (63910)	1017

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	sp	alc/w	25°C	95%	U		K1=2.28	1993GSa (64219)	1018

Medium: 95% w/w EtOH/H2O, 0.05 M Et4NClO4, by competitive spectrophotometry

Mg++	sp	non-aq	25°C	100%	U	I	K1=4.03 B2=6.33	1992GSa (64220)	1019

Medium: MeCN. In acetone:K1=2.25, K2=1.80; in MeOH:K1=2.01. By fluorimetry

Mg++	gl	diox/w	25°C	60%	U		K1=5.79 B2=11.02	1973SCd (64221)	1020

Medium: 60% dioxan, 0.1 M NaClO4

Mg++	kin	oth/un	25°C	0.10M	U	M	K1=4.48	1972HMb (64222)	1021
							K(MgA+L)=5.08		
							K(MgB+L)=3.05		

H3A=nitrilotriethanoic acid, H3B=uramildiethanoic acid.

Mg++	kin	oth/un	25°C	0.30M	U	M		1972HMb (64223)	1022
							K(MgA+L)=3.72		
							K(MgB+L)=3.70		
							K(MgC+L)=3.72		

H3A=adenosine diphosphate; H4B=ATP; H5C=tripolyphosphoric acid

Mg++	dis	R4N.X	20°C	1.0M	U		K1=4.08 B2=8.18	1969SRb (64224)	1023

17-20 C. Medium: 1 M NH4Cl

Mg++	sp	KNO3	16°C	0.10M	U		K1=4.35	1966HEb (64225)	1024
Mg++	gl	diox/w	30°C	75%	U		K1=8.8 B2=16.2	1954UFa (64226)	1025
Mg++	gl	oth/un	20°C	0.01M	U		K1=4.5	1953ALa (64227)	1026
Mg++	gl	diox/w	20°C	50%	U		K1=5.04 B2=9.33	1953NAb (64228)	1027

Medium: 50% dioxan, 0.3 M NaClO4

Mg++ gl diox/w 25°C 50% U K1=6.38 B2=11.81 1952JFa (64229)1028

Mg++ gl oth/un 20°C 0.0 U K1=4.74 1952NAa (64230)1029

Mg++ gl oth/un 20°C 0.0 U K1=3.27 1951NLa (64231)1030

Mg++ gl diox/w 25°C 70% U K1=6.88 B2=12.84 1949MMa (64232)1031

****

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

---

Mg++ gl diox/w 25°C 60% U K1=5.70 B2=10.49 1973SCd (64520)1032
Medium: 60% dioxan, 0.1 M NaClO4

Mg++ gl KNO3 25°C 0.10M U K1=4.06 B2=7.63 1959RGa (64521)1033

Mg++ gl oth/un 25°C 0.0 U K1=4.79 B2=8.19 1954NUa (64522)1034

Mg++ gl oth/un 20°C 0.01M U K1=4.8 B2=8.5 1953ALa (64523)1035

****

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

---

Mg++ gl alc/w 25°C 50% U 1967NPb (64694)1036
K(Mg+HL) < 3
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

---

Mg++ gl KCl 20°C 0.10M U K1=1.43 1957WSa (64781)1037

****

C9H8N2O HL CAS 17056-96-1 (3258)
8-Hydroxy-4-methylcinnoline;

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

---

Mg++ gl diox/w 20°C 50% U K1=3.66 B2=6.24 1954IRa (64790)1038
Medium: 50% dioxan, 0.3 M NaClO4

****

C9H8N2O2S HL (8279)
Dehydroxydemethyldesferrithiocin;

```
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Mg++       gl  KNO3   25°C 0.10M C        K1=2.5         1990ARa (64803)1039
********************************************************************************
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
--------------------------------------------------------------------------------
Mg++       vlt NaClO4 25°C 0.50M C T H    K1=6.22        1989GRb (64893)1040
Method: polarography. Medium: 0.50 M NH4ClO4, pH 4.8. Data for 25-45 C.
DH(K1)=-28.1 kJ mol-1, DS(K1)=24.6 J K-1 mol-1.
--------------------------------------------------------------------------------
Mg++       gl  NaClO4 37°C 0.15M C        K1=2.289       1978AKa (64894)1041
********************************************************************************
C9H8O4                H2L                     CAS 97652-17-0  (3855)
3-Carboxy-4-methyltropolone;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Mg++       sp  NaClO4   ?  0.20M U        K1=4.14        1967GDb (64932)1042
********************************************************************************
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
--------------------------------------------------------------------------------
Mg++       gl  alc/w  30°C  40%  M    M   K1=3.85   B2= 5.35  1995RRd (65147)1043
                                        K(MgL+A)=5.20
                                        K(MgL+en)=7.15
                                        K(MgL+pro)=5.03
                                        K(MgL+B)=3.27
Medium: 40% v/v EtOH/H2O, 0.10 M KNO3. K(MgL+ala)=2.75, K(MgL+gly)=2.54;
H2A is catechol, HB is hydroxyproline.
--------------------------------------------------------------------------------
Mg++       gl  alc/w  30°C  40%  M    M                  1995RRd (65148)1044
                                        K(Mg(phen)+L)=2.75
                                        K(MgA+L)=1.47
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
--------------------------------------------------------------------------------
Mg++       gl  alc/w  30°C  40%  M    M   K1=3.49   B2= 5.34  1995RRd (65214)1045
                                        K(MgL+A)=5.16
                                        K(MgL+en)=7.09
                                        K(MgL+pro)=4.85
```

```
                                        K(MgL+B)=3.08
Medium: 40% v/v EtOH/H2O, 0.10 M KNO3. K(MgL+ala)=2.63, K(MgL+gly)=2.47,
H2A is catechol, HB is hydroxyproline.
--------------------------------------------------------------------------------
Mg++       gl  alc/w  30°C  40%  M    M                  1995RRd (65215)1046
                                        K(Mg(phen)+L)=2.90
                                        K(MgA+L)=1.56
Medium: 40% v/v EtOH/H2O, 0.10 M KNO3. H2A is salicylic acid.
********************************************************************************
C9H10N2O2              HL                        (3265)
Salicylaldehyde acetylhydrazone; HO.C6H4.CH:N.NH.CO.CH3
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Mg++       gl  alc/w  20°C  50%  U        K1=4.2    B2=7.5    1959HOa (65237)1047
********************************************************************************
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
--------------------------------------------------------------------------------
Mg++       gl  NaClO4 22°C 0.10M U        K1=3.08        1964BBa (65265)1048
********************************************************************************
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
--------------------------------------------------------------------------------
Mg++       gl  diox/w 25°C  50%  U                       1969ZSa (65275)1049
                                        K(Mg+H2L)=2.15
                                        K(Mg+HL)=4.30
********************************************************************************
C9H10O2                HL                       CAS 699-91-2  (4594)
2-Hydroxy-3-methylacetophenone; HO(CH3).C6H3.CO.CH3
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Mg++       gl  diox/w 30°C  75%  U        K1=7.87        1970KDa (65320)1050
Medium: 50% v/v dioxan, 0.5 M NaClO4
********************************************************************************
C9H10O2                HL                       CAS 6921-64-8  (4595)
2-Hydroxy-4-methylacetophenone; HO(CH3).C6H3.CO.CH3
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Mg++       gl  diox/w 30°C  75%  U        K1=5.31        1970KDa (65326)1051
Medium: 50% v/v dioxan, 0.5 M NaClO4
********************************************************************************
C9H10O2                HL                       CAS 1450-72-2  (4596)
2-Hydroxy-5-methylacetophenone; HO(CH3).C6H3.CO.CH3
```

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl diox/w 30°C 75% U K1=6.09 B2=10.24 1970GMe (65333)1052
Medium: 50% v/v dioxan, 0.5 M NaClO4
****
C9H10O2 HL CAS 610-99-1 (4597)
2-Hydroxypropiophenone;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl diox/w 30°C 75% U K1=5.52 1970KDa (65343)1053
Medium: 75% dioxan, 0.1 M NaClO4
****
C9H10O2S HL CAS 21101-79-1 (3267)
2-Ethylthiobenzoic acid; CH3.CH2.S.C6H4.COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl diox/w 30°C 50% U K1=2.18 B2=5.47 1956IFa (65407)1054
****
C9H10O3 H2L CAS 1643-34-0 (4598)
2,6-Dihydroxy-4-methylacetophenone; (HO)2(CH3).C6H2.CO.CH3

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl diox/w 30°C 75% U K1=3.56 1970KDa (65429)1055
Medium: 75% dioxan, 0.1 M NaClO4
****
C9H10O3 HL CAS 118-61-6 (3858)
Salicylic acid ethyl ester; HO.C6H4.CO.OC2H5

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl diox/w 30°C 75% U K1=5.36 1964JVa (65492)1056
Medium: 75% dioxan, 0.1 M NaClO4
****
C9H10O4 H3L CAS 39223-40-0 (1825)
3,4-Dihydroxyphenylpropanoic acid; (HO)2.C6H3.CH2.CH2.COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl NaClO4 30°C 0.10M U K1=4.90 1966APb (65563)1057
****
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
---
Mg++ gl NaClO4 25°C 0.19M U K1=6.00 1986MSc (65637)1058

```
**************************************************************************
C9H11NO2              HL    Phenylalanine    CAS 63-91-2  (2)
2-Amino-3-phenylpropanoic acid; H2N.CH(CH2.C6H5)COOH
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Mg++       gl  NaCl   20°C 0.15M U    M   K1=1.63        1983VDb (65921)1059
**************************************************************************
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
--------------------------------------------------------------------------
Mg++       gl  oth/un 20°C 0.01M U                         1952ALa (66209)1060
                                    K(Mg+HL)=2
**************************************************************************
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
--------------------------------------------------------------------------
Mg++       gl  NaCl   25°C 0.12M U    M   K1=4.67        1978RMc (66390)1061
                                    K(Mg(ATP)+L)=3.67
--------------------------------------------------------------------------
Mg++       gl  KNO3   25°C  1.0M U        K1=4.71   B2=6.71   1972GJa (66391)1062
                                    K(Mg+H2L)=1
**************************************************************************
C9H11NO5              H2L                      CAS 57362-11-5  (3876)
N-(2'-Furfuryl)iminodiethanoic acid; C4H3O.CH2.N(CH2.COOH)2
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Mg++       gl  KNO3   20°C 0.10M U        K1=2.78        1963IFa (66449)1063
**************************************************************************
C9H11N3O7             H3L                        (3877)
N-(1-Methyl-2,4,6-trioxo-perhydropyrimidinyl)iminodiethanoic acid;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Mg++       gl  KNO3   20°C 0.10M U        K1=8.23   B2=11.95  1963IFb (66522)1064
**************************************************************************
C9H12N2O6              HL    Uridine          CAS 58-96-8  (828)
Uracil-1-beta-D-ribofuranoside;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Mg++       gl  KNO3   25°C 0.10M C T HM   K1=3.14   B2=6.12   1987KRa (66689)1065
--------------------------------------------------------------------------
Mg++       gl  KNO3   35°C 0.10M U    M   K1=2.71        1986RRa (66690)1066
Ternary complexes with glycine, oxalate, histidine and histamine
```

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

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl KNO3 25°C 0.1M U K1=7.15 1982KBe (66729)1067
****
C9H13NO2 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
---
Mg++ gl KNO3 22°C 0.25M U 1984GKa (66810)1068
K(Mg+HL)=2.64
****
C9H13NO3 H2L (-)Adrenaline CAS 51-43-4 (252)
4-(1-Hydroxy-2-(methylamino)ethyl)-1,2-dihydroxybenzene,
Epinephrine;CH3NHCH(OH)C6H3(OH)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl NaClO4 25°C 1.0M C 1997GCa (66855)1069
K(Mg+H2L=MgHL+H)=-6.94
K(Mg+H2L=MgL+2H)=-15.81
K(Mg+H2L=MgH-1L+3H)=-25.80
K(Mg+2H2L=MgL2+4H)=-31.74
Ligand defined as H2L. K(Mg+2H2L=MgH-1L+5H)=-42.6, K(MgHL=MgL+H)=-8.87,
K(MgL=MgH-1L+H)=-9.99 etc.

Mg++ gl KCl 25°C 0.10M U T H K1=6.00 B2= 8.19 1983CVa (66856)1070
Data for 0 and 37 C. DH(K1)=-40.5 kJ mol-1, DS(K1)=-38.2 J K-1 mol-1;
DH(K2)=-18.1, DS(K2)=-7.6.
****
C9H13NO6 H3L (3881)
2,6-Dicarboxypiperidyl-N-ethanoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl KNO3 25°C 0.10M U K1=5.06 1968KTd (66879)1071
****
C9H13NO8 H4L (7012)
1,3-Dicarboxypropane-1-iminodiethanoic acid; HOOC.CH(N(CH2COOH)2)CH2CH2COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl KNO3 25°C 0.10M U K1=5.93 1977GNb (66904)1072

Mg++ gl KNO3 25°C 0.1M U K1=5.18 1976NGb (66905)1073

****

C9H13N2O9P H3L UMP-5 CAS 58-97-9 (2948)
Uridine-5'-monophosphoric acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	R4N.X	25°C	0.1M	U	H	K1=1.56	1998HTa	(66962)1074

Medium: 0.10 M Me4NBr. By calorimetry: DH(K1)=12.0 kJ mol-1, DS=70 J K-1 mol-1.

Mg++	gl	KNO3	35°C	0.10M	U	M	1992RAd	(66963)1075
							K(Mg+HL)=1.80	
							K(Mg+HL+Gly)=2.07	
							K(Mg+HL+His)=7.12	
							K(Mg+HL+histamine)=6.50	
Mg++	gl	R4N.X	25°C	0.10M	C TIH	R	1991SMa	(66964)1076
							K(Mg+HL)=1.94	

IUPAC evaluation. DH(K2)=7.5 kJ mol-1 (tentative)

Mg++	gl	NaNO3	25°C	0.10M	C		1988MSa	(66965)1077
							K(Mg+HL)=1.56	
Mg++	gl	NaClO4	25°C	0.10M	C		1984SSe	(66966)1078
							K(Mg+HL)=1.48	
Mg++	cal	R4N.X	30°C	0.20M	U		1973SBb	(66967)1079
							K(Mg+HL)=1.70	

Medium: 0.2 M Me4NBr. micro-constants are also given

Mg++	ix	NaCl	23°C	0.10M	U		1958WAa	(66968)1080
							K(Mg+HL)=2.25	

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaNO3	25°C	0.50M	C		K1=0.12	1992KJa	(67046)1081
Mg++	gl	KNO3	35°C	0.10M	C	M	K1=2.42	1985RRc	(67047)1082
							B(MgHL(Gly))=11.78		
							B(MgL(oxalate))=8.81		
							B(MgHL(His))=11.48		
							B(MgHL(histamine))=11.44		
Mg++	gl	KNO3	45°C	0.10M	U		K1=2.53	1981TKa	(67048)1083

****

C9H13N4O4P H2L 3-deaza-PMEA CAS 121150-00-3 (6140)
9-[2-(Phosphonomethoxy)ethyl]-3-deazaadenine;

```
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Mg++       gl  NaNO3  25°C 0.10M C        K1=1.85        1998BHa (67097)1084
                                         K(MgL+H)=7.41
                                         K(Mg+HL)=1.43
Also data for the 1-deaza- and 7-deaza-adenine homologues
*******************************************************************************
C9H14NO4P            H2L                      (8075)
2-Amino-3-hydroxy-3-phenylpropane-3-phosphonic acid;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Mg++       gl  NaClO4 25°C  0.1M U        K1=1.52        1975SLa (67110)1085
*******************************************************************************
C9H14N2O9            H4L                    CAS 56360-11-3  (2576)
2-Hydroxy-1,3-diaminopropane-N,N'-di(1,3-propanedioic acid)
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Mg++       gl  KNO3   25°C 0.10M U        K1=3.96        1975KGa (67134)1086
                                         K(Mg+HL)=3.20
                                         K(Mg+MgL)=1.95
*******************************************************************************
C9H14N2O12P2         H4L    UDP            CAS 58-98-0  (3288)
Uridine-5'-diphosphoric acid;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Mg++       gl  NaNO3  25°C 0.10M M        K1=3.32        1999SSa (67155)1087
                                         K(Mg+H2L)=1.6
                                         K(MgHL+H)=4.65
-------------------------------------------------------------------------------
Mg++       gl  KNO3   25°C 0.10M U        K1=3.32        1995SBa (67156)1088
-------------------------------------------------------------------------------
Mg++       gl  R4N.X  25°C 0.10M C      T                1991SMa (67157)1089
                                         K(Mg+HL)=3.35
IUPAC evaluation
-------------------------------------------------------------------------------
Mg++       cal R4N.X  30°C 0.20M U                       1973SBb (67158)1090
                                         K(Mg+HL)=3.45
Medium: 0.2 M Me4NBr. micro-constants are also given
-------------------------------------------------------------------------------
Mg++       ix  NaCl   23°C 0.10M U        K1=3.17        1958WAa (67159)1091
*******************************************************************************
C9H14N3O7P           H2L    dCMP           CAS 1032-65-1  (5783)
Deoxycytidine-5'-monophosphoric acid;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
```

```
Mg++       gl  NaNO3  25°C 0.10M C    M   K1=1.58        1995SFa (67178)1092
                                           K(Mg+HL)=0.47
K(Mg+HA)=1.31, K(Mg+A)=1.98. A=H2(cis-(NH3)2Pt(dCMP)2)
**************************************************************************
C9H14N3O8P            H2L    CMP-5           CAS 63-37-6  (1243)
Cytidine-5'-monophosphoric acid, Cytidilic acid;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Mg++       gl  KNO3   25°C 0.10M C    M   K1=2.95        2001AAa (67242)1093
Also data for ternary complexes with MOPSO, TAPSO and ACES.
--------------------------------------------------------------------------
Mg++       gl  R4N.X  25°C  0.1M U   H    K1=1.54        1998HTa (67243)1094
Medium: 0.10 M Me4NBr. By calorimetry: DH(K1)=12.5 kJ mol-1,
DS=71 J K-1 mol-1.
--------------------------------------------------------------------------
Mg++       gl  R4N.X  25°C 0.10M C TI   R K1=1.93        1991SMa (67244)1095
IUPAC evaluation
--------------------------------------------------------------------------
Mg++       gl  NaNO3  25°C 0.10M C        K1=1.54        1988MSa (67245)1096
--------------------------------------------------------------------------
Mg++       gl  KNO3   35°C 0.10M U    M                  1986RRe (67246)1097
                                          K(Mg+HL+HA)=5.86
                                          K(Mg+HL+E)=6.36
                                          K(MgLE+H)=2.72
                                          K(Mg+L+HC)=5.31
K(MgLC+H)=2.36; K(Mg+L+HD)=5.27. HA is glycine; H2E is oxalic acid;
C is histamine; HD is histidine.
--------------------------------------------------------------------------
Mg++       gl  KNO3   15°C 0.10M U        K1=1.75        1972FSa (67247)1098
**************************************************************************
C9H14N4O3              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
--------------------------------------------------------------------------
Mg++       gl  KNO3   25°C 0.10M U        K1=3.10        1964LMa (67314)1099
**************************************************************************
C9H14N5O3P            H2L                    CAS 121149-93-7  (2512)
9-(4-Phosphonobutyl)adenine;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Mg++       gl  NaNO3  25°C 0.10M M        K1=1.84        2000GKa (67356)1100
                                          K(Mg+HL)=0.3
                                          *K(MgHL)=-6.2
**************************************************************************
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
Mg++	gl	KNO3	20°C	0.10M	U		K1=5.36	1974RMf	(67402)1101

****

C9H15NO6 H3L CAS 817-11-8 (3271)
3,3',3''-Nitrilotripropanoic acid; (HOOC.CH2.CH2)3N

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaClO4	25°C	0.50M	C		K1=2.96	1995CDa	(67430)1102
Mg++	gl	KCl	30°C	0.10M	U		K1=<1	1953CMa	(67431)1103

****

C9H15NO6 H3L CAS 95482-53-4 (3270)
N-(2-Carboxyethyl)-3,3-iminodipropanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KCl	30°C	0.10M	U		K1=3.6	1953CMa	(67441)1104

****

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
Mg++	gl	KCl	25°C	0.20M	C		K1=4.34	1999MKa	(67460)1105
							B(MgHL)=14.13		
							B(MgH2L)=19.03		
							B(MgH-1L)=-7.88		

****

C9H15N2O15P3 H5L UTP CAS 63-39-8 (407)
Uridine-5'-triphosphoric acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	R4N.X	25°C	0.10M	C	TIH R		1991SMa	(67520)1106
							K(Mg+HL)=4.43		
							K(Mg+H2L)=2.58		
IUPAC evaluation. DH(K1)=18.4 kJ mol-1 (tentative)									
Mg++	gl	NaNO3	25°C	0.10M	C			1987STb	(67521)1107
							K(Mg+HL)=4.27		
							K(MgL+H)=4.90		
							K(Mg+H2L)=2.72		
Mg++	gl	KNO3	25°C	0.10M	U	T H	K1=5.42	1983RRe	(67522)1108
Also data for 35 and 45 C. At 45 C: K1=5.61.									
DH(K1)=17.5 kJ mol-1, DS(K1)=161 J K-1 mol-1.									
Mg++	gl	NaClO4	25°C	0.10M	C			1977SIc	(67523)1109

```
                                        K(Mg+HL)=4.00
--------------------------------------------------------------------------------
Mg++       gl  KNO3   35°C 0.10M U                      1976KRa (67524)1110
                                        K(Mg+HL)=5.53
--------------------------------------------------------------------------------
Mg++       cal R4N.X  30°C 0.20M U                      1973SBb (67525)1111
                                        K(Mg+HL)=4.32
                                        K(Mg+H2L)=4.15
                                        K(Mg+H3L)=2.46
Medium: 0.2 M Me4NBr. micro-constants are also given
--------------------------------------------------------------------------------
Mg++       ix  NaCl   23°C 0.10M U                      1958WAa (67526)1112
                                        K(Mg+HL)=4.02
********************************************************************************
C9H15N3O11P2          H3L    CDP             CAS 63-38-7  (2187)
Cytidine-5'-diphosphoric acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Mg++       gl  NaNO3  25°C 0.10M M        K1=3.25        1999SSa (67583)1113
                                        K(Mg+HL)=1.6
                                        K(MgL+H)=4.74
--------------------------------------------------------------------------------
Mg++       gl  R4N.X  25°C 0.10M C      T K1=3.44        1991SMa (67584)1114
                                        K(Mg+HL)=1.62
                                        K(Mg+MgL)=1.0
IUPAC evaluation
--------------------------------------------------------------------------------
Mg++       gl  KNO3   15°C 0.10M U        K1=3.22        1972FSa (67585)1115
                                        K(Mg+HL)=1.60
--------------------------------------------------------------------------------
Mg++       sp  R4N.X    ?  0.05M U                      1961HBa (67586)1116
                                        K(?)=1.5
Medium: Me4NCl
********************************************************************************
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
--------------------------------------------------------------------------------
Mg++       gl  KCl    20°C 0.10M U        K1=2.68        1955SAa (67626)1117
********************************************************************************
C9H16N3O14P3          H4L    CTP             CAS 65-47-4  (406)
Cytidine-5'-triphosphoric acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Mg++       gl  R4N.X  25°C 0.10M C TI   R K1=4.44        1991SMa (67697)1118
                                        K(Mg+HL)=2.22
                                        K(Mg+MgL)=1.8
```

IUPAC evaluation

Mg++	gl	NaNO3	25°C	0.10M	C	K1=4.20 K(Mg+HL)=2.27 K(MgL+H)=4.62	1987STb (67698)1119
Mg++	gl	KNO3	25°C	0.10M	U T H	K1=4.19 K(Mg+HL)=3.85	1983RRe (67699)1120

Also data for 35 and 45 C. At 45 C: K1=4.30, K(Mg+HL)=3.98.
DH(K1)=10.0 kJ mol-1, DS(K1)=114 J K-1 mol-1; DH(Mg+HL)=-11.7, DS=113

Mg++	gl	NaClO4	25°C	0.10M	C	K1=4.08	1977SIc (67700)1121
Mg++	gl	KNO3	35°C	0.1M	C I	K1=4.21 K(Mg+HL)=3.93	1975TRc (67701)1122
Mg++	gl	KNO3	15°C	0.10M	U	K1=4.03 K(Mg+HL)=2.18	1972FSa (67702)1123
Mg++	sp	R4N.X	?	0.05M	U	K(?)=1.95	1961HBa (67703)1124

Medium: Me4NCl

Mg++	ix	NaCl	23°C	0.10M	U	K1=4.01	1958WAa (67704)1125

****

C9H16O4 H2L CAS 57218-62-9 (484)
Ethyl(2-methylpropyl)propanedioic acid; HOOC.C(C2H5)(CH2.CH(CH3)2).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	sp	none	25°C	0.0	U	T	K1=3.10	1976KOa	(67784)1126

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

****

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
Mg++	gl	NaClO4	25°C	1.0M	C		K1=2.58	1981ASb	(67829)1127

****

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
Mg++	gl	KCl	25°C	0.20M	C		K1=4.15 B(MgHL)=12.69	1999FEa	(67935)1128
Mg++	gl	NaNO3	25°C	0.10M	C		K1=4.37	1989EHa	(67936)1129

B(MgHL)=12.64

****

C9H19N2O4+ H2L (3277)

2-Di(carboxymethyl)aminoethyltrimethylammonium cation

+

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KCl	20°C	0.10M	U		K1=1.42	1955SAa (68000)	1130

****

C9H20N2O5S HL HEPPSO CAS 68399-78-0 (2011)

N-(2-Hydroxyethyl)piperazine-N'-(2-hydroxypropanesulfonic acid);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	25°C	0.10M	C		K1=3.69	2001AOa (68053)	1131

****

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
Mg++	gl	KCl	25°C	0.15M	U		K1=1.63	1962OSa (68075)	1132

****

C9H20O14P2 H3L (4662)

1-(Glycerylphosphoryl)-L-myoinositol-5-phosphate;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	R4N.X	20°C	0.10M	U		K1=2.19	1969HRa (68128)	1133

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
Mg++	gl	R4N.X	20°C	0.10M	U		K1=3.45	1969HRa (68224)	1134
							K(Mg+HL)=2.37		

Medium : 0.1 (C3H7)4NI

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	R4N.X	20°C	0.10M	U		K1=3.5	1965HFb (68225)	1135
							K(Mg+HL)=2.4		

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

```
Mg++       gl  KNO3   25°C 0.10M C        K1=5.36        1995BLa (68291)1136
                                          B(MgH-1L)=3.52
**************************************************************************
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
--------------------------------------------------------------------------
Mg++       gl  KNO3   25°C 1.00M U                         1988MKb (68307)1137
                                          B(Mg2L)=11.6
                                          K(Mg+MgL)=0.55
--------------------------------------------------------------------------
Mg++       gl  KCl    25°C  1.0M U        K1=11.01       1984KMa (68308)1138
                                          K(Mg+HL)=5.44
--------------------------------------------------------------------------
Mg++       gl  oth/un 25°C 1.00M U        K1=11.01       1982PSc (68309)1139
                                          K(Mg+HL)=5.44
**************************************************************************
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
--------------------------------------------------------------------------
Mg++       gl  KCl    25°C 0.10M U        K1=6.40        1967KDa (68404)1140
                                          K(Mg+HL)=5.40
                                          K(Mg+H2L)=4.70
                                          K(Mg+H3L)=3.94
                                          K(Mg+H4L)=3.13
K(Mg+H5L)=2.36
**************************************************************************
C10H6O8               H4L    Pyromellitic Ac  CAS 89-05-4  (519)
Benzene-1,2,4,5-tetracarboxylic acid; C6H2.(COOH)4
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Mg++       gl  oth/un 25°C  1.0M C        K1=2.63        1991DDb (68505)1141
                                          B(MgHL)=7.41
                                          B(MgH2L)=10.92
                                          B(MgH3L)=13.07
                                          B(Mg2L)=3.72
Medium: 1.0 M LiCl.
--------------------------------------------------------------------------
Mg++       con none   25°C  0.0  U        K1=3.69        1984TWa (68506)1142
**************************************************************************
C10H7NO2               HL                    CAS 131-91-9  (2668)
1-Nitroso-2-naphthol, alpha-Nitroso-beta-naphthol;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
```

Mg++ gl diox/w 30°C 75% U I K1=6.05 B2=10.77 1957CFa (68570)1143
In 50% dioxan K1=3.60, K2=3.47

Mg++ gl diox/w 30°C 75% U K1=6.2 B2=10.6 1954UFa (68571)1144
****
C10H7NO2 HL CAS 14510-06-6 (4715)
2-Formyl-8-hydroxyquinoline;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl diox/w 25°C 50% U K1=3.45 1972HUb (68608)1145
Medium: 50% v/v dioxan, 0.1 M KCl
****
C10H7NO2 HL CAS 132-53-6 (2524)
2-Nitroso-1-naphthol;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl diox/w 30°C 75% U K1=5.62 B2=9.97 1957CFa (68639)1146

Mg++ gl diox/w 30°C 75% U K1=5.80 B2=9.60 1954UFa (68640)1147
****
C10H7NO2 HL Quinaldic acid CAS 93-10-7 (2209)
Quinoline-2-carboxylic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl oth/un 25°C 0.0 U K1=1.37 B2=2.55 1955LUa (68698)1148
****
C10H7NO2 HL CAS 86-59-9 (873)
Quinoline-8-carboxylic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl oth/un 25°C 0.0 U K1=1.24 B2=3.73 1955LUa (68754)1149
****
C10H7O2F3 HL CAS 326-06-7 (196)
3-Benzoyl-1,1,1-trifluoroacetone; CF3.CO.CH2.CO.C6H5

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl oth/un ? 0.0 U B2=7.52 1951UFa (69133)1150
****
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
---
Mg++ cal KCl 25°C 0.25M U H K1=0.30 1997MKb (69519)1151
DH(K1)=-6.1 kJ mol-1; DS=-15 J K-1 mol-1

Mg++ gl oth/un 25°C 0.20M U TIH K1=0.47 1993DGa (69520)1152
DH(K1)=8 kJ mol-1, DS(K1)=36 J K-1 mol-1. Data for 5-45 C, 0.20-
0.75 M MgCl2

Mg++ sp alc/w 25°C 95% U K1=2.20 1993GSa (69521)1153
Medium: 95% w/w EtOH/H2O, 0.05 M Et4NClO4, by competitive spectrophotometry
---
Mg++ sp non-aq 25°C 100% U I K1=2.80 B2=5.04 1992GSa (69522)1154
Medium: MeCN. In acetone:K1=2.04, K2=1.02; in MeOH:K1=1.90.By fluorimetry
---
Mg++ gl KCl 25°C 0.25M U T H K1=0.32 1985CRa (69523)1155
K1=0.38(10 C);K1=0.26(40 C).
DH=-6.3 kJ mol-1, DS=-17 J mol-1 K-1

Mg++ sp non-aq 25°C 100% U I K1=-0.39 1985MKb (69524)1156
Medium: DMSO. In DMF: K1=-0.26; MeCN: 4.8; MeOH: 0.93

Mg++ sp NaClO4 25°C 0.20M U I K1=0.673 1983EBa (69525)1157

Mg++ sp oth/un 25°C 0.50M U K1=0.5 1955SKa (69526)1158
****
C10H8O4 H2L CAS 38489-70-2 (3297)
Benzoylpyruvic acid; C6H5.CO.CH2.CO.COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl diox/w 30°C 75% U K1=12.0 B2=17.0 1954UFa (69796)1159
****
C10H8O5S H3L DHNSA (877)
2,3-Dihydroxynaphthalene-6-sulfonic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl NaNO3 25°C 0.10M U K1=7.32 B2=11.53 1984NHa (69833)1160
****
C10H9NO HL 8-OH-Quinaldine CAS 826-81-3 (998)
2-Methyl-8-hydroxyquinoline;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ sp KCl 30°C 1.0M M K1=3.09 1996BTa (70039)1161

Mg++ dis R4N.X 20°C 1.0M U K1=1.98 B2=5.03 1969SRc (70040)1162
Medium: 1 M NH4Cl,HCl

Mg++ gl diox/w 20°C 50% U K1=3.73 B2=6.86 1954IRa (70041)1163
Medium: 50% dioxan, 0.3 M NaClO4

Mg++ gl diox/w 25°C 50% U K1=5.24 B2=9.64 1954JFa (70042)1164

****
C10H9NO HL CAS 5541-67-3 (999)
5-Methyl-8-hydroxyquinoline;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl diox/w 20°C 50% U K1=5.21 B2=9.68 1954IRa (70062)1165
Medium: 50% dioxan, 0.3 M NaClO4
****
C10H9NO HL CAS 5541-68-4 (1000)
7-Methyl-8-hydroxyquinoline;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl diox/w 20°C 50% U K1=4.64 B2=8.76 1954IRa (70075)1166
Medium: 50% dioxan, 0.3 M NaClO4
****
C10H9NO HL CAS 3846-73-9 (3320)
8-Hydroxy-4-methylquinoline;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl diox/w 25°C 50% U K1=6.45 B2=11.91 1954JFa (70094)1167
****
C10H9NO HL CAS 20984-33-2 (3321)
8-Hydroxy-6-methylquinoline;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl diox/w 20°C 50% U K1=5.09 B2=9.40 1954IRa (70100)1168
Medium: 50% dioxan, 0.3 M NaClO4
****
C10H9NO2 HL CAS 57334-35-7 (3905)
2-Hydroxymethyl-8-hydroxyquinoline;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ sp KCl 30°C 1.0M M K1=2.52 1996BTa (70117)1169

Mg++ gl diox/w 25°C 50% U K1=3.99 B2=8.08 1967SFa (70118)1170
****
C10H9NO8 H2L CAS 83785-11-9 (685)
2-Nitro-1,4-di(carboxymethoxy)benzene; O2N.C6H3.(OCH2COOH)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl oth/un 30°C ? U K1=3.42 1985TZa (70233)1171
****
C10H9O2Br HL CAS 4023-81-8 (1182)
4-Bromo-1-phenyl-1,3-butanedione; Br.C6H4.CO.CH2.CO.CH3

