```
SC-Database
Software version = 5.81 Data version = 4.62
Experiment list contains 899 experiments for
(no ligands specified)
Metal : Li+
(no references specified)
(no experimental details specified)
*******************************
                       Electron
                                      (442)
Electron:
              Metal Mtd Medium Temp Conc Cal Flags Lg K values
                                               Reference ExptNo
______
       EMF mixed 25°C 10% U I
                                            1974DKb (627) 1
                                K(Li+e=Li(s))=-51.40(-3041mV)
Medium: 10\% w/w DMSO/H2O; K=-51.30(-3.035V,20%), -50.97(-3.015V,40%),
-50.75(-3.002V,60%)
Li+
       oth mixed 25°C 0.0 U I
                                             1972C0a
                                                     (628)
                                K(Li+e+Li(s))=-50.73(3001mV)
Method: Estimated.K(Li+e=Li(s)).MeOH: -53.86(-3.186V).EtOH: -53.13(-3.143V)
BuOH: -54.21(-3.207V).PentylOH: -54.58(3.229V).Me2CO: -54.21(-3.207V)
______
        oth none 25°C 0.0 U I
Li+
                                             1972C0a
                                                     (629) 3
                                K(Li+e=Li(s))=-50.73(3001mV)
Method: Estimated. MeCN: -56.05(-3.316V).HCOOH: -59.72(-3.533V)
Also NH3 and N2H4
        con non-aq -71°C 100% U
                                             1972DBa (630)
                                K(Li + e(solv))=2.72
                                K(2Li=Li2)=1.95
Medium: NH3(liquid). Method:conductivity and magnetic susceptibility
______
Li+
       EMF mixed 25°C 30% U I
                                             1972KRb
                                                    (631)
                                K(Li+e=Li(s))=-51.32(-3036mV)
Med.:30% w/w ethylene glycol/H20; K=-51.18(-3.028V,50%), -50.95(-3.014V,70%)
-51.15(-3.026V,90%), -52.35(-3.097V,100%)
       EMF non-aq 25°C 100% U I
                                             1972KRc (632)
                                K(Li+e=Li(s))=-52.08(-3081mV)
Medium: 30% w/w propylene glycol/MeOH. 0% Pr Glycol: K=-52.30(-3.094V)
50%: -52.00(-3.076V). 70%: -51.96(-3.074V). 100%: -52.00(-3.076V)
-----
       EMF none 25°C 0.0 M
                                             1968HBb (633)
                                K(Li+e=Li(s))=-51.39,-3040.1mV
                                  1967BHc
        EMF none
                 25°C 0.0 U
                                                    (634)
                                K(Li+e=LiHg)=-36.99, -2188 mV
```

```
EMF none 25°C 0.0 M
Li+
                                 1967BHc (635) 9
                       K(Li+e=LiHg)=-37.13,-2196.3 \text{ mV}
-----
                                1966LCa (636) 10
     EMF non-aq 25°C 100% U
                       K' = -52.806, -3123.7 \text{ mV}
Medium: CH3NHCHO. K': Li + Cl + Ag(s) = Li(s) + AgCl(s)
_____
                   oth none 25°C 0.0 U
                                1952LAb (637) 11
                     K(Li+e)=-51.47(-3045 mV)
                        1923LRa (638) 12
    EMF none 25°C 0.0 U
                       K(Li+e=Li(s))=-50.02(-2957.8mV)
***********************************
                          (8856)
Tetrafluoroarsenate;
-----
     Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
     con non-ag 25°C 100% C K1=1.716 2002DDa (1040) 13
Medium: N,N-dimethylacetamide, 0.005-0.015 M LiAsF6.
********************************
            HL
                           (2497)
Tetrafluoroborate;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
     con non-ag 25°C 100% C K1=1.477 2002DDa (1195) 14
Medium: N,N-dimethylacetamide, 0.005-0.015 M LiBF4.
______
Li+ con non-aq 25°C 100% C T K1=2.50 2000VMa (1196) 15
Medium: 2-Methoxyethanol. Data for 15-35 C.
______
Li+ con non-aq 25°C 100% C K1=8.30 1997CHb (1197) 16
B(Li2BF4)=10.10
Medium: THF. By conductivity, species M2L and L2M are equivalent.
______
Li+ con non-aq 25°C 100% U K1=1.00 1991MHa (1198) 17
Medium: propylene carbonate
*********************************
            HL Borate CAS 10043-35-3 (991)
B04H4-
Borate; B(OH)4-
_____
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
-----
      EMF oth/un 25°C 0.0 C T H K1=1.09
                                 2000ZSb (1313) 18
Medium: 0.007-0.23 M LiCl. Method: Pt/H2 electrode. DH(K1)=0.64 kJ mol-1,
DS(K1)=22.9 \ J \ K-1 \ mol-1.
______
      sp oth/un 25°C 1.00M U I K1=0.73 1990RAa (1314) 19
Medium: LiCl. Data at I=0 M and at pressures to 2041 atmos.
```

```
Li+ gl NaCl 25°C 0.70M U K1=-0.05 1988RBa (1315) 20
HL Bromide
                         CAS 10035-10-6 (19)
Bromide;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
Li+ con non-ag 25°C 100% C K1=1.520
                                2002DDa (2083) 21
Medium: N,N-dimethylacetamide, 0.005-0.015 M LiBr.
______
                       K1=10.53 1997CHb (2084) 22
Li+ con non-ag 25°C 100% C
                       B(Li2Br)=13.33
                       K(2LiBr=Li2Br2)=1.70
Medium: THF. By conductivity, species M2L and L2M are equivalent.
_____
   con non-aq 25°C 100% U T K1=2.23 1993TAa (2085) 23
Medium: 2-methoxyethanol, -10 to 80 C
______
Li+ con non-aq 25°C 100% U K1=4.71 1982GRb (2086) 24
Medium: octanol
-----
Li+ con non-aq 25°C 100% U K1=0.76 1974HPb (2087) 25
Medium: hexamethylphosphotriamide. K1 by Pitts eqn. K1=1.13 (Fuoss-Hsia eqn)
______
  con mixed 25°C 0.10M U I K1=3.53 1973BHa (2088) 26
In 99.9% w/w acetone/H20. K1=3.62(100\%), 3.44(99.7\%), 3.38(99.4\%), 3.32(99\%),
3.21(98.5%),3.12(98%),2.96(97%),2.67(95%),2.15(90%),1.44(80%)
Li+ con mixed 25°C 0.1% U I K1=3.54 1973NIa (2089) 27
Medium: 0.1\% w/w MeOH/acetone. K1=3.42(0.3\%), 3.19(1\%), 3.03(2\%), 2.78(5\%),
2.50(=10%), 2.02(20%), 0.79(50%)
______
Li+ con non-aq 25°C 100% U K1=4.98 1973TKb (2090) 28
Medium: liquid SO2
______
     kin mixed 25°C 0.00 U I K1=3.56
                               1972HBa (2091) 29
In 99.995\% w/w acetone/H20.K1=3.54(99.894\%), 3.40(99.695\%), 3.32(99.395\%),
3.36(98.995%),3.28(98.495%). Data also by conductivity
______
Li+ con non-aq 25°C 100% U K1=1.26 1971BCa (2092) 30
Medium: tetramethylurea
-----
     kin non-aq 25°C 100% U K1=3.63 1970BIa (2093) 31
Medium: acetone. By conductivity:K1=3.67
-----
Li+ EMF non-aq 25°C 100% U K1=0.40
                               1970SAb (2094) 32
Medium: propene carbonate
con non-aq 25°C 100% U K1=1.28 1969MBf (2095) 33
```

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Medium: propene carbonate(0 corr)
-----
      con diox/w 25°C 50% U TI K1=1.11 1969SMe (2096) 34
In 50% w/w dioxan/H20. K1=1.78(70%),3.08(77.5%). At 50 C: K1=1.63(50%),
3.34(70%),4.76(77.5%). Also 30, 35 and 40 C
  con non-aq 40°C 100% U T K1=2.90 1967SMb (2097) 35
Li+
Medium: Me2CO. K1=2.80(25 C), 2.77(30 C), 2.85(35 C); also Me2CO-H2O mixtures
______
      con non-aq 25°C 100% U K1=3.66
                                1966SAa (2098) 36
Medium: acetone
______
      con alc/w 25°C 100% U K1=1.19
                                  1966SMc (2099) 37
Medium: MeOH, also K1 values for MeOH-H2O mixtures
------
   con non-aq 25°C 100% U
                      K1=3.18
                                   1965BFb (2100) 38
Medium: diaminoethane
-----
      oth non-aq 35°C 100% U
                                   1964TRb (2101) 39
                         K(2Li2Br2=Li4Br4)=1.3
Method:boiling point. Medium:Et20
______
Li+
   kin non-aq 0°C 100% U K1=0.41
                                1964WHa (2102) 40
Medium:DMF
   con non-aq 0°C 100% U
                          K1=4.58
                                  1960LRb (2103) 41
Medium: liquid SO2, I=0 corr., 0.22 C
______
    oth non-aq 16°C 100% U
                                   1959KEb (2104) 42
                         K(2LiBr=Li2Br2)=0.66
Method: freezing point; medium: CH3CO2H; m units.
      con non-aq 30°C 100% U K1=6.14 1954JGa (2105) 43
Medium: CH3CO2H
*******************************
Br03-
              HL
                             (6017)
                  Bromate
Bromate:
-----
Metal Mtd Medium Temp Conc Cal Flags Lg K values
                                     Reference ExptNo
-----
      sol NaClO4 25°C 0.15M U I K1=-0.77
                                  1963RSe (2422) 44
Medium: LiClO4. K1=-0.82 (I=0.20)
***********************************
             H2L Carbonate CAS 465-79-6 (268)
CO3--
Carbonate:
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
Li+ sol oth/un 40°C var U T
                                   1958MLa (3261) 45
                         K(Li2L+CO2(g)=2Li+2HL)=-0.23
```