```
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Mg++       gl  diox/w 20°C  75%  M T      K1=9.13   B2=15.25  1980GMd (70433)1172
*******************************************************************************
C10H10N2O              HL                     CAS 37920-81-3  (3323)
8-Hydroxy-2,4-dimethylquinazoline;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Mg++       gl  diox/w 20°C  50%  U        K1=3.81   B2=6.90   1954IRa (70539)1173
Medium: 50% dioxan, 0.3 M NaClO4
*******************************************************************************
C10H10N2O3S           H2L                     CAS 76045-30-2  (7218)
Desferriferrithiocin,
2-(3-Hydroxypyridin-2-yl)-4-methyl-4,5-dihydrothiazole-4-carboxylic acid;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Mg++       gl  KNO3   25°C 0.10M C        K1=5.10   B2= 9.16  1990ARa (70557)1174
*******************************************************************************
C10H10O2               HL    Benzoylacetone   CAS 93-91-4  (197)
1-Phenylbutane-1,3-dione; C6H5.CO.CH2.CO.CH3
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Mg++       gl  diox/w 20°C  17%  C        K1=7.60   B2=14.16  1976JWa (70703)1175
-------------------------------------------------------------------------------
Mg++       gl  diox/w 30°C  75%  U        K1=7.84   B2=14.04  1959MFa (70704)1176
-------------------------------------------------------------------------------
Mg++       gl  diox/w 30°C  75%  U        K1=7.69   B2=14.09  1953UFa (70705)1177
*******************************************************************************
C10H10O3               HL                     CAS 16636-62-7  (3298)
2-Hydroxybenzoylacetone; HO.C6H4.CO.CH2.CO.CH3
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Mg++       gl  diox/w 30°C  75%  U        K1=7.18   B2=13.23  1955HOa (70798)1178
*******************************************************************************
C10H10O6              H2L                     CAS 5411-14-3  (2394)
1,2-Phenylenedioxodiethanoic acid; C6H4(O.CH2.COOH)2
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Mg++       gl  NaClO4 25°C 0.10M U        K1=<1.5        1968SMb (70844)1179
*******************************************************************************
C10H11NO4             H2L                     CAS 1137-73-1  (2567)
N-Phenyliminodiethanoic acid; C6H5.N(CH2.COOH)2
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
```

Mg++ cal KNO3 25°C 0.1M C H 1991ANa (70997)1180
DH(K1)=5.9 kJ mol-1

Mg++ cal KNO3 25°C 0.10M U K1=1.15 1991Aa (70998)1181
DH(K1)=5.86 kJ mol-1, DS(K1)=41.84 J K-1 mol-1

Mg++ gl KCl 20°C 0.10M U K1=1.15 1955SAa (70999)1182

****

C10H11NO4S 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
Mg++	gl	KNO3	20°C	0.10M	U		K1=1.84 ?	1963IFb	(71021)1183

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	20°C	0.10M	U		K1=6.86 K(Mg+HL)=2.67	1963IFb	(71036)1184

****

C10H11NO5S H2L (3929)
N-(2-Thenoylmethyl)iminodiethanoic acid; C4H3S.CO.CH2.N(CH2.COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	25°C	0.10M	U		K1=2.80	1965AUa	(71061)1185

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	EMF	KCl	20°C	0.10M	C		K1=2.68	1947SWa	(71065)1186

****

C10H11NO7S 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
Mg++	EMF	KCl	20°C	0.10M	C		K1=1.26	1947SWa	(71072)1187

Method: H electrode

****

C10H11NO7S H3L (3337)
N-(4-Sulfophenyl)iminodiethanoic acid; HO3S.C6H4.N(CH2.COOH)2

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

---
Mg++ EMF KCl 20°C 0.10M C K1=1.15 1947SWa (71075)1188
Method: H electrode
****
C10H12N2O2 HL CAS 89314-29-4 (8507)
2-[(4-Methylphenyl)hydrazono]-propanoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl alc/w 30°C 40% M M K1=4.04 B2= 6.69 1995RRe (71192)1189
K(MgL+A)=5.00
K(MgL+en)=6.65
K(MgL+pro)=4.55
K(MgL+B)=2.90
Medium: 40% v/v EtOH/H2O, 0.10 M KNO3. K(MgL+ala)=2.50, K(MgL+gly)=2.35.
H2A is catechol, HB is hydroxyproline.

Mg++ gl alc/w 30°C 40% M M 1995RRe (71193)1190
K(Mg(phe)+L)=3.00
K(MgA+L)=2.05
Medium: 40% v/v EtOH/H2O, 0.10 M KNO3. H2A is salicylic acid.
****
C10H12N2O4 H2L CAS 16598-05-3 (967)
2-Pyridylmethyliminodiethanoic acid; C5H4N.CH2.N(CH2.COOH)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl NaNO3 20°C 0.10M C H K1=3.98 1981ANb (71247)1191
DH1=15.9 kJ mol-1 DS1=130.1 J K-1 mol-1

Mg++ gl KNO3 20°C 0.10M U K1=3.90 1963IFc (71248)1192
****
C10H12N4O6 H2L Xanthosine CAS 5968-90-1 (1176)
3,9-Dihydro-9-ribofuranosyl-1H-purine-2,6-dione;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl KNO3 25°C 0.10M U M 1990RRa (71477)1193
K(Mg(His)+H+L)=2.56
B(MgH2L(histamine))=7.14
B(MgH2L(catechol))=7.06
K(Mg(Gly)+H+L)=2.39

Mg++ gl NaNO3 25°C 0.10M C 1989KTa (71478)1194
K(Mg+H-1L) < 0.6

Mg++ gl KNO3 35°C 0.10M C M 1985RRh (71479)1195
K(Mg+HL)=2.23
K(Mg(gly)+HL)=2.5
K(Mg(his)+HL)=2.79

```
                                        K(Mg+HL+HA)=7.27
K(Mg+HL+B)=8.30. H2A is catechol, H2B is oxalic acid.
--------------------------------------------------------------------------------
Mg++       gl  KNO3   35°C 0.10M U    M                   1983RRb (71480)1196
                                        K(Mg+HL)=2.23
                                        K(Mg+2HL)=5.07
                                        K(MgGly+H2L=MgHLGly+H)=2.5
--------------------------------------------------------------------------------
Mg++       gl  KNO3   25°C 0.10M U T H                   1983RRc (71481)1197
                                        K(Mg+2HL)=5.00
DH=-7.9kJ mol-1. At 5 C: K=5..60; 35 C: 5.07; 45 C: 5.47
--------------------------------------------------------------------------------
Mg++       gl  KNO3   45°C 0.10M U    M                   1979RRb (71482)1198
                                        K(Mg+HL+TetraMeen)=5.26
                                        K(Mg+HL+Sulphosalicylate)=1.95
--------------------------------------------------------------------------------
Mg++       gl  KNO3   45°C 0.10M U    M                   1979RRb (71483)1199
                                        K(Mg+HL+bpy)=6.56
--------------------------------------------------------------------------------
Mg++       gl  KNO3   25°C 0.10M U T                     1978RRa (71484)1200
                                        K(Mg+HL)=2.22
********************************************************************************
C10H12N4O6             HL                      CAS 40281-74-1  (3910)
Purin-6-one 9-riboside N(1)-oxide    (Inosine N(1)-oxide)
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Mg++       sp  NaClO4 25°C 0.10M U        K1=1.7         1965SIa (71508)1201
********************************************************************************
C10H12O2               HL                      CAS 7624-24-2  (4702)
2-Hydroxy-4-methylpropiophenone; HO.C6H3(CH3).CO.CH2.CH3
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Mg++       gl  diox/w 30°C  75%  U        K1=5.51         1970KDa (71526)1202
Medium: 75% dioxan, 0.1 M NaClO4
********************************************************************************
C10H12O2               HL                      CAS 1946-74-3  (202)
3-Isopropyltropolone;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Mg++       gl  diox/w 30°C  50%  U        K1=6.2    B2=11.4   1954BFb (71569)1203
--------------------------------------------------------------------------------
Mg++       gl  diox/w 30°C  50%  U        K1=6.2    B2=11.0   1954BFb (71570)1204
                                        B3=14.0
********************************************************************************
C10H12O4               HL                      CAS 90-24-4  (4704)
2-Hydroxy-4,6-dimethoxyacetophenone; (HO)(CH3O)2.C6H2.CO.CH3
--------------------------------------------------------------------------------
```

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Mg++	gl	diox/w	30°C	75%	U		K1=8.44		1970KDa (71663)	1205

Medium: 75% dioxan, 0.1 M NaClO4

****

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
Mg++	gl	NaNO3	25°C	0.10M	M		K1=1.93		1991BSc (71790)	1206
							K(MgH-1L+H)=8.89			
Mg++	gl	NaNO3	25°C	0.10M	M	I			1991BSd (71791)	1207
							K(Mg+HL)=1.93			
							K(MgL+H)=8.89			

In 30% v/v dioxan/H2O: K(Mg+HL)=2.57, K(MgL+H)=9.32.

In 50% v/v dioxan/H2O: K1=2.96, K(MgL+H)=9.54

****

C10H13N3O7 H3L (3912)

1,3-Dimethyluramil-N,N-diethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Mg++	gl	KNO3	20°C	0.10M	U		K1=8.29	B2=12.07	1963IFb (71802)	1208

****

C10H13N4O8P H3L IMP CAS 131-99-7 (843)

Inosine-5'-monophosphoric acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Mg++	gl	KNO3	25°C	0.10M	C	M	K1=1.69		2001AAa (71854)	1209

Also data for ternary complexes with MOPSO, TAPSO and ACES.

Mg++	gl	R4N.X	25°C	0.1M	U	H	K1=1.68		1998HTa (71855)	1210
							K(Mg+HL)=<0			

Medium: 0.10 M Me4NBr. By calorimetry: DH(K1)=6.6 kJ mol-1,
DS=1 J K-1 mol-1.

Mg++	gl	NaNO3	25°C	0.10M	M				1994SMb (71856)	1211
							K(Mg+HL)=1.67			
							*K(MgHL)=-8.65			

****

C10H13N4O9P H3L (3930)

Inosine-5'-monophosphoric acid N(1)-oxide;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Mg++	sp	NaClO4	25°C	0.10M	U				1965SIa (71883)	1212
							K(Mg+HL)=2.1			

****

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
Mg++	nmr	non-aq	21°C	100%	U		K1=0.50	1973SFa	(71940)1213

Medium: (CH3)2SO

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	25°C	0.10M	C	T HM		1988KRa	(72005)1214
							K(Mg+HL)=2.31		
							K(MgHL+HL)=3.71		
Mg++	nmr	non-aq	21°C	100%	U			1973SFa	(72006)1215
							K(Mg+HL)=1.63		
Mg++	gl	oth/un	20°C	0.01M	U		K1=3.0	1953ALa	(72007)1216

Also data at 15, 35 and 45 C. DH(MgHL)=+17; DS=101. DH(MgH2L2)=+14.7; DS=120
Also ternary complexes with bpy, phen and 5-sulfosalicylic acid

Medium: (CH3)2SO

****

C10H14N4O11P2 H4L IDP CAS 86-04-2 (3932)
Inosine-5'-diphosphoric acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	sp	oth/un	?	0.05M	U		K1=3.76	1961HBa	(72136)1217
							K(Mg+HL)=2.38(?)		

Medium: Me4NCl. K1 by glass electrode

****

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
Mg++	gl	NaNO3	25°C	0.10M	M		K1=1.28	1997SSg	(72150)1218
Mg++	gl	KNO3	25°C	0.10M	U		K1=1.28	1995SSe	(72151)1219

****

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
Mg++	gl	R4N.X	25°C	0.10M	C	R	K1=1.98	1991SMa	(72180)1220

IUPAC evaluation

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaNO3	25°C	0.10M	C		K1=1.53 K1(open)=1.51	1989MSf	(72181)1221
Mg++	gl	KNO3	15°C	0.10M	U		K1=1.75	1972FSa	(72182)1222
Mg++	gl	KNO3	40°C	0.10M	U T H		K1=2.05	1967TMf	(72183)1223

K1=1.71(0.4 C),1.82(12 C),1.93(25 C). At 25 C: DH(K1)=14.6 kJ mol-1, DS=86

****

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
Mg++	gl	R4N.X	25°C	0.10M	C	T	K1=1.94	1991SMa	(72231)1224

IUPAC evaluation

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaNO3	25°C	0.10M	U		K1=1.49	1989MSf	(72232)1225
Mg++	gl	KNO3	40°C	0.10M	U T H		K1=2.01	1967TMf	(72233)1226

K1=1.68(0.4 C),1.78(12 C),1.86(25 C). At 25 C: DH(K1)=14.6 J K-1 mol-1,DS=86

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	25°C	0.10M	U		K1=1.89	1962TMa	(72234)1227
Mg++	gl	KCl	25°C	0.10M	U		K1=1.73	1958WSa	(72235)1228

****

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
Mg++	gl	NaNO3	25°C	0.10M	M		K1=1.62 K(MgL+H)=4.6 K(Mg+HL)=0.0	2003BSa	(72416)1229
Mg++	gl	KNO3	25°C	0.10M	C	M	K1=1.97 K(MgL+A)=1.31 B(MgLA)=3.28 K(MgL+B)=2.90 B(MgLB)=4.87	2001AOa	(72417)1230

K(MgL+C)=4.01, B(MgLC)=5.98. HA=MOPS, HB=POPSO and HC=HEPPSO.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	25°C	0.10M	C	M	K1=1.97 K(MgL+A)=4.40 B(MgLA)=6.37 K(MgL+B)=3.81 B(MgLB)=5.78	2000ADa	(72418)1231

HA=ACES, HB=MOPSO. Also data for CHES, TAPSO and DIPSO.

```
Mg++       gl  R4N.X  25°C  0.1M U   H    K1=1.61   B2= 3.45  1998HTa (72419)1232
                                          K(Mg+HL)=<0
Medium: 0.10 M Me4NBr. DH(K1)=11.1 kJ mol-1, DS=68 J K-1 mol-1.
DH(K2)=-10.2, DS=1.
--------------------------------------------------------------------------------
Mg++       gl  NaNO3  25°C 0.10M M        K1=1.62        1996SSd (72420)1233
--------------------------------------------------------------------------------
Mg++       nmr oth/un 25°C    ?  U        K1=1.26        1991COa (72421)1234
--------------------------------------------------------------------------------
Mg++       gl  R4N.X  25°C 0.10M C TIH  R K1=2.02        1991SMa (72422)1235
IUPAC evaluation. DH(K1)=7.5 kJ mol-1 (tentative). 37 C, I=0.15 M: K1=1.92
--------------------------------------------------------------------------------
Mg++       gl  NaNO3  25°C 0.10M U        K1=1.60        1989MSf (72423)1236
--------------------------------------------------------------------------------
Mg++       gl  KNO3   25°C 0.10M U    M   K1=2.36        1988MBa (72424)1237
--------------------------------------------------------------------------------
Mg++       gl  NaNO3  25°C 0.10M C        K1=1.60        1988SMb (72425)1238
--------------------------------------------------------------------------------
Mg++       gl  NaClO4 25°C 0.10M C   H    K1=2.10        1987SCa (72426)1239
DH(K1)=5.71 kJ mol-1, DS=59 J K-1 mol-1
--------------------------------------------------------------------------------
Mg++       gl  KCl    25°C 0.20M U        K1=67.4        1979TPb (72427)1240
--------------------------------------------------------------------------------
Mg++       ISE oth/un 25°C  0.0  C        K1=2.57        1976KRb (72428)1241
Method: Ca ion selective electrode. Self medium, pH 9.1.
--------------------------------------------------------------------------------
Mg++       gl  KNO3   15°C 0.10M U        K1=1.80        1972FSa (72429)1242
--------------------------------------------------------------------------------
Mg++       cal R4N.X  30°C 0.20M U        K1=1.81        1969BSc (72430)1243
Medium: Me4N4Cl, pH=8.5
--------------------------------------------------------------------------------
Mg++       gl  KNO3   40°C 0.10M U T H    K1=2.09        1967TMf (72431)1244
K1=1.75(0.4 C),1.85(12 C),1.97(25 C). At 25 C: DH(K1)=14.2 kJ mol-1, DS=85 J
--------------------------------------------------------------------------------
Mg++       gl  NaClO4 25°C 0.10M U        K1=1.63        1964SBa (72432)1245
--------------------------------------------------------------------------------
Mg++       gl  KNO3   25°C 0.10M U        K1=1.97        1962TMa (72433)1246
--------------------------------------------------------------------------------
Mg++       ix  NaCl   23°C 0.10M U        K1=1.95        1958WAa (72434)1247
--------------------------------------------------------------------------------
Mg++       gl  KCl    25°C 0.10M U        K1=2.14        1958WSa (72435)1248
--------------------------------------------------------------------------------
Mg++       ix  oth/un 23°C 0.10M U        K1=2.0         1957NAc (72436)1249
--------------------------------------------------------------------------------
Mg++       gl  KCl    20°C 0.10M U        K1=1.69        1956MSa (72437)1250
--------------------------------------------------------------------------------
Mg++       gl  R4N.X  25°C 0.20M U        K1=1.69        1956SAa (72438)1251
Medium: 0.2 M n-Pr4NCl
********************************************************************************
C10H14N5O7P           H2L    dGMP             CAS 902-04-5  (5781)
```

Deoxyguanosine-5'-monophosphoric acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaNO3	25°C	0.10M	U		K1=1.81	1998SSc (72513)	1252

****

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
Mg++	gl	NaClO4	25°C	0.10M	U			1964SBa (72521)	1253
							K(Mg+HL)=1.62		
							K(MgL+H) > 10.39		

By spectrophotometry: K1 < 3.72

****

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
Mg++	gl	KNO3	25°C	0.10M	C	M	K1=1.73	2001AAa (72580)	1254

Also data for ternary complexes with MOPSO, TAPSO and ACES.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	R4N.X	25°C	0.1M	U	H	K1=1.71	1998HTa (72581)	1255
							K(Mg+HL)=<0		

Medium: 0.10 M Me4NBr. By calorimetry: DH(K1)=5.3 kJ mol-1,
DS=-4 J K-1 mol-1.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaNO3	25°C	0.10M	M			1994SMb (72582)	1256
							K(Mg+HL)=1.70		
							*K(MgHL)=-9.02		

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	R4N.X	25°C	0.10M	C	R		1991SMa (72583)	1257
							K(Mg+HL)=1.99		

IUPAC evaluation

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	cal	R4N.X	30°C	0.20M	U			1973SBb (72584)	1258
							K(Mg+HL)=1.76		

Medium: Me4NI, pH=8.5

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KCl	20°C	0.10M	U		K1=6.75	1966IMa (72668)	1259

****

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
--------------------------------------------------------------------------------
Mg++       gl  R4N.X  25°C 0.10M C TI   R                1991SMa (72696)1260
                                        K(Mg+HL)=1.96
IUPAC evaluation
--------------------------------------------------------------------------------
Mg++       gl  NaNO3  25°C 0.10M C                       1988MSa (72697)1261
                                        K(Mg+HL)=1.55
********************************************************************************
C10H15N4O14P3         H5L    ITP             CAS 35908-31-7  (2148)
Inosine 5'-triphosphoric acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Mg++       gl  NaNO3  25°C 0.10M C                       2001SBc (72756)1262
                                        K(Mg+HL)=4.29
                                        K(MgHL+H)=4.6
                                        K(Mg+H2L)=2.4
For pyrimidine nucleoside 5'-triphosphoric acid, K1=4.21, K(Mg+HL)=2.3,
K(MgL+H)=4.6
--------------------------------------------------------------------------------
Mg++       gl  R4N.X  25°C 0.10M C      T                1991SMa (72757)1263
                                        K(Mg+HL)=4.44
                                        K(Mg+H2L)=2.34
IUPAC evaluation
--------------------------------------------------------------------------------
Mg++       gl  NaClO4 25°C 0.10M C                       1977SIc (72758)1264
                                        K(Mg+HL)=4.08
--------------------------------------------------------------------------------
Mg++       cal R4N.X  30°C 0.20M U  I     K1=4.07        1973SBb (72759)1265
                                        K(Mg+HL)=3.93
                                        K(Mg+H2L)=2.26
Medium: Me4NCl, pH=8.5. In 0.2 M Me4NBr K(Mg+HL)=3.93
--------------------------------------------------------------------------------
Mg++       gl  KNO3   25°C 0.10M U T                    1973TRb (72760)1266
                                        K(Mg+HL)=3.76
K(35 C)=4.08, K(45 C)=3.84
--------------------------------------------------------------------------------
Mg++       sp  R4N.X    ?  0.05M U                      1961HBa (72761)1267
                                        K(Mg+HL)=4.08
                                        K(Mg+H2L)=2.42 (?)
Medium: Me4NCl. K1 by glass electrode
--------------------------------------------------------------------------------
Mg++       ix  NaCl   23°C 0.10M U                       1958WAa (72762)1268
                                        K(Mg+HL)=4.04
********************************************************************************
C10H15N5O9P2S         H3L                  CAS 59286-20-3  (8421)
Adenosine-5'-(1-thiodiphosphoric acid);
--------------------------------------------------------------------------------
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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	nmr	KNO3	30°C	0.10M	C		K1=3.66 K(Mg+HL)=2.16 *K(MgL)=-5.27	1984PHc (72830)	1269

Method: 31P nmr.

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

Adenosine-5'-diphosphoric acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaNO3	25°C	0.10M	M		K1=3.36 K(MgL+H)=4.72 K(Mg+HL)=1.68	2003BSa (72944)	1270
Mg++	gl	KNO3	25°C	0.10M	C	M	K1=3.17 K(MgL+A)=2.38 B(MgLA)=5.55 K(MgL+B)=2.89 B(MgLB)=6.06	2001AOa (72945)	1271

K(MgL+C)=2.84, B(MgLC)=6.01, K(MgL+D)=4.83, B(MgLD)=8.00, K(MgL+E)=3.00, B(MgLE)=6.17. HA=PIPES, HB=MOPS, HC=POPSO, HD=HEPPSO and HE=AMPSO.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	25°C	0.10M	C	M	K1=3.17 K(MgL+A)=6.60 B(MgLA)=9.77 K(MgL+B)=4.12 B(MgLB)=7.29	2000ADa (72946)	1272

K(MgL+C)=3.80, B(MgLC)=6.97, K(MgL+D)=3.39, B(MgLD)=6.56, K(MgL+E)=3.40, B(MgLE)=6.57. HA=ACES, HB=MOPSO, HC=CHES, HD=TAPSO, HE=DIPSO.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaNO3	25°C	0.10M	C	M	K1=3.24 K(MgL+A)=3.43 B(MgLA)=6.67	2000KHa (72947)	1273

H2A=salicylhydroxamic acid.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	25°C	0.10M	U		K1=3.38	1995SBa (72948)	1274
Mg++	cal	none	75°C	0	M T H		K1=4.89 K(MgL+Mg)=2.10 K(2MgL=Mg2L2)=0.79	1995WOa (72949)	1275

DH(K1)=34.9 kJ mol-1, DS=194 J K-1 mol-1; DH(MgL+Mg)=18.3, DS=93; DH(dim)= =-0.4, DS=14. At 100 C: K1=5.29, K(MgL+Mg)=2.29, DH(K1)=44.5,DS=221

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	nmr	oth/un	25°C	?	U		K1=3.34 K(Mg+HL)=1.11	1991COa (72950)	1276
Mg++	gl	R4N.X	25°C	0.10M	C	TIH R	K1=3.43 K(Mg+HL)=1.61	1991SMa (72951)	1277

```
                                          K(Mg+MgL)=1.0
IUPAC evaluation. 37 C,0.15 NaCl: K1=3.22,K(Mg+HL)=1.57. DH(K1)=13.4 kJ m-1
-------------------------------------------------------------------------------
Mg++       cal NaCl   25°C 0.15M C   H                  1990MIa (72952)1278
DH(K1)=-13.3 kJ mol-1, DS(K1)=-74 J K-1 mol-1. Medium: 0.15 M NaCl,
0.015 M KCl, 0.003 M MgCl2, 0.02 M imidazole, pH 7.4
-------------------------------------------------------------------------------
Mg++       gl  KNO3   25°C 0.10M U    M   K1=3.20        1988MBa (72953)1279
-------------------------------------------------------------------------------
Mg++       gl  NaClO4 25°C 0.10M C   H    K1=3.28        1987SCa (72954)1280
                                          B(MgHL)=8.31
DH(K1)=17.53 kJ mol-1, DS=121 J K-1 mol-1
-------------------------------------------------------------------------------
Mg++       nmr R4N.X  22°C 0.10M U                       1985PHb (72955)1281
                                          K(Mg+H5L)=1.21
                                          K(2Mg+H5L)=-0.16
-------------------------------------------------------------------------------
Mg++       gl  KNO3   22°C 0.25M U        K1=2.53        1984GKa (72956)1282
-------------------------------------------------------------------------------
Mg++       nmr KNO3   30°C 0.10M C        K1=4.11        1984PHc (72957)1283
                                          K(Mg+HL)=2.94
                                          *K(MgL)=-5.46
Method: 31P nmr.
-------------------------------------------------------------------------------
Mg++       oth oth/un  RT   dil  C        K1=2.90        1980KRb (72958)1284
Method: effect of [Mg++] on ATP exchange activity. Medium: not stated.
-------------------------------------------------------------------------------
Mg++       ISE oth/un 25°C 0.01M C        K1=4.08        1978AMd (72959)1285
Method: divalent cation selective electrode. Medium: 0.01 M
triethanolamine/HCl buffer, pH 7.0-9.0.
-------------------------------------------------------------------------------
Mg++       gl  KNO3   15°C 0.10M U        K1=3.21        1972FSa (72960)1286
                                          K(Mg+HL)=1.55
-------------------------------------------------------------------------------
Mg++       cal R4N.X  30°C 0.20M U        K1=3.69        1969BSc (72961)1287
Medium: Me4NCl, pH=8.5
-------------------------------------------------------------------------------
Mg++       gl  KNO3   40°C 0.10M U T H    K1=3.30        1967TMf (72962)1288
                                          K(Mg+HL)=1.78
K1=2.94(0.4 C),3.05(12 C),3.17(25 C); K=1.39(0.4 C),1.51(12 C),1.64(25 C).
At 25 C:DH(K1)=15.0 kJ mol-1,DS=113 J K-1 mol-1; DH(Mg+HL)=16.3, DS=88
-------------------------------------------------------------------------------
Mg++       ix  R4N.X  25°C 0.17M U TIH    K1=3.33        1966PGa (72963)1289
Medium: Bu4NBr. At 5 C:K1=3.48(I=0.07),3.24(I=0.1),3.14(I=0.17). At 25 C:
K1=3.65(I=0.07),3.44(I=0.1). Expression for K1 as a function of I at 25 C
-------------------------------------------------------------------------------
Mg++       ix  R4N.X  65°C 0.17M U TIH    K1=3.64        1966PGa (72964)1290
Medium: Bu4NBr. At 45 C:K1=3.83(I=0.07),3.60(I=0.1),3.46(I=0.17). At 65 C:
K1=4.00(I=0.07),3.76(I=0.1). I=0,25 C,DH(K1)=18.0 kJ mol-1, DS=142 J K-1 m-1
-------------------------------------------------------------------------------
```

```
Mg++       ix  R4N.X  25°C  var  U  IH                  1966PGa (72965)1291
Medium: Bu4NBr. DH(Mg+HL)=4 kJ mol-1, DS=60. DH(MgL+H)=-8,DS=75. K(Mg+HL)=
2.45-2.03sqrtI+3.34I-2.04sqrtI/(1+6.02sqrtI). K(MgL+H)=5.38-0.51sqrtI+0.82I
--------------------------------------------------------------------------
Mg++       sp  oth/un 30°C 0.10M U       K1=3.6         1964OPa (72966)1292
Medium: 0.1 M buffer N-ethylmorpholine+HCl
--------------------------------------------------------------------------
Mg++       sp  oth/un 25°C  0.0  U   H   K1=4.10        1963GPb (72967)1293
DH(K1)=24.3 kJ mol-1, DS=159 J K-1 mol-1
--------------------------------------------------------------------------
Mg++       gl  KNO3   25°C 0.10M U       K1=3.17        1962TMa (72968)1294
                                         K(Mg+HL)=1.64
--------------------------------------------------------------------------
Mg++       sp  R4N.X    ?  0.05M U       K2=3.34        1961HBa (72969)1295
                                         K(Mg+HL)=1.5(?)
Medium: Me4NCl. K1 by glass electrode
--------------------------------------------------------------------------
Mg++       sp  R4N.X  25°C 0.10M U TI    K1=3.34        1959BUa (72970)1296
Medium: 0.1 M Bu3EtNBr. K1=3.48(35 C), 3.84(64 C). At I=0.22 M,25 C: K1=3.23
--------------------------------------------------------------------------
Mg++       ix  NaCl   23°C 0.10M U       K1=3.15        1958WAa (72971)1297
--------------------------------------------------------------------------
Mg++       gl  KCl    25°C 0.10M U       K1=3.23        1958WSa (72972)1298
                                         K(Mg+HL)=1.58
--------------------------------------------------------------------------
Mg++       ix  oth/un 23°C 0.10M U       K1=3.04        1957NAc (72973)1299
--------------------------------------------------------------------------
Mg++       gl  KCl    20°C 0.10M U       K1=3.11        1956MSa (72974)1300
                                         K(Mg+HL)=1.5
                                         K(MgL+H)=4.7
--------------------------------------------------------------------------
Mg++       gl  R4N.X  25°C 0.20M U       K1=3.01        1956SAa (72975)1301
                                         K(Mg+HL)=1.45
Medium: 0.2 M n-Pr4NCl
**************************************************************************
C10H15N5O11P2         H4L    GDP             CAS 146-91-8  (4792)
Guanosine-5'-diphosphoric acid;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Mg++       cal R4N.X  30°C 0.20M U                         1973SBb (73022)1302
                                         K(Mg+HL)=3.42
Medium: Me4NBr
**************************************************************************
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
--------------------------------------------------------------------------
Mg++       nmr NaClO4 27°C 3.00M U       K1=-1.0        1982SSb (73049)1303
```

Medium: D2O

****

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

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	25°C	0.50M	U		K1=5.61 K(Mg+HL)=1.47	1990KLa	(73107)1304

DH(K1)=23.8 kJ mol-1, DS=187.1 J K-1 mol-1

Mg++	cal	KNO3	25°C	0.50M	U	H		1989VKa	(73108)1305

DH(K1)=23.76 kJ mol-1, DS(K1)=194.6 J K-1 mol-1

Mg++	gl	KNO3	25°C	0.10M	U		K1=5.82 K(Mg+HL)=2.58 K(Mg+MgL)=2.06	1971GBc	(73109)1306

Mg++	gl	KNO3	20°C	0.10M	U		K1=6.09 K(Mg+HL)=1.78	1968MJa	(73110)1307

By paper electrophoresis: K1=5.6

****

C10H16N2O8 H4L EDTA CAS 60-00-4 (120)

1,2-Diaminoethane-N,N,N',N'-tetraethanoic acid, Sequestric acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	25°C	0.1M	U	I	K1=13.99 K(Mg+HL)=6.86	2004GKb	(73546)1308

In 1.0 mol/L KNO3 K1=13.60; K(Mg+HL)=6.77; K(MgL+H)=3.06

In 0.5 mol/L KNO3 K1=13.63; K(Mg+HL)=4.74; K(MgL+H)=3.04

Mg++	gl	NaCl	37°C	0.15M	C		K1=7.75	1984DMb	(73547)1309

Mg++	gl	R4N.X	25°C	0.15M	C	T H	K1=8.93	1983AMb	(73548)1310

Medium: 0.15-0.77 M Me4NCl. At 10 C, K1=8.86.

DH(K1)=12.1 kJ mol-1, DS(K1)=213 J K-1 mol-1.

Mg++	EMF	KCl	20°C	0.10M	C		K1=9.1	1981SFa	(73549)1311

Method: Pt/H2 electrode.

Mg++	gl	KNO3	20°C	0.10M	C	I	R	K1=8.65	1978ANa	(73550)1312

IUPAC evaluation

Mg++	gl	KNO3	20°C	0.10M	U		K1=8.69	1978NLb	(73551)1313

Mg++	cal	KNO3	25°C	0.5M	U	IH	K1=8.06 DH1=11.97 kJ/mol	1976VBc	(73552)1314

For15 C: K1=8.00, DH1=10.59; 35 C: K1=8.14, DH1=13.68

for 25 C and I=0.3 M K1=8.15; for 25 C and I=1.0 M K1=7.87

```
--------------------------------------------------------------------------------
Mg++       cal KNO3   25°C  0.3M U TI     K1=8.15        1975VBa (73553)1315
                                          DH(K1)=16.3 kJ mol-1
For 15 C DH1=18.04 kJ/mol;
For 35 C DH1=14.9 kJ/mol
--------------------------------------------------------------------------------
Mg++       oth KNO3   20°C 0.10M U        K1=11          1965JMb (73554)1316
Method: electrophoresis
--------------------------------------------------------------------------------
Mg++       gl  KNO3   20°C 0.10M U        K1=8.69        1964ANa (73555)1317
                                          K(Mg+HL)=2.28
--------------------------------------------------------------------------------
Mg++       cal KNO3   20°C 0.10M U   H                   1963ANf (73556)1318
DH(K1)=14.6 kJ mol-1, DS=213 J K-1 mol-1
--------------------------------------------------------------------------------
Mg++       gl  KNO3   25°C 0.10M U T H  T K1=8.64        1960BMc (73557)1319
K1=8.49(0.5 C), 8.57(13.4 C), 8.73(42.4 C); DH(K1)=8 kJ mol-1, DS=197
--------------------------------------------------------------------------------
Mg++       cal none   25°C  0.0  U   H    K1=9.1         1957JAb (73558)1320
DH(K1)=23.0 kJ mol-1, DS=251 J K-1 mol-1
--------------------------------------------------------------------------------
Mg++       ix  none     ?   0.0  U        K1=9.72        1957KFa (73559)1321
--------------------------------------------------------------------------------
Mg++       cal KNO3   20°C 0.10M U   H                   1956CSb (73560)1322
DH(K1)=13.1 kJ mol-1, DS=211 J K-1 mol-1
--------------------------------------------------------------------------------
Mg++       EMF oth/un 25°C  0.0  U   H                   1956MAa (73561)1323
Method: H electrode. DG(K1)=-51.9 kJ mol-1.
--------------------------------------------------------------------------------
Mg++       EMF NaClO4 25°C 0.10M U        K1=8.9         1956SRb (73562)1324
--------------------------------------------------------------------------------
Mg++       cal oth/un 25°C 0.05M U   H                   1954CHa (73563)1325
Medium: Mg(NO3)2. DH(K1)=12.9 kJ mol-1, DS=217 J K-1 mol-1
--------------------------------------------------------------------------------
Mg++       EMF KCl    20°C 0.10M U        K1=8.69        1954SGa (73564)1326
                                          K(Mg+HL)=2.28
Method: H electrode
--------------------------------------------------------------------------------
Mg++       EMF oth/un 20°C  0.0  U   H  T K1=9.12        1947SAa (73565)1327
Method: H electrode. DH(K1)=-12.1 kJ mol-1
********************************************************************************
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
--------------------------------------------------------------------------------
Mg++       gl  KNO3   25°C 0.10M U        K1=5.09        1978SGc (74359)1328
                                          K(Mg+HL)=1.57
                                          K(Mg+MgL)=2.10
********************************************************************************
```

C10H16N2O9 H4L CAS 616-90-0 (2615)
Bis-(2-aminoethylether)-N,N'di(1,3-propanedioic acid); ((HOOC)2CH.NH.CH2.CH2)2O

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	25°C	0.10M	U		K1=3.24	1979KBd	(74374)1329
							K(Mg+HL)=1.96		

****
C10H16N2O11P2 H4L CAS 491-97-4 (7674)
Thymidine-5'-diphosphoric acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaNO3	25°C	0.10M	M			1999SSa	(74387)1330
							K(Mg+HL)=3.34		

****
C10H16N5O12P3S H4L CAS 58976-48-0 (8420)
Adenosine-5'-(1-thiotriphosphoric acid);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	nmr	KNO3	30°C	0.10M	C		K1=4.47	1984PHc	(74400)1331
							K(Mg+HL)=2.94		
							*K(MgL)=-5.12		

Method: 31P nmr. For adenosine-5'-(2-thiophosphoric acid), K1=4.04,
K(Mg+HL)=2.45, *K(MgL)=-5.05.
****
C10H16N5O13P3 H4L ATP CAS 56-65-5 (403)
Adenosine-5'-triphosphoric acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	25°C	0.10M	C	M	K1=3.99	2001AOa	(74643)1332
							K(MgL+A)=1.46		
							B(MgLA)=5.45		
							K(MgL+B)=3.05		
							B(MgLB)=7.04		

K(MgL+C)=2.22, B(MgLC)=6.21. HA=POPSO, HB=HEPPSO and HC=AMPSO.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	25°C	0.10M	C	M	K1=3.99	2000ADa	(74644)1333
							K(MgL+A)=3.48		
							B(MgLA)=7.47		
							K(MgL+B)=3.82		
							B(MgLB)=7.81		

K(MgL+C)=3.43, B(MgLC)=7.42. HA=ACES, HB=MOPSO, HC=CHES.
Also data for TAPSO and DIPSO.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaNO3	25°C	0.10M	C	M	K1=4.30	2000KHa	(74645)1334
							K(MgL+A)=3.49		
							B(MgLA)=7.79		

H2A=salicylhydroxamic acid.

Mg++ gl KCl 25°C 0.25M C T K1=4.48 1996IFa (74646)1335
B(MgHL)=8.9
At 37 C: K1=4.61, B(MgHL)=9.0, B(MgH2L)=11.90, B(Mg2L)=6.21

Mg++ nmr oth/un 25°C 0.02M C H 1996OCa (74647)1336
Method: 25Mg nmr. Medium: 0.02 M Tris, pH 7.5. DH(K1)=15.9 kJ mol-1.

Mg++ cal none 50°C 0 M T H K1=6.17 1995WOa (74648)1337
K(MgL+Mg)=2.82
K(2MgL=Mg2L2)=0.53
DH(K1)=31.6 kJ mol-1, DS=216 J K-1 mol-1; DH(MgL+Mg)=26.2, DS=135; DH(dim)=
=-5.5, DS=-7. At 100 C: K1=7.12, K(MgL+Mg)=3.50, K(dim)=0.41. Also at 125 C

Mg++ nmr oth/un 25°C ? U K1=3.48 1991COa (74649)1338
K(Mg+HL)=0.78

Mg++ gl R4N.X 25°C 0.10M C TIH R K1=4.55 1991SMa (74650)1339
K(Mg+HL)=2.32
K(Mg+MgL)=1.7
IUPAC evaluation. DH(K1)=18.8 kJ mol-1, DH(Mg+HL)=9.6
37 C, 0.15 NaCl: K1=4.34, K(Mg+HL)=2.39

Mg++ gl KCl 25°C 0.10M U M K1=3.60 1990DSb (74651)1340
B(Mg(OH)L)=6.39
K(Mg+HL)=1.62
B(MgL(NTA))=8.84

Mg++ cal NaCl 25°C 0.15M C H 1990MIa (74652)1341
DH(K1)=-18.7 kJ mol-1, DS(K1)=-91J K-1 mol-1. Medium: 0.15 M NaCl,
0.015 M KCl, 0.003 M MgCl2, 0.02 M imidazole, pH 7.4

Mg++ gl NaNO3 25°C 0.50M U TI K1=4.50 1988GDa (74653)1342
B(MgHL)=9.08
B(MgH2L)=12.72
B(Mg2L)=5.53
At 25 C, I=0, K1=6.0, B(MgHL)=10.9, B(MgH2L)=14.6, B(Mg2L)=7.7. At 37 C,
I=0.16 M, K1=4.6, B(MgHL)=9.1, B(MgH2L)=12.6, B(Mg2L)=5.7.

Mg++ gl NaClO4 25°C 0.10M C H K1=4.03 1987SCa (74654)1343
B(MgHL)=8.63
DH(K1)=18.08 kJ mol-1, DS=138 J K-1 mol-1

Mg++ gl NaNO3 25°C 0.10M C K1=4.29 1987STb (74655)1344
K(Mg+HL)=2.42
K(MgL+H)=4.60

Mg++ gl NaClO4 25°C 0.10M U K1=4.365 1986CCc (74656)1345
B(MgHL)=8.57

```
                                        B(MgH2L2)=18.33
-------------------------------------------------------------------------------
Mg++       gl  oth/un 25°C 0.25M U   H    K1=4.54   B2=6.0    1986RSa (74657)1346
                                        B(CoHL)=8.96
-------------------------------------------------------------------------------
Mg++       nmr R4N.X  22°C 0.10M U                    1985PHb (74658)1347
                                        K(Mg+H3L)=2.78
                                        K(Mg+H2L)=3.845
-------------------------------------------------------------------------------
Mg++       gl  KNO3   22°C 0.25M U        K1=2.21        1984GKa (74659)1348
-------------------------------------------------------------------------------
Mg++       ix  NaCl   30°C 0.10M C        K1=3.92        1984JMb (74660)1349
Method: anion exchange. Medium: 0.10 M NaCl, 0.01 M Tris buffer, pH 8.2.
-------------------------------------------------------------------------------
Mg++       nmr KNO3   30°C 0.10M C        K1=4.70        1984PHc (74661)1350
                                        K(Mg+HL)=2.79
                                        *K(MgL)=-4.72
Method: 31P nmr.
-------------------------------------------------------------------------------
Mg++       sp  oth/un 25°C 0.05M C        K1=4.72        1981BKf (74662)1351
                                        K(MgL+Mg)=1.52
Method: by competition with 8-hydroxyquinoline.
Medium: 0.05 M Tris buffer, pH 7.5. K(MgL+Mg) determined by 31P nmr.
-------------------------------------------------------------------------------
Mg++       nmr NaCl   25°C 0.15M C                    1981WPa (74663)1352
                                        K1eff=4.46 (pH=7.0)
Method: 31P nmr.
-------------------------------------------------------------------------------
Mg++       oth oth/un  RT   dil  C        K1=3.90        1980KRb (74664)1353
Method: effect of [Mg++] on ATP exchange activity. Medium: not stated.
-------------------------------------------------------------------------------
Mg++       kin oth/un 25°C 0.02M C                    1980MCd (74665)1354
                                        K1eff=4.81 (pH=8.85)
Method: spectrophotometry. Medium: 0.02 M (NH4)2SO4.
-------------------------------------------------------------------------------
Mg++       gl  R4N.X  70°C 0.20M U  I                 1980RMb (74666)1355
                                        K(MgL+H)=5.36
                                        K(MgHL+H)=3.9
Medium: Me4NCl. In 50% acetonitrile/H2O, K(MgL+H)=5.78
-------------------------------------------------------------------------------
Mg++       sp  oth/un 25°C 0.10M C                    1979MKb (74667)1356
                                        K1eff=4.49
Method: divalent cation selective electrode. Medium: 0.1 M triethanolamine
/HCl buffer, pH 8.0.
-------------------------------------------------------------------------------
Mg++       gl  KNO3   35°C 0.10M C        K1=4.50        1979MTb (74668)1357
                                        K(Mg+HL)=2.77
-------------------------------------------------------------------------------
Mg++       ISE oth/un 25°C 0.01M C        K1=5.15        1978AMd (74669)1358
Method: divalent cation selective electrode. Medium: 0.01 M
```

triethanolamine/HCl buffer, pH 7.0-9.0.

Mg++ gl NaClO4 25°C 0.10M C K1=4.24 1978MSd (74670)1359
B(Mg(phen)L)=6.10
K(Mg(phen)+L)=4.65
K(MgL+phen)=1.86

Mg++ gl NaCl 25°C 0.12M U M K1=4.01 1978RMc (74671)1360
K(MgL+DOPA)=3.67
H3DOPA=3,4-dihydroxyphenylalanine

Mg++ gl R4N.X 20°C 0.10M M K1=4.72 1976PSe (74672)1361
K(Mg+HL)=2.72
Medium: 0.1 M Me4NClO4

Mg++ kin oth/un 20°C 0.00 U K1=4.68 1973LJa (74673)1362
Medium: 0.001 M Tris HCl. tris buffer, pH=8.5

Mg++ gl R4N.X 39°C 0.20M U T K1=4.74 1973SRa (74674)1363
Medium: Me4NBr. K1(3 C)=4.34, K1(17 C)=4.53, K1(26 C)=4.62, K1(30 C)=4.66

Mg++ oth KNO3 15°C 0.10M U 1972FBa (74675)1364
K(2Mg+HL)=1.77

Mg++ gl KNO3 15°C 0.10M U K1=4.05 1972FSa (74676)1365
K(Mg+HL)=2.18

Mg++ sp oth/un 25°C 0.02M U K1=4.50 1971HRa (74677)1366
K(Mg+HL)=1.7
Medium: 0.02 M MgCl2, 0.02 M H4L. Raman spectra

Mg++ ix KCl 25°C 0.10M U 1971YBa (74678)1367
K1eff=3.65
pH=7.4. At pH 8.5: K1eff=4.17

Mg++ sp oth/un 37°C 0.06M U I K1=4.54 1970NOa (74679)1368
tris buffer. I=0.24 M: K1=3.54

Mg++ cal oth/un 30°C 0.20M U K1=4.69 1969BSc (74680)1369
pH=8.5

Mg++ ix R4N.X 25°C 0.17M U TIH K1=4.54 1966PGa (74681)1370
Medium: Bu4NBr. At 5 C:K1=4.46(I=0.07),4.45(I=0.1),4.38(I=0.17); 25 C:4.60
(I=0.07),4.63(I=0.1). At 25 C, I=0: DH(K1)=21.3 kJ mol-1, DS=184 J K-1 mol-1

Mg++ ix R4N.X 25°C var U IH 1966PGa (74682)1371
Medium: Bu4NBr. K(MgL+H)=5.44-1.52sqrtI+2.52I; DH=-5 kJ mol-1,DS=88 J K-1m-1
K(Mg+HL)=3.59-4.06srI+6.36I-2.04srI/(1+6.02srI); DH=8, DS=100

Mg++ gl KNO3 40°C 0.10M U T H K1=4.28 1966TMb (74683)1372

K(Mg+HL)=2.29
K1=3.97(0.4 C),4.10(12 C),4.22(25 C); K=1.95(0.4 C),2.16(12 C),2.24(25 C).
At 25 C:DH(K1)=10.9 kJ mol-1, DS=115 J K-1 mol-1; DH(KMg+HL)=14.2, DS=90

Mg++ gl R4N.X 30°C 0.10M U I K1=4.88 1964OPa (74684)1373
K(Mg+HL)=2.7
Medium: Et4NBr. In 0.1 M N-ethylmorpholine buffer: K1=4.90

Mg++ oth oth/un 23°C 0.10M U K1=4.9 1962AMa (74685)1374
Method: interferometer. Medium: (HOCH2)3CNH2

Mg++ gl KCl 20°C 0.10M U K1=3.84 1962HBa (74686)1375
K(Mg+HL)=2.09
K(Mg+H2L)=1.58

Mg++ gl KNO3 25°C 0.10M U K1=4.22 1962TMb (74687)1376
K(Mg+HL)=2.24

Mg++ sp R4N.X ? 0.50M U K1=3.90 1961HBa (74688)1377
K(Mg+HL)=2.23(?)
Medium: Me4NCl. K1 by glass electrode

Mg++ gl R4N.X 25°C 0.10M U K1=4.43 1961NAa (74689)1378
Medium: Et4NBr. By ion exchange: K1=4.37

Mg++ gl R4N.X 30°C 0.10M U I K1=5.02 1961OPa (74690)1379
K(Mg+HL)=2.90
Medium: Et4NBr. K1=4.30(0.1 M tris buffer), 4.89(triethanolamine buffer),
4.93(N-ethylmorpholine buffer)

Mg++ sp R4N.X 64°C 0.10M U TI K1=4.99 1959BUa (74691)1380
Medium: Bu3EtNBr. K1=4.58(25 C),4.74(37 C). At I=0.2: K1=4.35(25 C)
In 0.1 M KCl: K1=4.25(25 C)

Mg++ ix NaCl 23°C 0.10M U K1=4.04 1958WAa (74692)1381

Mg++ gl KCl 25°C 0.10M U K1=4.04 1958WSa (74693)1382
K(Mg+HL)=2.16

Mg++ ix oth/un 23°C 0.10M U H K1=3.61 1957NAc (74694)1383
DH(K1)=17.2 kJ mol-1, DS=122 J K-1 mol-1

Mg++ gl KCl 20°C 0.10M U K1=4.00 1956MSa (74695)1384
K(Mg+HL)=2.00

Mg++ gl R4N.X 25°C 0.20M U K1=3.47 1956SAa (74696)1385
K(Mg+HL)=1.49
Medium: 0.2 M n-Pr4NCl
****
C10H16N5O14P3 H5L GTP CAS 86-01-1 (404)

Guanosine-5'-triphosphoric acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaNO3	25°C	0.10M	C			2001SBc	(74875)1386
							K(Mg+HL)=4.31		
							K(MgHL+H)=4.8		
							K(Mg+H2L)=2.6		
Mg++	gl	R4N.X	25°C	0.10M	C	T		1991SMa	(74876)1387
							K(Mg+HL)=4.49		
							K(Mg+H2L)=2.31		
IUPAC evaluation									
Mg++	gl	NaClO4	25°C	0.10M	C			1977SIc	(74877)1388
							K(Mg+HL)=4.13		
Mg++	cal	R4N.X	30°C	0.20M	U I	T	K1=4.11	1973SBb	(74878)1389
							K(Mg+HL)=3.93		
							K(Mg+H2L)=2.23		
Medium: Me4NCl. pH=8.5. In 0.2 M Me4NBr K(Mg+HL)=3.93. Also micro constants									
Mg++	gl	KNO3	25°C	0.10M	U	T		1973TRb	(74879)1390
							K(Mg+HL)=4.98		
K(35 C)=5.20, K(45 C)=5.03									
Mg++	ix	NaCl	23°C	0.10M	U			1958WAa	(74880)1391
							K(Mg+HL)=4.02		

****

C10H17NO4 H2L CAS 2848-06-8 (3916)
N-(Cyclohexyl)iminodiethanoic acid; C6H11.N(CH2.COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	20°C	0.10M	U		K1=3.46	1963IFb	(74973)1392

****

C10H17NO5 H2L CAS 6243-06-7 (3326)
N-(2-Hydroxycyclohexyl)iminodiethanoic acid; HO.C6H10.N(CH2.COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KCl	20°C	0.10M	U		K1=4.27	1955ASb	(74985)1393

****

C10H17NO5 H2L (3917)
N-(Tetrahydropyran-2-ylmethyl)iminodiethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	20°C	0.10M	U		K1=3.70	1963IFa	(74999)1394

****

C10H17N2O14P3 H3L TTP CAS 365-08-2 (402)
Thymidine-5'-triphosphoric acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	R4N.X	25°C	0.10M	C	T		1991SMa (75050)	1395
							K(Mg+HL)=4.50		

IUPAC evaluation

Mg++	gl	NaNO3	25°C	0.10M	C			1987STb (75051)	1396
							K(Mg+HL)=4.23		
Mg++	gl	NaClO4	25°C	0.10M	C			1977SIc (75052)	1397
							K(Mg+HL)=4.18		

****

C10H17N3O6S H3L Glutathione CAS 70-18-8 (333)
Glutamyl-cysteinyl-glycine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaClO4	25°C	0.10M	U	TIH	K1=6.385	2001SGd (75112)	1398

Data for 0.05-0.2 M NaClO4 and 15-45 C. DH(K1)=-30.1 kJ mol-1, DS(K1)=-30 J K-1 mol-1. At I=0, K1=6.840. Also data for MeOH/H2O, EtOH/H2O, DMF/H2O.

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C10H17N5O16P4 H7L CAS 228218-4-6 (8418)
Adenosine-3'-(diphosphoric acid)-5'-(diphosphoric acid);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	sp	oth/un	25°C	0.10M	C			1979MKb (75154)	1399
							K1eff=5.10		

Method: divalent cation selective electrode. Medium: 0.1 M triethanolamine /HCl buffer, pH 8.0.

****

C10H17N5O16P4 H5L AQP CAS 1062-98-2 (3341)
Adenosine-5'-tetraphosphoric acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KCl	20°C	0.10M	U		K1=4.22	1957SAa (75157)	1400
							K(Mg+HL)=2.7		
							K(MgL+H)=5.3		

****

C10H17N6O12P3 H4L CAS 4209-30-7 (4795)
Adenyl-5'-yl-imidodiphosphoric acid; adenosine-O.PO(OH).O.PO(OH).NH.PO(OH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	R4N.X	20°C	0.10M	M	T H	K1=5.05	1976PSe (75169)	1401
							K(Mg+HL)=2.84		

Medium: 0.1 M Me4NClO4. At 0 C: K1=5.26, K(Mg+HL)=2.91. DH(K1)=-16 kJ mol-1, DS=12 J K-1 mol-1; DH(Mg+HL)=-5, DS=11

Mg++ ix KCl 25°C 0.10M U 1971YBa (75170)1402
K1eff=4.58
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
Mg++	cal	NaClO4	25°C	0.10M	U	H	K1=4.0	1985EHa	(75202)1403

DH(K1)=6.1 kJ mol-1, DS=97.6 J K-1 mol-1

****

C10H18N2O5 H2L (5608)
1-Oxa-4,7-diazacyclononane-N,N'-diethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	25°C	0.10M	U		K1=3.68	1990CCa	(75230)1404
Mg++	cal	NaClO4	25°C	0.10M	U	H	K1=5.2	1985EHa	(75231)1405

DH(K1)=23.8 kJ mol-1, DS=179.0 J K-1 mol-1

****

C10H18N2O7 H3L HEDTA CAS 150-39-0 (392)
N-(Hydroxyethyl)diaminoethane-N,N',N'-triethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaClO4	30°C	0.10M	U		K1=6.41	1981MMc	(75324)1406
Mg++	cal	KNO3	25°C	0.10M	U	H		1965WHa	(75325)1407

DH(K1)=14.2 kJ mol-1, DS=180 J K-1 mol-1

Mg++	EMF	KNO3	25°C	0.10M	U		K1=7.0	1960HRa	(75326)1408

Mg++	gl	KCl	20°C	0.10M	U		K1=5.78	1959KRa	(75327)1409
							K(Mg+HL)=1.43		

Mg++	gl	oth/un	25°C	0.10M	U		K1=5.2	1953KPb	(75328)1410

****

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
Mg++	gl	KCl	25°C	0.20M	C		K1=3.46	1999FEa	(75567)1411
							B(MgHL)=11.72		
							B(MgH-1L)=-8.21		

****

C10H18N4O8 H4L CAS 35048-92-5 (4751)
Ethylenedinitrilo-N,N'-diacetohydroxamic-N,N'-diethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	25°C	0.10M	U			1971MMe	(75582)1412
							K(Mg+H2L)=3.29		
							K(MgL+H)=8.73		
							K(MgHL+H)=7.54		

****

C10H18N5O19P5 H7L CAS 53951-06-7 (8419)
Adenosine-3'-(diphosphoric acid)-5'-(triphosphoric acid);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	sp	oth/un	25°C	0.10M	C			1979MKb	(75584)1413
							K1eff=5.70		

Method: divalent cation selective electrode. Medium: 0.1 M triethanolamine /HCl buffer, pH 8.0.

****

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
Mg++	gl	KNO3	25°C	0.10M	U		K1=1.4	1974MSa	(75617)1414

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KCl	20°C	0.10M	U		K1=3.6	1955SAa	(75637)1415

****

C10H19N3O4 H2L (8095)
1,4,7-Triazacyclononane-1,4-diethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KCl	25°C	1.0M	U		K1=6.07	2000LKc	(75655)1416

****

C10H20N2O4 H2L CAS 58534-57-9 (2113)
Hexamethylenediamine-N,N-diethanoic acid; H2N(CH2)6.N(CH2.COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	25°C	0.10M	U			1977TIa	(75775)1417
							K(Mg+HL)=2.65		

****

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
Mg++	gl	NaNO3	25°C	0.10M	C		K1=4.34 B(MgHL)=12.47	1989EHa (75797)	1418

****
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
Mg++	gl	KNO3	20°C	0.10M	U		K1=2.8	1970DKa (75833)	1419

****
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
Mg++	sp	oth/un	20°C	0.10M	U		K1=2.8	1972DKa (75844)	1420

****
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
Mg++	gl	oth/un	25°C	0.10M	U		K1=4.8	1953KPb (75851)	1421

****
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
Mg++	con	mixed	25°C	20%	C		K1=4.74	2003SIa (75966)	1422

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	nmr	non-aq	27°C	100%	C		K1=4.74	2000SMg (75967)	1423

Medium: acetonitrile. Method: competitive 7Li nmr technique.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	cal	non-aq	25°C	100%	C	H	K1=3.46	1992BSc (75968)	1424

Medium: propylene carbonate. DH(K1)=-27.5 kJ mol-1, DS(K1)=-26
J K-1 mol-1

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	con	non-aq	25°C	100%	C		K1=4.32	1992STa (75969)	1425

Medium: propylene carbonate.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	vlt	alc/w	25°C	100%	C		K1=2.30	1987CBd (75970)	1426

Medium: methanol, 0.10 M Et4NI or Bu4NClO4. Method: polarography.

****

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
Mg++	gl	NaCl	25°C	0.15M	C		K1=2.34 B(MgH-1L)=-8.54	1990JKa (76430)1427	

****
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
Mg++	con	non-aq	25°C	100%	C	H	K1=2.06	1992BSc (76437)1428	

Medium: propylene carbonate. By calorimetry, DH(K1)=-15.6 kJ mol-1, DS(K1)=-13 J K-1 mol-1.
****
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
Mg++	gl	R4N.X	25°C	1.0M	U		K1=<1 K(Mg+HL) < 1	1962IMb (76714)1429	

****
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
Mg++	gl	oth/un	25°C	0.10M	U		K1=6.40	1959BYa (76756)1430	

****
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
Mg++	gl	NaCl	25°C	0.0	C		K1=1.69 K(Mg+HL)=0.79 K(Mg+H2L)=0.11 K(Mg+H3L)=-0.6 K(Mg+MgL)=0.1	1999SFc (76794)1431	

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
Mg++	gl	KCl	25°C	0.10M	C		K1=7.9	1998BRa (76801)1432	

*K(MgL)=-9.5

****

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
Mg++	gl	NaClO4	25°C	0.10M	U				1976CJa	(76817)1433

K(Mg+H2L)=3.93

****

C11H8N6O8S2 H5L CAS 74385-48-1 (897)
2-(1H-Tetrazol-5-ylazo)chromotropic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Mg++	sp	NaClO4	25°C	0.10M	U				1982PRa	(76948)1434

K(Mg+H2L=MgHL+H)=-5.21

****

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
Mg++	gl	KNO3	30°C	0.15M	U	IH	K1=4.22	B2=8.09	1976SSc	(77111)1435

****

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
Mg++	gl	diox/w	30°C	75%	U		K1=8.10	B2=15.07	1953UFe	(77155)1436

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Mg++	gl	diox/w	35°C	50%	U		K1=2.00	B2=3.76	1971MAa	(77169)1437

Medium: 50% dioxan, 0.01 M NaClO4

****

C11H9NO2 HL CAS 92609-55-3 (4827)
5-Acetyl-8-hydroxyquinoline;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Mg++	gl	diox/w	25°C	60%	U		K1=4.91	B2=9.39	1973SCd	(77326)1438

Medium: 60% dioxan, 0.1 M NaClO4

****

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
---
Mg++ gl diox/w 25°C 70% U K1=7.27 B2=13.43 1992DAc (77347)1439
For N-m-Cl derivative, K1=7.34, K2=6.20; for N-p-Cl, K1=7.64, K2=6.44.
****
C11H9NO3 H2L CAS 80690-05-7 (872)
3-Hydroxy-2-methyl-1,4-naphthoquinone monoxime;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl diox/w 30°C 0.10M U K1=2.43 1981KSa (77362)1440
****
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
---
Mg++ gl diox/w 25°C 70% U K1=7.00 B2=12.87 1992DAc (77389)1441
For N-p-tolyl derivative, K1=7.80, K2=6.62, for N-m-Cl, K1=7.18,
K2=6.03; for N-p-Cl, K1=7.46, K2=6.34.
****
C11H9NO4 H2L CAS 4321-82-7 (4829)
3-Acetyl-4-hydroxycoumarin oxime;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl diox/w 35°C 50% U 1971MAa (77411)1442
K(Mg+HL)=2.37
K(Mg+2HL)=4.37
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
---
Mg++ gl NaNO3 25°C 0.50M M K1=0.09 1998KSa (77667)1443
****
C11H11NO2 HL CAS 35385-27-4 (8689)
8-Hydroxy-(2-hydroxyethyl)quinoline;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ sp KCl 30°C 1.0M M K1=3.60 1996BTa (77767)1444
****
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

---
Mg++ EMF KCl 20°C 0.10M U K1=3.91 1947SWa (77820)1445
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
---
Mg++ EMF KCl 20°C 0.10M C K1=1.38 1947SWa (77843)1446
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
---
Mg++ EMF KCl 20°C 0.10M C K1=1.3 1947SWa (77848)1447
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
---
Mg++ gl alc/w 25°C 0.1M U K1=6.61 2004GMc (77874)1448
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
---
Mg++ gl alc/w 25°C 0.1M U K1=6.60 2004GMc (77887)1449
Medium: 0.1 mol/L KCl in 3:7 EtOH/H2O mixture
****
C11H11N2O2I HL (9227)
3-[4-Iodophenylazo]penta-2,4-dione;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl alc/w 25°C 0.1M U K1=6.71 2004GMc (77898)1450
Medium: 0.1 mol/L KCl in 3:7 EtOH/H2O mixture
****
C11H11N3O4 HL (9230)
3-[4-Nitrophenylazo]penta-2,4-dione;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl alc/w 25°C 0.1M U K1=6.04 2004GMc (77958)1451

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.CH2.CH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Mg++	gl	diox/w	20°C	75%	M	T	K1=9.28	B2=15.81	1980GMd (77965)	1452

****

C11H12N2O2 HL Tryptophan CAS 73-22-3 (3)

2-Amino-3-(3-indolyl)propanoic acid; H2N.CH(CH2.C8H6N)COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Mg++	gl	KNO3	25°C	0.10M	U	M	K1=2.02		1988MBa (78186)	1453
Mg++	gl	KNO3	35°C	0.10M	C	M	K1=2.09		1983KSc (78187)	1454
							K(MgHA+L)=3.06			

A is adenine.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Mg++	gl	NaCl	20°C	0.15M	U	M	K1=1.70		1983VDb (78188)	1455
Mg++	gl	oth/un	20°C	0.01M	U		K2=<4		1950ALa (78189)	1456

****

C11H12N2O2 HL (9226)

3-[Diphenylazo]penta-2,4-dione;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Mg++	gl	alc/w	25°C	0.1M	U		K1=7.22		2004GMc (78249)	1457

Medium: 0.1 mol/L KCl in 3:7 EtOH/H2O mixture

****

C11H12N2O5S HL CAS 56475-09-3 (8410)

3-(4'-Sulfophenylhydrazo)-pentane-2,4-dione;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Mg++	gl	KCl	25°C	0.10M	U	T	K1=6.36		2005ACa (78315)	1458

For 35 C K1=6.26; for 45 C K1=6.14

****

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
Mg++	gl	KNO3	25°C	0.10M	U		K1=2.65		1962ANa (78334)	1459

****

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
Mg++	gl	KNO3	25°C	0.10M	U		K1=1.6		1962ANa	(78337)1460

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
Mg++	gl	KCl	20°C	0.10M	U		K1=6.85		1952SAb	(78341)1461
							K(Mg+HL)=1.84			

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
Mg++	gl	diox/w	20°C	75%	M	T	K1=9.50	B2=15.91	1980GMd	(78371)1462

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Mg++	gl	diox/w	30°C	75%	U		K1=8.65	B2=15.65	1954UFa	(78396)1463

C11H13NO4 H2L CAS 83070-98-8 (3944)
N-Benzylaminobutanedioic acid (N-Benzylaspartic acid)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Mg++	gl	KCl	30°C	0.10M	U		K1=1.74		1966SHc	(78554)1464

C11H13NO4 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
Mg++	gl	oth/un	?	?	U		K1=2.6		1975DTa	(78584)1465
Mg++	gl	KCl	30°C	0.10M	U		K1=3.02		1966SHc	(78585)1466
Mg++	gl	KNO3	25°C	0.10M	U		K1=2.63		1962ANa	(78586)1467

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
Mg++	gl	KCl	20°C	0.10M	U		K1=7.28		1952SAb	(78614)1468

****

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
Mg++	EMF	oth/un	?	?	U		K(Mg+HL)=7.4	1975DTa	(78659)1469

****

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
Mg++	gl	oth/un	25°C	0.0	U		K(Mg+HL)=7.63	1970TTb	(78674)1470

****

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
Mg++	EMF	oth/un	?	?	U		K(Mg+HL)=5.2	1975DTa	(78690)1471

****

C11H14N2O4 H2L (1880)
N-(6-Methyl-2-pyridylmethyl)iminodiethanoic acid; CH3C5H3NCH2N(CH2COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaNO3	20°C	0.10M	C	H	K1=3.0	1981ANb	(78876)1472

DH(K1)=20.1 kJ mol-1 DS=131.4 J K-1 mol-1

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaNO3	25°C	0.50M	C		K1=-0.05	2002KSb	(78956)1473
Mg++	gl	NaNO3	25°C	0.50M	M		K1=-0.01	1991JCa	(78957)1474

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaNO3	25°C	0.10M	C		K1=1.54	1988SMb	(79068)1475
							K(Mg+HL)=0.5		

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Mg++	gl	KCl	25°C	0.10M	U T H		K1=4.55	B2= 6.72	1988CVa (79155)	1476

Data for 0 and 37 C. DH(K1)=-29.3 kJ mol-1, DS(K1)=-10.5 J K-1 mol-1;
DH(K2)=-5.48, DS(K2)=23.5.

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KCl	20°C	0.10M	U		K1=5.3	1966IMa (79164)	1477

****

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
Mg++	gl	KCl	25°C	0.10M	C			1984RFd (79174)	1478
							K(Mg+HL)=3.53		

****

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
Mg++	gl	KNO3	25°C	0.10M	U		K1=9.20	1980KBb (79257)	1479
Mg++	gl	KNO3	20°C	0.10M	U		K1=9.95	1978NLb (79258)	1480
Mg++	gl	KCl	25°C	0.10M	U		K1=10.08	1970AIa (79259)	1481

DL-isomer. For D-isomer, K1=10.05

Mg++	gl	KCl	30°C	0.10M	U		K1=10.29	1963GHa (79260)	1482

****

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
Mg++	cal	KNO3	20°C	0.10M	U	H		1964ANa (79417)	1483

DH(K1)=38.0 kJ mol-1, DS=247 J K-1 mol-1

Mg++	gl	KNO3	20°C	0.10M	U		K1=6.21	1964LAa (79418)	1484
							K(Mg+HL)=3.05		
Mg++	gl	KCl	20°C	0.10M	U		K1=6.02	1948SAa (79419)	1485