```
K=-2.63(200 C), -3.68(250 C), -4.91(290 C), m units
-----
     sol oth/un 20°C var U
                                1958VGa (3262) 46
                      Kso(Li2CO3(s)) = -1.6
***********************************
                          (2191)
Hexacyanoferrate (II); Fe(II)(CN)6----
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
Li+ gl oth/un 25°C 0.10M C TIH K1=1.37 1986CDc (3584) 47
                       B(Li2Fe(CN)6)=1.69
                       B(LiHFe(CN)6)=4.38
Data for 10-35 C and 0.05-1.0 M LiCl. DH(K1)=23.4 kJ mol-1, DS(K1)=117
J K-1 mol-1; DH(Li2Fe(CN)6)=9.62, DS=88; DH(LiHFe(CN)6)=20.1, DS=176.
______
Li+ EMF oth/un 25°C U K1=1.95 1969NSa (3585) 48
Assuming K(Li+Fe(CN)6)=1.3
_____
Li+ oth oth/un 25°C 0.0 U K1=1.78 1966NSa (3586) 49
Medium: 0 corr. Method: electrical migration or transference number
Chloride
C1-
            HL
                        CAS 7647-01-0 (50)
Chloride:
-----
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
-----
Li+ con non-aq 25°C 100% C K1=1.660 2002DDa (5163) 50
Medium: N,N-dimethylacetamide, 0.005-0.015 M LiCl.
------
Li+ con non-aq 25°C 100% U I K1=1.5
                              1982GCb (5164) 51
Medium: DMF
______
Li+ con diox/w 25°C ? U K1=-0.092 1975MFa (5165) 52
Data for dioxan/H2O solution with a dielectric constant of 78.35
Further data available for solutions with varying dielectric constants
______
Li+ ISE non-aq 25°C 100% U K1=5.3 1974BMf (5166) 53
Medium: tributylphosphate
______
      oth non-aq 25°C 100% U
                                1974GRa (5167) 54
Li+
                 Kd(2LiCl=Li2Cl2)=2.26
Medium: octanoic acid. Method: permittivity
-----
     con non-aq 25°C 100% U K1=1.27 1974HPb (5168) 55
Medium: hexamethylphosphotriamide, using Pitts equation. Using Fuoss-Hsia
equation, K1=1.24
-----
  con non-aq 25°C 100% U K1=0.61 1972SKb (5169) 56
Medium: isopentylalcohol
```

Li+ Medium: ac	con non-aq 25°C 100% etone	U	K1=5.55	1971BHa	(5170)	57
	con non-aq 25°C 100% ifluoroethanol, K1=2.1			1971ENa	(5171)	58
	con non-aq 25°C 100% opanol, also acetone-p				•	
	oth non-aq 37°C 100% hanoic acid. Method: v		Kd(2LiCl=Li2Cl2 e osmometry	1971HMb )=0.4	(5173)	60
	con non-aq 25°C 100% methylformamide	U	K1=0.18	1971PGa	(5174)	61
	EMF non-aq 25°C 100% opene carbonate	U	K1=1.70	1970SAb	(5175)	62
	kin non-aq 25°C 100% etone. By conductivity			1969BEa	(5176)	63
Medium: 43	con alc/w 25°C 43% .5% w/w EtOH/H2O. K1=0 ), 1.20(92.3%), 1.43(1	.49(57.1%				64
	con non-aq 25°C 100% opene carbonate	U	K1=2.75	1969MBf	(5178)	65
Method: fr	oth alc/w 25°C 100% om literature data. Me ), 3(acetone)					66
Li+ Medium: ac	con non-aq 25°C 100% etone	U	K1=5.48	1966SAa	(5180)	67
	oth non-aq 18°C 100% ezing point. Medium: [	MSO	K1=0.7		, ,	
Medium:DMF	kin non-aq 0°C 100%	U	K1=0.74	1964WHa	(5182)	69
Li+ Medium:TBP	con non-aq 20°C 100% ,(BuO)3PO	U	K1=5.3	1963MSd	(5183)	
Li+	gl diox/w 25°C 70%	U	K1=2.54	1963PGb	(5184)	71
Li+	con non-aq 25°C 100% 3COOH. By EMF K1=3.98					72

	con 90% ace			90%			K1=2.3			73
	oth freezin	·			U	1	K(2LiCl=Li2Cl2	1959KEb		74
Medium:	EtOH						K1=1.75			75
Li+ Medium:		non-aq	25°C	100%	U		K1=7.08	1956BKa	(5189)	76
Li+		non-aq		100%			K1=7.13	1953SEa	(5190)	77
Medium:	cyclohe	xanol.	K1=4.	21(35	υ <sup>-</sup> 5 C)	Γ	K1=4.14 ******			
ClO3- Chlorate	e;		HL	Chl	.orat	te	CAS 7790-	93-4 (971	)	
						Flags	Lg K values		ence Exp	tNo
K1=1.42	(64.5% d	ioxan)				I	K1=6.42	1966CKa	(6046)	79
C104-										
Perchlo	rate;		ПL	Per	CUTO	orace	CAS 7001-	90-3 (287	)	
							Lg K values			 tNo
Metal Li+	Mtd con	 Medium  non-aq	Temp 25°C	Conc 100%	Cal Cal	 Flags 		Refer	ence Exp	
Metal Li+ Medium: Li+ Medium:	Mtd con N,N-dim con con	Medium non-aq ethylac non-aq non-aq	Temp 25°C cetami  25°C	Conc 100% de, 6	Cal C C 0.00!	Flags  5-0.01	Lg K values  K1=1.349  M LiClO4.  K1=1.26	Refer  2002DDa  1999DSd	 ence Exp  (6290)  (6291)	80
Metal Li+ Medium: Li+ Medium: Li+ Medium: Li+ Medium:	Mtd con N,N-dim con acetoni con	Medium non-aq ethylac non-aq trile. non-aq	Temp 25°C cetami 25°C 25°C	Conc 100% de, 6 100%	Cal C C O.00! M	Flags  5-0.01	Lg K values  K1=1.349 5 M LiClO4.	Refer 2002DDa  1999DSd  1997CHb 9 quivalent.	ence Exp (6290)  (6291)  (6292)	80  81
Metal Li+ Medium: Li+ Medium: Li+ Medium: Also da: Li+ Medium: DH(K1)=	Mtd con N,N-dim con acetoni con THF. By ta for d Glacial 52 kJ m	Medium non-aq trile non-aq conductimethox non-aq acetic	Temp  25°C  25°C  25°C  tivit  xyetha  25°C  acid	Conc 100% de, 6 100%	Cal CO.00! M Coecie	Flags 5-0.01 I es M2L l acet H ative	Lg K values  K1=1.349  M LiClO4.  K1=1.26  K1=7.34  B(Li2ClO4)=8.9  and L2M are e	Refer 2002DDa 1999DSd 1997CHb 9 quivalent. ethyl-1-he 1981TMb	ence Exp (6290) (6291) (6292)  xanol (6293)	80 81 82 83

Li+ con non-aq 25°C 100% U Medium: Acetonitrile	K1=1.20	1978CAa	(6295)	85 85
Li+ con non-aq 25°C 100% U Medium: - tributylphosphate	K1=5.09	1977BIb	(6296)	86
Li+ con non-aq 25°C 100% U Medium: hexamethylphosphotriamide. K1 by				
Li+ con non-aq 25°C 100% U T  Medium: THF. At -15 C: K1=7.18, KT=2.14;	KT=K(LiL+Li)=2.1	L8	(6298)	88
Li+ oth non-aq 25°C 100% U T H Medium: acetone. DH(K1)=3.68 kJ mol-1. K -0.64(-25 C), -0.57(0 C), -0.39(45 C). M	1=-0.92(-90 C),	-0.70(-45	•	89
Li+ con mixed 25°C 15% U I Medium 15% w/w THF/H2O. K1=2.59(30%),2.5 2.57(80%),3.16(90%),3.97(95%),4.36(97%),	6(40%),2.24(50%)	,2.39(60%)	` '	
Li+ con alc/w 25°C 100% U Medium: MeOH	K1=1.14	1972DAa	(6301)	91
Li+ con non-aq 25°C 100% U Medium: isopentylalcohol	K1=0.51	1972SKb	(6302)	92
Li+ con non-aq 25°C 100% U Medium: acetone	K1=3.23	1971BHa	(6303)	93
Li+ con non-aq 25°C 100% U Medium: N-methylformamide	K1=0.18	1971PGa	(6304)	94
Li+ con mixed 25°C 80% U I Medium: 80% w/w t-butanol/H20. K1=2.25(8	K1=1.75 5%),3.08(90%),3.8	1970ALa 37(95%),4	(6305) .12(97%)	95
Li+ EMF mixed 25°C 0.10M U I Medium: dimethoxy-1,2-ethane, 0.1 M H2O.			(6306)	96
Li+ EMF non-aq rt 100% U Medium: CF3COOH				97
Li+ EMF non-aq 25°C 100% U Method: H electrode. Medium: pyridine	K1(Li+)/K1(H+)=	1968MKa L.12	(6308)	98
Li+ EMF non-aq 20?°C 100% U Method: H electrode. Medium:C4H8O, 0.1 M				99

Medium: MeCN	on non-aq 25°C 100% U T , also at 20 C, 30 C	K1=1.54	1966MWb (6310) 100
	on non-aq 25°C 100% U	K1=1.83	•
	th non-aq 16°C 100% U	K(2LiL=Li2L2)=0	1959KEb (6312) 102
	zing point. Medium: CH3CO2H, *************		******
CrO4 Chromate;	H2L Chromate	CAS 7738-9	4-5 (2382)
Metal M	td Medium Temp Conc Cal Flags	Lg K values	Reference ExptNo
	th oth/un 25?°C 0.0 U ***********		1966MBb (6496) 103
F- Fluoride;	HL Fluoride		
Metal M	td Medium Temp Conc Cal Flags	Lg K values	Reference ExptNo
	p oth/un 25°C 1.0M U I er a range of pressures and i		1993MAa (6997) 104
	SE NaClO4 25°C 1.0M U TI		1984CTd (6998) 105
Li+ IS	SE NaClO4 25°C 1.00M C I M KNO3 (K1=-0.03) and 1.0 M N	K1=-0.12	1984HCa (6999) 106
Li+ of	th oth/un 25°C ? U	K1=0.25	1981ASa (7000) 107
	SE NaNO3 25°C 1.0M U mbrane electrode	K1=2.90 B2=3	.67 1968SRd (7001) 108
		Kd=1.81	1964KYa (7002) 109
Kd: Li+F=Li(:	in BuOH)+F(in BuOH). Kd=3.84( 	Na+),3.86(K+),3	.53(Cs+),3.69(NH4+)
Li+ ca	al oth/un 25°C 0.0 U H	Kso=-2.77	1964SHb (7003) 110
DH(so)=4.5 k			*****
H2O Water	L Water		8-5 (6115)
Metal M	td Medium Temp Conc Cal Flags	Lg K values	Reference ExptNo
	th non-aq 25°C 100% U I ial pressure. Medium: propene		

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K2=0.5. In DMSO, K1=-0.7 (by N.M.R.)
______
     nmr non-aq 36°C 100% U
                      K1=0.81 B2=1.24 1971CBc (7597) 112
                      K3 = 0.28
Method:N.M.R., Medium: Propene carbonate
______
      sol non-aq 25°C 100% U K1=0.5 B2=0.7 1967CKa (7598) 113
Medium: MeCN
______
Li+ sp alc/w 25°C 100% U I K1=0.18 1953BJa (7599) 114
Medium: MeOH. Maximum value of n is 3 or 4. In EtOH K1=-0.3
************************************
I-
                         CAS 10034-85-2 (20)
            HL
                Iodide
Iodide;
______
     Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
                            2002DDa (8219) 115
     con non-ag 25°C 100% C K1=1.478
Medium: N,N-dimethylacetamide, 0.005-0.015 M LiI.
______
Li+ oth diox/w 25°C 80% U I K1=2.23
                               1981ASa (8220) 116
K1=-0.21 in water
______
     oth diox/w 25°C ? U K1=-0.21
                               1975MFa (8221) 117
Data for dioxan/H2O solution with a dielectric constant of 78.35
Further data available for solutions with varying dielectric constants
______
Li+ con non-aq 25°C 100% U K1=0.48 1974HPb (8222) 118
Medium: hexamethylphosphotriamide. Calculated using Pitts eqn. By Fuoss-Hsia
K1=1.11
______
Li+ con non-aq 25°C 100% U K1=4.22
                               1973TKb (8223) 119
Medium: liquid SO2
______
                          1967RMe (8224) 120
   dis oth/un 25?°C 0.0 U
                       Kd(Li+I=Li(TBP)+I(TBP))=-0.54
In (i-amyl0)2MePO: Kd=-1.03
-----
  dis oth/un 25?°C 0.0 U
Li+
                                1967RMe (8225) 121
                      Kd(Na+I=Na(TBP)+I(TBP))=-1.32
In (i-amyl0)2MePO: Kd=-1.52
______
Li+ con diox/w 25°C 40% U I K1=-0.82 1966AMb (8226) 122
K1=0.40(60% dioxan), 1.38(70%), 2.28(80%), 2.82(87%), 3.85(91%), 4.50(95%)
______
      con non-aq 25°C 100% U K1=2.16
                             1966SAa (8227) 123
Li+
Medium: acetone
------
     con non-aq 25°C 100% U K1=2.97 1965BFb (8228) 124
Medium: diaminoethane
```