```
                                          K(Mg+HL)=2.91
**************************************************************************
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
--------------------------------------------------------------------------
Mg++       gl  KNO3   25°C  0.1M U  I     K1=9.02        2004GKb (79534)1486
                                          K(Mg+HL)=4.79
                                          K(MgL+H)=5.41
In 1.0 mol/L KNO3 K1=8.58; K(Mg+HL)=4.50; K(MgL+H)=5.34
In 0.5 mol/L KNO3 K1=8.64; K(Mg+HL)=4.50; K(MgL+H)=5.36
--------------------------------------------------------------------------
Mg++       gl  KCl    25°C  0.1M C        K1=4.98        2000VGb (79535)1487
Also for I=0.5 M K1=4.24; for I=1.0 M K1=4.10
--------------------------------------------------------------------------
Mg++       oth KNO3   20°C 0.10M U        K1=4.5         1965JMb (79536)1488
Method: electrophoresis
--------------------------------------------------------------------------
Mg++       gl  KCl    20°C 0.10M U        K1=4.93        1964DSc (79537)1489
By polarography: K1=5.25
--------------------------------------------------------------------------
Mg++       gl  KCl    30°C 0.10M U        K1=5.3         1963GHa (79538)1490
--------------------------------------------------------------------------
Mg++       gl  KCl    20°C 0.10M U        K1=4.35        1959KRa (79539)1491
                                          K(Mg+HL)=1.63
**************************************************************************
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
--------------------------------------------------------------------------
Mg++       gl  KNO3   25°C 0.10M U        K1=3.67        1974KGa (79589)1492
                                          K(Mg+HL)=2.44
**************************************************************************
C11H18N5O12P3         H4L                    CAS 5085-65-4  (4875)
Adenylylmethylenediphosphoric acid;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Mg++       ix  KCl    25°C 0.10M U                        1971YBa (79640)1493
                                          K1eff=4.11
pH=7.4. At pH 9.2, K1eff=4.58
**************************************************************************
C11H20N2O5            H2L                      (5609)
1-Oxa-4,8-diazacyclodecane-N,N'-diethanoic acid;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Mg++       cal NaClO4 25°C 0.10M U   H    K1=3.8         1985EHa (79719)1494
```

DH(K1)=13.3 kJ mol-1, DS=118.0 J K-1 mol-1
****
C11H20N4O6 H2L ICRF 198 CAS 108430-47-3 (8369)
N,N'-(1-Methyl-1,2-ethanediyl)bis[N-(2-amino-2-oxoethyl)glycine];

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl NaCl 37°C 0.15M C K1=5.801 B2= 6.91 1982HMb (79728)1495
B(MgHL)=8.896
****
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
---
Mg++ dis non-aq 25°C 100% U K1=1.9 1969PKb (80069)1496
Medium: nitrobenzene
****
C12H6O2Cl4S H2L CAS 97-18-7 (4944)
Bithionol; Cl2.C6H2(OH).S.C6H2(OH).Cl2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl alc/w 25°C 75% U K1=1.6 1970FGa (80098)1497
Medium: 75% EtOH, 1.0 M NaClO4
****
C12H6O12 H6L Mellitic acid (7400)
Benzenehexacarboxylic acid; (C(COOH))6

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ ISE R4N.X 25°C 0 C I K1=6.39 1996RSb (80110)1498
B(MgHL)=13.13
B(MgH3L)=21.7
B(MgH4L)=24.3
B(Mg2H2L)=20.47
B(Mg3L)=12.65. 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
---
Mg++ cal KCl 25°C 0.25M U H K1=1.60 1997MKb (80407)1499
DH(K1)=-7.2 kJ mol-1; DS=7 J K-1 mol-1

Mg++ sp alc/w 25°C 95% U K1=2.93 1993GSa (80408)1500
Medium: 95% w/w EtOH/H2O, 0.05 M Et4NClO4, by competitive spectrophotometry
using murexide as indicator

```
Mg++       sp  non-aq 25°C 100%  U  I     K1=5.11   B2=8.56   1992GSa (80409)1501
Medium: MeCN. In acetone:K1=4.22, K2=2.40; in MeOH:K1=2.14. By fluorimetry
-------------------------------------------------------------------------------
Mg++       EMF KCl    25°C 0.25M U T H    K1=1.55        1985CRa (80410)1502
K1=1.61(10 C);K1=1.49(40 C). DH(K1)=-7.1 kJ mol-1, DS=4 J K-1 mol-1
-------------------------------------------------------------------------------
Mg++       sp  NaClO4 25°C 0.20M U  I     K1=2.48        1983EBa (80411)1503
-------------------------------------------------------------------------------
Mg++       gl  KNO3   35°C 0.10M C        K1=2.21        1979MTb (80412)1504
-------------------------------------------------------------------------------
Mg++       gl  NaClO4 25°C 0.10M C    M   K1=1.45        1978MSd (80413)1505
                                          B(MgL(ATP))=6.10
-------------------------------------------------------------------------------
Mg++       gl  KNO3   20°C 0.10M U        K1=1.2         1963ANg (80414)1506
*******************************************************************************
C12H10N2O2            H2L                    CAS 2050-14-8  (3378)
2,2'-Dihydroxyazobenzene; HO.C6H4.N:N.C6H4.OH
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Mg++       sp  KCl     rt  0.10M U                        1960DEa (80698)1507
                                          K1eff=4.85 (pH 10)
*******************************************************************************
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
-------------------------------------------------------------------------------
Mg++       sp  KCl     rt  0.10M U                        1960DEa (80719)1508
                                          K1eff=3.50 (pH 10)
*******************************************************************************
C12H10O2               HL                     CAS 830-81-9  (3371)
2-Acetyl-1-hydroxynaphthalene;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Mg++       gl  diox/w 30°C  75%  U        K1=7.15   B2=12.70  1954UFa (80797)1509
*******************************************************************************
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
-------------------------------------------------------------------------------
Mg++       gl  diox/w 25°C  70%  U        K1=8.02   B2=14.88  1992DAc (80833)1510
*******************************************************************************
C12H11NO9              H5L                      (3975)
N-(2',5'-Dicarboxy-4'-hydroxyphenyl)iminodiethanoic acid;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
```

Mg++ gl KNO3 25°C 0.10M U 1967UKa (80852)1511
K(Mg+HL)=4.59

****

C12H11N3OS HL (6787)
2-Hydroxy-1-naphthaldehyde thiosemicarbazone;

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

---

Mg++ gl diox/w 20°C 75% U K1=3.39 B2=6.70 1992SSc (80885)1512
Medium: 75% v/v dioxan/H2O and other mixtures, 0.1 M NaClO4

****

C12H11N3O2 HL CAS 50536-09-5 (6323)
2-Hydroxy-1-naphthaldehyde-semicarbazone; HO.C10H6.CH:N.NH.CO.NH2

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

---

Mg++ gl diox/w 20°C 75% U K1=3.21 B2=6.25 1992SSc (80913)1513
Medium: 75% v/v dioxan/H2O and other mixtures, 0.1 M NaClO4

****

C12H12NO6Cl H3L (4004)
(alpha-Carboxy-4'-chlorobenzyl)iminodiethanoic acid;

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

---

Mg++ gl KCl 20°C 0.10M U K1=4.45 1966IMb (80982)1514

****

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

---

Mg++ gl NaCl 37°C 0.15M U K1=3.05 B2=5.95 1984CGb (81065)1515
B(MgH-1L)=-4.65

Mg++ sp KCl 25°C 0.10M U K1=3.0 1978TSb (81066)1516

****

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

---

Mg++ gl NaNO3 25°C 0.50M M K1=-0.04 1998KSd (81101)1517

****

C12H12O4 HL (3374)
Ethyl benzoylpyruvate; C6H5.CO.CH2.CO.CO.O.CH2.CH3

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

---

Mg++ gl diox/w 30°C 75% U K1=7.85 B2=13.90 1954UFa (81169)1518

****

C12H13NO5 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
Mg++	gl	KNO3	25°C	0.10M	U		K1=3.06	1965AUa (81233)	1519

****
C12H13NO5 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
Mg++	gl	KCl	30°C	0.10M	U		K1=3.11	1966SHc (81238)	1520

****
C12H13NO6 H3L CAS 17335-88-5 (3981)
1-(Carboxybenzyl)iminodiethanoic acid; C6H5.CH(COOH).N(CH2.COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KCl	20°C	0.10M	U		K1=4.64	1966IMb (81242)	1521

****
C12H13N2O5Br H2L (4005)
(2'-(4''-Bromoanilino)-2'-oxoethyl)iminodiethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KCl	30°C	0.10M	U		K1=2.06	1966SHc (81260)	1522

****
C12H13N5O4 L Ethenoadenosine CAS 39007-51-7 (6331)
N6-Ethenoadenosine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaNO3	25°C	0.10M	C		K1=<0.3	1983SSc (81318)	1523

Also studied using spoecrophotometry and nmr

****
C12H13O10S H5L (8082)
3-Bis(N,N-carboxymethyl)aminomethyl-2-hydroxy-5-sulphobenzoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KCl	25°C	0.1M	U		K1=8.2	1978TZa (81325)	1524

****
C12H14N5O7P H2L e-AMP CAS 361-99-9 (6334)
1,N6-Ethenoadenosine-5'-monophosphoric acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaClO4	25°C	0.10M	C		K1=1.61	1984SSe (81383)	1525

****

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
Mg++	gl	KCl	25°C	0.10M	C		K1=4.53	1989MMd	(81414)1526
							K(MgL+H)=5.44		
							K(MgL+MgL)=0.1		

****

C12H15NO4 H2L CAS 36369-62-7 (4928)
(Phenethylimino)diethanoic acid; C6H5.CH2.CH2.N(CH2.COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KCl	20°C	0.10M	U		K1=3.12 B2=4.12	1971KTl	(81463)1527
							K(Mg+HL)=1.47		

****

C12H15NO5 H3L (4930)
1-Hydroxy-4-methylphenyl-2-methyleneiminodiethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	oth/un	25°C	0.0	U		K1=6.73	1970TTb	(81495)1528

****

C12H15NO5 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
Mg++	gl	KCl	30°C	0.10M	U		K1=3.03	1966SHc	(81503)1529

****

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
Mg++	gl	KCl	20°C	0.10M	U			1971KTl	(81508)1530
							K(Mg+HL)=3.21		
							K(Mg+2HL)=4.21		
							K(Mg+H2L)=1.51		

****

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
Mg++	gl	KCl	25°C	0.10M	U		K1=3.31	1979TSa	(81600)1531
							K(Mg+HL)=2.81		
							K(Mg+MgL)=2.6		

****
C12H16N5O13P3 H4L e-ATP CAS 37482-17-0 (5714)
1,N6-Ethenoadenosine 5'-triphosphoric acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl NaNO3 25°C 0.10M U K1=4.24 1986SSb (81629)1532
K(Mg+HL)=2.3
K(MgL+H)=4.6
****
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
---
Mg++ sp non-aq 25°C 100% U K1=3.45 2000EGa (81671)1533
Method: fluorescence emission spectroscopy. Medium: acetonitrile.
****
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
---
Mg++ gl NaCl 23°C 0.15M U K1=1.99 1989DBb (81770)1534

Mg++ gl KNO3 45°C 0.10M U T K1=2.62 1981TTa (81771)1535
K(MgL+H)=2.00
5 C: K1 = 2.15

Mg++ gl KNO3 35°C 0.10M U K1=2.84 1978KBa (81772)1536
(Mg+HL)=2.38
****
C12H18N2O5S H2L CAS 80459-15-0 (1595)
2-Nitroso-5-(N-propyl-3-sulfopropylamino)phenol;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl KNO3 25°C 0.10M C K1=2.16 1988YSc (81804)1537
****
C12H18N2O8 H2L CAS 93031-52-8 (5829)
1,4-Dioxa-7,10-diazayclododecane-5,12-dione-7,10-diethanoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl R4N.X 25°C 0.10M C K1=3.67 2002DCb (81830)1538
K(MgL+H)=5.18
Medium: 0.10 M Me4NNO3.
****
C12H18N2O8 H4L CAS 77441-50-0 (2930)
cis-1,4-Diaminocyclohexane-N,N'-di(propanedioic acid)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	25°C	0.10M	U		K1=3.82	1982SGb	(81849)1539

****

C12H18N2O8 H4L (8011)
trans-1,4-Diaminobuten-2-N,N,N',N'-tetraethanoic acid

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KCl	20°C	0.10M	U		K1=3.83	1976TTb	(81890)1540
							K(Mg+HL)=3.15		
							K(MgL+Mg)=2.9		

****

C12H18N2O8 H4L CAS 82481-42-3 (2931)
trans-1,4-Diaminocyclohexane-N,N'-di(propanedioic acid)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	25°C	0.10M	U		K1=2.55	1982SGb	(81898)1541

****

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
Mg++	gl	NaCl	23°C	0.15M	U		K1=3.26	1989DBb	(81939)1542
Mg++	gl	KNO3	45°C	0.10M	U	T	K1=3.55	1981TTa	(81940)1543
							K(MgL+H)=2.46		

5 C: K1 = 2.84

Mg++	gl	KNO3	35°C	0.10M	U		K1=3.68	1978KBa	(81941)1544
							K(Mg+HL)=2.52		

****

C12H18O8S4 H4L CAS 51865-19-1 (1140)
(Butanediylidenetetrathio)tetraethanoic acid; ((HOOC.CH2.S)2.CH.CH2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	EMF	NaClO4	25°C	0.10M	U		K1=3.24	1975JBa	(81965)1545
							K(Mg+HL)=2.48		

****

C12H19NO6 H3L (3991)
N-(2'-Carboxycycloheptyl)iminodiethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KCl	20°C	0.10M	U		K1=6.15	1966IMa	(81980)1546

****

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
Mg++	gl	KNO3	20°C	0.10M	U		K1=10.15	1969NDa	(82019)1547

****
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
Mg++	gl	KNO3	20°C	0.10M	U		K1=3.90	1973DSc	(82055)1548
							K(Mg+HL)=1.4		
Mg++	gl	KNO3	25°C	0.10M	U		K1=3.0	1972GBe	(82056)1549
							K(Mg+HL)=1.26		
							K(Mg+MgL)=2.74		

****
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
Mg++	gl	KNO3	20°C	0.10M	U		K1=8.58	1966MKb	(82124)1550
Mg++	gl	KCl	30°C	0.10M	U		K1=9.41	1963GHa	(82125)1551

****
C12H20N2O8 H4L CAS 40623-42-5 (3388)
1,2-Diaminoethane-N,N'-diethanoic-N,N'-dipropanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KCl	30°C	0.10M	U		K1=6.9	1952CMc	(82157)1552

****
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
Mg++	gl	KNO3	20°C	0.10M	U	H		1964ANa	(82209)1553
							K(Mg+HL)=3.50		

By calorimetry: DH(K1)=35.5 kJ mol-1, DS=226 J K-1 mol-1

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	20°C	0.10M	U		K1=6.23	1964LAa	(82210)1554
Mg++	EMF	KCl	20°C	0.10M	C			1948SAa	(82211)1555
							K(Mg+HL)=3.44		

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
Mg++	gl	KCl	25°C	0.10M	U		K1=11.41(DL) K1=11.38(D)	1970AIa	(82279)1556
Mg++	gl	KCl	20°C	0.10M	U		K1=11.33	1966IPa	(82280)1557
Mg++	gl	KCl	20°C	0.10M	U		K1=11.44	1963MDa	(82281)1558

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	25°C	0.10M	U		K1=5.75 K(Mg+HL)=2.02 K(Mg+MgL)=2.23	1978SGc	(82350)1559

****

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
Mg++	gl	KCl	20°C	0.10M	U		K1=8.84	1966IPa	(82380)1560
Mg++	oth	KNO3	20°C	0.10M	U		K1=10.5	1965JMb	(82381)1561
Method: electrophoresis									
Mg++	gl	KCl	20°C	0.10M	U		K1=8.85 K(Mg+HL)=2.07	1963MDa	(82382)1562

****

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
Mg++	gl	KNO3	20°C	0.10M	U	H	K1=4.61 K(Mg+HL)=3.2	1964ANa	(82446)1563
By calorimetry: DH(K1)=17.3 kJ mol-1, DS=147 J K-1 mol-1									
Mg++	gl	KCl	20°C	0.10M	U		K1=4.61 K(Mg+HL)=3.20	1964PCa	(82447)1564

****

C12H20N2O8S2 H4L (3395)
2,2'-Dithiobisethyleneiminodiethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	25°C	0.10M	U		K1=4.83 K(MgL+H)=8.68 K(Mg+HL)=3.88 B(Mg2L)=7.94	1988PGb	(82486)1565

****

C12H20N2O8Se H4L (4007)
((2,2'-Selenodiethylene)dinitrilo)tetraethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	oth/un	25°C	0.10M	U		K1=6.15 K(Mg+HL)=3.17	1966KLc	(82491)1566

****

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
Mg++	cal	KNO3	25°C	0.10M	U	H		1965WHa	(82520)1567
DH(K1)=15.0 kJ mol-1, DS=209 J K-1 mol-1									
Mg++	gl	KNO3	20°C	0.10M	U	H	K1=8.32 K(Mg+HL)=3.8	1964ANa	(82521)1568
By calorimetry: DH(K1)=14.7 kJ mol-1, DS=209 J K-1 mol-1									
Mg++	gl	KCl	20°C	0.10M	U		K1=8.31 K(Mg+HL)=3.75	1964PCa	(82522)1569

****

C12H20N2O10 H4L CAS 10258-50-1 (3993)
(2,3-Dihydroxytetramethylenedinitrilo)tetraethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	20°C	0.10M	U		K1=4.11 K(Mg+HL)=3.3 K(MgL+Mg)=2.95	1967DSb	(82583)1570

****

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
Mg++	gl	KNO3	20°C	0.10M	C		K1=9.65	1978NLa	(82668)1571

****

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
Mg++	gl	KNO3	20°C	0.10M	U		K1=5.44	1985LBc	(82691)1572

****

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
Mg++	gl	NaNO3	25°C	0.10M	C	T H	K1=9.69 K(MgL+H)=4.6	1987BGc	(82727)1573

DH(K1)=1.7 kJ mol-1. DH(MgL+H)=-32.2 kJ mol-1; DS=20.9 J K-1 mol-1

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	EMF	NaNO3	25°C	0.10M	C		K1=8.93	1985MBb	(82728)1574

****

C12H21N3O6 H3L CAS 111769-28-9 (8145)
Azetidine-2-carboxy-1-(4-azaheptane-1-amino-1,5-dicarboxylic acid);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	oth/un	25°C	0.10M	M		K1=ca.4.5	1983BSd	(82749)1575

Medium: 0.10 M KClO4.

****

C12H22N2O6 H2L (6394)
1,7-Dioxa-4,10-diazacyclododecan-4,10-diethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	R4N.X	25°C	0.10M	C		K1=5.62	1992ADa	(82790)1576

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
Mg++	gl	R4N.X	25°C	0.10M	C		K1=4.79	1992ADa	(82804)1577

Medium: 0.1 M Me4NNO3

****

C12H22N4O6 H2L ICRF 243 (5772)
DL-NN'-Dicarboxamidomethyl-NN'-dicarboxymethyl-2,3-diaminobutane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaCl	37°C	0.15M	U		K1=5.874	1985HCa	(82832)1578

****

C12H22N4O6 H2L ICRF 226 CAS 83266-80-2 (8370)
N,N'-(1-Ethyl-1,2-ethanediyl)bis[N-(2-amino-2-oxoethyl)glycine];

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaCl	37°C	0.15M	C		K1=4.876	1982HMb (82842)	1579

****
C12H22N4O6 H2L ICRF 236 (5771)
meso-NN'-Dicarboxamidomethyl-NN'-dicarboxymethyl-2,3-diaminobutane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaCl	37°C	0.15M	U		K1=2.912	1985HCa (82850)	1580

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	R4N.X	25°C	0.10M	C		K1=6.80 B(MgHL)=13.82	1992ADa (82971)	1581

Medium: 0.1 M Me4NNO3

****
C12H24N2O4 H2L (9225)
5,8-Diaza-4,9-dicarboxydodecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	25°C	0.5M	U		K1=4.78 K(Mg+HL)=4.23	2004FCa (83044)	1582

For 1.0 mol/L KNO3 K1=4.64; K(Mg+HL)=4.17
For 1.5 mol/L KNO3 K1=4.60; K(Mg+HL)=4.17

****
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
Mg++	gl	KCl	25°C	0.10M	C	T H	K1=8.9 B(MgHL)=14.8	1996HSb (83062)	1583

Data for 37 C. By 31P nmr, DH(K1)=4 kJ mol-1; DH(Mg+HL=MgL+H)=57.

****
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
Mg++	gl	KCl	25°C	0.10M	C		K1=5.40	1997HTa (83078)	1584

****

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
Mg++	cal	non-aq	25°C	100%	C	H	K1=<1	1992BSc	(83131)1585

Medium: propylene carbonate. DH(K1)=-3.2 kJ mol-1.

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	EMF	alc/w	25°C	100%	C		K1=3.36	2004ZTa	(83251)1586

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

Mg++	con	mixed	25°C	20%	C		K1=4.61	2003SIa	(83252)1587

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

Mg++	nmr	non-aq	27°C	100%	U	I	K1=2.31	2000SMd	(83253)1588

Competitive method by 7Li nmr. Medium: acetonitrile (AN). Also data for 50% w/w AN/nitrobenzene (K1=2.62) and 50% w/w AN/nitromethane (K1=3.05).

Mg++	con	alc/w	25°C	90%	C	TIH T	K1=2.70	1999SSc	(83254)1589

Medium: 90% w/w MeOH/H2O. Data for 5-40C. DH(K1)=-4.67 kJ mol-1, DS(K1)=35.94 J K-1 mol-1.

Mg++	cal	non-aq	25°C	100%	C	H	K1=1.99	1999WBa	(83255)1590

Medium: N,N-dimethylformamide. DH(K1)=-0.7 kJ mol-1.

Mg++	ISE	mixed	10°C	52%	U	T	K1=2.10	1997BEa	(83256)1591

Medium: 52% w/w CH3CN/H2O. Data for MeCN/H2O mixtures 283-318 K. For 20%, 283K: K1=1.42; 52%, 293 K: K1=1.28; 20%, 293 K: K1=2.04

Mg++	dis	non-aq	25°C	100%	U			1993INa	(83257)1592
							B(MgPL)=3.99		

K is the equilibrium constant for extraction of the metal picrate (P) into CH2Cl2. For extraction from D2O, B=4.07.

Mg++	cal	non-aq	25°C	100%	C	H	K1=2.94	1992BSc	(83258)1593

Medium: propylene carbonate. DH(K1)=-30.2 kJ mol-1, DS(K1)=-45.3 J K-1 mol-1.

Mg++	con	non-aq	25°C	100%	C		K1=4.42	1992STa	(83259)1594

Medium: propylene carbonate.

Mg++	nmr	non-aq	30°C	100%	U	I	K1=3.08	1991ASc	(83260)1595

Medium: nitromethane. In MeCN, K1=2.77.

Mg++ vlt non-aq 25°C 100% C K1=2.63 1991SSb (83261)1596
Method: competitive complexation with Tl+; use of Tl(Hg)/Tl couple.
Medium: acetonitrile, 0.05 M Et4NClO4.

Mg++ sp alc/w 25°C 100% U I K1=3.61 1989KSc (83262)1597
In MeOH. In DMF K1=2.50; in DMSO K1=2.22

Mg++ vlt alc/w 25°C 100% C K1=2.26 1987CBd (83263)1598
Medium: methanol, 0.10 M Et4NI or Bu4NClO4. Method: polarography.

Mg++ nmr non-aq 25°C 100% U K1=2.33 1985BPa (83264)1599
Medium: DMF
****
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
---
Mg++ sp alc/w 25°C 100% U I K1=3.40 1989KSc (83810)1600
In MeOH. In DMF K1=2.37; in DMSO K1=2.06

Mg++ gl R4N.X 25°C 0.10M C K1=1.3 1975ANa (83811)1601
Medium: Me4NCl
****
C12H26O4S HL SDS CAS 151-21-3 (2522)
Dodecyl sulfate; CH3(CH2)11.OSO3H

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ sol oth/un 21°C ? U B2=5.0 1979KBb (83978)1602
B(Mg2L4)=6.6
B(Mg3L6)=7.1
****
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
---
Mg++ con non-aq 25°C 100% C H K1=2.47 1992BSc (83990)1603
Medium: propylene carbonate. By calorimetry, DH(K1)=-17.2 kJ mol-1,
DS(K1)=-11 J K-1 mol-1. By calorimetry, K1=2.57.
****
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
---
Mg++ gl KCl 25°C 0.10M C T H K1=8.0 1996HSb (84095)1604
B(MgHL)=14.5
At 37 C, K1=8.1. By 31P nmr, DH(K1)=11 kJ mol-1; DH(Mg+HL=MgL+H)=62.

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C12H30N3O6P3 H3L (6467)
1,4,7-Tris(methylenemethylphosphinate)-1,4,7-triazacyclononane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KCl	25°C	0.10M	C		K(MgL+H)=5.2	1996HSa (84270)	1605
Mg++	gl	KCl	25°C	0.10M	C	T H	K1=6.66 B(MgHL)=12.76	1996HSb (84271)	1606

Data for 37 C. By 31P nmr, DH(K1)=15 kJ mol-1, DS(K1)=178 J K-1 mol-1;
DH(Mg+HL=MgL+H)=62, DS(Mg+HL=MgL+H)=126.

****

C12H30N3O9P3 H6L DOPHET CAS 123325-12-2 (227)
1,4,7-Tris(beta-dioxyphosphorylethyl)-1,4,7-triazacyclononane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	25°C	1.0M	U		K1=6.10 K(Mg+HL)=2.9	1988MKa (84277)	1607

****

C12H32N4O8P4 H4L (7111)
1,4,7,10-Tetraazacyclododecane-1,4,7,10-tetrayltetramethylenetetrakis(phosphinic acid);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	25°C	0.10M	C		K1=3.50	1995BLa (84388)	1608

****

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
Mg++	gl	R4N.X	25°C	0.10M	M		K1=9.38 B(MgHL)=20.57 B(MgH2L)=30.60 B(MgH3L)= 39.53 B(MgH4L)=46.09	1990DSa (84403)	1609

Medium: Me4NNO3. Binuclear complexes also observed

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	25°C	1.0M	U		K1=7.3 K(Mg+HL)=6.0 K(Mg+H2L)=3.2 K(Mg+H3L)=3.1 K(Mg+H4L)=2.2	1984KMb (84404)	1610

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C13H8O3 HL CAS 719-41-5 (3397)
1-Hydroxyxanthone (1-Hydroxy-9-xanthenone)

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--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Mg++       gl  KCl    25°C 0.10M U        K1=3.75        1986DDa (84493)1611
********************************************************************************
C13H9NOBrCl            HL                        (6173)
N-(2-Hydroxy-5-bromobenzylidene)-4-chloroaniline; Cl.C6H4.N:CH.C6H3(OH)Br
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Mg++       gl  mixed  28°C  75%  U        K1=3.64        1988MNb (84533)1612
********************************************************************************
C13H9NOS               HL                     CAS 3411-95-8  (1683)
2-(2-Hydroxyphenyl)benzothiazole;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Mg++       gl  alc/w  20°C  50%  U        K1=3.1         1959HOa (84549)1613
--------------------------------------------------------------------------------
Mg++       gl  diox/w 39°C  50%  U        K1=3.06        1954CFa (84550)1614
********************************************************************************
C13H9NO2               HL                        (3403)
2-(2'-Hydroxyphenyl)benzoxazole;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Mg++       gl  alc/w  20°C  50%  U        K1=5.2         1959HOa (84563)1615
--------------------------------------------------------------------------------
Mg++       gl  diox/w 40°C  50%  U        K1=4.96   B2=9.08   1954CFa (84564)1616
********************************************************************************
C13H9N3O8S3           H3L                     CAS 28467-51-8  (898)
2-(2-Thiazolylazo)chromotropic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Mg++       sp  NaClO4 25°C 0.10M U                         1982PRa (84662)1617
                                          K(Mg+H2L=MgL+2H)=-12.53
********************************************************************************
C13H10NOBr             HL                        (6171)
N-(2-Hydroxy-5-bromobenzylidene)aniline; C6H5.N:CH.C6H3(OH)Br
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Mg++       gl  diox/w 28°C  75%  U        K1=3.72        1988MNb (84674)1618
********************************************************************************
C13H10N2O              HL                     CAS 5496-07-1  (3404)
2-(2'-Hydroxyphenyl)benzimidazole;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
```

```
Mg++       gl  alc/w  20°C  50%  U        K1=3.5         1959HOa (84825)1619
********************************************************************************
C13H10N2O4            H2L                      CAS 62437-12-1  (4013)
4-(Phenylamino)pyridine-2,6-dicarboxylic acid; C6H5.NH.C5H2N(COOH)2
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Mg++       gl  NaClO4 22°C 0.10M U        K1=2.85        1964BBa (84875)1620
********************************************************************************
C13H10N2O5S           H2L                      CAS 98789-35-6  (5012)
4-Hydroxy-3-formylazobenzene-4'-sulfonic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Mg++       EMF alc/w  25°C  42%  U                        1972DSc (84920)1621
                                        K(Mg+HL=MgL+H)=3.19
                                        K(MgL+HL=MgL2+H)=2.96
Medium: 42% EtOH, 0.2 M NaClO4
********************************************************************************
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
--------------------------------------------------------------------------------
Mg++       gl  KNO3   25°C 0.10M U        K1=4.45   B2=7.49   1964MTc (84936)1622
********************************************************************************
C13H10O3               HL                       CAS 5910-23-6  (3399)
Benzoyl-2-furoylmethane; C6H5.CO.CH2.CO.C4H3O
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Mg++       gl  diox/w 30°C  75%  U        K1=8.37   B2=15.67  1953UFe (84999)1623
********************************************************************************
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
--------------------------------------------------------------------------------
Mg++       sp  non-aq 20°C 100%  C                        1998FLb (85004)1624
                                        K(Mg+HL=MgL+H)=3.54
                                        K(MgL+HL=MgL2+H)=2.80
Method: absorption and fluoroscence spectroscopy. Medium: acetonitrile.
********************************************************************************
C13H11NO               HL                       CAS 779-84-0  (3406)
N-Salicylideneaniline; HO.C6H4.CH:N.C6H5
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Mg++       gl  alc/w  20°C  50%  U        K1=3.4         1959HOa (85034)1625
********************************************************************************
```