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kin non-aq 0°C 100% U K1=0.26 1964WHa (8229) 125
Li+
______
Li+ oth non-ag 16°C 100% U
                                 1959KEb (8230) 126
                      K(2LiI=Li2I2)=1.11
Method: freezing point. Medium: CH3CO2H, m units
______
      con non-aq 25°C 100% U I K1=2.56 1957HUa (8231) 127
Medium: EtCOMe. In PhCOMe K1=2.17
**********************************
           H2L Molybdate
                           (443)
Molybdate;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
-----
Li+ sp oth/un 25°C ? U M
                                 1997STa (8740) 128
                       K(H2L+2Li=Li2L+2H)=-3.3
Ligand: nano-Molibdenomanganate, MnMo9032-----
*********************************
NH3
              L
                Ammonia
                         CAS 7664-41-7 (414)
Ammonia
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
                       K1=-0.01 B2=-0.06 1992MPa (9175) 129
Li+ gl diox/w 25°C 2.0M U
                       K1=-0.28(100\%H20)
                        K3=-1.10(100\%H20)
                        K2=-0.76(100\% H20)
                        K4=-1.50 (100%H20)
Medium: NH4NO3 in 40% v/v dioxane/H2O; for 20% K1=-0.13; K2=-0.65
For 2 M NH4NO3 in40%v/v ethanol/H2O K1=-0.10; K2=-0.58
______
      gl oth/un 25°C 2.0M U H K1=-0.28 B2=-1.04 1991MPa (9176) 130
                       K3 = -1.1
Medium: NH4NO3; the same measured by cal. K1=-0.3; K2=-0.8; K3=-1.3
Also by extraction: K1=-0.32; K2=-0.8; K3=-1.2; K4=-1.6
______
      cal oth/un rt dil U H
                                1952FYa (9177) 131
DH(B3?)=-2.1 \text{ kJ mol-1; } DS(B3?)=-52.7.
______
Li+ gl R4N.X 23°C 2.0M U
                       K1=-0.3 B2=-1.1 1941BJa (9178) 132
                       K3 = -1.3
Medium: NH4NO3.
**********************************
NO2-
                       CAS 7782-77-6 (635)
             HL
                Nitrite
Nitrite:
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
```

\_\_\_\_\_\_

Li+ con oth/un 25°C 0.0 U K1=-0.04 1964PSh (9386) 133 ***********************************
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
Li+ con non-aq 25°C 100% C I K1=10.88 1997CHb (9747) 134 B(Li2NO3)=14.17
Medium: THF. Also data for dimethoxyethane and THF/2-ethyl-1-hexanol mixtures. By conductivity, species M2L and L2M are equivalent.
Li+ sp non-aq 25°C 100% U K1=-0.187 1979ITa (9748) 135 Medium: N,N-Dimethylacetamide. Method: Raman spectroscopy
Li+ con non-aq 25°C 100% U K1=0.72 1974HPb (9749) 136 Medium: Hexamethylphosphotriamide. Using Pitts equation. Using Fuoss-Hsia eq K=1.18
Li+ con non-aq 25°C 100% U K1=3.35 1974PHb (9750) 137 Medium: MeCN
Li+ con non-aq 25°C 100% U K1=9.77 1973WHa (9751) 138 K(LiL+Li)=2.3
Medium: THF
Li+ con non-aq 25°C 100% U K1=0.58 1972SKb (9752) 139 Medium: Isopentyl alcohol
Li+ con non-aq 25°C 100% U K1=2.22 1971BCa (9753) 140 Medium: Tetramethylurea
Li+ sp oth/un var U K1=-0.6 1971INb (9754) 141 Method: Raman spectra
Li+ con diox/w 25°C 72% U I K1=1.59 1969SBe (9755) 142 In 74.6% dioxan: K1=2.12, 75.9%: 2.43, 77.8%: 2.76
Li+ EMF non-aq 25°C 100% U 1968MKa (9756) 143 K1(Li+)/K1(H+)=0.91
Method: H electrode. Medium: C5H5N
Li+ ix mixed 23°C 90% U K1=-0.54 1966WFa (9757) 144 Medium: 90% i-PrOH, 0.5 M HL
Li+ con alc/w 25°C 100% U K1=1.28 1963PSa (9758) 145 Medium: EtOH, I=0 corr.
Li+ con non-aq 25°C 100% U K1=3.39 1961KBa (9759) 146 Medium: MeCN

Li+	oth	non-aq	16°C	100%	U		K(3LiL=Li3L3)=1	1959KEb	(9760)	147
Method: Fr	eezin	g point	t. Med	dium:C	СНЗС	02H				
							K1=-1.45 *******	1928HEa	(9761)	148
OH- Hydroxide;						ide	(57)			
Metal	Mtd	Medium	Temp	Conc	Cal		Lg K values		rence Exp	otNo
Li+ method: NM Medium: 3.	R Li-	7			1 C		K1=-0.1	2002PLa	(11701)	149
Li+ Medium: TH	F, 0.	1 M Bu <sup>2</sup>	4NC104	1. H €	elec	trode	K1=11.0			
	EMF	NaClO4			1 U		K1=-0.18			151
Li+	EMF	NaClO4	25°C	3.0			K1=-0.2 *K1=-14.4			152
Method: H	elect	rode 								
							K1=0.89 9(227 C),1.76(2		(11705)	153
							K1=0.17 5 C). Method: H			154
							K1=-0.08 ******			
PO4 Phosphate;			H3L	Pho	sph	ate	CAS 7664-3	8-2 (176	5)	
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Refer	rence Exp	otNo
Li+	J						K1=0.95 K(Li+HL)=0.79 K(Li+H2L)=0.2			156
Li+	gl	R4N.X	25°C	0.20	1 U	T HM	K(Li+HL)=0.72	1956SAc	(13239)	157
Medium: Pr ******	4NCl, ****	K=0.32	2(0 C) *****	). DH( *****	(K)= ****	25.1 k *****	J mol-1, DS=100 *******	J K-1 mc ******	)1-1 ******	****
P206 Hypophosph			H4L				e CAS 9803-6			

Metal	Mtd Medium	n Temp Conc Cal Fla	gs Lg K values	Reference ExptNo
Ligand: 03	POPH02,	Medium: Me4NCl		1967CMc (13415) 158
P207		H4L Pyrophosph 0)2P0.0.PO(OH)2		
Metal	Mtd Medium	n Temp Conc Cal Fla	gs Lg K values	Reference ExptNo
Li+ Medium: Me		5°C 1.00M U H (1)=1.3 kJ mol-1. 3		1973VAa (13615) 159 =4.2. DH(Li+HL)=-0.8
Li+ K1=3.3(40	•			1959WOa (13616) 160
			K1=2.39 K(Li+HL)=1.03	1957LWa (13617) 161
Medium: Me		*******	*******	*******
P208 Peroxodiph	osphate, al	H4L lso cyclic metaposp		-81-5 (2402) hates etc.;
Metal	Mtd Medium	n Temp Conc Cal Fla	gs Lg K values	Reference ExptNo
Li+	kin NaNO3	65°C 1.0M C	K(I; HD200) 0	1985GGb (13692) 162
Ligand is	peroxydisu]	lfate, S208	K(Li+HP208)=0.	
		25°C 1.00M U		1960CEa (13693) 163
Medium: Me		******	******	******
		Polytungst o-polytungstate (us		mer)
Metal	Mtd Medium	n Temp Conc Cal Fla	gs Lg K values	Reference ExptNo
Li+	gl R4N.X	25°C 1.0M U	K1=3.61 K(Li+HL)=3.77 K(Li+H2L)=2.0	1982CCb (13724) 164
		lpha1 isomer, K1>3.	7, K(Li+HL)=1.6,	K(Li+H2L)=0.6 *********
P3010		H5L om (H0)2P0.0.P0(OH)	CAS 10380	-08-2 (1001)
Metal	Mtd Medium	n Temp Conc Cal Fla	gs Lg K values	Reference ExptNo
Li+ K1=3.8(40	_	25°C 0.0 U T	K1=3.9	1959WOa (13878) 165

```
gl R4N.X 25°C 1.00M U
                       K1=2.87 1957WLa (13879) 166
                       K(Li+HL)=0.88
Medium: Me4NCl
**********************************
            H6L
                Tetraphosphate (1102)
Tetraphosphate;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
  gl R4N.X 25°C 1.0M U
                      K1=2.64 1967WMa (14049) 167
                       K(Li+HL)=1.59
Medium: Me4NCl
**********************************
            H6L
                          CAS 25268-83-1 (6590)
Dodecaoxohexaphosphate(III); anion of (PO.OH)6
______
     Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
Li+ gl R4N.X 25°C 1.0M U K1=1.34 1960CEa (14061) 168
                       K(Li+HL)=0.70
Medium: Me4NCl
******************************
             HL Thiocyanate CAS 463-56-9 (106)
Thiocyanate;
______
     Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
Li+ sp non-aq 25°C 100% U K1=0.93 1994GGa (15130) 169
Medium: DMF
______
    sp non-aq 20°C 100% U I
                       K1=3.87
                                1989GGa (15131) 170
                       K1out=3.05
Medium: MeCN, by IR spectroscopy. Also data for MeCN containing R4NX salts
______
Li+
     cal NaClO4 25°C 0.50M U H
                        K1=1.00
                              B2=1.07 1988ISb (15132) 171
                       B4=3.12
Medium: LiClO4 + 10%w/w Triton X-100. DH(K1)=-11.0 kJ mol-1, DH(B2)=-31,
DH(B4)=-32.6. DS(K1)=-18 J K-1 mol-1, DS(B2)=-84, DS(B4)=-50.
______
      sp non-aq 25°C 100% U
                        K1=-0.125 B2=0.26 1979ITa (15133) 172
Medium: N,N-Dimethylacetamide. Method: Raman spectroscopy
______
      con non-aq 25°C 100% U K1=0.15
                             1971PGa (15134) 173
Medium: MeHNCHO
______
      sp non-aq 20°C 100% U
                        K1=2.9
                                1970SSa (15135) 174
*********************************
S04--
            H2L Sulfate
                          CAS 7664-93-9 (15)
```

S		٦	£	_	+	^	
2	u	1	1	а	L	C	,

Sulfate;		
Metal	Mtd Medium Temp Conc Cal Flags Lg K values Reference	ce ExptNo
	gl NaCl 37°C 0.10M C I K1=0.77 1982DRb (16 0.03-0.50 M NaCl. At I=0.0 M, K1=1.12	5304) 175
	oth oth/un 25°C 0.50M U TI K1=0.77 1980GAb (16 rasonic absorption. Medium: Na2SO4	5305) 176
	con none 25°C 0.0 U 1978FFa (16 K(Li+LiSO4)=0.096	5306) 177
	oth oth/un 25°C .244M U K1=0.77 1975REa (16	5307) 178
Li+	oth none 25?°C 0.0 M K1=0.7 1966MBb (16	5308) 179
	con oth/un 18°C 0.0 U K1=0.64 1930RDa (16************************************	
Metal	Mtd Medium Temp Conc Cal Flags Lg K values Reference	ce ExptNo
Medium: ac	sp non-aq 20°C 100% U K1=2.4 1970SSa (16 tonitrile ************************************	
SiW11039	H8L (2464) osilicon-polytungstate;	
Metal	Mtd Medium Temp Conc Cal Flags Lg K values Reference	ce ExptNo
V04	gl R4N.X 25°C 1.0M U K1=4.1 1982CCb (17 ************************************	******
Metal	Mtd Medium Temp Conc Cal Flags Lg K values Reference	ce ExptNo
Li+	gl NaClO4 25°C 1.00M U 1975KIc (17 K(Li+H7PV12O36)=1.92	7381) 183
	gl R4N.X 20°C 0.10M U	·
CH202	HL Formic acid CAS 64-18-6 (37) cid; H.COOH	

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
Li+ con non-aq 30°C 100% U K1=7.06 1954JGa (17622) 185 Medium: ethanoic acid ************************************
CH3NO L Formamide CAS 75-12-7 (3536) Methanoic acid amide; HCO.NH2
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
Li+ ISE non-aq 25°C 100% C K1=1.3 B2=2.0 1975NAa (17678) 18 Medium: CH3CN, 0.01 M Et4NCl04 ************************************
CH40 L Methyl alcohol CAS 67-56-1 (597) Methanol; CH3.OH
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
Li+ ISE non-aq 25°C 100% C K1=0.65 B2=0.83 1975NAa (17884) 18 Medium: CH3CN, 0.01 M Et4NClO4  ***********************************
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
Li+ gl R4N.X 25°C 0.10M U K1=0.72 1972WFa (18149) 188 Medium: (CH3)4NCl ************************************
CH606P2 H4L Medronic acid CAS 1984-15-2 (2384) Methanediphosphonic acid; CH2(P03H2)2
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
Li+ gl R4N.X 25°C 0.50M U K1=2.48 1967CIa (18285) 189 K(Li+HL)=0.82
Medium: Me4NCl ************************************
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
Li+ gl oth/un 37°C 0.15M C I K1=0.79 1983DRb (18946) 190 Medium: 0.15 M LiNO3. Method: determination of protonation constant in LiNO3 and [Et4N]NO3 media. Data for I=0.0-1.0 M LiNO3. At I=0.0, K1=1.17.  *********************************
C2H4O2 HL Acetic acid CAS 64-19-7 (36) Ethanoic acid; CH3.COOH

Metal	Mtd Medium Temp Conc Cal Flags	s Lg K values	Reference ExptNo
Li+ I=0.02-1 M		K1=0.13	, ,
	gl R4N.X 25°C 0.16M U I (I=0.04); -0.13 (0.25); -0.09 (6	K1=-0.13	1985RSa (20032) 192
	con alc/w 25°C 100% U I n water. In 50% dioxan/H20: K1=1		· · ·
Medium: Gl	gl non-aq 25°C 100% U H lacial acetic acid. Alternative 9.0 kJ mol-1	method: Spectrop	hotometry.
Also data	con none 35°C 0.0 C I for MeOH (K1=1.834), 50% dioxar ne/H2O (K1=2.874).	K1=1.295	1979ASc (20035) 195 and
Li+	gl oth/un 25°C 0.0 U		
	gl non-aq 25°C 100% U chanoic acid	K1=6.78	1964KLa (20037) 197
	con oth/un 18°C 0.10M U I i ethanoate. K1=-0.54(I=0.2), -6		·
Medium: et	sp non-aq 25°C 100% U chanoic acid		,
Li+	EMF non-aq 25°C 100% U nloranil electrode. Medium: etha		
Medium: et	con non-aq 30°C 100% U  Chanoic acid  ***********************************		
C2H5NO		nide CAS 123-39-	
Metal	Mtd Medium Temp Conc Cal Flags	s Lg K values	Reference ExptNo
Medium: CH	ISE non-aq 25°C 100% C H3CN, 0.01 M Et4NClO4		
C2H5NO2		CAS 56-40-6	
Metal	Mtd Medium Temp Conc Cal Flags	s Lg K values	Reference ExptNo
Li+	sp oth/un 25°C 1.0M U	K1=1.2	 1987НАа (21603) 203

C2H6OS	**************************************	
Metal	Mtd Medium Temp Conc Cal Flags Lg K value	s Reference ExptNo
	ISE non-aq 25°C 100% M K1=1.69 CN, 0.01 M Et4NClO4	B2=2.99 1988NHa (22105) 204
Li+ Medium: Me	ISE non-aq 25°C 100% U T H K1=1.70	
Li+	ISE non-aq 25°C 100% C K1=1.7 B3=3.5	B2=3.0 1975NAa (22107) 206
******** C2H8N2	H3CN, 0.01 M Et4NClO4  ***************  L Ethylenediamine CAS 10  noethane; H2N.CH2.CH2.NH2	
Metal	Mtd Medium Temp Conc Cal Flags Lg K value	s Reference ExptNo
Medium: 95	sp alc/w 25°C 95% U K1=0.87 % w/w EtOH/H2O, 0.05 M Et4NClO4, by compet	
Li+ Medium: 0. ******** C2H806P2	gl oth/un 25°C 0.10M C I K1=-0.20 K(Li+HL)=-0 10 M LiCl. Data for I=0.25-1.0 M.	1990CDb (23187) 208 .65
Metal	Mtd Medium Temp Conc Cal Flags Lg K value	s Reference ExptNo
Li+	gl R4N.X 25°C 0.50M U K1=3.1 K(Li+HL)=0.	` ,
C2H807P2	**************	09-21-4 (436)
Metal	Mtd Medium Temp Conc Cal Flags Lg K value	s Reference ExptNo
Li+ Medium: (C	gl R4N.X 25°C 0.10M U K(Li+HL)=1. B(2Li+L)=4.	
Li+ Medium: Me	gl R4N.X 25°C 0.50M U K1=3.35 K(Li+HL)=1.	•

C3H4O4	**************************************	Malonic aci	**************************************	
Metal	Mtd Medium Tem	p Conc Cal Flag	s Lg K values	Reference ExptNo
Li+ I=0.02-1 M		C 0.25M C TI	K1=0.95 19 B(LiHL)=5.63	985DRa (24488) 212
Medium: 0. LiNO3 and ************************************	15 M LiNO3. Met [Et4N]NO3 media	hod: determinat . Data for I=0. ******* L-Lactic ac	ion of protonation 0-1.0 M LiNO3. At I ********** id CAS 79-33-4	=0.0, K1=1.05.
Metal	Mtd Medium Tem	p Conc Cal Flag	s Lg K values	Reference ExptNo
Method: H ******** C3H7NO	electrode *******	**************************************	K1=0.20 19 ************************************	******
Metal	Mtd Medium Tem	p Conc Cal Flag	s Lg K values	Reference ExptNo
Li+ Method: IS			K1=1.14 B2= 2.2 B3=1.66 B4=1.75 upled to polyacryla	0 1999NMa (25659) 215
	etonitrile, 0.0			
	ISE non-aq 25° CN, 0.01 M Et4N		K1=1.20 B2=3.04	1988NHa (25660) 216
Li+ Medium: Me	CN		K1=1.37 19	
	ISE non-aq 25°	C 100% C	K1=1.2 B2=2.0 B3=1.8	1975NAa (25662) 218
********* C3H1006P2	3CN, 0.01 M Et4 *************** H4L 2-diphosphonic	************* acid; CH3.C(PO3	**************************************	
Metal	Mtd Medium Tem		s Lg K values	
Li+	gl R4N.X 25°	C 0.50M U	K1=3.8 19 K(Li+HL)=1.38	67CIa (28401) 219

```
Medium: Me4NCl
*********************************
                          CAS 110-16-7 (111)
                 Maleic acid
cis-Butenedioic acid; HOOC.CH:CH.COOH
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
     gl R4N.X 37°C 0.25M C TI K1=0.91 1985DRa (29099) 220
B(LiHL)=5.9
                        B(LiHL)=5.9
I=0.02-1 M Et4NI
-----
Li+ gl oth/un 37°C 0.15M C I K1=0.72 1983DRb (29100) 221
Medium: 0.15 M LiNO3. Method: determination of protonation constant in
LiNO3 and [Et4N]NO3 media. Data for I=0.0-1.0 M LiNO3. At I=0.0, K1=1.08.
******************************
                           CAS 108-32-7 (6267)
Propylene carbonate, 1,2-Propanediol cyclic carbonate, 4-Methyl-1,3-dioxolan-2-one;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
-----
      ISE non-aq 25°C 100% C K1=0.5
                                1975NAa (29752) 222
Medium: CH3CN, 0.01 M Et4NCl04
********************************
            H2L Succinic acid CAS 110-15-6 (112)
1,4-Butanedioic acid; HOOC.CH2.CH2.COOH
______
     Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
    gl R4N.X 37°C 0.25M C TI K1=0.70 1985DRa (29991) 223
                        B(LiHL)=5.38
I=0.02-1 M Et4NI
______
Li+ gl oth/un 37°C 0.15M C I K1=0.42 B2= 0.60 1983DRb (29992) 224
Medium: 0.15 M LiNO3. Method: determination of protonation constant in
LiNO3 and [Et4N]NO3 media. Data for I=0.0-1.0 M LiNO3. At I=0.0, K1=0.84.
*********************************
            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
______
   ISE oth/un 25°C 0.10M U K1=0.38 1964RZa (30669) 225
-----
      gl R4N.X ? 0.28M U K1=0.45 1963EDa (30670) 226
Medium: Me4NBr
************************
                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
```

```
gl R4N.X 25°C 0.25M C TIH K1=0.70
                                1985DRa (30892) 227
Li+
                         B(LiHL)=3.91
0.02-1 M NEt4I. 12.5-48 C. DH(K1)=4 kJ mol-1, DS=35; DH(LiHL)=10, DS=119
   oth oth/un 30°C 1.00M U K1=-0.62 19730Ea (30893) 228
Method: Raman spectroscopy. medium: LiCl
*************************
            L THF CAS 109-99-9 (2537)
Tetrahydrofuran; cyclo(-CH2.CH2.O.CH2.CH2-)
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values
______
Li+ sp diox/w 25°C 100% U M
                                  1990TPa (33188) 229
                         K(Li(picrate)+L)=-0.02
With 2-methyltetrahydrofuran K=-0.47; 2,5-dimethyl- K=-0.09; tetrahydropyran
K=-0.54; dioxalane K=-0.47; hexamethyleneoxide -0.55
*****************************
                           CAS 127-19-5 (477)
N,N-Dimethylacetamide; CH3.CO.N(CH3)2
______
     Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
Li+ ISE non-aq 25°C 100% U T H K1=1.76 1982NYa (33762) 230
Medium: MeCN
______
      ISE non-aq 25°C 100% U
                        K1=1.39 B2=2.27 1976CWc (33763) 231
                         B3=2.34
                         B4=2.3
Medium: propylene carbonate
______
    ISE non-aq 25°C 100% C
                        K1=1.8 B2=2.9 1975NAa (33764) 232
                        B3 = 3.3
Medium: CH3CN, 0.01 M Et4NCl04
**********************************
                 t-Butanol CAS 75-65-0 (1740)
              HL
C4H100
tert-Butanol, (CH3)3C.OH
-----
      Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
_____
      con non-aq 25°C 100% U K1=8.0
                                  1974ESa (34659) 233
Medium: DMSO
***********************************
              L
                            CAS 111-46-6 (3579)
2,2'-Oxydiethanol; (HO.CH2.CH2)2.0 (Diethylene glycol)
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
- - - '
      con non-ag 25°C 100% C K1=2.7 1992MSe (34702) 234
Medium: 100% MeOH. Anion: picrate. Also data for nitrophenolate anions.
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***********************************
C4H11N
              L
                             (6678)
Dimethylethylamine; (CH3)2NCH2CH3
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
-----
      kin non-aq 20°C 100% U M
                                 1993BCd (34823) 235
                        K = 0.740
Metal:Li(0). Medium:Tetrahydrofuran. K:0.5Li2A2B2+L=0.5Li2A2L2+B.
A:Di(iso-propyl)amine. B:N,N,N',N'-Tetramethylethylenediamine.
****************************
           L Tris buffer
C4H11N03
                          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
-----
      gl R4N.X 25°C 1.00M C I K1=-0.23
                                 1982SSf (35058) 236
In 90 % (v/v) DMSO/water mixture: K1=0.37
*********************************
                 Pyridine CAS 110-86-1 (31)
C5H5N
Pyridine, Azine;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      ISE non-aq 25°C 100% C K1=0.72 B2=0.43 1975NAa (36648) 237
Medium: CH3CN, 0.01 M Et4NCl04
************************************
                 2-Aminopyridine CAS 504-29-0 (1478)
C5H6N2
2-Aminoazine, 2-Pyridylamine; C5H4N.NH2
-----
     Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      sp alc/w 25°C 95% U K1=0.76 1993GSa (37128) 238
Medium: 95% w/w EtOH/H2O, 0.05 M Et4NClO4, by competitive spectrophotometry
**********************
                 Acetylacetone CAS 123-54-6 (164)
C5H802
              HL
Pentane-2,4-dione; CH3.CO.CH2.CO.CH3
-----
     Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
-----
      sp non-aq 25°C 100% U K1=4.76 1984AMa (38012) 239
In Dimethyl Sulfoxide (DMSO);
Data also for other di- and triketones and esters and their alkali enolates
-----
Li+ gl diox/w 30°C 75% U K1=4.75 B2=8.72 1975MMa (38013) 240
      gl alc/w 25°C 100% U K1=2.8 1965LIa (38014) 241
Medium: MeOH, 0.1 M LiClO4. In EtOH: K1=4.6
*********************************
              HL Picric acid CAS 88-89-1 (593)
C6H3N307
```

```
2,4,6-Trinitrophenol; HO.C6H2(NO2)3
-----
     Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
Li+ dis non-aq 25°C 100% C K1=3.04 1999KKb (42122) 242
Medium: MIBK. Method: distribution of metal picrates into MIBK
containing HO(CH2.CH2.O)n.C12H25, n=4, 6 or 8.
______
Li+ dis oth/un 25°C dil C
                                 1998TKa (42123) 243
                       K(LiA+L)=2.53
Self medium, I<0.03 M. Method: Extraction of LiAL into dichloromethane.
A is 18-crown-6.
_____
  con non-aq 25°C 100% C I
                       K1=8.07 1997CHb (42124) 244
                       B(Li2L)=10.03
Medium: THF. By conductivity, species M2L and L2M are equivalent.
Also data for dimethoxyethane and ethyl acetate.
______
Li+ con non-aq 25°C 100% C I K1=2.99 1996HHc (42125) 245
Medium: acetonitrile. Also data for benzonitrile and DMF.
______
Li+ sp non-aq 25°C 100% U K1=3.97 1980GRa (42126) 246
Medium: 2-butanol
______
Li+ con alc/w 30°C 100% U I M K1=2.72 1979PSa (42127) 247
Medium: isoPrOH. K(LiL+diethyleneglycol)=2.51; K(LiL+trien-glycol)=2.41.
In H20: K1=1.11
______
   dis none 25°C 0.00 U K1=1.13
                                1972IWc (42128) 248
-----
     dis oth/un 25°C var U K1=2.2 1970SSb (42129) 249
Method: paper chromatography
***********************
                         CAS 50-28-5 (505)
2,4-Dinitrophenol; HO.C6H3(NO2)2
______
    Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
Li+ con non-aq 25°C 100% C I K1=4.29
                              1996HHc (42232) 250
                       B(Li2L)=6.71
Medium: acetonitrile. By conductivity, species M2L and L2M are equivalent.
Also data for benzonitrile and DMF.
______
      con non-aq 25°C 100% U K1=3.54 1973FGa (42233) 251
Medium: tetrahydrofuran
*******************************
                          CAS 329-71-5 (507)
2,5-Dinitrophenol; HO.C6H3(NO2)2
______
     Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
```

```
con non-aq 25°C 100% C I
                         K1=5.33
Li+
                                  1996HHc (42244) 252
                        B(Li2L)=8.48
                        K(2LiL=Li2L2)=1.72
Medium: acetonitrile. By conductivity, species M2L and L2M are equivalent.
Also data for DMF.
************************
                 2-Nitrophenol
                          CAS 88-75-5 (510)
             HL
2-Nitrohydroxybenzene; HO.C6H4.NO2
-----
      Mtd Medium Temp Conc Cal Flags Lg K values
-----
      con non-aq 25°C 100% C
Li+
                         K1=6.51
                                  1996HHc (42737) 253
                        B(Li2L)=10.60
                        K(2LiL=Li2L2)=3.01
Medium: acetonitrile. By conductivity, species M2L and L2M are equivalent.
**********************
C6H5N03
             HL
                 4-Nitrophenol
                          CAS 100-02-7 (454)
4-Nitrohydroxybenzene; HO.C6H4.NO2
  -----
      Mtd Medium Temp Conc Cal Flags Lg K values
                                    Reference ExptNo
______
Li+
     con non-aq 25°C 100% C
                         K1=4.96
                                  1996HHc (42810) 254
                        B(Li2L)=8.30
                        K(2LiL=Li2L2)=3.18
Medium: acetonitrile. By conductivity, species M2L and L2M are equivalent.
______
      con non-aq 25°C 100% U
                         K1=6.99
                                  1991AMa (42811) 255
Li+
Medium: THF
***********************************
                 4-Chlorophenol CAS 106-48-9 (1631)
4-Chlorophenol; HO.C6H4.Cl
______
      Mtd Medium Temp Conc Cal Flags Lg K values
-----
Li+
      con non-aq 25°C 100% U
                         K1=9.13
                                  1991AMa (43054) 256
Medium: THF
*******************************
                 Phenol
                           CAS 108-95-2 (457)
Hydroxybenzene, phenol; C6H5.OH
______
     Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      con non-aq 25°C 100% U
Li+
                         K1=10.16
                                  1991AMa (43542) 257
Medium: THF
************************
             H2L
                 Catechol
                           CAS 120-80-9 (534)
1,2-Dihydroxybenzene, pyrocatechol; HO.C6H4.OH
______
      Mtd Medium Temp Conc Cal Flags Lg K values
                                   Reference ExptNo
Metal
```