C13H11NO2 HL CAS 1761-56-4 (3408)
2-(Salicylideneamino)phenol, Salicylaldehyde-2-hydroxyanil; HO.C6H4.CH:N.C6H4.OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Mg++	gl	alc/w	20°C	50%	U		K1=3.4		1959HOa (85069)	1626

****

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
Mg++	sp	KCl	25°C	0.10M	U		K1=3.3		1978TSb (85216)	1627

****

C13H11N3O5S H3L (5019)
4-Hydroxy-3-oximinomethylazobenzene-4'-sulfonic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Mg++	gl	alc/w	25°C	50%	U		K1=3.40	B2=6.35	1973DSa (85297)	1628

Medium: 42% EtOH, 0.2 M NaClO4

****

C13H12O5 HL CAS 17426-76-5 (3401)
O,O-Dimethylpurpurogallin

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Mg++	gl	diox/w	30°C	50%	U		K1=4.9	B2=8.8	1954BFc (85485)	1629

****

C13H13NO HL CAS 24403-51-8 (3410)
1,2,3,4-Tetrahydro-9-hydroxyacridine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Mg++	gl	diox/w	20°C	50%	U		K1=3.98	B2=7.54	1954IRa (85491)	1630

Medium: 50% dioxan, 0.3 M NaClO4

****

C13H14NO3P H2L CAS 19316-85-7 (1466)
2-Hydroxyphenyl-N-phenylaminomethylphosphinic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Mg++	gl	NaClO4	20°C	0.10M	U		K1=4.60		1985SIb (85561)	1631

****

C13H14N3O5P H2L CAS 80767-75-5 (1467)
2-Hydroxy-4-nitrophenyl-N-(2-pyridylmethyl)aminemethylphosphinic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Mg++	gl	NaClO4	20°C	0.10M	U		K1=5.40		1985SIb (85638)	1632

****

C13H14N3O5P H2L CAS 80767-76-6 (1468)
2-Hydroxy-4-nitrophenyl-N-(3-pyridylmethyl)aminemethylphosphinic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaClO4	20°C	0.10M	U		K1=5.50	1985SIb	(85651)1633

****

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
Mg++	sp	NaNO3	25°C	0.15M	U		K1=0	1953KMa	(85682)1634

****

C13H15NO6 H3L (4999)
2-Benzylnitrilotriethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	oth	oth/un	25°C	0.10M	U		K2=5.44	1962HKa	(85733)1635

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KCl	20°C	0.10M	U		K1=5.17	1966IMa	(85750)1636

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KCl	20°C	0.10M	U		K1=4.74	1966IMb	(85756)1637

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KCl	20°C	0.10M	U		K1=4.75	1966IMb	(85765)1638

****

C13H15N2O3P H2L CAS 80767-72-2 (1460)
2-Hydroxyphenyl-(N-2-pyridylmethylamino)methylphosphinic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaClO4	20°C	0.10M	U		K1=4.70	1985SIa	(85778)1639

****

C13H15N2O3P H2L CAS 80767-73-3 (1461)
2-Hydroxyphenyl-(N-3-pyridylmethylamino)methylphosphinic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaClO4	20°C	0.10M	U		K1=4.60	1985SIa	(85791)1640

****
C13H15N2O3P H2L CAS 80767-74-4 (1462)
2-Hydroxyphenyl-(N-4-pyridylmethylamino)methylphosphinic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaClO4	20°C	0.10M	U		K1=4.72	1985SIa	(85804)1641

****
C13H15N2O4P H3L CAS 80767-78-8 (1463)
2-Hydroxyphenyl-(N-2-pyridylmethylamino)methylphosphonic acid;
C6H4(OH)CH(PO3H2).NH.CH2.C5H4N

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaClO4	20°C	0.10M	U		K1=6.00	1985SIa	(85817)1642

****
C13H15N2O4P H3L CAS 85946-85-6 (1464)
2-Hydroxyphenyl-(N-3-pyridylmethylamino)methylphosphonic acid;
C6H4(OH)CH(PO3H2).NH.CH2.C5H4N

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaClO4	20°C	0.10M	U		K1=6.00	1985SIa	(85830)1643

****
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
Mg++	gl	NaClO4	20°C	0.10M	U		K1=6.05	1985SIa	(85843)1644

****
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
Mg++	gl	KCl	20°C	0.10M	U		K1=3.25 B2=4.25 K(Mg+HL)=1.54	1971KTl	(85979)1645

****
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
-------------------------------------------------------------------------
Mg++       gl  NaClO4 25°C  1.0M C        K1=2.35        1981ASb (85991)1646
*************************************************************************
C13H18N2O4            H2L                     CAS 13933-94-3  (4028)
Pyridoxylidenevaline;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Mg++       sp  oth/un 25°C 0.10M U        K1=<3.5        1961DRa (86042)1647
*************************************************************************
C13H20NO4P            H3L                       (1471)
2-Hydroxyphenyl-N-(cyclohexylamino)methylphosphonic acid;
C6H4(OH)CH(PO3H2).NH.C6H11
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Mg++       gl  NaClO4 20°C 0.10M U        K1=6.05        1985SIb (86088)1648
*************************************************************************
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
-------------------------------------------------------------------------
Mg++       gl  oth/un 20°C 0.10M U        K1=9.05        1960KGa (86109)1649
-------------------------------------------------------------------------
Mg++       gl  KCl    20°C 0.10M U        K1=9.07        1959KRa (86110)1650
                                         K(Mg+HL)=4.32
*************************************************************************
C13H20O8S4            H4L                     CAS 51865-20-4  (1139)
(Pentanediylidenetetrathio)tetra-ethanoic acid; ((HOOCCH2S)2CHCH2)2.CH2
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Mg++       gl  NaClO4 25°C 0.10M U        K1=3.29        1975JBa (86155)1651
*************************************************************************
C13H22N2O8            H4L                     CAS 1798-14-7  (921)
(Pentamethylenedinitrilo)tetraethanoic acid; ((HOOC.CH2)2N.CH2.CH2)2CH2
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Mg++       gl  KNO3   20°C 0.10M U        K1=5.2         1964ANa (86187)1652
                                         K(Mg+HL)=3.6
-------------------------------------------------------------------------
Mg++       EMF KCl    20°C 0.10M C                       1948SAa (86188)1653
                                         K(Mg+HL)=3.63
Method: H electrode
*************************************************************************
C13H22N2O8            H4L                     CAS 1198-14-7  (5004)
1,2-Diaminopentane-N,N,N',N'-tetraethanoic acid; (HOOCCH2)2NCH2CH(C3H7)N(CH2COOH)2
```

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	20°C	0.10M	U		K1=10.15	1969NDa	(86221)1654

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	20°C	0.10M	U		K1=8.27	1981NSc	(86248)1655
							K(MgL+H)=2.92		

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	20°C	0.10M	U		K1=10.30	1969NDa	(86276)1656

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	EMF	KCl	20°C	0.10M	C		K1=7.31	1957SSa	(86394)1657
							K(Mg+HL)=2.92		

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
Mg++	gl	R4N.X	25°C	0.10M	C		K1=2.38	1998CCd	(86408)1658
							*K(MgL)=-10.9		

Medium: 0.10 M Me4NNO3.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	cal	NaClO4	25°C	0.10M	U	H	K1=4.2	1985EHa	(86409)1659

DH(K1)=6.6 kJ mol-1, DS=102.0 J K-1 mol-1

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
Mg++	gl	R4N.X	25°C	0.10M	M			1990DSa	(86584)1660
							B(MgHL)=19.34		
							B(MgH2L)=30.42		
							B(MgH3L)=38.86		

B(MgH4L)=45.43
Medium: Me4NNO3. Binuclear complex 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
---
Mg++ gl KCl 25°C 0.1M U K1=7.17 B2=13.52 2004ACa (86609)1661
****
C14H8O4 H2L Quinizarin CAS 81-64-1 (1060)
1,4-Dihydroxyanthraquinone;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ sp alc/w 20°C 50% U 1982KMd (86663)1662
K(Mg+HL)=4.1
Medium: 50% v/v EtOH/H2O
****
C14H8O5 H3L Purpurine CAS 81-54-9 (8759)
1,2,4-Trihydroxy-9,10-anthraquinone;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ sp alc/w 20°C 50% C 2001ISb (86677)1663
K(Mg+H2L=MgHL+H)=-6.30
*K(MgHL)=-9.82
K(Mg+H2L=MgH2L)=3.97
K(Mg+HL+OH)=8.15
Medium: 50% v/v EtOH/H2O, 0.10 M NaClO4. K(MgHL(OH)+Mg=Mg2L(OH)+H)=-11.59.
K(2Mg+L+OH)=10.55.
****
C14H9NO2 HL CAS 641-63-4 (4038)
2-(2'-Pyridyl)indan-1,3-dione;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl diox/w 30°C 75% U K1=6.36 B2=11.63 1964CMb (86787)1664
****
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
---
Mg++ sp NaCl 25°C 0.50M U 1990DOa (86907)1665
K(Mg+H2L=MgHL+H)=-6.97
K(2Mg+H2L=Mg2L+2H)=-14.7
****
C14H11N5O8S2 H5L CAS 1105-53-9 (5084)
1,5-Bis(2-hydroxy-5-sulfophenyl)-3-cyanoformazan;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaNO3	20°C	0.10M	U		K1=5.29	1971SEa (87016)	1666

C14H12NOBr HL CAS 20772-74-1 (6172)
N-(2-Hydroxy-5-bromobenzylidene)-4-methylaniline; HO(Br)C6H3.CH:N.C6H4.CH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	mixed	28°C	75%	U		K1=4.32	1988MNb (87041)	1667

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
Mg++	sp	KCl	rt	0.10M	U			1960DEa (87209)	1668
							K1eff=3.68 (pH 10)		
Mg++	gl	diox/w	30°C	75%	U			1957SFb (87210)	1669
							K(Mg+H2L=MgL+2H)=-12.6		

C14H13NO2 HL CAS 3290-98-0 (3434)
N-Salicylidene-2-methoxyaniline; HO.C6H4.CH:N.C6H4.OCH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	alc/w	20°C	50%	U		K1=3.1	1959HOa (87520)	1670

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
Mg++	gl	KNO3	25°C	0.10M	U		K1=5.25	1973UWb (87670)	1671

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaClO4	25°C	0.50M	C		K1=6.09	1995CDa (87744)	1672
Mg++	gl	KCl	25°C	0.10M	U		K1=6.16	1990MDa (87745)	1673
							B(MgHL)=9.25		

C14H16NO3P H2L CAS 25881-35-0 (1469)
Phenyl-N-(benzylamino)methylphosphonic acid; C6H5.CH(PO3H2).NH.CH2.C6H5

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaClO4	20°C	0.10M	U		K1=6.00	1985SIb	(87807)1674

C14H16NO4P H3L CAS 61146-25-6 (1470)
2-Hydroxyphenyl-N-(benzylamino)methylphosphonic acid; C6H4(OH)CH(PO3H2).NH.CH2.C6H5

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaClO4	20°C	0.10M	U		K1=6.00	1985SIb	(87820)1675

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaClO4	25°C	0.50M	C		K1=6.40	1995CDa	(87939)1676
Mg++	gl	NaClO4	25°C	1.00M	C	H	K1=6.48	1992NSa	(87940)1677

By calorimetry: DH(K1)=34.3 kJ mol-1, DS=239 J K-1 mol-1

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KCl	30°C	0.10M	U		K1=7.1 K(Mg+HL)=2.6	1963GHa	(87941)1678

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaCl	25°C	0.50M	C		K1=1.298 B(MgHL)=6.436 B(MgH2L)=10.533	1989FRa	(87990)1679

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
Mg++	gl	NaCl	25°C	0.50M	C		K1=1.23	1984RFe	(88011)1680

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
Mg++	gl	NaClO4	20°C	0.10M	U		K1=6.10	1985SIb	(88040)1681

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
Mg++	con	mixed	25°C	20%	C		K1=4.41	2003SIa (88235)1682	

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

Mg++	sp	non-aq	25°C	100%	U		K1=10.78	2000EGa (88236)1683	

Method: fluorescence emission spectroscopy. Medium: acetonitrile.

Mg++	nmr	non-aq	27°C	100%	C		K1=4.48	2000SMg (88237)1684	

Medium: acetonitrile. Method: competitive 7Li nmr technique.

Mg++	sp	non-aq	rt	100%	U		K1=>7	1992BFa (88238)1685	

Medium: CH3CN

Mg++	vlt	non-aq	25°C	100%	C		K1=2.46	1991SSb (88239)1686	

Method: competitive complexation with Tl+; use of Tl(Hg)/Tl couple.
Medium: acetonitrile, 0.05 M Et4NClO4.

Mg++	sp	alc/w	25°C	100%	U	I	K1=2.27	1989KSc (88240)1687	

In MeOH. In DMF, K1 <2; in DMSO, K1<2

****

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
Mg++	gl	KCl	20°C	0.10M	U		K1=8.39	1959KRa (88428)1688	
							K(Mg+HL)=2.12		

****

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
Mg++	gl	alc/w	25°C	99%	U		K1=10.2	1972RBa (88565)1689	

Medium: 99% MeOH, 0.1 M NaClO4

Mg++	cal	KNO3	25°C	0.10M	U	H		1965WHa (88566)1690	

DH(K1)=6.7 kJ mol-1, DS=217 J K-1 mol-1

Mg++	cal	KNO3	20°C	0.10M	U	T H		1963ANb (88567)1691	

DH(K1)=15.9 kJ mol-1, DS=264 J K-1 mol-1

Mg++	cal	KNO3	20°C	0.10M	U	H	K1=10.97	1963ANf (88568)1692	

DH(K1)=15.9 kJ mol-1, DS=264 J K-1 mol-1

Mg++	gl	KNO3	25°C	0.10M	U	T H	K1=10.41	1960BMb (88569)1693	

K1=10.45(0 C), 10.31(42.4 C). DH(K1)=-6.3 kJ mol-1, DS=180 J K-1 mol-1

Mg++ EMF KCl 20°C 0.10M C K1=10.32 1954SGa (88570)1694
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
---
Mg++ EMF KCl 20°C 0.10M C K1=4.64 1949SAa (88832)1695
K(Mg+HL)=3.14
K(Mg+MgL)=2.42
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
---
Mg++ EMF KCl 20°C 0.10M C K1=4.30 1949SAa (88848)1696
K(Mg+HL)=3.04
K(Mg+MgL)=2.32
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
---
Mg++ gl diox/w 24°C 50% U K1=7.1 1979ACa (88991)1697
****
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
---
Mg++ gl NaClO4 25°C 0.10M U K1=1.92 1975PJa (88999)1698
****
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
---
Mg++ gl KNO3 25°C 0.1M C TI R K1=9.3 2005AAa (89137)1699
IUPAC recommended value. Provisional value, 37 C, 0.15 NaCl: K1=8.56,
K(MgL+H)=6.98, K(MgHL+H)=4.64, K(MgH2L+H)=3.74

Mg++ gl NaCl 37°C 0.15M C K1=8.56 B2=10.63 1984DMb (89138)1700
B(MgHL)=15.53
B(MgH2L)=20.20
B(MgH3L)=23.94

```
------------------------------------------------------------------------------
Mg++       cal KNO3   27°C 0.10M U   H                  1968CLd (89139)1701
DH(K1)=10.9 kJ mol-1, DS=209 J K-1 mol-1
------------------------------------------------------------------------------
Mg++       gl  KNO3   25°C 0.10M U       K1=9.3         1968WRa (89140)1702
------------------------------------------------------------------------------
Mg++       cal KNO3   20°C 0.10M U T H                  1965ANa (89141)1703
DH(K1)=12.5 kJ mol-1, DS=219 J K-1 mol-1
------------------------------------------------------------------------------
Mg++       cal KNO3   25°C 0.10M U   H                  1965WHa (89142)1704
DH(K1)=15.0 kJ mol-1, DS=226 J K-1 mol-1
------------------------------------------------------------------------------
Mg++       gl  KNO3   25°C 0.10M C       K1=9.3         1960WAa (89143)1705
                                         K(MgL+H)=6.9
******************************************************************************
C14H24N2O7            H3L                      (3440)
N-(2-Hydroxycyclohexyl)ethylenediamine-N,N',N'-triethanoic acid;
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Mg++       gl  KCl    20°C 0.10M U       K1=4.35         1959KRa (89491)1706
                                         K(Mg+HL)=1.63
******************************************************************************
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
------------------------------------------------------------------------------
Mg++       gl  KNO3   20°C 0.10M U       K1=7.83         1969NDc (89503)1707
******************************************************************************
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
------------------------------------------------------------------------------
Mg++       gl  KNO3   25°C 0.10M U       K1=4.21         1969GKb (89563)1708
                                         K(Mg+HL)=3.36
                                         B(Mg2L)=2.30
------------------------------------------------------------------------------
Mg++       gl  KNO3   20°C 0.10M U       K1=4.8          1964ANa (89564)1709
                                         K(Mg+HL)=3.66
******************************************************************************
C14H24N2O8            H4L                     CAS 1633-00-7  (5076)
4-Methyl-1,2-diaminopentane-N,N,N',N'-tetraethanoic acid;
(HOOCCH2)2NCH2CH(N(CH2COOH)2CH2CH(CH3)2
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Mg++       gl  KNO3   20°C 0.10M U       K1=10.16        1969NDa (89627)1710
******************************************************************************
```

C14H24N2O8 H4L EDTP (2936)
Diaminoethane-N,N,N',N'-tetrapropanoic acid; (HOOC.CH2CH2)2N.CH2CH2.N(CH2CH2.COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KCl	30°C	0.10M	U		K1=1.8	1953CCb	(89676)1711

****

C14H24N2O9 H4L CAS 87720-52-3 (1593)
2,2'-Oxybis(propyliminodiethanoic acid)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KCl	20°C	0.10M	U		K1=4.8 K(Mg+HL)=3.92	1961ISa	(89706)1712
Mg++	gl	KCl	20°C	0.10M	U		K1=7.92 K(Mg+HL)=4.51	1961KGa	(89707)1713
Mg++	gl	oth/un	25°C	0.10M	U		K1=6.9 K(Mg+HL)=4.5	1953KPa	(89708)1714

****

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
Mg++	gl	KCl	20°C	0.10M	U		K1=4.8 K(Mg+HL)=3.92	1961ISa	(89723)1715

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KCl	20°C	0.10M	C		K1=5.30 K(Mg+HL)=3.47	1985SMg	(89827)1716
Mg++	gl	KNO3	25°C	0.10M	U		K1=4.72 K(MgL+H)=9.5 K(MgL+2H)=7.2	1982JGa	(89828)1717
Mg++	gl	NaCl	25°C	0.70M	U		K1=5.40 Medium: seawater	1974JAb	(89829)1718
Mg++	gl	alc/w	25°C	99%	U		K1=6.3 Medium: 99% MeOH, 0.1 M NaClO4	1972RBa	(89830)1719
Mg++	gl	KNO3	25°C	0.10M	U		K1=5.2	1968WRa	(89831)1720
Mg++	cal	KCl	25°C	0.10M	U	H		1965BBe	(89832)1721

DH(K1)=23.0 kJ mol-1, DS=178 J K-1 mol-1

Mg++ cal KNO3 25°C 0.10M U H 1965WHa (89833)1722
DH(K1)=18.4 kJ mol-1, DS=167 J K-1 mol-1

Mg++ gl KNO3 20°C 0.10M U H K1=5.2 1964ANa (89834)1723
K(Mg+HL)=3.4
By calorimetry: DH(K1)=21.7 kJ mol-1, DS=174 J K-1 mol-1

Mg++ EMF KCl 20°C 0.10M C K1=5.21 1964PCa (89835)1724
K(Mg+HL)=3.37
Method: H electrode

Mg++ gl oth/un 25°C 0.10M U K1=5.4 1957SRa (89836)1725

****

C14H24N2O10 H4L (2655)
N,N'-Bis(2-hydroxyethane)-N,N'-ethanediaminedibutanedioic acid;

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

---

Mg++ gl KNO3 25°C 0.1M U K1=5.85 1985MGb (89975)1726

****

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

---

Mg++ gl R4N.X 25°C 0.10M U K1=10.25 1988ADa (90078)1727
K(Mg+HL)=4.31

****

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

---

Mg++ cal R4N.X 25°C 0.10M U H 1989DSa (90171)1728
DH(MgL)=15.9 kJ mol-1; DS=197.

Mg++ gl R4N.X 25°C 0.10M C K1=7.534 1987DDb (90172)1729

Mg++ gl R4N.X 25°C 0.10M M K1=7.42 1986COb (90173)1730

****

C14H26N4O6 H3L DOTRA (6701)
1,4,7,10-Tetraazacyclododecane-1,4,7-triethanoic acid;

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

---

Mg++ gl R4N.X 25°C 0.10M M K1=9.79 1996CHc (90243)1731
Medium: 0.1 M Me4NCl.

****

C14H26N4O6 H2L (4690)
Hexanoic acid bis(3-hydroxycarbamoyl-propyl)amide;
HONHCO(CH2)3NHCO(CH2)4CONH(CH2)3COHNOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KCl	25°C	0.20M	C		K1=4.11 B(MgHL)=12.51 B(MgH-1L)=-7.65	1999FEa	(90263)1732

****
C14H28N2O4 L Cryptand 2,1,1 CAS 31250-06-3 (836)
1,10-Diaza-4,7,13,18-tetraoxabicyclo[8,5,5]eicosane (2,1,1);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	R4N.X	25°C	0.05M	C	I	K1=2.5	1975LSc	(90344)1733

In 95% MeOH, 0.05 M Me4NBr: K1=4.0
****
C14H30N2O4 L CAS 31255-13-7 (2448)
N,N'-Dimethyl-cyclo-1,10-diaza-4,7,13,16-tetraoxaoctadecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	alc/w	25°C	95%	C		K1=3.18	2004KVa	(90571)1734

Medium: 95% MeOH/H2O, 0.01 M Et4NClO4.
****
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
Mg++	gl	R4N.X	25°C	0.10M	C		K1=2	1995LLa	(90625)1735

Medium: Et4NClO4
****
C14H30O7 L CAS 1072-40-8 (2499)
2,5,8,11,14,17,20-Heptaoxaheneicosane; CH3.O.(CH2.CH2.O)6.CH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	con	non-aq	25°C	100%	C	H	K1=2.11	1992BSc	(90684)1736

Medium: propylene carbonate. By calorimetry, DH(K1)=-22.8 kJ mol-1,
DS(K1)=-36.2 J K-1 mol-1.
****
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
Mg++	gl	KCl	25°C	0.10M	C		K1=<3	1998BRa	(90840)1737

****

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
Mg++	gl	R4N.X	25°C	0.10M	M		B(MgHL)=19.07 B(MgH2L)=30.35 B(MgH3L)=38.48 B(MgH4L)=45.43	1990DSa (90869)	1738

Medium: Me4NNO3

****

C15H11NO2 HL CAS 55022-23-6 (4061)
2-(6'-Methyl-2'-pyridyl)indan-1,3-dione;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	diox/w	30°C	75%	U		K1=6.86 B2=13.30	1964CMb (91061)	1739

****

C15H11N3 L CAS 1148-79-4 (488)
2,2':6'2"-Terpyridine; C5H4N.C5H3N.C5H4N

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	sp	NaClO4	25°C	0.20M	U	I	K1=0.844	1983EBa (91150)	1740
Mg++	ISE	oth/un	25°C	0.10M	C	I	K1=0.77	1980ELb (91151)	1741

****

C15H11N3O2 L CAS 74378-23-7 (2745)
Phenanthrenequinone monosemicarbazone; C14H8(:O)(:N.NH.CO.NH2)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaClO4	25°C	0.10M	C	TIH	K1=5.75 B2=10.20	1985SMa (91303)	1742

****

C15H12OS HL (1261)
mono-Thiodibenzoylmethane; C6H5.CO.CH2.CS.C6H5

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	diox/w	25°C	75%	U		B2=6.1	1968MSa (91486)	1743

Medium: 75% dioxan, 0.05 M NaClO4

****

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
Mg++	gl	diox/w	20°C	17%	C		K1=7.86 B2=14.83	1976JWa (91535)	1744

Mg++ gl diox/w 30°C 75% U K1=8.54 B2=16.21 1953UFe (91536)1745
****
C15H12O3 H2L CAS 1469-94-9 (3445)
2-Hydroxydibenzoylmethane; HO.C6H4.CO.CH2.CO.C6H5

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl diox/w 30°C 75% U K1=8.14 B2=15.14 1955HOa (91604)1746
****
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
---
Mg++ gl diox/w 30°C 75% M K1=4.61 2000ANa (91687)1747
Medium: 75% v/v dioxan/H2O, 0.10 M NaClO4. Data for an extensive series of
4'-substituted phenylimino derivatives.
****
C15H14N2O5S HL (9232)
3-(5-Sulphonylnaphthylazo)penta-2,4-dione;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl KCl 25°C 0.1M U H K1=6.70 2004ACb (91734)1748
for 35 C K1=6.60; for 45 C K1=6.46
****
C15H14O3 HL (5102)
2-Hydroxy-4-benzyloxy acetophenone; C6H5.CH2.O.C6H3(OH).CO.CH3

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl diox/w 30°C 75% U K1=3.03 1970KDa (91779)1749
Medium: 75% dioxan, 0.1 M NaClO4
****
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
---
Mg++ sp KCl 22°C 0.14M C 2000RGa (91971)1750
K1eff=2.11
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
---
Mg++ oth oth/un 25°C 0.10M U K1=3.4 1969RMa (92061)1751

****

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
Mg++	gl	NaClO4	25°C	0.50M	C		K1=6.80	1995CDa (92081)1752	

****

C15H18N2O8 H4L (6114)
2,5-Toluenediamine-N,N'-disuccinic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaCl	25°C	0.50M	C		K1=0.934	1989FRa (92093)1753	

****

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
Mg++	gl	KCl	25°C	0.10M	U		K1=9.5	1984VOb (92130)1754	

For the 4-methoxy derivative: K1=7.3; for the 4-dimethylamino derivative, K1=7.4.

****

C15H20N2O6 H3L BEDTA CAS 65311-06-0 (2944)
N-Benzyldiaminoethane-N,N',N'-triethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KCl	25°C	0.10M	U		K1=6.72	2003SVa (92146)1755	
							K(Mg+HL)=1.79		

****

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
Mg++	gl	KCl	25°C	0.10M	C		K1=8.4	1995KHa (92245)1756	

****

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
Mg++	gl	KNO3	25°C	0.10M	U		K1=9.21	1968MMb (92318)1757	
							K(Mg+HL)=6.46		
							K(Mg+H2L)=2.8		

****

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
--------------------------------------------------------------------------------
Mg++       gl  NaClO4 25°C 0.10M U        K1=2.20        1975PJa (92352)1758
********************************************************************************
C15H27N3O6            H3L                        (6514)
1,5,9-Triazacyclododecane-N,N',N"-triethanoic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Mg++       gl  R4N.X  25°C 0.10M M        K1=7.1         1990CBc (92464)1759
Medium: Me4NCl
********************************************************************************
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
--------------------------------------------------------------------------------
Mg++       gl  NaCl   25°C 0.15M U        K1=<2          1995BGa (92494)1760
********************************************************************************
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
--------------------------------------------------------------------------------
Mg++       gl  R4N.X  25°C 0.10M C  I     K1=2.3         1991DLa (92516)1761
In 95% v/v MeOH/H2O: K1=3.25
********************************************************************************
C15H36N3O9P3          H3L                        (6749)
1,4,7-Triazacyclononane-N,N'N''-tris(methylenephosphonatemonoethylester)
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Mg++       gl  R4N.X  25°C 0.10M C        K1=6.2         1992LRa (92610)1762
********************************************************************************
C15H36N6                L                      CAS 82261-26-5  (587)
15-(4-Aminobutyl)-1,4,7,10,13-pentazacyclohexadecane;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Mg++       gl  NaClO4 25°C 0.10M U        K1=2.5         1982FKa (92622)1763
********************************************************************************
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
--------------------------------------------------------------------------------
Mg++       gl  mixed  25°C  75%  U        K1=5.72        1972MCb (92646)1764
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
---
Mg++ gl mixed 25°C 75% U K1=6.54 1972MCb (92696)1765
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
---
Mg++ gl mixed 25°C 75% U K1=6.03 1972MCb (92711)1766
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
---
Mg++ gl mixed 25°C 75% U K1=6.42 1972MCb (92726)1767
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
---
Mg++ gl mixed 25°C 75% U K1=6.73 1972MCb (92741)1768
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
---
Mg++ gl diox/w 30°C 75% U K1=11.05 1957SFb (92758)1769
K(Mg+H2L=MgL+2H)=-12.9
****
C16H11N3O3 HL CAS 6410-09-9 (5151)
1-(2-Nitrophenylazo)-2-hydroxynaphthalene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl mixed 25°C 75% U K1=3.07 1972MCb (92795)1770
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
-------------------------------------------------------------------------------
Mg++       gl  mixed  25°C  75%  U        K1=3.88        1972MCb (92810)1771
Medium: 75% acetone, 0.1 M KNO3
*******************************************************************************
C16H11N3O3S            HL                    CAS 35778-69-9  (4090)
Diphenylthiovioluric acid;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Mg++       gl  diox/w 30°C  75%  U        K1=2.79        1973CSb (92824)1772
Medium: 75% dioxan, 0.1 M NaClO4
*******************************************************************************
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
-------------------------------------------------------------------------------
Mg++       gl  diox/w 30°C  75%  U        K1=10.34       1957SFb (92844)1773
                                         K(Mg+H2L=MgL+2H)=-10.9
*******************************************************************************
C16H11N3O10S2          H4L    Chromotrope 2B   CAS 548-80-1  (896)
2-((4-Nitrophenyl)azo)chromotropic acid;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Mg++       sp  NaClO4 25°C 0.10M U                         1982PRa (92860)1774
                                         K(Mg+H2L=MgHL+H)=-5.27
*******************************************************************************
C16H12N2O              HL                    CAS 842-07-9  (5156)
1-Phenylazo-2-hydroxynaphthalene;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Mg++       gl  mixed  25°C  75%  U        K1=7.29        1972MCb (92916)1775
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
-------------------------------------------------------------------------------
Mg++       gl  mixed  25°C  75%  U                       1972MCb (92947)1776
                                         K(Mg+HL)=7.26
Medium: 75% acetone, 0.1 M KNO3
-------------------------------------------------------------------------------
Mg++       sp  KCl     rt  0.10M U                       1960DEa (92948)1777
                                         K1eff=4.59 (pH 10)
-------------------------------------------------------------------------------
```