```
sp alc/w 25°C 95% U K1=1.31
Li+
                                    1993GSa (43783) 258
Medium: 95% w/w EtOH/H2O, 0.05 M Et4NClO4, by competitive spectrophotometry
***********************************
                             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
       sp alc/w 25°C 95% U K1=1.12
                                    1993GSa (45271) 259
Medium: 95% w/w EtOH/H2O, 0.05 M Et4NClO4, by competitive spectrophotometry
***********************************
                  Tricarballylic CAS 99-14-9 (1620)
              H3L
1,2,3-Propanetricarboxylic acid; HOOC.CH2.CH(COOH).CH2.COOH
-----
      Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      gl oth/un 25°C 0.0 C I
                          K1=1.473
                                    1994DFc (45567) 260
                          B(LiHL) = 7.322
                          B(LiH2L)=11.504
                          B(Li2L)=2.083
                          B(Li2HL)=6.923
Values at I=0 calculated from data for 0.04-1.0 M LiCl.
************************************
                 Citric acid CAS 77-92-9 (95)
C6H807
             H3L
2-Hydroxypropane-1,2,3-tricarboxylic acid; HOOCCH2.CH(OH)(COOH).CH2COOH
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
                          K1=1.10
      gl oth/un 25°C 0.50M U H
                                    1990DRa (46158) 261
                          B(LiHL)=6.49
                          B(Li2L)=1.66
DH(K1)=-3.0, DH(LiHL)=-3.6 and DH(Li2L)=-5.0 kJ mol-1.
-----
   gl KCl 37°C 0.15M C K1=0.88 B2=1.13 1981CDb (46159) 262
______
      ISE oth/un 25°C 0.10M U K1=0.83 1964RZa (46160) 263
*********************************
                            CAS 139-13-9 (191)
              H3L
Nitrilotriethanoic acid; N(CH2.COOH)3
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      gl oth/un 25°C 0.10M C TIH
                          K1=2.56
                                    1985DRb (46894) 264
                          B(LiHL)=9.62
Data at 10-45 C and I=0.02-1.0 M in LiNO3. DH(K1)=8 kJ mol-1; DS=(K1)=74.
DH(LiHL)=15; DS(LiHL)=232 (by T coeff.)
______
  sp R4N.X 25°C 0.10M C K1=2.35 1985HAd (46895) 265
______
```

Li+ Medium: Me	_	20°C 0.10	M U	T K1=2.51	1963IFb (46896) 266
Method: H	electrode			K1=3.28	, ,
C6H1002	ent-2,4-dic	HL		CAS 815-5	**************************************
Metal	Mtd Medium	Temp Conc	Cal Flag	s Lg K values	Reference ExptNo
Li+ Medium: CE ******	)30D	-60°C 1005			1979RHa (47948) 268
C6H14O3 bis-2-Meth	noxyethyl et		~ .	CAS 111-90	6-6 (6769) CH2.O.CH2CH2.O.CH3
Metal	Mtd Medium	Temp Conc	Cal Flag	s Lg K values	Reference ExptNo
********** C6H15NO3	00% MeOH. Ar	ion: picra ******** Tr	te. Also ******	data for nitrop	1992MSe (51051) 269 henolate anions. ************************************
Metal	Mtd Medium	Temp Conc	Cal Flag	s Lg K values	Reference ExptNo
Li+ In 90 % (\	•			K1=-0.48 9 (I=0.25 M)	1982SSf (51297) 270
Li+		•		K1=4.70 K(LiA+L)=2.34	, ,
	•	•	•	late. Medium: To	etrahydrofuran ********
C6H15O15P3	3 sitol 1,2,6-				-62-5 (6479)
Metal	Mtd Medium	Temp Conc	Cal Flag	s Lg K values	Reference ExptNo
Li+	gl R4N.X	25°C 0.10	M U	K1=2.38 B(LiHL)=11.24 B(LiH2L)=17.83 B(Li2L)=3.60	1991BSa (51537) 272
**************************************	*********			**************************************	**************************************
	Tetramethyl			(CH3)2N.CH2.CH	
Metal	Mtd Medium	Temp Conc	Cal Flag	<del>-</del>	Reference ExptNo
Li+	kin non-ac	0°C 100%			1993BCd (51648) 273

```
K(Li2A2B2+2L=Li2B2L2+2A)=0.204
Metal:Li(0). Medium:Hexane. A:di(iso-propyl)amine. B:Tetrahydrofuran.
*****************************
                            (2075)
Di(dimethylphosphinylmethyl) ether; Me2P(0)CH2.O.CH2.P(0)Me2
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
Li+ con non-aq 25°C 100% U K1=4.04 1989KSa (51773) 274
Medium: tetrahydrofuran/CHCl3 4:1 (vol)
_____
Li+ sp non-ag 25°C 100% U K1=1.83 1983YSb (51774) 275
Medium: tetrahydrofurane + CHCl3 (4:1); Li as 2,4-dinitrophenolate.
In (CH3CN+CHCl3 1:1) K1=2.69. Data also for other phosphine oxides
______
Li+ con non-aq 25°C 100% U K1=4.04 1982YSa (51775) 276
Medium: tetrahydrofuran+CHCl3 4:1(vol); M is 2,4-dinitrophenolate
*****************************
       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
Li+ ISE non-aq 25°C 100% M K1=3.32 B2=5.51 1988NHa (51981) 277
Medium: MeCN, 0.01 M Et4NClO4
-----
     con non-ag 25°C 100% U M
                                 1982GJb (51982) 278
                        Kout(LiL+A)=5.8
Medium: 1,2-dichloroethane. A=tetraphenylborate
-----
      ISE non-aq 25°C 100% U T H K1=3.31 1982NYa (51983) 279
Li+ ISE non-aq 25°C 100% C K1=3.3 B2=5.5 1975NAa (51984) 280
Medium: CH3CN, 0.01 M Et4NCl04
***********************************
                          CAS 767-00-0 (1632)
4-Cyanophenol; HO.C6H4.CN
-----
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
     con non-aq 25°C 100% U K1=8.04 1991AMa (52582) 281
Medium: THF
**********************************
                          CAS 303-38-8 (1398)
            H3L
2,3-Dihydroxybenzoic acid; C6H3(OH)2.COOH
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
-----
Li+ gl NaClO4 25°C 0 C I K1=1.67
                              1992CRa (54468) 282
```

```
K(Li+LiL)=0.77
K(Li+HL)=0.75
K(Li+H2L)=-0.7
```

Extrapolated to I=0 form I=0.04		((L1+H2L)=-0./	
**************************************	******	**************************************	
Metal Mtd Medium Temp Conc	: Cal Flags	Lg K values	Reference ExptNo
Li+ con non-aq 25°C 100% Medium: THF. With 4-t-butylphen ************************************	ol K=10.87,	2-t-butylphen	ol K=10.13
C7H8O8P2 H4L 1,2-((Phenylenedioxo)methylene)		(6892)	
Metal Mtd Medium Temp Conc	Cal Flags	Lg K values	Reference ExptNo
Li+ gl R4N.X 25°C 0.50 Medium: 0.5 M Me4NCl ************************************			1985GMb (56169) 284
C8H5N5O6 H3L Mu Purpuric acid (Murexide is ammo	ırexide	(453)	
Metal Mtd Medium Temp Conc	Cal Flags	Lg K values	Reference ExptNo
Li+ sp non-aq 25°C 100% Medium: 10% w/w DMF/MeCN. DH(K1 Data also for 20 30, 40 w/w% DM	.)=-5.0 kJ m		• • •
Li+ sp alc/w 25°C 95% Medium: 95% w/w EtOH/H2O, 0.05		K1=2.44	1993GSa (58519) 286
Li+ sp non-aq 20°C 100% Medium: DMF, 0.01 M Me4NI ************************************			, ,
C8H5O2F3S HL TT 4,4,4-Trifluoro-1-(2-thienyl)bu	·A	CAS 326-91	-0 (165)
Metal Mtd Medium Temp Conc	_	-	Reference ExptNo
Li+ dis non-aq 25°C 100%	C M		2002IIa (58639) 288
Medium: chlorobenzene. For extr K(Li+HL(o)=LiL(o)+H)=-10.34; K(	action from		
Li+ gl alc/w 25°C 0.10 Medium: MeOH, 0.1 M LiClO4. In ************************************	EtOH: K1=5.	3	1965LIa (58640) 289
		I CAS 88-99-	

```
Benzene-1,2-dicarboxylic acid; C6H4(COOH)2
_____
    Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
Li+ gl R4N.X 37°C 0.25M C TI K1=0.85 1985DRa (58985) 290
B(LiHL)=5.03
Medium: 0.02-1 M NEt4I
-----
Li+ gl oth/un 37°C 0.15M C I K1=0.65 B2= 0.65 1983DRb (58986) 291
Medium: 0.15 M LiNO3. Method: determination of protonation constant in
LiNO3 and [Et4N]NO3 media. Data for I=0.0-1.0 M LiNO3. At I=0.0, K1=1.00.
********************************
                 Phenoxyacetic CAS 122-59-8 (1153)
              HL
Phenoxyethanoic acid; C6H5.O.CH2.COOH
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
25°C 0.0 C TIH K1=0.07 1985CDb (60038) 292
      gl none
Calculated from protonation data for I=0.04-0.9 M LiCl. Data for 10-45 C.
DH(K1)=7.7 \text{ kJ mol-1}, DS(K1)=28 \text{ J K-1 mol-1}.
**********************************
            H2L Uramildiacetic CAS 13055-06-5 (185)
C8H9N307
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
______
    cal R4N.X 20°C 0.1M C
                                  1976ANb (60637) 293
                        DH1= -7.61 \text{ kJ/mol}
in Me4NCl
-----
      gl R4N.X 39°C 0.10M U TIH K1=4.60 1963IFb (60638) 294
Medium: Me4NNO3. K1=4.90(20 C), 4.70(27 C), 4.57(34 C); DH(K1)=-29.3 kJ mol-1
DS=-4 J K-1 mol-1. At I=0 corr:K1=5.61(20 C)
______
  ISE oth/un 20°C 0.0 U K1=5.40 1948SBa (60639) 295
*********************************
                          CAS 576-26-1 (1498)
2,6-Dimethylphenol; HO.C6H3(CH3)2
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      nmr non-aq 22°C 100% U T H
                                  1991JRa (60826) 296
Medium: dioxolane. 90-22 C. DH(Li2L+2LiCl04=2Li2LCl04)=0 kJ mol-1, DS=58
In THF: DH=0, DS=28. In dioxalane DH(LiL2+2LiBPh4=2Li2LBPh4)=-5, DS=-5
******************************
C8H1102F3
              HL
                           CAS 22767-90-4 (1249)
1,1,1-Trifluoro-5,5-dimethyl-2,4-hexanedione; F3C.CO.CH2.CO.CH(CH3)3
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
```

```
Li+ oth diox/w 25°C 75% U K1=4.61 B2=8.05 1979MMa (61304) 297
*******************************
                Dimedone
                         CAS 126-81-8 (1137)
5,5-Dimethyl-1,3-cyclohexanedione;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
    gl alc/w 25°C 100% U I K1=1.5 1965LIa (61687) 298
Medium: MeOH, 0.1 M LiClO4. In EtOH: K1=2.1
*******************************
                12-Crown-4 CAS 294-93-9 (174)
1,4,7,10-Tetraoxacyclododecane; cyclo(-0.(CH2.CH2.0)3.CH2.CH2-)
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
  nmr non-aq 25°C 100% C I K1=1.89 2001KZb (62683) 299
Method: 7Li nmr. Medium: acetonitrile.
Data for 20-80% w/w nitrobenzene/acetonitrile.
______
Li+ nmr non-aq 27°C 100% C K1=3.91 2000SMg (62684) 300
Medium: acetonitrile. Method: 7Li nmr.
_____
Li+ cal non-aq 25°C 100% C IH K1=3.52 1996DNa (62685) 301
Medium: CH3CN. Data for LiX where X=AsF6-,BF4-,CF3SO3-,Cl04-. DH(K1)=
-21.35 kJ mol-1, DS=-4.6. In PC, K1=2.84, DH(K1)=-17.05, DS(K1)=-2.8.
-----
     nmr non-aq 27°C 1.0M C I K1=3.12 1996KAb (62686) 302
Method: 7Li nmr. Medium: acetonitrile. Also data for nitromethane and
20-80% w/w acetonitrile/nitromethane.
-----
     con alc/w 25°C 100% U I K1=1.320 1995DSb (62687) 303
Medium : MeOH. In MeCN K1=3.140
______
Li+ con non-aq 25°C 100% U K1=3.2
                                1993EVa (62688) 304
Medium: THF+CHCl3 (4:1 vol)
______
Li+ nmr non-aq 25°C 100% U K1=1.0
                                1989MGc (62689) 305
Medium: tetrahydrofurane
------
     con alc/w 25°C 100% U H T B2=2.73
                                1987BUa (62690) 306
Medium: MeOH. DH(B2)=0 kJ mol-1; DS=52.0 J K-1 mol-1
______
Li+ con non-aq 25°C 100% C K1=<0.0 1987ZBb (62691) 307
Medium: MeOH.
-----
Li+ con non-aq 25°C 100% U K1=3.40 1980HNa (62692) 308
-----
Li+ vlt non-aq 25°C 100% U K1=2.93 1980MDa (62693) 309
Medium: propylene carbonate
```

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Li+ nmr non-aq 27°C 100% C IH K1=4.25 1980SPb (62694) 310
Method 7Li nmr. Medium: CH3CN. Also data for CH3NO2, PC, MeOH, acetone, PY
DMSO, TMG, H2O.By calorimetry, DH(K1)=-16 kJ mol-1, DS(K1)=27 J K-1 mol-1.
**************************
                           CAS 41775-76-2 (6751)
10-Aza-1,4,7-trioxacyclododecane;
-----
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
Li+ vlt non-aq 25°C 100% C K1=4.5 2000HHa (62764) 311
Medium: acetonitrile, 0.1 M Et4NClO4. Method: dc polarography.
______
Li+ cal non-aq 25°C 100% C IH K1=4.24 1994DTa (62765) 312
Medium: CH3CN. Data are for LiBF4. Data for LiAsF6 and Li(CF3SO3). DH(K1)=
-19.91 kJ mol-1, DS=14.4. In propylene carbonate, K1=3.69, DH=-14.63, DS=22
***************************
C8H18N2O2
                            CAS 294-92-8 (654)
1,7-Dioxo-4,10-diazacyclododecane;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      vlt non-aq 25°C 100% C K1=5.3 2000HHa (62844) 313
Medium: acetonitrile, 0.1 M Et4NClO4. Method: dc polarography.
______
      sol non-ag 20°C 100% C K1=4.03 1983SLa (62845) 314
Medium: CHCl3
**********************************
         L
                 Triglyme
                            CAS 112-49-2 (2358)
1,2-Bis(methoxyethoxy)ethane; CH30.C2H40.CH2.CH2.OC2H4.OCH3
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
Li+ con non-aq 25°C 100% U K1=2.9 1993EVa (62988) 315
Medium: THF+CHCl3 (4:1 vol)
______
     con non-aq 25°C 100% U M
                                    1982GJb (62989) 316
                          Kout(LiL+A)=7.0
Medium: 1,2-dichloroethane. A=picrate
******************************
                  Tetra-Et-Glycol CAS 112-60-7 (5664)
2,2'-(Oxybis(2,2-ethanediyloxy))-bis-ethanol; O(CH2.CH2.O.CH2.CH2.OH)2
_____
    Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
       con non-aq 25°C 100% C K1=3.3 1992MSe (63004) 317
Medium: 100% MeOH. Anion: picrate. Also data for nitrophenolate anions.
************************************
                  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
______
     gl R4N.X 25°C 1.00M C I K1=-0.28
                                 1982SSf (63062) 318
In 90 % (v/v) DMSO/water mixture: K1=0.61 (I=0.25 M)
**********************************
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
Li+ EMF non-ag 25°C 100% U I K1=6.90
                                1996WPa (63294) 319
Medium: acetonitrile, 0.05 M NEt4ClO4. In propylene carbonate K1=5.6; in
dimethylformamide K1=2.1
CAS 86536-56-3 (2076)
1,2-Bis(2-dimethylphosphinylmethoxy)ethane; Me2P(0)CH2.O.CH2.CH2.O.CH2.P(0)Me2
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      con non-aq 25°C 100% U
                        K1=4.38 1989KSa (63311) 320
Medium: tetrahydrofuran/CHCl3 4:1 (vol)
*************************
                         CAS 521-74-4 (3279)
5,7-Dibromo-8-hydroxyquinoline;
_____
     Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
Li+ sp alc/w ? 100% U K1=5.54 1970PMc (63520) 321
***********************************
                         CAS 148-24-3 (504)
                0xine
8-Hydroxyquinoline (8-quinolinol);
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      nmr non-aq 27°C 100% U I K1=1.96 B2= 2.36 1996MAb (64302) 322
Method: 7Li nmr. Medium: acetonitrile, 0.05 M LiClO4. Data for acetone
(K1<0.5) and nitromethane (K1=1.87, K2=1.22).
-----
     sp alc/w 25°C 95% U K1=1.80 1993GSa (64303) 323
Medium: 95% w/w EtOH/H2O, 0.05 M Et4NClO4, by competitive spectrophotometry
______
      sp non-ag 25°C 100% U I K1=2.82 B2=4.54 1992GSa (64304) 324
Li+
Medium: MeCN. In acetone: K1=1.98; in MeOH: K1=0.91. By fluorimetry
*********************************
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
______
```

Li+ gl R4N.X 20°C 0.10M U K1=4.86 1963IFb (66526) 325 Medium: Me4NNO3 ***********************************	
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo	
Li+ oth diox/w 25°C 75% U K1=4.84 B2=8.23 1979MMa (66536) 32	26
C9H16O2 HL CAS 18362-64-6 (1134) 2,6-Dimethyl-3,5-heptanedione; (CH3)2.CH.CO.CH2.CO.CH(CH3)2	
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo	
Li+ gl diox/w 30°C 75% U K1=9.23 B2=15.76 1975MMa (67746) 32 ************************************	27
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo	
Li+ con non-aq 22°C 100% U K1=1.11 1981SKd (68123) 328  Medium: CH3CN  ***********************************	
Methylenedi(phosphonic acid diethyl ester) CH2(PO.(OC2H5)2)2	
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo	
Li+ con non-aq 22°C 100% U K1=1.62 1981SKd (68260) 329 Medium: CH3CN	
**************************************	
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo	
Metal Med Medium Temp Conc Cal Tlags Lg R Values Reference Expend	
Li+ con non-aq 25°C 100% C K1=10.07 1997CHb (68444) 330 B(Li2L)=14.00	
Li+ con non-aq 25°C 100% C K1=10.07 1997CHb (68444) 330	
Li+ con non-aq 25°C 100% C K1=10.07 1997CHb (68444) 330 B(Li2L)=14.00  Medium: THF. By conductivity, species M2L and L2M are equivalent.  ***********************************	

```
B(LiH3L)=13.00
B(Li2L)=2.50
```

Medium: 1	.0 M Et4NI.	B(Li2HL)=6.87.		
	•		I K1=1.44 B(LiHL)=6.33 B(LiH2L)=10.0 B(LiH3L)=12.1 B(Li2HL)=6.15	1990DDb (68521) 332 4 2
Medium: 0 ******	).25 M Et4NI. *******	Data for 0.08-	0.99 M. B(Li2L)=1. *******	97 ********
C10H8N2 2,2'-Bipy	ridine; (C5H	•	pyridyl CAS 366-	, ,
Metal	Mtd Medium	Temp Conc Cal	Flags Lg K values	Reference ExptNo
Method: 7	Li nmr. Med		le, 0.05 M LiClO4.	= 2.97 1996MAb (69596) Data for acetone
Medium: 9		H2O, 0.05 M Et4		1993GSa (69597) 334 ive spectrophotometry
Medium: M ******* C10H10O2	leCN. In acet	one:K1=1.85; in ******	MeOH:K1=0.45. By ************************************	********
Metal	Mtd Medium	Temp Conc Cal	Flags Lg K values	Reference ExptNo
Medium: a	cetonitrile			1988YSb (70745) 336
Li+ Medium: M	gl alc/w HeOH, 0.1 ML	25°C 100% U iClO4. In EtOH:	I K1=3.1 K1=3.2	1965LIa (70746) 337
C10H11NO5 N-(2-Hydr		H3L inodiethanoic a	CAS 1008 cid; HO.C6H4.N(CH2	44-86-8 (2108) .СООН)2
Metal	Mtd Medium	Temp Conc Cal	Flags Lg K values	Reference ExptNo
	******			1963IFb (71042) 338 ********
N-(2-Sulf	ophenyl)imin	odiethanoic aci	d; HO3S.C6H4.N(CH2	.COOH)2
				Reference ExptNo
Li+	EMF KCl	20°C 0.10M C	K1=2.26	1947SWa (71067) 339

```
************************************
C10H1102F7
                         CAS 17587-22-3 (1252)
1,1,1,2,2,3,3-Heptafluoro-7,7-dimethyl-4,6-octanedione;
  -----
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
-----
     oth diox/w 25°C 75% U K1=4.75 B2=8.32 1979MMa (71111) 340
C10H12N2O4
                         CAS 16598-05-3 (967)
           H2L
2-Pyridylmethyliminodiethanoic acid; C5H4N.CH2.N(CH2.COOH)2
______
     Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
Li+ gl KNO3 20°C 0.10M U K1=1.71 1963IFc (71264) 341
****************************
                          (3912)
C10H13N307
           H3L
1,3-Dimethyluramil-N,N-diethanoic acid;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
_____
     gl R4N.X 20°C 0.10M U K1=4.91
                              1963IFb (71806) 342
Medium: Me4NNO3
***********************
            L Adenosine
                        CAS 58-61-7 (2154)
Adenosine, Adenine-9-beta-D-ribofuranoside;
______
     Mtd Medium Temp Conc Cal Flags Lg K values
                                Reference ExptNo
______
     nmr non-aq 25°C 100% U M
                               1976PSc (71945) 343
Li+
                      K(LiCl+L)=0.8
Medium: DMSO
**********************************
C10H14N507P
                AMP-5
                         CAS 18422-05-4 (842)
Adenosine-5'-monophosphoric acid, 5-Adenylic acid;
_____
     Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
-----
     gl R4N.X 25°C 0.10M C T K1=1.22 1991SMa (72459) 344
IUPAC evaluation
************************************
C10H140
                         CAS 98-54-4 (458)
4-(t-Butyl)-1-hydroxybenzene; C4H9.C6H4.OH
______
     Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
                       K1=10.87 1991AMa (72610) 345
      con non-aq 25°C 100% U
Medium: THF. With 2-t-butylphenol K=10.13
**********************************
                ADP
                        CAS 20398-34-9 (2181)
C10H15N5O10P2
Adenosine-5'-diphosphoric acid;
```