Mg++ gl diox/w 30°C 75% U K1=10.93 1957SFb (92949)1778
K(Mg+H2L=MgL+2H)=-13.7
****
C16H12N2O2 H2L CAS 14934-27-1 (5157)
1-(4-Hydroxyphenylazo)-2-hydroxynaphthalene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl mixed 25°C 75% U 1972MCb (92968)1779
K(Mg+HL)=7.02
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
---
Mg++ gl mixed 25°C 75% U K1=3.52 1972MCb (92995)1780
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
---
Mg++ sp oth/un 25°C 0.0 U K1=8.6 B2=13.6 1962CRa (93020)1781
****
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
---
Mg++ gl KNO3 25°C 0.10M U 1971KMb (93057)1782
K(Mg+HL)=3.64

Mg++ gl KNO3 25°C 0.10M U 1968NMb (93058)1783
K(Mg+HL)=3.64
****
C16H12N2O9S2 H5L CAS 26197-92-2 (4094)
2-(2'-Hydroxyphenylazo)chromotropic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl KNO3 25°C 0.10M U 1968NMb (93074)1784
K(Mg+HL)=6.15
****
C16H12N2O11S3 H5L (4095)
2-(2'-Sulphophenylazo)chromotropic acid;

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

---
Mg++ gl KNO3 25°C 0.10M U 1968NMb (93081)1785
K(Mg+HL)=3.58
****
C16H12N2O12S3 H6L CAS 25849-37-0 (4096)
2-(2'-Hydroxy-5'-sulfophenylazo)chromotropic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ sp NaNO3 20°C 0.20M U 1966BBd (93102)1786
B(MgH3L2)=46.6
****
C16H13N2OCl HL CAS 36458-49-8 (5181)
2-(4-Chlorophenylaminomethyl)-8-hydroxyquinoline;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl diox/w 25°C 50% U K1=4.5 1972HUb (93167)1787
Medium: 50% v/v dioxan, 0.1 M KCl
****
C16H13N2O10AsS2 H5L Thorin I CAS 3688-92-4 (2609)
1-((2-Arsonophenyl)azo)-2-hydroxy-3,6-naphthalyldisulfonic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl KNO3 25°C 0.10M U K1=5.20 1971KTc (93182)1788

Mg++ gl oth/un 30°C ? U K1=5.9 1964PCa (93183)1789
****
C16H13N2O10AsS2 H5L (5204)
2-(2-Arsonophenylazo)-1-hydroxynaphthalene-3,6-disulfonic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl KNO3 25°C 0.10M U K1=5.35 1971KTc (93224)1790
****
C16H13N2O10PS2 H5L (5205)
1-(2-Phosphonophenylazo)-2-hydroxynaphthalene-3,6-disulfonic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl KNO3 25°C 0.10M U K1=4.83 1971KMa (93229)1791
****
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
---
Mg++ gl KNO3 25°C 0.10M U K1=5.53 1971KTc (93245)1792

Mg++ gl KNO3 25°C 0.10M U 1968NMb (93246)1793
K(Mg+HL)=5.58
****
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
---
Mg++ sp KCl ? 0.10M U K1=3.81 1960DEa (93290)1794
****
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
---
Mg++ sp KCl rt 0.10M U 1960DEa (93293)1795
K1eff=4.50 (pH 10)
****
C16H14N2O2 H2L CAS 36458-47-6 (5158)
2-(2-Hydroxyphenylaminomethyl)-8-hydroxyquinoline;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl diox/w 25°C 50% U K1=5.17 1972HUa (93426)1796
K(Mg+HL)=4.52
Medium: 50% v/v dioxan, 0.1 M KCl
****
C16H14N4O2 H2L (3467)
5-Hydroxy-4-(2-hydroxyphenylazo)-3-methyl-1-phenylpyrazole;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl diox/w 30°C 75% U K1=10.94 1952SNa (93471)1797
K(Mg+H2L=MgL+2H)=-12.8
****
C16H14N4O4S HL (5183)
3-Methyl-1-phenyl-4-(2-sulfophenylazo)-5-pyrazolone;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl diox/w 30°C 75% U K1=5.10 1969SSc (93493)1798
****
C16H14N4O4S HL (5184)
5-Methyl-1-phenyl-4-(2-sulfophenylazo)-3-pyrazolone;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl diox/w 30°C 75% U K1=5.37 1969SSc (93505)1799
****
C16H14O3 HL CAS 41126-22-1 (3457)

2-Methoxydibenzoylmethane; CH3.O.C6H4.CO.CH2.CO.C6H5

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	diox/w	30°C	75%	U		K1=8.71 B2=15.83	1955HOa (93550)	1800

****

C16H15NO7 H4L (4082)
N-(3-Carboxy-2-hydroxynaphthy-1-ylmethyl)iminodiethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KCl	25°C	0.10M	U		K1=9.1	1975TRb (93629)	1801

****

C16H16N2O6S2 HL Cephalothin CAS 153-61-7 (9104)
3-(Acetoxylmethyl)-8-oxo-7-(2-thienylacetylamino)-5-thia-1-azabicyclo[4.2.0]oct-2-ene-carboxylic

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaClO4	25°C	0.10M	C		K1=5.070 B2= 8.15	2001SGe (93711)	1802

****

C16H18O8S4 H4L CAS 51865-21-5 (239)
1,2-Dimethylbenzene-tetrathioethanoic acid; C6H4(CH(S.CH2.COOH)2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	EMF	NaClO4	25°C	0.10M	U		K1=3.78	1975JBa (93886)	1803
							K(Mg+HL)=3.45		

****

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
Mg++	gl	KNO3	20°C	0.10M	U		K1=9.40	1989SLa (94028)	1804
Mg++	gl	KNO3	20°C	0.10M	U		K1=9.40	1969NDb (94029)	1805
Mg++	gl	KCl	25°C	0.10M	U		K1=9.14	1967OTb (94030)	1806

****

C16H20N2O10 H6L (704)
1,2-Dihydroxy-3,6-di-(methyleneiminodiethanoic acid)-benzene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	25°C	0.10M	C		K1=8.24	1988ZHa (94063)	1807
							K(Mg+H2L)=5.62		
							K(Mg+HL)=7.47		
							K(MgHL+H)=9.29		
							K(MgL+H)=11.10		

B(Mg2L)=14.81

****

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
Mg++	gl	oth/un	25°C	0.0	U		K(Mg+HL)=6.8 K(Mg+H2L)=5.0 K(Mg+H3L)=1.8 K(2Mg+HL)=15.2	1970TTb (94075)	1808

****

C16H22N2O4P2 H2L (7262)
1,2-Diaminoethane-N,N'-bis(methylenephenylphosphinic acid); (CH2NHCH2PO(OH)C6H5)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	R4N.X	25°C	0.10M	M		K1=3.14	1996BCa (94126)	1809

Medium: 0.1 M Me4NNO3.

****

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
Mg++	gl	NaNO3	25°C	0.10M	U		K1=6.36	1979PBa (94317)	1810

****

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
Mg++	gl	R4N.X	25°C	0.10M	M		K1=3.3 B(MgHL)=8.0	1991FGb (94489)	1811

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
Mg++	sp	non-aq	RT	100%	C		K1=2.51	2001AVa (94511)	1812

Method: spectrophotometric titration. Medium: acetonitrile.

****

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

Mg++ gl R4N.X 25°C 0.10M C K1=3.02 2002DCb (94563)1813
K(MgL+H)=5.67
Medium: 0.10 M Me4NNO3.
****
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
---
Mg++ gl NaClO4 25°C 0.10M U K1=2.20 1975PJa (94638)1814
****
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
---
Mg++ gl KCl 25°C 0.10M C K1=4.61 1995IOa (94663)1815
****
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
---
Mg++ gl KNO3 20°C 0.10M U K1=5.20 1969NDc (94705)1816
****
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
---
Mg++ gl KNO3 20°C 0.10M U K1=7.96 1969NDc (94731)1817
****
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
---
Mg++ gl KNO3 20°C 0.10M U K1=10.16 1979MBd (94757)1818
****
C16H28N2O8 H4L (2850)
1,8-Diaminooctane-N,N,N',N'-tetraethanoic acid; ((HOOCCH2)2N(CH2)4)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl KNO3 20°C 0.10M U K1=4.8 1964ANa (94790)1819
K(Mg+HL)=3.66
****
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
--------------------------------------------------------------------------------
Mg++       gl  R4N.X  25°C 0.10M M        K1=11.79       1996CHc (94870)1820
Medium: 0.1 M Me4NCl.
--------------------------------------------------------------------------------
Mg++       gl  KCl    25°C 0.10M C        K1=11.15       1991CMb (94871)1821
--------------------------------------------------------------------------------
Mg++       cal R4N.X  25°C 0.10M C   H                   1984DFa (94872)1822
Medium: 0.10 M Me4NNO3. DH(K1)=7.9 kJ mol-1, DS(K1)=255 J K-1 mol-1.
--------------------------------------------------------------------------------
Mg++       gl  R4N.X  25°C 0.10M C        K1=13.64       1982DSa (94873)1823
                                          K(Mg+HL)=3.917
--------------------------------------------------------------------------------
Mg++       EMF KCl    20°C 0.10M C        K1=11.0        1981SFa (94874)1824
Method: Pt/H2 electrode.
--------------------------------------------------------------------------------
Mg++       gl  KCl    20°C 0.10M U        K1=11.03       1976SFb (94875)1825
********************************************************************************
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
--------------------------------------------------------------------------------
Mg++       gl  R4N.X  25°C 0.10M C        K1=7.34        2000CDd (94961)1826
Medium: 0.10 M (Me4N)NO3.
********************************************************************************
C16H30N4O8            H4L                        (3473)
N,N'-Dimethyl-2,2'-ethylenedi-iminobis(ethylenediethanoic acid);
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Mg++       gl  KCl    20°C 0.10M U        K1=4.31        1964PCa (95081)1827
                                          K(Mg+HL)=3.30
********************************************************************************
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
--------------------------------------------------------------------------------
Mg++       gl  R4N.X  25°C 0.05M C  I     K1=<2          1975LSc (95174)1828
In 95% MeOH: K1 < 2
********************************************************************************
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
--------------------------------------------------------------------------------
Mg++       gl  KCl    25°C 0.10M C        K1=7.0         1997HTa (95326)1829
********************************************************************************
```

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
---
Mg++ gl NaClO4 25°C 0.50M U K1=<2 1981KMb (95333)1830
****
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
---
Mg++ gl R4N.X 25°C 0.10M C K1=2 1995LLa (95411)1831
Medium: Et4NClO4
****
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
---
Mg++ gl R4N.X 25°C 0.10M C K1=2 1995LLa (95444)1832
Medium: Et4NClO4

Mg++ gl NaClO4 25°C 0.50M U K1=<2 1981KMb (95445)1833
****
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
---
Mg++ gl R4N.X 25°C 0.10M U K1=2.4 1978LMa (95469)1834
****
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
---
Mg++ gl R4N.X 25°C 0.10M C K1=2.86 2000DFb (95568)1835
Medium: 0.10 M Et4NClO4.
****
C17H12N2O3 H2L (2040)
1-(2-Carboxyphenylazo)-2-hydroxynaphthalene; HOOC.C6H4.N:N.C10H6.OH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ sp KCl rt 0.10M U 1960DEa (95701)1836
K1eff=2.10 (pH 10)
****
C17H12N2O10S2 H5L CAS 3440-76-4 (4119)
2-(2'-Carboxyphenylazo)chromotropic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	25°C	0.10M	U			1971KMb	(95717)1837
							K(Mg+HL)=4.53		
Mg++	gl	KNO3	25°C	0.10M	U			1968NMb	(95718)1838
							K(Mg+HL)=4.55		

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	mixed	25°C	75%	U		K1=7.26	1972MCb	(95793)1839

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
Mg++	gl	mixed	25°C	75%	U		K1=7.76	1972MCb	(95808)1840

Medium: 75% acetone, 0.1 M KNO3

C17H14N2O2 HL CAS 1229-55-6 (5216)
1-(2-Methoxyphenylazo)-2-hydroxynaphthalene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	mixed	25°C	75%	U		K1=7.96	1972MCb	(95827)1841

Medium: 75% acetone, 0.1 M KNO3

C17H14N2O2 HL CAS 13441-91-1 (5217)
1-(4-Methoxyphenylazo)-2-hydroxynaphthalene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	mixed	25°C	75%	U		K1=7.55	1972MCb	(95842)1842

Medium: 75% acetone, 0.1 M KNO3

C17H14N2O8S2 H4L CAS 15475-90-8 (2605)
2-(2-Tolylazo)-chromotropic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	25°C	0.10M	U			1971KMb	(95939)1843
							K(Mg+HL)=3.47		

C17H14N2O9S2 H4L (5228)

2-(2-Methoxyphenylazo)chromotropic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Mg++	gl	KNO3	25°C	0.10M	U				1971KMb (95943)	1844
							K(Mg+HL)=3.95			

****

C17H16N2O HL CAS 36458-48-7 (5219)
2-(4-Tolylaminomethyl)-8-hydroxyquinoline;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Mg++	gl	diox/w	25°C	50%	U		K1=4.2		1972HUb (96024)	1845

Medium: 50% v/v dioxan, 0.1 M KCl

****

C17H16O4 H2L CAS 58134-82-0 (6193)
Benzoyl-2-hydroxy-4-methoxy-3-methylacetophenone;
C6H5.CO.CH2.CO.C6H2(OH)(OCH3)(CH3)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Mg++	gl	mixed	30°C	60%	M	I	K1=4.34	B2=7.88	1991GDb (96145)	1846

Medium: 60%v/v acetone/water; 0.1M NaClO4; data also for 65% and 75%; for
75% v/v dioxane/water and EtOH/water.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Mg++	gl	mixed	30°C	60%	M	I	K1=4.34	B2=7.88	1991GDc (96146)	1847

Medium: 60%v/v acetone/water; 0.1M NaClO4; data also for 65% and 75%; for
75% v/v dioxane/water and EtOH/water

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Mg++	gl	alc/w	30°C	75%	M	TI	K1=4.66	B2=8.05	1990DGc (96147)	1848

Medium: 75% v/v EtOH/H2O

****

C17H16O4 HL CAS 18362-51-1 (3485)
Di-2-methoxybenzoylmethane; CH3.O.C6H4.CO.CH2.CO.C6H4.O.CH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Mg++	gl	diox/w	30°C	75%	U		K1=8.55		1955HOa (96171)	1849

****

C17H16O6 HL (4111)
2-Hydroxy-2',4',4-trimethoxydibenzoyl; HO.C6H4.CO.CO.C6H2(OCH3)3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Mg++	gl	NaClO4	?	0.10M	U		K1=3.61	B2=6.84	1963DSa (96181)	1850

****

C17H20N4O6 HL Riboflavin CAS 83-88-5 (1438)
7,8-Dimethyl-10(D-1'-ribityl)isoalloxazine, Vitamin B2, Vitamin H

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

```
------------------------------------------------------------------------------
Mg++       sol oth/un 22°C       U        K1=0.47        1980LDa (96335)1851
Medium: variable Mg(ClO4)2 content 0.1-0.9 M
The same constant measured spectrophotometrically: K1=-0.69
******************************************************************************
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
------------------------------------------------------------------------------
Mg++       ix  NaCl   23°C 0.10M U        K1=2.03        1958WAa (96386)1852
******************************************************************************
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
------------------------------------------------------------------------------
Mg++       EMF KCl    20°C 0.10M C        K1=8.0         1952SAb (96403)1853
                                          K(Mg+HL)=6.8
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
------------------------------------------------------------------------------
Mg++       gl  R4N.X  25°C 0.10M C        K1=11.82       1997DQa (96451)1854
                                          K(MgL+H)=3.70
Medium:Me4NNO3
------------------------------------------------------------------------------
Mg++       EMF KCl    20°C 0.10M C        K1=7.2         1981SFa (96452)1855
Method: Pt/H2 electrode.
******************************************************************************
C17H27NO5               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
------------------------------------------------------------------------------
Mg++       sp  alc/w   RT   10%  C        K1=0.9         2002GNe (96543)1856
Medium: 10% v/v MeOH/H2O, pH 7.4 (0.1M Tris buffer), 0.1 M Me4NCl.
******************************************************************************
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
------------------------------------------------------------------------------
Mg++       gl  NaClO4 25°C 0.10M U        K1=2.21        1975PJa (96563)1857
******************************************************************************
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
---
Mg++ gl KCl 25°C 0.10M C K1=8.18 1991CMb (96637)1858
K(MgL+H)=8.12

Mg++ gl KNO3 25°C 0.10M C K1=7.620 1982DSa (96638)1859
K(Mg+HL)=2.781

Mg++ EMF KCl 20°C 0.10M C K1=6.4 1981SFa (96639)1860
Method: Pt/H2 electrode.

Mg++ gl KCl 20°C 0.10M U K1=6.36 1976SFb (96640)1861
****
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
---
Mg++ sp alc/w RT 80% C K1=3.64 1994HWc (96670)1862
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
---
Mg++ gl R4N.X 25°C 0.10M C K1=3.46 2000CDd (96680)1863
Medium: 0.10 M (Me4N)NO3.
****
C17H32N4O6 H3L (7253)
1,4,7,10-Tetraazacyclododecane-1-propyl-4,7,10-triethanoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl R4N.X 25°C 0.10M M K1=9.35 1996CHc (96693)1864
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
---
Mg++ gl R4N.X 25°C 0.10M M K1=9.70 1996CHc (96710)1865
Medium: 0.1 M Me4NCl.
****
C17H32N4O8 H3L (7255)
1,4,7,10-Tetraazacyclododecane-1-(2,3-dihydroxypropyl)-4,7,10-triethanoic acid;

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

---
Mg++ gl R4N.X 25°C 0.10M M K1=9.72 1996CHc (96724)1866
Medium: 0.1 M Me4NCl
****
C17H34N4O4S L CAS 503465-04-1 (9247)
4,7,13,16-Tetraoxa-1,10,21,23-tetraazabicyclo[8.8.7]pentacosane-22-thione;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl alc/w 25°C 95% C K1=2.12 2004KVa (96755)1867
Medium: 95% MeOH/H2O, 0.01 M Et4NClO4.
****
C18H11NO2 HL CAS 83-08-9 (4126)
2-(2'-Quinolyl)indan-1,3-dione;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl diox/w 30°C 75% U K1=7.33 1964CMb (96840)1868
****
C18H12N2O11S2 H5L (5251)
2-(2'-Oxalophenylazo)chromotropic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl KNO3 25°C 0.10M U 1971KMb (96867)1869
K(Mg+HL)=4.45
****
C18H14N2O3 H3L (4127)
2-(2',4'-Dihydroxyphenylazo)-4-phenylphenol;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ sp KCl rt 0.10M U 1960DEa (96916)1870
K1eff=3.68 (pH 10)
****
C18H14N2O9S2 H4L (5252)
2-(2'-Methyl-benzoylazo)chromotropic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl KNO3 25°C 0.10M U 1971KMb (96934)1871
K(Mg+HL)=3.66
****
C18H14N2O10S2 H5L (5253)
2-(2-Phenylethanoic acidazo)chromotropic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl KNO3 25°C 0.10M U 1971KMb (96938)1872
K(Mg+HL)=4.00

****

C18H14N2O11S2 H5L (4132)
2-(2'-(Carboxyhydroxymethyl)phenylazo)chromotropic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	25°C	0.10M	U			1971KMb	(96944)1873
							K(Mg+HL)=3.96		

****

C18H14N2O11S2 H5L (4133)
2-(2'-(Carboxymethoxy)phenylazo)chromotropic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	25°C	0.10M	U			1971KMb	(96951)1874
							K(Mg+HL)=4.31		

****

C18H16N4O3S HL (3505)
(2-(4,5-Dihydro-3-methyl-5-oxo-1-phenyl-1H-pyrazol-4-yl)azophenylthio)ethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	diox/w	30°C	75%	U		K1=3.9	1962SCc	(97198)1875

****

C18H16N4O4 H2L (3500)
2-(4,5-Dihydro-3-methyl-5-oxo-1-phenyl-1H-pyrazol-4-ylazo)phenoxyethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	diox/w	30°C	75%	U		K1=5.71	1962SCc	(97209)1876

****

C18H18O8 H2L (5631)
1,4-bis(2-Carboxymethoxyphenyl)-1,4-dioxabutane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	alc/w	25°C	90%	M		K1=1.27	1998KLa	(97302)1877