Metal	Mtd	Medium	Temp	Conc Ca	l Flags	Lg K valu	ies	Refe	rence Ex	ptNo
IUPAC eval	uatio	n				Γ K1=1.32				
C10H16N2O8			H4L	EDTA		CAS 6 acid, Seq	60-00-4 Juestrio	(120) acid;		ጥ ጥ ጥ ጥ ጥ
					_	s Lg K valu	ies	Refe	rence Ex	
						K1=2.90 B(LiHL)=10 B(Li2L)=3.	1 0.85			
Data at 10 DH(LiHL)=-						3. DH(K1)=2	kJ mol	l-1; DS:	=60.	
						K1=2.66 DH1= 3.26	kJ/mol	L976ANb	(73928)	348
						0.84 kJ/mol				
Medium: (C	H3)4N	IC1				K1=2.43				
	vlt	R4N.X		0.10M U		K1=3.15	1	1972BZc	(73930)	
Li+ Medium: Cs		oth/un	25°C	0.32M U		K1=2.85 K(Li+HL)=0	B2=3.6	58 196	65BCa (7	3931) :
					Н	54.3 J K-1	1			352
Method: H	elect	rode				Κ1=2.79				
**************************************	3P3		H4L	ATP		·*************************************			*****	****
Metal	Mtd	Medium	Temp	Conc Ca	l Flags	Lg K valu	ies	Refe	rence Ex	ptNo
IUPAC eval	uatio	n. DH(	(1)=-4	kJ mol		R K1=1.78 ntatitive)	1	1991SMa	(74755)	354
Li+					Н	K(Li+LiHL) B(LiHL)=6.	=1.35	1986RSa	(74756)	355
Li+	gl	oth/un	25°C	0.32M U		K1=1.7	B2=2.2	23 196	65BCa (7	4757)

```
Medium: CsCl
**********************************
                         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
______
Li+ gl KNO3 20°C 0.10M U K1=1.74 1963IFb (74975) 357
*******************************
                         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
______
           20°C 0.10M U K1=2.19 1963IFb (74989) 358
Li+ gl KNO3
*************************
C10H17N05
            H2L
                          (3917)
N-(Tetrahydropyran-2-ylmethyl)iminodiethanoic acid;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
-----
Li+ gl KNO3 20°C 0.10M U K1=1.7 1963IFa (75002) 359
******************************
C10H17N5O16P4
               AQP
                        CAS 1062-98-2 (3341)
           H5L
Adenosine-5'-tetraphosphoric acid;
-----
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
Li+ gl R4N.X 25°C 0.10M C T K1=2.22 1991SMa (75159) 360
IUPAC evaluation
****************************
C10H18N2O5
                          (5608)
1-0xa-4,7-diazacyclononane-N,N'-diethanoic acid;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
Li+ gl KNO3 25°C 0.10M U K1=1.42 1990CCa (75235) 361
*******************************
               15-Crown-5 CAS 33100-27-5 (576)
1,4,7,10,13-Pentaoxacyclopentadecane; cyclo(-(0.CH2.CH2)5-)
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
-----
      ISE alc/w 25°C 100% C I T K1=1.24
                               2003ADa (76036) 362
IUPAC Tentative. Medium: 0-0.1 M various.
Li+ nmr non-aq 25°C 100% C I K1=3.58 2001KZb (76037) 363
Method: 7Li nmr. Medium: acetonitrile.
Data for 20-80% w/w nitrobenzene/acetonitrile.
```

```
Li+ nmr non-aq 27°C 100% C K1=4.76 2000SMg (76038) 364
Medium: acetonitrile. Method: 7Li nmr.
_____
Li+ vlt non-aq 25°C 100% C I K1=4.2 1999WKb (76039) 365
Medium: acetonitrile, 0.10 M Et4NClO4. Also data for TMS, propylene
carbonate, acetone, formamide, DMF, DMA, DMSO, MeOH, EtOH.
______
Li+ nmr non-aq 27°C 1.0M C I K1=4.8 1996KAb (76040) 366
Method: 7Li nmr. Medium: acetonitrile. Also data for nitromethane and
20-80% w/w acetonitrile/nitromethane.
-----
Li+ con alc/w 25°C 100% U I K1=1.314 1995DSb (76041) 367
Medium : MeOH. In MeCN K1=3.580
_____
   vlt non-ag 25°C 100% C K1=7.2 1995KTb (76042) 368
Method: ion transfer polarography. Medium: nitrobenzene, 0.05 M
tetrabutylammonium tetraphenylborate.
-----
Li+ cal non-aq 25°C 100% M H K1=3.42 1994BCd (76043) 369
Medium: acetone. DH(K1)=-12.9 kJ mol-1, TDS=6.5
______
Li+ cal non-aq 25°C 100% C IH K1=4.44 1994DTa (76044) 370
Medium: CH3CN. Data are for LiBF4. Data for LiAsF6 and Li(CF3SO3). DH(K1)=
-25.34 kJ mol-1, DS=0.0. In propylene carbonate, K1=4.21, DH=-20.44, DS=12
_____
Li+ con non-aq 25°C 100% C T K1=5.3 1988TKa (76045) 371
Medium: MeCN
_____
Li+ con non-aq 25°C 100% C I K1=1.21 1987ZBb (76046) 372
Medium: MeOH. In 70% w/w MeOH/H2O, K1=1.02.
______
Li+ con non-aq 25°C 100% U K1=3.60 1980HNa (76047) 373
Medium: MeCN
-----
     nmr non-aq 27°C 100% C IH K1=>4 1980SPb (76048) 374
Method 7Li nmr. Medium: CH3CN. Also data for CH3NO2, PC, MeOH, acetone, PY
DMSO, TMG, H2O.By calorimetry, DH(K1)=-21 kJ mol-1, DS(K1)=>6 J K-1 mol-1.
______
Li+ dis non-aq 25°C 100% U K1=4.2 1980TYa (76049) 375
Medium: propylene carbonate
*******************************
C10H21N04 L CAS 66943-05-3 (5818)
1-Aza-4,7,10,13-tetraoxacyclopentadecane;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
Li+ vlt non-aq 25°C 100% C K1=5.2 2000HHa (76185) 376
Medium: acetonitrile, 0.1 M Et4NClO4. Method: dc polarography.
*********************************
```

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L Cryptand 2,1 CAS 31249-95-3 (835)
C10H22N2O3
4,7,13-Trioxa-1,10-diazacyclopentadecane (Trioxa(2,1)cryptand);
Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
Li+ vlt non-aq 25°C 100% C K1=5.4 2000HHa (76323) 377
Medium: acetonitrile, 0.1 M Et4NClO4. Method: dc polarography.
______
Li+ cal non-aq 25°C 100% M H K1=3.13 1994BCd (76324) 378
Medium: acetone. DH(K1)=-9.1 kJ mol-1, TDS=8.7
_____
   sp non-aq 20°C 100% U K1=2.3 1992PSa (76325) 379
Medium: DMF, 0.01 M Me4NI
************************
           L Tetraglyme CAS 143-24-8 (121)
C10H22O5
2,5,8,11,14-Pentaoxapentadecane; (CH3.0.CH2.CH2.0.CH2.CH2.)20
-----
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
Li+ dis non-aq 25°C 100% C K1=4.69 1998KSc (76456) 380
Medium: 1,2-dichloroethane.
______
     con non-aq 25°C 100% U K1=3.2 1993EVa (76457) 381
Medium: THF+CHCl3 4:1(vol)
-----
Li+ con non-aq 25°C 100% U M
                                 1982GJb (76458) 382
                        Kout(LiL+A)=5.7
Medium: 1,2-dichloroethane. A=tetraphenylborate
********************************
       H3L CAS 1147-65-5 (425)
C11H11N06
N-(2'-Carboxyphenyl)iminodiethanoic acid; HOOC.C6H4.N(CH2.COOH)2
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
-----
Li+ gl R4N.X 20°C 0.10M U K1=2.05
                                 1963IFb (77829) 383
Medium: Me4NNO3
Li+ EMF KCl 20°C 0.10M U K1=2.18 1950WIa (77830) 384
Method: H electrode
************************************
            H4L PDTA
                          CAS 4408-81-5 (1655)
C11H18N2O8
1,2-Diaminopropane-N,N,N',N'-tetraethanoic acid;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
Li+ oth R4N.X 25°C 0.50M U K1=4.01 1971CSb (79306) 385 Method: polarimetry. Medium: Me4NOH
**********************************
                 Dipivaloylmeth. CAS 1118-71-4 (363)
2,2,6,6-Tetramethyl-3,5-heptanedione; (CH3)3C.CO.CH2.CO.C(CH3)3
```

```
Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
Li+ gl diox/w 30°C 75% U K1=5.76 B2=10.37 1975MMa (79750) 386
*******************************
                  16-Crown-5 CAS 55477-28-8 (1592)
1,4,7,10,13-Pentaoxacyclohexadecane; cyclo(-(0.CH2.CH2)5.CH2.CH2-)
-----
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
      con none 25°C 0.0 C K1=1.05
                                2001KMb (79859) 387
______
      dis none 25°C 0.0 C M
                                   1989TKc (79860) 388
Method: extraction of metal picrate/L from H2O into benzene.
K(Li+HA(org)+L(org)=LiAL(org)+H)=-1.74. HA is picric acid.
-----
Li+ con non-aq 25°C 100% C I K1=4.5
                                1988TKa (79861) 389
Medium: MeCN. In propylene carbonate K1=3.3
*******************************
               L Dipicrylamine CAS 131-73-7 (1942)
C12H5N7012
Di(2,4,6-trinitrophenyl)amine; HN(C6H2(NO2)3)2
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
      dis non-aq 25°C 100% C K1=3.9
                                   1998KSc (80078) 390
Medium: 1,2-dichloroethane.
______
      dis oth/un 25°C var U K1=1.7 1970SSb (80079) 391
Method: paper chromatography
*************************
                 Mellitic acid (7400)
             H6L
Benzenehexacarboxylic acid; (C(COOH))6
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
-----
Li+
      ISE R4N.X 25°C 0 C I
                          K1=2.95
                                   1996RSb (80113) 392
                         B(NaHL)=10.13
                         B(NaH2L)=15.57
                         B(NaH3L)=20.06
                         B(NaH4L)=22.80
B(Li2L)=4.80, B(Li2HL)=11.33 B(Li2H2L)=17.13, BLi2H3L)=20.84
B(LI3L)=6.43,B(Li3HL)=12.95, B(Li4L)=7.83. I=0-3 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
______
      nmr non-aq 27°C 100% U I K1=2.28 B2= 3.98 1996MAb (80474) 393
Method: 7Li nmr. Medium: acetonitrile, 0.05 M LiClO4.
```

```
Also data for acetone: K1=2.20, K2=1.93.
_____
     sp alc/w 25°C 95% U K1=2.24 1993GSa (80475) 394
Medium: 95% w/w EtOH/H2O, 0.05 M Et4NClO4, by competitive spectrophotometry
_____
Li+ sp non-aq 25°C 100% U I K1=3.01 B2=4.88 1992GSa (80476) 395
Medium: MeCN. In acetone:K1=3.11, K2=2.00; in MeOH:K1=0.95. By fluorimetry
***********************************
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
______
Li+ sp non-aq 25°C 100% U K1=1.16 2000EGa (81675) 396
Method: fluorescence emission spectroscopy. Medium: acetonitrile.
-----
Li+ cal non-aq 25°C 100% U H K1=1.05 1989SSd (81676) 397
Medium: CH3CN
Li+ cal non-aq 25°C 100% U H K1=1.05 B2=2.80 1988SSc (81677) 398
Medium: MeCN
______
Li+ cal alc/w 25°C 100% U H K1=1.34 1985LWa (81678) 399
**********************************
        H4L BDTA
C12H20N2O8
                          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
______
Li+ oth R4N.X 25°C 0.50M U
                                 1973CSa (82313) 400
                        K1=5.26(D)
                        K1=2.60(meso)
                        K(Li+HL)=1.68
Method: polarimetry. Medium: Me4NCl
********************
                          CAS 82154-47-0 (2915)
1,2-Di((2-dimethylphosphinyl)methoxy)benzene; C6H4(OCH2PO(CH3)2)2
_____
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
      con non-aq 25°C 100% U K1=4.31 1982YSa (82642) 401
Medium: tetrahydrofuran+CHCl3 4:1(vol); M is 2,4-dinitrophenolate
*******************************
                          CAS 93269-15-9 (1250)
2,2,4,6,6-Pentamethyl-3,5-heptanedione; (CH3)3C.CO.CH(CH3).CO.C(CH3)3
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
-----
     oth diox/w 25°C 75% U K1=6.85 B2=10.54 1979MMa (82859) 402
```

```
***********************************
C12H23N05
             L
                           (6793)
10-Methoxycarbonylethyl-1,4,7-trioxa-10-azacyclododecane;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
-----
      cal alc/w 25°C 100% U H K1=2.71
                                1990KMb (82946) 403
Medium: MeOH. DH=-3.0 kJ mol-1
*********************************
             L Cryptand 1,1,1 CAS 37095-49-1 (6636)
4,10,15-Trioxa-1,7-diazabicyclo[5.5.5]heptadecane;
_____
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
Li+ sp non-aq 20°C 100% U K1=1.7 1992PSa (83018) 404
Medium: DMF, 0.01 M Me4NI
*********************************
C12H2402
             HL
                Lauric acid CAS 143-07-7 (2540)
Dodecanoic acid, CH3.(CH2)10.COOH
  -----
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
_____
     gl oth/un 26°C 0.00 U K1=4.12 1976HYa (83113) 405
B(LiHL2)=9.06
*********************************
                         CAS 26996-94-3 (2541)
C12H2404
Tetramethyl-12-crown-4
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      con non-aq 25°C 100% U K1=3.46 1980HNa (83124) 406
Medium: MeCN
************************************
        L 18-Crown-6
                         CAS 17455-13-9 (577)
1,4,7,10,13,16-Hexaoxacyclooctadecane;
______
    Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      nmr non-aq 27°C 100% C I K1=4.96
                                2001KZa (83454) 407
Method: 7Li nmr. Medium: nitromethane. In acetonitrile, K1=2.25
-----
     nmr non-ag 25°C 100% C I K1=1.92 2001KZb (83455) 408
Method: 7Li nmr. Medium: acetonitrile.
Data for 20-80% w/w nitrobenzene/acetonitrile.
______
      dis non-aq 25°C 100% U K1=8.20 2000KSa (83456) 409
Medium: 1,2-dichloroethane
_____
   nmr non-aq 27°C 100% U I K1=2.52 2000SMd (83457) 410
Method: 7Li nmr. Medium: acetonitrile (AN). Also data for 50% w/w AN/
```