Medium: 90% v/v MeOH/H2O, 0.1 M Me4NCl

****

C18H20N2O6 H4L CAS 10328-28-6 (3501)
Ethylenedinitrilo-N,N'-bis(2'-hydroxyphenyl)-N,N'-diethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	25°C	0.10M	C		K1=14.4	1992GVa	(97391)1878
							K(Mg+HL)=10.3		
							K(Mg+H2L)=6.0		
							*K(MgH2L)=-7.2		
							*K(MgHL)=-9.5		

```
--------------------------------------------------------------------------------
Mg++       gl  KNO3   25°C 0.10M U        K1=8.0         1958FFa (97392)1879
                                          K(Mg+HL)=5.2
                                          K(Mg+H2L)=2.9
********************************************************************************
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
--------------------------------------------------------------------------------
Mg++       gl  KCl    25°C 0.10M C        K1=8.9         1995KHa (97470)1880
********************************************************************************
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
--------------------------------------------------------------------------------
Mg++       gl  KNO3   25°C 0.10M U        K1=10.28       1970YKa (97526)1881
********************************************************************************
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
--------------------------------------------------------------------------------
Mg++       gl  oth/un 25°C 0.10M U        K1=5.5         1965LCa (97538)1882
********************************************************************************
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
--------------------------------------------------------------------------------
Mg++       gl  diox/w 24°C  50%  U        K1=6.6         1979ACa (97559)1883
********************************************************************************
C18H24N6O9            H3L    BAMTPH           CAS 87834-24-0  (5915)
N,N',N"-Tris(3-(hydroxyamino)-3-oxopropyl)-1,3,5-benzenetricarboxamide;
C6H3(CONHCH2CH2CONHOH)3
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Mg++       gl  NaNO3  25°C 0.10M C        K1=6.42        1989EHa (97619)1884
                                          B(MgHL)=15.11
********************************************************************************
C18H26N6                L                          (6628)
3,6,14,17,23,24-Hexaazatricyclo[17.3.1.1]tetracosa-1(23),8,10,12(24),19,21-hexaene;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Mg++       gl  KCl    25°C 0.10M M        K1=2.6         1996MBb (97711)1885
********************************************************************************
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
Mg++	gl	KNO3	25°C	0.10M	C		K1=7.95 K(Mg+H2L)=3.04 K(MgL+H)=11.05 K(MgHL+H)=9.10	1975MMc (97740)	1886

****

C18H28N4O4 H2L (7378)
7-Methyl-3,7,11,17-tetraazabicyclo[11.3.1]heptadeca-1(17),13,15-triene-3,11-diethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	R4N.X	25°C	0.10M	C		K1=5.3 K(Mg(OH)L+H)=8.74	1997CDb (97783)	1887

Medium: NMe4NO3

****

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
Mg++	EMF	non-aq	25°C	100%	U		K1=6.72	1982MRb (97800)	1888

Medium: anhydrous propylene carbonate, 0.1M Et4NClO4

****

C18H28O6 H2L O(EAcAcE)2O CAS 73199-63-0 (2251)
1,11-Dioxacycloeicosane-5,7,15,17-tetraone;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	diox/w	24°C	50%	U		K1=7.2	1979ACa (97829)	1889

****

C18H28O10 H2L (OEOAcAcOE)2 CAS 62950-36-1 (2254)
1,4,10,13,16,22-Hexaoxacyclotetracosa-6,8,18,20-tetraone;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	diox/w	24°C	50%	U		K1=7.4	1979ACa (97867)	1890

****

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
Mg++	gl	NaCl	25°C	0.15M	U		K1=2.53	1995BGa (97925)	1891

****

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
Mg++	EMF	KCl	20°C	0.10M	C		K1=7.5 K(Mg+HL)=5.5	1964PCa (97940)	1892

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
Mg++	ISE	KNO3	25°C	0.10M	U		K1=8.43	1970HAa (98003)	1893
By glass electrode : K1=8.10, K(MgL+H)=9.30, B(Mg2L)=5.95									
Mg++	gl	KNO3	25°C	0.10M	U		K(MgHL+H)=4.65 K(MgL+H)=9.31 B(Mg2L)=13.9	1967BMd (98004)	1894
Mg++	gl	KNO3	25°C	0.10M	U		K1=8.43 K(Mg+H2L)=2.81 K(Mg+HL)=7.55 K(MgL+Mg)=5.5 K(Mg2L+Mg)=3.10	1965BMf (98005)	1895
Mg++	gl	KCl	30°C	0.10M	U		K1=8.47 K(Mg+H2L)=1.9 K(Mg+HL)=7.39 K(MgL+Mg)=5.94	1963GHa (98006)	1896

****

C18H31N5O8 H3L CAS 165196-67-8 (8858)
1,4,7-Tris(carboxymethyl)-1,4,7,10,15-pentaazacycloheptane-9,16-dione;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KCl	25°C	0.10M	C		K1=4.88	1995IOa (98128)	1897

****

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
Mg++	gl	KCl	25°C	0.10M	C		K1=3.01	1991CMb (98183)	1898
Mg++	gl	KNO3	25°C	0.10M	C		K1=1.967 K(Mg+HL)=1.743	1982DSa (98184)	1899
Mg++	EMF	KCl	20°C	0.10M	C		K1=3.0	1981SFa (98185)	1900

Method: Pt/H2 electrode.

Mg++ gl KCl 20°C 0.10M U K1=3.02 1976SFb (98186)1901
****
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
---
Mg++ EMF KCl 20°C 0.10M C K1=7.5 1981SFa (98244)1902
Method: Pt/H2 electrode. For the 3-ethyl- derivative, K1=6.4;
for the 3,3-dimethyl- derivative, K1=4.5
****
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
---
Mg++ gl R4N.X 25°C 0.10M C K1=7.31 1999CDb (98254)1903
K(MgL+Mg)=2.5
Medium: 0.10 M NMe4NO3.
****
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
---
Mg++ gl R4N.X 25°C 0.10M M K1=9.71 1996CHc (98367)1904
Medium: 0.1 M Me4NCl
****
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
---
Mg++ gl alc/w 25°C 95% M K1=<2 1990LNa (98412)1905
Medium: 95% MeOH, 0.05 M Bu4NBr. For the 9,16-dihydroxy- analogue: K1=4.32
****
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
---
Mg++ EMF non-aq 25°C 100% C H K1=10.73 1992BSc (98511)1906
Medium: propylene carbonate. Method: disproportionate titration with Ag.
By calorimetry, DH(K1)=-39 kJ mol-1, DS(K1)=73.8 J K-1 mol-1.

Mg++ gl R4N.X 25°C 0.05M C I K1=<2 1975LSc (98512)1907
In 95% MeOH: K1 < 2
****

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
---
Mg++ gl KCl 25°C 0.10M C K1=8.0 1997HTa (98788)1908
****
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
---
Mg++ gl R4N.X 25°C 0.10M C K1=2 1995LLa (98836)1909
Medium: Et4NClO4
****
C18H38N4O8P2 H6L CAS 187240-55-7 (7347)
1,4,7,10-Tetraazacyclododecane-1,7-bis(ethanoic
acid)-4,10-bis(methylene-ethylphosphinic acid);

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl KCl 25°C 0.10M C K1=7.63 1997HTa (98866)1910
****
C18H38N4O10P2 H6L CAS 187240-54-6 (7346)
1,4,7,10-Tetraazacyclododecane-1,7-bis(ethanoic
acid)-4,10-bis(ethylmethyenephosphonic acid);

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl KCl 25°C 0.10M C K1=7.5 1997HTa (98870)1911
****
C18H40N4O4 L CAS 89066-60-2 (867)
N,N',N",N"'-Tetrakis(2-hydroxyethyl)-1,4,8,11-tetraazacyclotetradecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl NaNO3 25°C 0.10M U K1=1.86 1984MMc (98921)1912
****
C19H16N2O2 HL CAS 29126-31-6 (8348)
N-[4-[[(2-Hydroxy-1-naphthalenyl)methylene]amino]phenyl] acetamide;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl diox/w 25°C 75% U K1=5.20 B2= 9.83 1981MGb (99157)1913
Medium: 75% dioxane/H2O, 0.10 M NaClO4.
****
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

---
Mg++ gl NaClO4 25°C 0.10M U T M K1=4.48 B2= 7.13 2000CCe (99191)1914
K(MgL+ala)=4.16
Also data at 35 C.
****
C19H18N4O3S H2L (4145)
4-(2'-(2''-Carboxyethylthio)Phe-azo)-3-Me-1-Phe-pyrazole-5(2H)-one;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl diox/w 30°C 75% U K1=3.4 1965SMh (99228)1915
****
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
---
Mg++ gl diox/w 30°C 75% U K1=4.6 1965SMh (99248)1916
****
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
---
Mg++ gl alc/w 20°C 50% U K1=1.21 1957WSa (99294)1917
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
---
Mg++ gl NaCl 25°C 0.10M C K1=8.81 2004SGb (99326)1918
B(MgHL)=17.33
B(MgH2L)=25.57
Additional method: UV-visible spectrometry
****
C19H28N4O6 H3L CAS 106967-44-6 (8973)
3,7,11-Tris(carboxymethyl)-3,7,11,17-tetraazabicyclo[11.3.1]heptadeca-1(17),13,15-t
riene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl R4N.X 25°C 0.10M C K1=2.89 1998CDa (99406)1919
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

---
Mg++ gl R4N.X 25°C 0.10M U K1=1.9 1978LMa (99488)1920
****
C20H13N3O7S H3L Eriochrome Bl T CAS 1787-61-7 (997)
1-(1-Hydroxy-2-naphthylazo)-6-nitro-2-naphthol-4-sulfonic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ sp non-aq 25°C 100% U 1973PCa (99557)1921
K(Mg+HL=MgL+H)=5.02
K(Mg+H2L=MgL+2H)=3.97
Medium: CH3CN

Mg++ sp oth/un 18°C 0.08M U K1=7.0 1948SBa (99558)1922
****
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
---
Mg++ sp oth/un 18°C 0.08M U K1=7.2 1948SBa (99583)1923
****
C20H14N2O HL (5291)
1-(1-Naphthylazo)-2-hydroxynaphthalene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl mixed 25°C 75% U K1=6.44 1972MCb (99597)1924
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
---
Mg++ gl mixed 25°C 75% U K1=7.10 1972MCb (99612)1925
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
---
Mg++ gl diox/w 30°C 75% U 1957SFb (99626)1926
K(Mg+H2L=MgL+2H)=-12.8
****
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
Mg++	vlt	NaCl	25°C	0.20M	C			1985GSb (99642)	1927
							K1eff=3.36		

Method: polarography. Data for 10-40 C. Medium: 0.2 M NH3/0.2 M NH4Cl, pH 10.9

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	sp	oth/un	18°C	0.08M	U		K1=7.4	1948SBa (99643)	1928

****

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
Mg++	sp	oth/un	25°C	0.10M	U		K1=7.64	1957HRa (99684)	1929
Mg++	sp	oth/un	18°C	0.08M	U		K1=7.56	1948SBa (99685)	1930

****

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
Mg++	sp	none	25°C	0.0	U			1980WNa (99723)	1931
							K(Mg+HL=MgL+H)=6.83		

Data for similar ligands also included

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	sp	none	25°C	0.0	U			1978BRb (99724)	1932
							K1eff=3.43		

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
Mg++	gl	diox/w	25°C	50%	U		K1=4.6	1972HUb (99762)	1933

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
Mg++	gl	mixed	25°C	80%	C		K1=6.28	1997HMc (99772)	1934
							B(MgHL)=14.56		

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
--------------------------------------------------------------------------------
Mg++       gl  diox/w 30°C  75%  U                        1957SFb (99794)1935
                                          K(Mg+H2L=MgL+2H)=-12.0
********************************************************************************
C20H17NO               HL                        (6215)
N-(2-Hydroxy-5-phenylbenzylidene)-2-methylaniline; C6H5.C6H3(OH).CH:N.C6H4.CH3
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Mg++       gl  diox/w 30°C  75%  U        K1=3.544        1986MBd (99810)1936
********************************************************************************
C20H19NO8               L                        (2558)
4-Dedimethylamino-tetracycline;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Mg++       gl  NaCl   37°C 0.15M C        K1=4.744  B2=7.642  1988LVa (99853)1937
********************************************************************************
C20H19N3O3S            HL                      CAS 380496-12-8  (9100)
1,3-Di(3-ethylphenyl)-4,5,6-pyrimidinetrione-2-thio-5-oxime;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Mg++       gl  diox/w 25°C  75%  U T      K1=3.00         2001SSd (99873)1938
Medium: 75% v/v dioxan/H2O, 0.10 NaClO4. Data for 30 and 35 C.
********************************************************************************
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
--------------------------------------------------------------------------------
Mg++       sp  none   25°C  0.0  U        K1=7.2          1984WNa (99913)1939
********************************************************************************
C20H21N6O8P           H2L                     CAS 155933-76-9  (8687)
3'-Adenylic acid, mono[(8-hydroxy-2-quinolinyl)methyl] ester;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Mg++       sp  KCl    30°C  1.0M M        K1=3.03         1996BTa (99916)1940
********************************************************************************
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
--------------------------------------------------------------------------------
Mg++       gl  NaCl   25°C 0.10M C        K1=7.52         2004SGb (99959)1941
                                          B(MgHL)=16.15
                                          B(MgH2L)=25.14
```

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
Mg++	gl	KNO3	25°C	0.10M	U		K1=10.51 K(Mg+HL)=6.20 K(Mg+H2L)=2.21	1967LMd	(99986)1942

****

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
Mg++	EMF	alc/w	25°C	100%	C		K1=3.15	2004ZTa	(100078)1943

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	con	mixed	25°C	20%	C		K1=4.40	2003SIa	(100079)1944

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	con	non-aq	25°C	100%	C		K1=4.52	1992STa	(100080)1945

Medium: propylene carbonate.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	vlt	non-aq	25°C	100%	C		K1=<2.5	1991SSb	(100081)1946

Method: competitive complexation with Tl+; use of Tl(Hg)/Tl couple.
Medium: acetonitrile, 0.05 M Et4NClO4.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	sp	alc/w	25°C	100%	U	I	K1=2.33	1989KSc	(100082)1947

In MeOH. In DMF K1 <2, in DMSO K1 <2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	vlt	alc/w	25°C	100%	C		K1=2.10	1987CBd	(100083)1948

Medium: methanol, 0.10 M Et4NI or Bu4NClO4. Method: polarography.

****

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
Mg++	EMF	KCl	20°C	0.10M	C		K1=2.9	1981SFa	(100574)1949

Method: Pt/H2 electrode. For the 3,3,10,10-tetramethyl- homologue, K1=2.9

****

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
Mg++	EMF	alc/w	25°C	100%	C		K1=3.57	2004ZTa	(100621)1950

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

Mg++ con mixed 25°C 20% C K1=4.21 2003SIa (100622)1951
Medium: 20% w/w propylene carbonate/ethylene carbonate.

Mg++ con non-aq 25°C 100% C K1=4.55 1992STa (100623)1952
Medium: propylene carbonate.

Mg++ vlt non-aq 25°C 100% C K1=3.46 1991SSb (100624)1953
Method: competitive complexation with Tl+; use of Tl(Hg)/Tl couple.
Medium: acetonitrile, 0.05 M Et4NClO4.
****
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
---
Mg++ gl alc/w 25°C 95% M K1=<2 1990LNa (100782)1954
Medium: 95% MeOH, 0.05 M Bu4NBr. For the 12,19-dihydroxy- analogue: K1=3.63
****
C20H40N2O6 L Cryptand 3,2,1H (6589)
1,7-Diaza-4,11,14,17,23,26-hexaoxabicyclo[13.8.5]octacosane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl alc/w 25°C 95% M K1=<2 1990LNa (100791)1955
Medium: 95% MeOH, 0.05 M Bu4NBr. For the 9,19-dihydroxy- analogue: K1=3.24
****
C20H40N2O7 L Cryptand 3,2,2 CAS 31255-22-8 (1763)
Cryptand 3,2,2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl R4N.X 25°C 0.05M C I K1=<2.0 1975LSc (100806)1956
In 95% MeOH: K1 < 2
****
C20H42N4O4 L CAS 39678-14-3 (1543)
4,7-Dimethyl-1,4,7,10-tetraaza-13,16,21,24-tetraoxa-bicyclohexacosane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl R4N.X 25°C 0.10M U K1=2.6 1978LMa (100884)1957
****
C20H44N4O4 L (6730)
1,4,7,10-Tetra-(2-methoxyethyl)-1,4,7,10-tetrazacyclododecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl R4N.X 25°C 0.10M C K1=2.47 1993SFb (100936)1958

Medium: 0.1 M Et4NClO4.
****
C20H48N4O8P4 H4L (6569)
1,4,7,10-Tetraazacyclododecane-1,4,7,10-tetrakis(methyleneethylphospinic acid);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KCl	25°C	0.10M	C		K1=4.41	1997HTa (100991)	1959
Mg++	gl	KNO3	25°C	0.10M	C		K1=4.41	1991LSc (100992)	1960

****
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
Mg++	sp	alc/w	20°C	25%	U		K1=7.64	1971KBc (101028)	1961

Medium: 25% MeOH, 0.1 M KCl
****
C21H14N4O2 HL CAS 194480-84-7 (8524)
2-Hydroxy-1-naphthalenecarboxaldehyde benzofuro[2,3-d]pyrimidin-4-ylhydrazone;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	diox/w	30°C	10%	U		K1=5.006	1997HVa (101034)	1962

Medium: 10% v/v dioxane/H2O, 0.10 M NaClO4.
****
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
Mg++	gl	mixed	25°C	80%	C		K1=6.90 B(MgHL)=15.19	1997HMa (101115)	1963

In 80 % (wt/wt) DMSO-H2O, I= 0.5 M NaClO4
****
C21H19NO HL (6216)
N-(2-Hydroxy-5-phenylbenzylidene)-2,6-dimethylaniline;
C6H5.C6H3(OH).CH:N.C6H3(CH3)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	diox/w	30°C	75%	U		K1=3.669	1986MBd (101137)	1964

****
C21H21N2O8Cl H2L Demeclocycline CAS 64-73-3 (5759)
7-Chloro-6-demethyltetracycline;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaCl	37°C	0.15M	U			1985LBb (101181)	1965

B(MgH2L2)=23.592
B(MgHL2)=15.416
B(MgHL)=11.852
B(Mg2L)=7.605

Mg++ gl KNO3 25°C 0.10M C K1=5.15 1979DDd (101182)1966
K(Mg+HL)=3.47

Also data for other tetracycline analogues.

****

C21H22O10 L G-Rubrofusarin CAS 63174-98-1 (7067)
2-Methyl-5,6-dihydroxy-6-O-B-D-galactosyl-8-methoxy-naphtho-pyrone;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	sp	NaClO4	25°C	1.00M	U		K1=3.97	1995PDa (101212)1967	

****

C21H23NO6 HL Colchiceine (7054)
Colchiceine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	diox/w	20°C	75%	U	I	K1=5.22 B2=9.37	1994SHc (101221)1968	

****

C21H23N6O8P H2L CAS 183793-02-4 (8688)
3'-Adenylic acid, mono[2-(8-hydroxy-2-quinolinyl)ethyl] ester;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	sp	KCl	30°C	1.0M	M		K1=2.60	1996BTa (101228)1969	

****

C21H24N3O4SF HL CAS 215190-91-3 (9102)
6-Fluoro-7-(5-nonyl-1,3,4-oxadiazol-2-ylsulphanyl)-4-quinolone-3-carboxylic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	mixed	25°C	20%	C		K1=4.81	2001SCc (101236)1970	

Medium: 20% DMF/H2O, 0.1 M NaClO4.

****

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
Mg++	gl	diox/w	25°C	13%	C		K1=5.32	2001CLa (101284)1971	
							B(MgHL)=15.00		
							B(MgH-2L)=-14.95		

Medium: 13% v/v dioxane/H2O, 0.10 M KNO3.

****

C21H27N7O14P2 H2L beta-NAD CAS 53-84-9 (5577)
beta-Nicotinamide adenine dinucleotide;

```
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Mg++       nmr R4N.X  22°C 0.10M U        K1=1.40        1985PHb (101296)1972
******************************************************************************
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
------------------------------------------------------------------------------
Mg++       nmr none    RT     0  U                        1995MMf (101373)1973
                                        K1eff=1.88
Medium: D2O, pH 8.5-9.5.  Coordination site is the adenine phosphate. For
the ribose phosphate site, K1eff=1.95; for nicotinamide phosphate, K1=1.50
******************************************************************************
C21H30N7O17P3         H4L    NADP             CAS 50443-29-3  (2783)
Nicotinamide adenine dinucleotide phosphate;
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Mg++       nmr none    RT     0  U                        1995MMf (101379)1974
                                        K1eff=1.98
Medium: D2O, pH 8.5-9.5.  Coordination site is the adenine phosphate. For
the nicotinamide phosphate, K1=0.91
******************************************************************************
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
------------------------------------------------------------------------------
Mg++       gl  R4N.X  25°C 0.10M M        K1=9.53        1996CHc (101406)1975
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-tetraethan
oic acid;
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Mg++       EMF KCl    20°C 0.10M C        K1=4.7         1981SFa (101415)1976
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
------------------------------------------------------------------------------
Mg++       gl  alc/w  25°C  95%  C        K1=2.26        2004KVa (101460)1977
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
Mg++	sp	KCl	rt	0.10M	U			1960DEa	(101527)1978
							K1eff=4.29 (pH 10)		

****
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
Mg++	sp	KNO3	25°C	0.20M	U			1967BMc	(101576)1979
							B(MgH4L)=47.4		

****
C22H19NO7S 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
Mg++	gl	KCl	37°C	0.10M	C			2002CSa	(101683)1980
							K1eff=2.28		

Method: fluorimetry. Medium pH 7.05-7.40
****
C22H22N2O8 L Methacycline CAS 3963-95-9 (6020)
Methacycline;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaCl	37°C	0.15M	C		K1=5.142	1988LBa	(101723)1981
							B(MgH2L2)=25.196		
							B(MgHL2)=17.233		
							B(MgHL)=12.373		

****
C22H22N4O2 H2L CAS 75651-32-0 (5318)
N,N'-Bis(8-hydroxy-2-quinolylmethyl)ethylenediamine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	diox/w	25°C	50%	U		K1=10.2	1972HUa	(101732)1982

Medium: 50% v/v dioxan, 0.1 M KCl
****
C22H23N2O8Cl H2L Aureomycin CAS 56235-18-8 (3515)
Chlorotetracycline;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaCl	37°C	0.15M	U			1985LBb	(101757)1983
							B(MgH2L2)=23.995		

B(MgHL)=11.515

****

C22H24N2O8 L Deoxycycline CAS 564-25-0 (2204)
Deoxycycline, 6-Deoxy-5-hydroxytetracycline;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaCl	37°C	0.15M	C		K1=12.988 B(MgH2L2)=25.559 B(Mg2L)=8.546 B(MgHL2)=17.420	1983BBc (101765)	1984

****

C22H24N2O8 H2L Tetracycline CAS 60-54-8 (2201)
Tetracycline;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaClO4	25°C	0.10M	C		B(MgHL)=9.30	1996SJa (101803)	1985
Mg++	cal	oth/un	25°C	?	U	T H	Keff(Mg+L)=-3.01	1995OCa (101804)	1986

Medium: 20mM Tris(hydroxymethyl)aminomethane, pH 9.5. DH=-11.76 kJ mol-1, DS=56.07 J K-1 mol-1

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaNO3	25°C	0.10M	C	M	K1=8.40 K(MgL+Gly)=4.20	1989GAb (101805)	1987
Mg++	gl	NaCl	37°C	0.15M	C		B2=8.698 B(MgHL)=12.657 B(MgH2L2)=25.275 B(MgHL2)=17.597 B(Mg2L)=7.740	1983BBc (101806)	1988

****

C22H24N2O8 H4L CAS 91044-24-5 (1920)
meso-1,2-Diphenyl-1,2-diaminoethane-N,N,N',N'-tetraethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	20°C	0.10M	U		K1=4.66	1989SLa (101838)	1989

****

C22H24N2O8 H4L CAS 91044-25-6 (1921)
rac-1,2-Diphenyl-1,2-diaminoethane-N,N,N',N'-tetraethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	20°C	0.10M	U		K1=10.33	1989SLa (101853)	1990
Mg++	gl	KCl	25°C	0.10M	U		K1=10.40	1967OTb (101854)	1991

****

C22H24N2O9 H2L Oxotetracycline CAS 79-57-2 (2202)
Oxytetracycline, 5-Hydroxy-tetracycline;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaCl	37°C	0.15M	C		K1=4.874 B2=9.560 B(MgH2L2)=24.095 B(MgHL2)=17.423 B(Mg2HL)=14.970 B(Mg2L)=8.346	1983BBc (101879)1992	
Mg++	gl	oth/un	20°C	0.01M	U		K1=3.8	1956ARd (101880)1993	

****

C22H24N2O10 H4L CAS 132796-79-3 (8113)
1,2-Bis(2-aminophenoxy)ethane-N,N,N',N'-tetraethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	sp	KCl	22°C	0.10M	C		K1=1.77	1980TSb (101892)1994	

****

C22H25O3P L CAS 97745-35-2 (2069)
Adamantyl(diphenoxy)phosphonyl

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	sol	non-aq	25°C	100%	U		K1=3.84	1987TCa (101922)1995	

Medium: CH2Cl2, 2% MeCN. Metal as picrate

****

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
Mg++	gl	alc/w	25°C	95%	M		K1=<2	1990LNa (102412)1996	

Medium: 95% MeOH, 0.05 M Bu4NBr. For the 12,22-dihydroxy- analogue: K1=3.71

****

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
Mg++	gl	R4N.X	25°C	0.05M	C		K1=<2	1975LSc (102425)1997	

****

C22H44N6O5S2 L CAS 503465-08-5 (9241)
9,20,23,28,31-Pentaoxa-1,4,6,12,14,17-hexaazabicyclo[15.8.8]tritriacontane-5,13-dithione;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	alc/w	25°C	95%	C		K1=2.54	2004KVa (102435)1998	

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

****

C23H18O9S H4L Eriochrome cyan CAS 3564-18-9 (433)
4'-Hydroxy-3,3'-dimethyl-2''-sulfofuchsone-5,5'-dicarboxylic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	sp	oth/un	25°C	0.10M	U		B(MgHL)=8.65	1975EPa (102624)	1999

****

C23H23NO5 L CAS 218619-58-0 (7808)
Dibenzo-pyridino-18-crown-6;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	EMF	alc/w	25°C	100%	C		K1=2.84	2004ZTa (102654)	2000

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

****

C23H25NO5S L CAS 464185-98-6 (9292)
4'-[(2-Benzothiazole)ethenyl]-2:3-benzo-15-crown-5;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	sp	non-aq	20°C	100%	C		K1=5.5	2003FFa (102689)	2001

Medium: CH3CN.

****

C23H26N2O7 H2L (2559)
6-Desoxy-6-dimethyl-tetracycline;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	NaCl	37°C	0.15M	C		K1=5.495 B2=9.307 B(MgHL)=13.074 B(MgL2)=19.325 B(MgH2L2)=26.566	1988LVa (102707)	2002

****

C23H27N2O8I H2L CAS 6602-90-0 (361)
4-Methyltetracycline Iodide;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KNO3	25°C	0.10M	U		K1=3.78 B2=6.36	1979HFa (102718)	2003

****

C23H27N3O7 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
Mg++	gl	NaCl	37°C	0.15M	C		K1=5.886	1983BBc (102726)	2004

B(MgHL)=13.088
B(MgH2L2)=26.728
B(MgHL2)=17.905
B(Mg2HL)=15.824

****

C23H30N2O4 L CAS 361454-16-2 (8960)
N-(Phenylmethylene)-4-(1,4,7,10-tetraoxa-13-azacyclopentadec-13-yl)benzamine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	sp	non-aq	RT	100%	C		K1=2.64	2001AVa (102747)	2005

Method: spectrophotometric titration. Medium: acetonitrile.

****

C23H30N4O4Br2 H2L CAS 354154-85-1 (8979)
N,N'-Bis-(3-N"-2-hydroxy-5-bromobenzyl)aminopropyl malondiamide;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	diox/w	25°C	13%	C		K1=5.55	2001CLa (102764)	2006
							B(MgHL)=15.33		
							B(MgH-2L)=-14.83		

Medium: 13% v/v dioxane/H2O, 0.10 M KNO3.

****

C24H20N4O14Cl2P2S2 H8L (4165)
2,7-Bis(4'-chloro-5'-methyl-2'-phosphonophenylazo)chromotropic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	sp	KNO3	25°C	0.20M	U			1967BMc (102914)	2007
							B(MgH4L)=47.7		

****

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
Mg++	gl	NaCl	25°C	0.10M	C		K1=7.35	2004SGb (102944)	2008
							B(MgHL)=16.59		
							B(MgH2L)=24.85		

Additional method: UV-visible spectrometry

****

C24H24N2O8 H4L CAS 89593-26-0 (8632)
N,N'-[1,2-Ethynediylbis(2,1-phenylenemethylene)]bis[N-(carboxymethyl)]glycine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	KCl	20°C	0.10M	U		K1=5.0	1984VSc (102948)	2009

****

C24H25O7P L (2067)
Phenylphosphonyldibenzo-17-crown-6

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ sol non-aq 25°C 100% U K1=2.78 1987TCa (102963)2010
Medium: CH2Cl2, 2% MeCN. Metal as picrate
****
C24H26N2O8 H4L CAS 89561-09-1 (8633)
N,N'-[1,2-Ethenediylbis(2,1-phenylenemethylene)]bis[N-(carboxymethyl)]glycine;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl KCl 20°C 0.10M U K1=3.4 1984VSc (102973)2011
****
C24H26N2O8 H4L CAS 89561-11-5 (8635)
N,N'-[1,2-Ethenediylbis(4,1-phenylenemethylene)bis[N-(carboxymethyl)]glycine;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl KCl 20°C 0.10M U K1=2.4 1984VSc (102978)2012
****
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
---
Mg++ sp diox/w 25°C 40% C K1=3.04 2003GHb (103003)2013
Method: fluorescence spectroscopy. Medium: 40% w/w dioxane/H2O, 0.05 M
Et4NClO4.
****
C24H28N2O8 H4L CAS 89561-10-4 (8634)
N,N'-[1,2-Ethanediylbis(2,1-phenylenemethylene)]bis[N-(carboxymethyl)]glycine;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl KCl 20°C 0.10M U K1=3.7 1984VSc (103006)2014
****
C24H32O8 L DiBz-24-Crown-8 CAS 14174-09-5 (580)
2,3:14,15-Dibenzo-1,4,7,10,13,16,19,22-octaoxacyclotetracosa-2,14-diene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ con mixed 25°C 20% C K1=4.83 2003SIa (103107)2015
Medium: 20% w/w propylene carbonate/ethylene carbonate.

Mg++ vlt alc/w 25°C 100% C K1=2.37 1987CBd (103108)2016
Medium: methanol, 0.10 M Et4NI or Bu4NClO4. Method: polarography.
Additional method conductivity in methanol: K1=2.71.
****
C24H35NO9 L CAS 330462-64-1 (8032)
6,7-Dimethoxy-4-(1,4,7,10,13-pentaoxa-16-azacyclooctadec-16-ylmethyl)-2H-1-benzopyr

an-2-one;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ sp mixed 25°C 10% C K1=5.12 2001LWa (103240)2017
Method: fluorimetry. Medium: 10%v/v acetonitrile/H2O.
****
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
---
Mg++ gl R4N.X 25°C 0.10M M K1=2.8 1991FGb (103306)2018
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
---
Mg++ gl NaClO4 25°C 0.20M C K1=8.3 1985KFa (103368)2019

Mg++ EMF KCl 20°C 0.10M C K1=6.5 1981SFa (103369)2020
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
---
Mg++ con mixed 25°C 20% C K1=4.46 2003SIa (103425)2021
Medium: 20% w/w propylene carbonate/ethylene carbonate.
****
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
---
Mg++ gl R4N.X 25°C 0.05M C K1=<2 1975LSc (103462)2022
****
C24H48N6O6S2 L CAS 503465-10-9 (9242)
9,12,23,26,31,34-Hexaoxa-1,4,6,15,17,20-hexaazabicyclo[18.8.8]hexatricontane-5,16-dithione;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl alc/w 25°C 95% C K1=2.70 2004KVa (103502)2023
Medium: 95% MeOH/H2O, 0.01 M Et4NClO4.
****

C25H21N3O3 H2L Xylidyl blue II (5334)
4-Hydroxy-3-(2-hydroxy-3-(2,4-dimethylaminophenylaminocarbonyl)-1-naphthylaao)benze
ne;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ sp alc/w ? 50% U B2=9.79 1971SCb (103608)2024
****
C25H22O2P2 L CAS 207-21-8 (2099)
Methylenebis(diphenylphosphine oxide); Ph2P(O)CH2P(O)Ph2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ con non-aq 25°C 100% U 1971SYc (103626)2025
K(MgI+L=MgL+I)=-0.96
Medium: CH3CN
****
C25H28N4O10 L CAS 752-13-6 (2940)
Tetraacetylriboflavine;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ nmr non-aq 38°C 100% U K1=1.74 1975LHa (103674)2026
Medium: acetone. Using spectrophotometry. 25 C: K1=1.1
****
C25H29NO7 L FQC CAS 215095-38-8 (8804)
4'-(Dimethylamino)-2,7-(3,6,9-trioxaundecane-1,11-dioxy)flavone;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ sp non-aq ns 100% C K1=2.98 2000LXa (103679)2027
Medium: acetonitrile. By fluorescence, K1=3.19.
****
C25H48N6O8 H3L Desferrioxamine CAS 70-51-9 (2488)
Desferrioxamine B; NH2.((CH2)5.NOH.CO.C2H4.CO.NH)2.(CH2)5.NOH.CO.CH3

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl KCl 25°C 0.20M C K1=2.8 1999FEa (103798)2028
B(MgHL)=14.66
B(MgH2L)=23.85

Mg++ gl NaNO3 20°C 0.1M U 1963AEa (103799)2029
K(Mg+HL)=4.30
****
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

---
Mg++ gl alc/w 25°C 95% C K1=3.16 2004KVa (103841)2030
Medium: 95% MeOH/H2O, 0.01 M Et4NClO4.
****
C26H25NO9S H4L Semi-Xylenol O (426)
3-(N,N-Di(carboxymethyl)aminomethyl)-2-cresolsulfonephthalein;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ sp KNO3 25°C 0.10M U K1=6.89 1974YOa (103941)2031
B(MgHL)=10.90
K(MgL+OH)=2.43
****
C26H28N2O5 L (2155)
1,13-Di-(8-quinolyl)-1,4,7,10,13-tetraoxatridecane; C9H6N.O.(CH2.CH2.O)4.C9H6N

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ sp alc/w 25°C 100% U K1=4.99 B2=9.82 1977TMa (103977)2032
K3=4.63
K4=4.40
Medium: MeOH
****
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
---
Mg++ gl diox/w 24°C 50% U K1=5.5 1979ACa (104019)2033
****
C26H31NO8S2 L CAS 136195-71-6 (6832)
Crown Ether Styryl Dye;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ sp non-aq 25°C 100% U 1992BFa (104033)2034
K(Mg+cis-L) > 9.15
K(Mg+trans-L)=7.00
Medium:CH3CN. Ligand:2-[2-(2,3,5,6,8,9,11,12-octahydro-1,4,7,10,13-benzopent
aoxacyclopentadecin-16-yl)ethenyl]-3-(3-sulfopropyl)benzothiazolium betain
****
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
---
Mg++ sp diox/w 25°C 40% C K1=4.96 2003GHb (104037)2035
K(MgL+Mg)=3.08
Method: fluorescence spectroscopy. Medium: 40% w/w dioxane/H2O, 0.05 M
Et4NClO4.

****
C26H32N2S2 L CAS 677034-81-0 (9064)
4-(2-{10-[2-(1,4-Thiazinan-4-yl)ethyl]-9-anthryl}ethyl)thiomorpholine;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ sp non-aq 25°C 100% C K1=5.08 2003GHa (104043)2036
K(MgL+Mg)=2.92
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
---
Mg++ sp non-aq 25°C 100% C K1=>7 2003GHa (104072)2037
K(MgL+Mg)=ca. 6
Method: fluorescence spectroscopy. Medium: acetonitrile, 0.05 M Et4NClO4.
****
C26H34N6O8 H4L CAS 132709-65-0 (8941)
3,6,14,17,23,24-Hexaazatricyclotetracosa-1,8,10,12,19,21-hexaene-3,6,14,17-tetraace
tic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl KCl 25°C 0.10M M K1=3.2 1996MBb (104091)2038
****
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
---
Mg++ gl alc/w 25°C 90% M K1=1.08 1998KLa (104105)2039
Medium: 90% v/v MeOH/H2O, 0.1 M Me4NCl
****
C26H52N6O7S2 L CAS 503465-16-5 (9245)
4,12,20,26,29,34,37-Heptaoxa-1,7,9,15,17,23-hexaazabicyclo[21.8.8]nonatriacontane-8
,16-dithione;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl alc/w 25°C 95% C K1=3.11 2004KVa (104336)2040
Medium: 95% MeOH/H2O, 0.01 M Et4NClO4.
****
C26H52N6O7S2 L CAS 503465-12-1 (9243)
9,12,15,26,29,34,37-Heptaoxa-1,4,6,18,20,23-hexaazabicyclo[21.8.8]nonatricontane-5,
19-dithione;

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

Mg++ gl alc/w 25°C 95% C K1=2.77 2004KVa (104346)2041
Medium: 95% MeOH/H2O, 0.01 M Et4NClO4.
****
C27H29NO10 H2L Daunorubicine CAS 23541-50-6 (5660)
Daunomycin;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ sp oth/un 20°C 0.15M U 1982KMd (104438)2042
K(Mg+HL)=3.7
****
C27H32NO5S+ L CAS 423763-94-4 (8997)
3-Ethyl-2-[4-(2,3,5,6,8,9,11,12-octahydro-1,4,7,10,13-benzopentaoxacyclopentadecin-15-yl)butadien
---
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ sp non-aq 25°C 100% C K1=5.95 2002GVc (104514)2043
Medium: acetonitrile, 0.01 M Et4NClO4.
****
C27H33NO7 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
---
Mg++ sp non-aq ns 100% C K1=3.38 2000LXa (104524)2044
Medium: acetonitrile. By fluorescence, K1=3.27.
****
C27H33N9O15P2 H2L FAD CAS 146-14-5 (3521)
Flavin adenine dinucleotide;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ ix NaCl 23°C 0.1M U K1=2.02 1958WAa (104545)2045
****
C27H47N3O6 L (8029)
Tripodal ionophore 3;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ sp non-aq 25°C 100% C 2001LFa (104622)2046
K(MgP+L=LiPL)=4.98
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
---

Mg++ cal oth/un 25°C 0.10M C H 2001BIa (104692)2047
K(Mg+H4L)=3.30
Medium: 0.10 m Na4H4L, pH=2. DH(Mg+H4L)=4.7 kJ mol-1.
****
C28H34N2O6 HL CAS 83874-22-0 (6920)
Cezomycin;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl alc/w 25°C 100% C K1=5.2 B2=11.8 1994ABc (104755)2048
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
---
Mg++ sp non-aq RT 100% C K1=2.75 1998ABc (104760)2049
Medium: acetonitrile. Method: fluorescence spectroscopy.
****
C28H35O7P L CAS 90275-27-7 (2068)
Adamantylphosphonyldibenzo-17-crown-6

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ sol non-aq 25°C 100% U K1=3.62 1987TCa (104766)2050
Medium: CH2Cl2, 2% MeCN. Metal as picrate
****
C28H36N2O2 L CAS 588691-42-3 (9067)
4-{3-[10-(3-Morpholinopropyl)-9-anthryl]propyl}morpholine;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ sp diox/w 25°C 40% C K1=7.08 2003GHb (104775)2051
K(MgL+L)=6.76
Method: fluorescence spectroscopy. Medium: 40% w/w dioxane/H2O, 0.05 M
Et4NClO4.
****
C28H36N2O7S2 HL CAS 150196-54-6 (7735)
3-(3-Sulfopropyl)-2-[4-[N-(1,4,7,10,13-pentaoxa-16-azacyclooctadeca)]]styryl-benzot
hiazolium;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ sp non-aq 18°C 100% C K1=1.6 1997LHa (104781)2052
Medium: acetonitrile.
****
C28H40O6 L CAS 29471-17-8 (1262)
2,3:11,12-Bis(4'-tert-butylbenzo)-1,4,7,10,13,16-hexaoxacyclooctadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ EMF non-aq 25°C 100% U K1=<1 1982MRb (104833)2053
Medium: anhydrous propylene carbonate, 0.1M Et4NClO4
****
C28H40O10 L DiBz-30-crown10 CAS 104946-67-0 (1776)
2,3:17,18-Dibenzo-1,4,7,10,13,16,19,22,25,28-decaoxacyclotriaconta-2,17-diene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ vlt non-aq 25°C 100% C K1=3.20 1991SSb (104869)2054
Method: competitive complexation with Tl+; use of Tl(Hg)/Tl couple.
Medium: acetonitrile, 0.05 M Et4NClO4.

Mg++ EMF non-aq 25°C 100% U K1=2.89 1982MRb (104870)2055
Medium: anhydrous propylene carbonate, 0.1M Et4NClO4
****
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
---
Mg++ gl alc/w 25°C 95% C K1=2.04 2004KVa (105037)2056
Medium: 95% MeOH/H2O, 0.01 M Et4NClO4.
****
C28H56N6O8S2 L CAS 503465-14-3 (9244)
9,12,15,18,29,32,37,40-Octaoxa-1,4,6,21,23,26-hexaazabicyclo[24.8.8]dotetratriconta
ne-5,22-dithio

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl alc/w 25°C 95% C K1=2.15 2004KVa (105047)2057
Medium: 95% MeOH/H2O, 0.01 M Et4NClO4.
****
C29H35NO5 L CAS 201154-06-5 (7825)
N-(1-Pyrenylmethyl)-1,4,7,10,13-pentaoxa-16-azacyclooctadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ sp mixed 25°C 90% C 1997KKa (105097)2058
K(Mg(SCN)2+L)=2.71
Method: fluorescence emission. Medium: MeOH/CHCl3 (9:1 v/v).
****
C30H27N3O18S3 H9L TRIMCAMS CAS 77069-63-7 (5468)
1,3,5-Tris(2,3-dihydroxy-5-sulfobenzoyl)carbamido)benzene;

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

```
Mg++       gl  KNO3   25°C 0.10M C                        1982KRb (105203)2059
                                        B(MgHL)=22.3
                                        B(MgH2L)=27.9
**************************************************************************
C30H30O5P2              L                      CAS 68402-79-9  (2624)
1,2:7,8-Dibenzo-3,6-diphospho-3,6-dioxo-3,6-diphenyl-15-crown-5
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Mg++       con non-aq 22°C 100%  U        K1=2.88        1980YKa (105224)2060
Medium: MeCN
**************************************************************************
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
--------------------------------------------------------------------------
Mg++       sp  non-aq 25°C 100%  U   H    B2=11.1        1996AAb (105250)2061
Medium: MeCN
tacyclo[12.12.12.1(6,9).1(19,22).1(31,34]hentetetraconta-4,6,8.....dodecaene
**************************************************************************
C31H32N2O13S          H6L    Xylenol orange   CAS 63721-85-5  (432)
5,5'-Bis-N,N-bis(carboxymethyl)aminomethyl-4'-hydroxy-3,3'-dimethylfuchsone-2"-sulf
onic acid;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Mg++       gl  KNO3   25°C 0.10M C    M   K1=8.96        1998GBa (105448)2062
                                        K(MgL+H)=10.08
                                        K(MgL+Mg)=5.28
                                        K(Mg2L+H)=8.15
--------------------------------------------------------------------------
Mg++       sp  KNO3   25°C 0.10M U        K1=9.02        1974YOa (105449)2063
                                        K(Mg+HL)=7.10
                                        K(Mg+H2L)=3.09
                                        K(Mg+MgL)=6.14
                                        K(Mg+MgHL)=2.6
**************************************************************************
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
--------------------------------------------------------------------------
Mg++       gl  KCl    25°C 0.10M U        K1=3.7         1982LVa (105587)2064
**************************************************************************
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
--------------------------------------------------------------------------------
Mg++       gl  KCl    25°C 0.10M U        K1=4.2         1982LVa (105592)2065
********************************************************************************
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
--------------------------------------------------------------------------------
Mg++       gl  oth/un 25°C 0.10M U         K1=8.32        1981GMd (105607)2066
                                          B(MgHL)=18.47
                                          B(Mg2L)=12.05
--------------------------------------------------------------------------------
Mg++       gl  KCl    20°C  0.1M U         K1=8.9         1954AGb (105608)2067
                                          K(Mg+HL)=7.5
                                          K(Mg+H2L)=3.6
                                          K(Mg+H3L)=2.2
                                          K(Mg+MgL)=3.0
K(Mg+MgHL)=1
********************************************************************************
C32H37NO9S            H4L    SemiMeThymolBlu    (427)
3-(N,N-Di(carboxymethyl)-aminomethyl)thymolsulfonephthalein;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Mg++       sp  KNO3   25°C 0.10M U         K1=7.05        1974YOa (105662)2068
                                          B(MgHL)=14.60
                                          K(MgL+OH)=2.35
********************************************************************************
C32H38N4O6Cl2         H2L                        (7214)
7,16-Bis((5-chloro-8-hydroxy-7-quinolinyl)methyl)-1,4,10,13-tetraoxa-7,16-diazacycl
ooctadecane;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Mg++       cal alc/w  25°C 100%  U   H                    1996BBf (105688)2069
                                          K(Mg+H2L)=6.82
Medium: MeOH; 0.1 M Me4NCl. DH(K)=-2.5 kJ mol-1. Data also for similar
lariat ligands with substituted oxine side chains
********************************************************************************
C32H40N4O4              L                     CAS 340963-90-8  (8926)
8,8'-[1,4,10,13-Tetraoxa-7,16-diazacyclooctadecane-7,16-diylbis(methylene)bisquinol
ine;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Mg++       cal alc/w  25°C 100%  C   H    K1=4.02         2001DXa (105712)2070
Medium: MeOH. DH(K1)=9.9 kJ mol-1, DS(K1)=110 J K-1 mol-1.
********************************************************************************
```

C32H40N4O6 H2L CAS 254900-30-6 (8916)
7,16-Bis(8-hydroxyquinoline-7-ylmethyl)-1,4,10,13-tetraoxa-7,16-diazacyclooctadecan
e;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ cal alc/w 25°C 100% C H 1999SBg (105722)2071
K(Mg+H2L)=5.7
Medium: MeOH. DH(K)=10.7 kJ mol-1, DS(K)=145 J K-1 mol-1.
****
C32H43N2O7S HL CAS 189057-31-6 (7756)
3-(4-Carboxybutyl)-2-[4-[N-(1,4,7,10,13-pentaoxa-16-azacyclooctadeca)]]styryl-benzo
thiazolium;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ sp non-aq 18°C 100% C K1=2.1 1997LHa (105754)2072
Medium: acetonitrile.
****
C32H49N9O7 HL KLAHFG CAS 188184-11-4 (5653)
Lysyl-leucyl-alanyl-histidyl-phenylalanyl-glycine;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl NaCl 20°C 0.15M U M K1=1.45 1983VDb (105810)2073
****
C33H39N11 L Pyr-cryptand CAS 141258-00-6 (7452)
1,4,12,15,18,26,31,39,42,43,44-Undecaazapentacyclo[13.13.13.1.1.1]tetratetetraconta
pentadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ sp non-aq 25°C 100% U H B2=12.6 1996AAb (105915)2074
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
---
Mg++ sp non-aq 25°C 100% C 2001LFa (105921)2075
K(MgP+L=LiPL)=4.04
Method: Analyses by spectrophotometry. Medium: chloroform. P is picrate.
****
C34H38N2O14 H2L (7072)
7,16-Bis(3-carboxy-6-methoxy-2-oxo-2H-1-benzopyran-7-yl)-1,4,10,13-tetraoxa-diazacy
clooctadecane;

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

---
Mg++ sp none RT 0 U K1=2.10 1994CGa (106027)2076
Method: fluorimetry
****
C34H38N4O6 H4L (3525)
Haematoporphyrin IX;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ sp oth/un 25°C var U T H 1973ACb (106032)2077
K1eff=1.34
Additional method: spectroscopy. pH=7.4, K1(30 C)=1.40, K1(35 C)=1.40, K1(40 C)=1.42, DH=4.76 kJ mol-1

Mg++ sp oth/un 25°C var U T H 1973ACb (106033)2078
K1eff=1.17
Additional method: spectroscopy. pH=8.2, K1(30 C)=1.27, K1(35 C)=1.44, K1(40 C)=1.51, DH=40.88 kJ mol-1

Mg++ sp oth/un 25°C var U T H 1973ACb (106034)2079
K1eff=1.10
Additional method: spectroscopy. pH=9.0. K1(30 C)=1.04, K1(35 C)=0.88, K1(40 C)=0.75, DH=39.71 kJ mol-1
****
C34H44N4O6 H2L CAS 254900-31-7 (8917)
7,16-Bis(5-methyl-8-hydroxyquinoline-7-ylmethyl)-1,4,10,13-tetraoxa-7,16-diazacyclooctadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ cal alc/w 25°C 100% C H 1999SBg (106072)2080
K(Mg+H2L)=5.02
Medium: MeOH. DH(K)=13.9 kJ mol-1, DS(K)=143 J K-1 mol-1.
****
C34H53O8Br H2L CAS 38784-08-6 (2336)
5-Bromolasalocid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl alc/w 25°C 100% M 1988JTa (106095)2081
K(Mg+HL)=3.89
K(Mg+2HL)=6.3
Medium: MeOH
****
C34H54O8 H2L Lasalocid CAS 25999-20-6 (2335)
Lasalocid acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ nmr non-aq 20°C 100% C 1998MLa (106118)2082

```
                                        K(Mg+HL)=-1.0
Medium: CD3OD. Method: 13C nmr.
-------------------------------------------------------------------------
Mg++       dis non-aq 25°C 100%  U                      1993LPa (106119)2083
                                        K(Mg+2HL=MgL2+2H)=-9.7
Method: extraction into CHCl3.  K is for Mg(aq)+2HL(org)=MgL2(org)+2H(aq).
-------------------------------------------------------------------------
Mg++       gl  alc/w  25°C 100%  M                      1988JTa (106120)2084
                                        K(Mg+HL)=4.20
                                        K(Mg+2HL)=6.7
-------------------------------------------------------------------------
Mg++       cal alc/w  25°C 100%  U   H                  1988PPa (106121)2085
Medium: MeOH. DH(MgL)=27.5 kJ mol-1; DS=173. DH(MgL2)=27.4; DS=172
-------------------------------------------------------------------------
Mg++       gl  alc/w  25°C 100%  U                      1982BDc (106122)2086
                                        K(Mg+4HL)=4.12
                                        K(Mg+5HL)=6.07
Medium: MeOH
*************************************************************************
C35H45N9                L                       CAS 312304-65-7  (7962)
29,32,35-TriMe-1,14,29,32,35,38,39,40,41-Nonaazahexacyclohentetraconta-3,5,7,8,10,1
2,16,18,20,21,
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Mg++       gl  R4N.X  25°C 0.10M U        K1=4.1         2001BBa (106200)2087
                                        K(MgL+H)=9.9
                                        K(MgHL+H)=9.1
Medium: 0.10 M NMe4NO3.
*************************************************************************
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
-------------------------------------------------------------------------
Mg++       sp  non-aq 25°C 100%  U        K1=4.26        1996AAd (106316)2088
                                        B(Mg2L)=7.5
Medium: CH3CN. L is 11,4,12,15,18,26,31-Octaazapentacyclo[13.13.13.1(6,10).
1(20,24).1(33,37)]tetratetraconta-4,6,8,10(44),11,18,20,22,24(43).....
*************************************************************************
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
-------------------------------------------------------------------------
Mg++       cal non-aq 25°C 100%  U        K1=3.33   B2=4.82   1991SGa (106331)2089
Medium: CH3CN; Mg as Mg(NCS)2
*************************************************************************
C36H46N4                L                          (9018)
```

2,3,6,7,11,12,17,18-Octaethylcorphycene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ sp non-aq RT 100% C M 2002FSa (106351)2090
K(MgL+py)=3.00
K(Mg(py)+py)=<0
Medium: toluene.
****
C36H46N4 L CAS 130351-26-7 (9017)
2,3,6,7,12,13,16,17-Octaethylporphycene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ sp non-aq RT 100% C M 2002FSa (106355)2091
K(MgL+py)=3.34
K(Mg(py)+py)=<0
Medium: toluene.
****
C36H46N4 L (9019)
2,3,7,8,11,12,17,18-Octaethylhemiporphycene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ sp non-aq RT 100% C M 2002FSa (106359)2092
K(MgL+py)=3.46
K(Mg(py)+py)=<0
Medium: toluene.
****
C36H46N4 H2L Octaethylporph. CAS 2683-82-1 (1794)
2,3,7,8,12,13,17,18-Octaethyl-21H,23H-porphine;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ sp non-aq RT 100% C M 2002FSa (106366)2093
K(MgL+py)=3.66
K(MgL(py)+py)=<0
Medium: toluene.
****
C36H47N3O6 L (8028)
Tripodal ionophore 2;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ sp non-aq 25°C 100% C 2001LFa (106372)2094
K(MgP+L=LiPL)=3.82
Method: Analyses by spectrophotometry. Medium: chloroform. P is picrate.
****
C36H58N10O10S4 H5L CAS 136685-24-0 (6875)
(1-Cys-,1'-Cys,4-Cys-,4'-Cys)-dithiobis(Ac-1-Cys-Pro-D-Val-4-Cys-NH2);

```
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Mg++       gl  non-aq 20°C 100%  U        K1=4.07        1993EAa (106440)2095
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
--------------------------------------------------------------------------------
Mg++       ISE alc/w  25°C 100%  M        K1=5.20        1984CTa (106488)2096
Medium: MeOH. In EtOH K1=9.10
--------------------------------------------------------------------------------
Mg++       ISE non-aq 25°C 100%  M        K1=6.88        1984CTa (106489)2097
Medium: N,N-dimethylformamide. In DMSO K1=5.40
********************************************************************************
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
--------------------------------------------------------------------------------
Mg++       sp  R4N.X  25°C 0.10M U         K1=10.4        1996BGa (106579)2098
                                          K(Mg+HL)=7.1
                                          K(Mg+H2L)=2.8
                                          K(MgHL+Mg)=1.5
                                          K(MgL+Mg)=5.6
Medium: Me4NCl
--------------------------------------------------------------------------------
Mg++       sp  oth/un 20°C 0.01M U                        1986VDa (106580)2099
                                          Keff=9.54
Medium: ammonia buffer. Method: FIA
--------------------------------------------------------------------------------
Mg++       sp  KNO3   25°C 0.10M U         K1=8.87        1974YOa (106581)2100
                                          B(MgHL)=19.67
                                          B(MgH2L)=26.71
                                          K(Mg+MgL=Mg2L)=5.80
                                          K(Mg+MgHL=Mg2HL)=2.3
--------------------------------------------------------------------------------
Mg++       sp  oth/un   ?     ?  U                       1971ANb (106582)2101
                                          K(Mg+H3L)(?)=4.09
********************************************************************************
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
--------------------------------------------------------------------------------
Mg++       gl  KNO3   25°C 0.10M C                       1982KRb (106669)2102
                                          B(MgH4L)=50.5
                                          B(MgH3L)=42.5
```

B(MgH2L)=34.3
B(Mg2L)=19.9
****
C40H36O4P2 HL CAS 126763-08-4 (7791)
1,2-Bis[2-(diphenylphophinylmethyl)phenoxy]-ethane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ EMF non-aq 25°C 100% C K1=9.21 1997PKc (106729)2103
Medium: nitrobenzene
****
C40H36O5P2 L CAS 86341-96-0 (5724)
1,7-Di(2-diphenylphosphinyl)phenyl-1,4,7-trioxaheptane;Ph2PO.C6H4.O.C2H4.O.C2H4.O.C6H4.POPh2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ EMF non-aq 25°C 100% C K1=11.21 1997PKc (106740)2104
Medium: nitrobenzene

Mg++ EMF non-aq 25°C 100% C K1=12.82 1997PKc (106741)2105
Medium: nitrobenzene
****
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
---
Mg++ EMF non-aq 25°C 100% C K1=9.86 1997PKc (106921)2106
Medium: nitrobenzene
****
C44H30N4O12S4 H4L (6422)
5,10,15,20-Tetra(p-phenylsulfonic acid)porphin;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ sp mixed 25°C 80% U 1991JJa (107082)2107
K(Mg+H2L=MgL+2H)=-3.96
In 80% v/v DMSO/H2O, 0.1 M (KClO4+KOH).
****
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
---
Mg++ EMF non-aq 25°C 100% C K1=8.39 B2=13.34 1997PKc (107125)2108
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
---
Mg++ gl non-aq 25°C 100% C K1=6.42 2000ABb (107140)2109
B(Mg2L)=9.97
B(Mg2HL2)=25.13
Medium: MeOH, 0.05 M Et4NClO4.
****
C44H52N4O8 L CAS 246035-33-6 (2925)
25,27-Bis(N,N-diethylaminocarbonylmethoxy)-26,28-bis(aminocarbonylmethoxy)calix[4]a
rene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ sp non-aq 25°C 100% C K1=1.1 1999USa (107155)2110
Medium: MeOH, 0.10 M Et4NCl
****
C45H39O3P3 L CAS 73218-92-5 (5679)
1,3,5-Tris(diphenylphosphinylmethyl)-benzene; C6H3(CH2.PO(C6H5)2)3

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ con non-aq 25°C 100% U I M 1984YSb (107210)2111
K(MgI+L)=2.5
Medium: tetrahydrofuran:CHCl3 1:1
****
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
---
Mg++ con non-aq 25°C 100% U I 1984YSb (107223)2112
K(MgI+L)=2.9
Medium: tetrahydrofuran:CHCl3 1:1. In CH3CN:CHCl3 1:1 K=2.8
****
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
---
Mg++ sp mixed 25°C 90% C 1997KKa (107246)2113
K(Mg(SCN)2+L)=3.15
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-diazacy
clooctadecane;

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

---
Mg++ sp none RT 0 U K1=1.40 1994CGa (107255)2114
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
---
Mg++ EMF non-aq 25°C 100% C K1=9.21 1997PKc (107275)2115
Medium: nitrobenzene
****
C46H58O6 HL (6716)
Calix[4]arene-O(1)-ethanoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl alc/w 25°C 100% C K1=6.4 1993ABb (107294)2116
B(MgHL)=18.4
B(MgH2L)=30.8
B(MgH3L)=41.8
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
---
Mg++ sol mixed 25°C 1% U K1=2.87 B2=4.45 1985BOa (107337)2117
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
---
Mg++ EMF non-aq 25°C 100% C K1=8.54 1997PKc (107369)2118
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
---
Mg++ EMF non-aq 25°C 100% C K1=11.57 1997PKc (107373)2119
Medium: nitrobenzene
****
C48H60O8 H2L R-Bu-Calixarene CAS 147513-53-9 (6705)
4-tert-Butylcalix[4]arenedicarboxylic acid;

```
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Mg++       gl  alc/w  25°C 100%  C        K1=7.3         1993ABb (107398)2120
                                         B(Mg2L)=11.0
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
-------------------------------------------------------------------------
Mg++       sp  non-aq 25°C 100%  C        K1=3.03        2004BCb (107419)2121
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
-------------------------------------------------------------------------
Mg++       ISE oth/un 21°C 100%  C        K1=9.7         1999CPa (107445)2122
Medium: PVC/DOS ion selective electrode membrane (DOS: bis(2-ethylhexyl)-
sebacate). Data for structurally related ionophores.
*************************************************************************
C52H64O12            H4L    R-Bu-Calixarene  CAS 113215-72-8  (6704)
5,11,17,23-Tetra-(t-butyl)-25,26,27,28-tetrakis[(hydroxycarbonyl)methoxy]calix[4]ar
ene;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Mg++       gl  alc/w  25°C 100%  C        K1=11.02       1993ABb (107486)2123
                                         B(MgHL)=21.43
                                         B(MgH2L)=30.52
                                         B(MgH3L)=37.96
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
-------------------------------------------------------------------------
Mg++       sp  non-aq 25°C 100%  C        K1=<1          1999USa (107496)2124
Medium: MeOH, 0.10 M Et4NCl.
*************************************************************************
C52H68N4O8             L                       (4823)
25,27-Bis(N,N-diethylaminocarbonylmethoxy)-26,28-bis(N-butylaminocarbonylmethoxy)ca
lix[4]arene;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Mg++       sp  non-aq 25°C 100%  C        K1=<1          1999USa (107504)2125
```

Medium: MeOH, 0.10 M Et4NCl
****
C52H69N3O6 H2L CAS 136158-03-7 (9132)
Tetra-t-butyl-calix[4]azacrown dione;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ sp non-aq 20°C 100% C K1=5.13 2003OAa (107521)2126
Medium: 100% acetonitrile, 0.01 M Et4NClO4.
****
C54H90N6O18 L Valinomycin CAS 2001-95-8 (2142)
Valinomycin, Potassium Ionophore

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ dis non-aq 25°C 100% U M 1996BSa (107545)2127
K(Mg2+,2A-+L=Mg2+,L,2A-)=3.87
Medium: CHCl3; 0.1 M picrate. Host-guest complex. A=(O2N)3C6H2O
Also data for host-guest complexes with several other salts, and L=nonactin.
****
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
---
Mg++ sp non-aq 25°C 100% C K1=3.27 2004BCb (107611)2128
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
---
Mg++ sp alc/w 25°C 100% C K1=4.1 2001MAa (107619)2129
Medium: MeOH, 0.01 M Et4NCl.
****
C58H80O10 L (9264)
5,11,17,23-Tetra-t-butyl-25,27-di(2-methoxyethoxy)-26,28-di(ethylacetate)calix[4]ar
ene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ sp non-aq 25°C 100% C K1=3.01 2004BCb (107628)2130
Medium: acetonitrile, 0.01 M Et4NClO4.
****
C60H82N2O10 L CAS 155377-20-1 (8806)
5,11,17,23-Tetra-butyl-25,27-bis(carboxymethoxy)-bis[(N,N-diethylaminocarbonyl)meth
oxy]calix[4]ar

```
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Mg++       gl  non-aq 25°C 100%  C                        2000ABb (107663)2131
                                          B(Mg2L)=11.62
Medium: MeOH, 0.05 M Et4NClO4.
*************************************************************************
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
-------------------------------------------------------------------------
Mg++       sp  non-aq 25°C 100%  C        K1=1.5         1999USa (107676)2132
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
-------------------------------------------------------------------------
Mg++       sp  non-aq 25°C 100%  C        K1=2.2         1991ACc (107690)2133
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
-------------------------------------------------------------------------
Mg++       oth non-aq 25°C 100%  C        K1=4.7    B2= 8.70  2003CGa (107716)2134
Method: CD spectroscopy. Medium: acetonitrile. Alternative model:
K1=4.8, K2=4.4.
*************************************************************************
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
-------------------------------------------------------------------------
Mg++       sp  non-aq 25°C 100%  C        K1=<1          1999USa (107801)2135
Medium: MeOH, 0.10 M Et4NCl
*************************************************************************
C69H102N4O9             L                     CAS 116352-85-3  (9286)
para-t-Butyldihomooxacalix[4]arene tetra(diethyl)amide;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Mg++       sp  alc/w  25°C 100%  C        K1=2.6         2004MFa (107830)2136
Medium: MeOH, 0.01 M Et4NCl.
*************************************************************************
```

C77H82O9 L CAS 253317-20-3 (9288)
p-Tert-butyldihomooxacalix[4]arene tetraphenyketone;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ sp alc/w 25°C 100% C I K1=4.0 1999MAb (107890)2137
Medium: MeOH, 0.01 M Et4NCl. In acetonitrile, K1=4.4.
****
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
---
Mg++ dis non-aq 25°C 100% U 1995FDa (107961)2138
K=4.24
Medium: CDCl3. Method: by H2O/CDCl3 extraction of picrate salt.
K: MA(org)+L(org)=MLA(org) where A=picrate.
****
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
---
Mg++ ISE NaCl rt 0.01M C K1=14.4 2003MGa (107989)2139
Method: segmented sandwich membrane ISE.
Phosphonic acid diethyl ester derivative: K1=16.5
****
C114H198N6O73 L CAS 571203-66-2 (9254)
4,13-Bis(8-(6-deoxy-beta-cyclodextrin-6-yl)aminooctylamidomethyl)-4,13-diazatrioxac
yclopentadecan

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Mg++ gl R4N.X 25°C 0.10M C K1=2.95 2003WWa (107998)2140
K(Mg+HL)=2.53
K(Mg+H2L)=ca.2
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
---
Mg++ dis non-aq 25°C 100% U 1995FDa (108004)2141
K=4.28
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
Mg++	dis	non-aq	25°C	100%	U				1995FDa (108015)	2142
							K=5.73			

Medium: CDCl3. Method: by H2O/CDCl3 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
Mg++	gl	KNO3	25°C	0.10M	U		K1=4.19		1980YTb (108045)	2143

(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
Mg++	EMF	oth/un	?	?	U		K1=2.11		1966HEa (108051)	2144

****

Polymer H2L X-14885A (4547)
Antibiotic X14885A, calcium ionophore

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Mg++	gl	alc/w	25°C	100%	U		K1=7.1		1989ABb (108073)	2145

Medium: MeOH, I=0 M. When I=0.1 M, K=5.2

****

Polymer H2L (8999)
Bacteriorhodopsin;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Mg++	ISE	oth/un	22°C	dil	C				1995YAa (108081)	2146
							K1eff=4.48			

Method: Ca ion selective electrode. Competition with Ca. Medium pH 3.9.

****

Polymer Calmodulin CAS 73298-54-1 (2957)
Calmodulin

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Mg++	ISE	KCl	25°C	0.11M	C	H	K1=4.36	B2=7.49	1989HGa (108105)	2147
							K3=3.13			
							K4=2.70			

In PIPES buffer, pH 7.0. DH(B4)=31.6 kJ mol-1; DS(B4)=360.9.

****

Polymer DNA (4185)
Deoxyribonucleic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	sp	NaClO4	25°C	0.10M	C	I	K1eff=3.30	1994SDb (108139)	2148

At pH 7.0. For I=0.01 M NaClO4, pH 7.0, K1eff=4.11.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	sp	NaCl	?	.002M	U		*K=5.3(calf thymus)	1959SBa (108140)	2149

*K decreases greatly with increasing Na+ concentration, not clearly defined

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	oth	NaCl	5°C	0.20M	U		K'=2.45(calf thymus)	1958ZDa (108141)	2150

Method: dialysis. See reference for definitions

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	oth	NaCl	25°C	0.20M	U	T	K'=1.92(calf thymus)	1957WNa (108142)	2151

Method: dialysis. K'=2.10(I=0.15). See reference for definitions

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Polymer (5379)
Dextran derivative of N-propyliminodiethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	oth/un	20°C	0.10M	U		K1=3.74	1968VGa (108161)	2152

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Polymer (4181)
Phosphatidic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	oth/un	24°C	0.10M	U		K1=4.1	1966AKa (108269)	2153

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Polymer (4183)
Phosphatidylserine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Mg++	gl	R4N.X	20°C	0.10M	U		K1=4.3 K(Mg+HL)=3.8	1965HFb (108276)	2154

Medium: Pr4NI

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Polymer (1642)
Polymethacrylic acid;

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

Mg++ gl NaNO3 20°C 0.05M U 1964MLa (108375)2155
*K'=-6.2
See reference for definitions
****
Polymer Elastase CAS 39445-21-1 (7314)
Porcine pancreatic elastase;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
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Mg++ oth oth/un 25°C 0.15M U 1980JMb (108386)2156
K1eff=3.48
Medium: 0.1 M KCl, 0.05 M MOPS, pH 6.85. Method: enhancement of Tb lumin-
escence
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Polymer (4204)
Pyruvate kinase;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
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Mg++ sp R4N.X 25°C 0.10M U 1966SSc (108399)2157
K'=3.04
Medium: Me4NCl

Mg++ nmr oth/un 24°C 0.10M U 1965MCc (108400)2158
K'=3.42
Medium: 0.1 M KCl,0.02 Tris. By kinetics: K'=3.4. See reference for defn.

Mg++ sp R4N.X 25?°C 0.10M U 1963SMb (108401)2159
K'=3.28
Medium: 0.1 M KCl,0.05 Tris
****
Polymer RNA (4205)
Ribonucleic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
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Mg++ nmr oth/un 25°C 0.02M C H 1996OCa (108413)2160
K1eff=4.41
Method: 25Mg nmr. Medium: 0.02 M Tris, pH 7.5. Ligand is Poly(A)xPoly(U)-
-RNA. DH=-65.3 kJ mol-1, DS=-117 J K-1 mol-1. Data for other RNA variants.

Mg++ oth NaCl 25°C 0.20M U 1957WNa (108414)2161
K'=2.09(calf liver)
Method: dialysis. See reference for definition
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Polymer (4182)
Triphosphoinositide;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
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Mg++ gl R4N.X 20°C 0.10M U K1=5.1 1965HFb (108419)2162
K(Mg+HL)=3.8

Medium: Pr4NI. Ligand assumed as H2L

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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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