```
nitrobenzene (K1=2.80) and 50% w/w AN/nitromethane (K1=2.98).
_____
      cal non-aq 25°C 100% C H K1=2.50 1999WBa (83458) 411
Medium: N,N-dimethylformamide. DH(K1)=-0.7 kJ mol-1.
-----
   dis non-aq 25°C 100% C I
                                   1998TKa (83459) 412
                         K(Li+A+L(org)=LiAL(org))=2.440
Method: Extraction from aqueous phase (I<0.03, pH 10.6-11.8) into
dichloromethane. Data for many non-aqueous phases. HA is picric acid.
______
Li+ cal non-aq 25°C 100% C K1=4.74 1997DZa (83460) 413
Medium: benzonitrile. DH(K1)=-38.48 \text{ kJ mol}-1, DS(K1)=-38.3 \text{ J K}-1 \text{ mol}-1.
______
Li+ nmr non-aq 27°C 1.0M C I K1=2.30 1996KAb (83461) 414
Method: 7Li nmr. Medium: acetonitrile. Also data for nitromethane and
20-80% w/w acetonitrile/nitromethane.
      vlt non-aq 25°C 100% C K1=7.5 1995KTb (83462) 415
Method: ion transfer polarography. Medium: nitrobenzene, 0.05 M
tetrabutylammonium tetraphenylborate.
______
Li+ cal non-aq 25°C 100% M H K1=2.41 1994BCd (83463) 416
Medium: acetone. DH(K1)=-19.8 kJ mol-1, TDS=-6.1
______
Li+ dis non-aq 25°C 100% U B(Li2P2L)=7.43
                                   1993INa (83464) 417
K is the equilibrium constant for extraction of the metal picrate (P) into
CH2Cl2. For extraction from D2O, B=7.53
______
Li+ con non-aq 25°C 100% C K1=2.782 1990SAb (83465) 418
Medium: propylene carbonate.
______
Li+ con non-aq 25°C 100% U K1=3.73 1980HNa (83466) 419
Medium: MeCN
-----
      nmr non-aq 27°C 100% C IH K1=2.34 1980SPb (83467) 420
Method 7Li nmr. Medium: CH3CN. Also data for CH3NO2, PC, MeOH, acetone, PY
DMSO, TMG, H2O.By calorimetry, DH(K1)=ca.0 kJ mol-1,DS(K1)=45 J K-1 mol-1.
**************************
C12H25N05 L CAS 33941-15-0 (4939)
1,4,7,10,13-Pentaoxa-16-azacyclooctadecane;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
-----
      vlt non-aq 25°C 100% C K1=3.2
                                   2000HHa (83707) 421
Medium: acetonitrile, 0.1 M Et4NClO4. Method: dc polarography.
********************************
                         (7849)
N,N-Diethylcarbamoylmethyl-(dipropylphosphineoxide;
______
```

	Mtd Medium	Temp	Conc	Cal	Flags	Lg K value	Reference ExptNo
In tetrahy ********** C12H26N2O4	drofuran; a	lkali ***** L	meta] **** Cry	l is **** ptar	used a ****** nd 2,2	as 2,4-dini ********** CAS 23	1999ESa (83720) 422 trophenolate ************************************
Metal	Mtd Medium	Temp	Conc	Cal	Flags	Lg K value	s Reference ExptNo
Li+ Medium: 10	sp alc/w 90% MeOH. Me						2002NFa (83860) 423 ass spectrometry.
	cal non-aqeetone. DH(K					K1=1.52	1994BCd (83861) 424
	sp non-aq IF, 0.01 M M		100%	U		K1=1.2	1992PSa (83862) 425
Li+ Medium: Me	-	25°C	100%	U	I	K1=6.98	1983CFa (83863) 426
Medium: CH						K1=4.08	1983SLa (83864) 427
C12H2606		L	Per	ntag]	Lyme	CAS 11	91-87-3 (2498) H2.CH2.O.CH2.)2
Metal	Mtd Medium	Temp	Conc	Cal	Flags	Lg K value	Reference ExptNo
Li+	con non-aq		100%	U		K1=3.2	
**************************************	IF+CHC13 (4:	****** L	***** THE	**** ETAC	*****	other sol ************************************	********
**************************************	F+CHC13 (4: ************************************	***** L yl)-1,	***** THE 4,7-t	**** ETAC :riaz	****** zacyclo	r other sol ******* (719 ononane	/ents *********
********* C12H27N3O3 1,4,7-Tris Metal Li+ Medium: Me Method: Ag	<pre>HF+CHCl3 (4: ********** (hydroxyeth Mtd Medium EMF non-aq OH, 0.05M E J/Ag+ electr</pre>	******  y1)-1, Temp 25°C t4NClC	****** THE .4,7-t Conc 100%	***** ETAC Eriaz Cal Cal	<pre>****** zacyclo Flags ition v</pre>	r other solution of the component of the	/ents ************************************
********* C12H27N3O3 1,4,7-Tris Metal Li+ Medium: Me Method: Ag ********* C12H32N4O1	######################################	******  L y1)-1, Temp 25°C t4NC1C ode; b *****	****** THE 4,7-t Conc 100% 04. Dy con *****	***** ETAC Criaz Cal C npeti	****** zacyclo  Flags  ition v	r other solution of the control of t	/ents ************************************
********* C12H27N3O3 1,4,7-Tris Metal Li+ Medium: Me Method: Ag ********* C12H32N4O1	##********  (hydroxyeth  Mtd Medium  EMF non-aq OH, 0.05M E  (/Ag+ electr ************************************	******  L y1)-1, Temp 25°C t4NC1C ode; b ***** H8L ododec	******  THE ,4,7-t Conc .100% )4. by con ***** DOT cane-N	<pre>***** ETAC Eriaz Cal Cal  C mpeti ***** FPH N,N',</pre>	zacyclo Flags ition v *****	r other solutions of the control of	/ents /************************************

```
B(Li3TmDOTP)=4.31
B(LiTmDOTPH)=9.16
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B(LiTmDOTPH2)=16.0, B(Li2TmDOTPH)=10.57, B(Li3TmDOTPH)=11.79
mixed-metal complexes in the Li(I)-Tm(III)-DOTP terner system
*****************************
                              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
Li+ sp non-aq 20°C 100% C
                                      1998FLb (85005) 431
                          K(Li+HL=LiL+H)=-3.01
Method: absorption and fluoroscence spectroscopy. Medium: acetonitrile.
*******************************
C13H1804
               L Bz-13-crown-4 CAS 62150-58-7 (552)
2,3,6,7,9,10-Hexahydro-5H-1,4,8,11-Benzotetraoxacyclotridecane;
_____
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
Li+ cal alc/w 25°C 100% U H K1=1.26 1985LWa (86047) 432
       sol non-aq 25°C 100% U I K1=3? K2=1.26 19810Ja (86048) 433
Medium: CH2Cl2: K1=5(?), K2=1.70. In CH3CN: K1=2.40
**********************************
C13H2605
                               (6410)
15,15-Dimethyl-1,4,7,10,13-pentaoxacyclohexadecane;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
Li+ con none 25°C 0.0 C K1=1.15 2001KMb (86477) 434
       con non-ag 25°C 100% C I
                          K1=4.1
                                     1992TFa (86478) 435
Medium: acetonitrile. In propylene carbonate, K1=3.13.
****************************
             L 19-Crown-6 CAS 55471-27-7 (8943)
C13H2606
1,4,7,10,13,16-Hexaoxacyclononadecane;
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
       con non-aq 25°C 100% C I K1=3.73
                                      2000TMb (86498) 436
Medium: CH3CN. In other media, K1=2.29 (propylene carbonate), 1.72 (DMSO).
______
       con oth/un 25°C dil C K1=0.79 1999TMa (86499) 437
Li+
Self medium (LiCl). For LiNO3, K1=0.72; for LiClO4, K1=0.77.
**********************************
                   Anthraquinone CAS 84-65-1 (2781)
C14H802
Anthraguinone;
               Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
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Li+ vlt R4N.X 25°C 0.20M U K1=1.06 1975PTc (86623) 438
********************************
                          CAS 129-43-1 (2778)
1-Hydroxyanthraquinone;
-----
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
_____
     vlt R4N.X 25°C 0.20M U K1=2.94 B2=5.49 1975PTc (86629) 439
***********************
C14H16N2O8
                           CAS 40774-59-2 (1901)
1,2-Diaminobenzene-N,N,N',N'-tetraethanoic acid; C6H4(N(CH2.COOH)2)2
______
    Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
Li+ gl R4N.X 25°C 0.10M C H K1=2.02
                                 1990NNa (87956) 440
                        K(LiL+H)=5.63
Medium: Et4NClO4. DH(K1)=10.4 kJ mol-1. DS(K1)=73 J mol-1 K-1.
______
                        K1=2.39 1985MHb (87957) 441
Li+ gl R4N.X 25°C 0.10M U
                        K(LiL+H)=6.34
                        K(Li+HL)=1.81
                        K(LiHL+H)=4.44
Medium: 0.10 M Me4NCl.
*********************************
        L Benzo15-crown-5 CAS 14098-44-3 (608)
C14H2005
2,3-Benzo-1,4,7,10,13-pentaoxacyclopentadeca-2-ene;
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
     dis none 25°C dil C I M
                                  2002THb (88294) 442
                        K(LiL+A)=-0.32
                        K(Li+A+L(org)=LiAL(org))=1.720
HA is picric acid. Data for several aryl and alkyl solvents.
Method: extraction of metal picrate into dichloromethane/L.
-----
     con none 25°C 0.0 C K1=0.76 2002TTa (88295) 443
______
Li+ nmr non-aq 25°C 100% C I K1=3.22 2001KZb (88296) 444
Method: 7Li nmr. Medium: acetonitrile.
Data for 20-80% w/w nitrobenzene/acetonitrile.
-----
     con non-aq 25°C 100% C K1=5.60 2000ICa (88297) 445
Medium: nitromethane.
______
     nmr non-aq 27°C 100% C
                        K1=4.56
                                 2000SMg (88298) 446
Medium: acetonitrile. Method: 7Li nmr.
Li+ vlt non-aq 25°C 100% C I K1=3.8 1999WKb (88299) 447
Medium: acetonitrile, 0.10 M Et4NClO4. Also data for TMS, propylene
carbonate, acetone, formamide, DMF, DMA, DMSO, MeOH, EtOH.
```

Li+ nmr non-aq 27°C 1.0M C I K1=4.51 1996KAb (88300) 448 Method: 7Li nmr. Medium: acetonitrile. Also data for nitromethane and 20-80% w/w acetonitrile/nitromethane.
Li+ cal non-aq 25°C 100% U H K1=3.20 1989SSd (88301) 449 Medium: CH3CN
Li+ con non-aq 25°C 100% C I K1=4.46 1988TKb (88302) 450 Medium: MeCN. In propylene carbonate K1=3.77; in MeOH 2.31
Li+ sp non-aq 22°C 100% U K1=6.09 1987CCc (88303) 451 In deuterochloroform
Li+ con non-aq 25°C 100% U K1=3.77 1982TAa (88304) 452 Medium: propylene carbonate ************************************
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
Li+ oth R4N.X 25°C 0.50M U K1=6.11 1971CSa (88710) 453 K(Li+HL)=1.15
Method: polarimetry. Medium: Me4NOH
Li+ vlt KNO3 30°C 0.10M U K1=4.13 1967SSe (88711) 454 **********************************
C14H23N3O10 H5L DTPA CAS 67-43-6 (238) Diethylenetriamine-pentaethanoic acid; H0OC.CH2.N(CH2.CH2.N(CH2.COOH)2)2
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
Li+ gl KNO3 25°C 0.10M C K1=3.1 1960WAa (89308) 455 ***********************************
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
Li+ kin KCl 25°C 1.50M U K1=1.17 1968TFb (89891) 456 ************************************
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
Li+ gl R4N.X 25°C 0.10M C K1=2.139 1987DDb (90195) 457 ************************************

```
Cyclohexyl-15-crown-5, 2,3-Cyclohexyl-1,4,7,10,13-pentaoxacyclopentadecane;
-----
    Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
Li+ ISE oth/un 25°C dil A K1=<1 1971FRa (90272) 458
**********************************
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
______
Li+ ISE non-ag 25°C 100% C H K1=6.66 1999WBa (90387) 459
Medium: N,N-dimethylformamide. Method: competitive titration against
Ag+, using Ag+ ISE. By calorimetry: DH(K1)=-38.0 kJ mol-1.
-----
Li+ gl R4N.X 25°C 0.05M C H K1=6.6 1996BCh (90388) 460
Medium: 0.05 M Et4NClO4. By calorimetry: DH(K1)=-20.2 kJ mol-1.
-----
Li+ cal non-aq 25°C 100% M H K1=11.80 1994BCd (90389) 461
Medium: acetone. DH(K1)=-63.0 kJ mol-1, TDS=4.0
-----
Li+ EMF non-aq 25°C 100% U K1=6.44 1993LRa (90390) 462
Medium: triethylphosphate, 0.05 M Et4NClO4
______
Li+ sp non-aq 20°C 100% U K1=6.6 1992PSa (90391) 463
Medium: DMF, 0.01 M Me4NI
-----
Li+ gl R4N.X 25°C 0.05M U K1=6.98 1991LRc (90392) 464
______
Li+ cal alc/w 25°C 100% U H K1=7.90 1986BUd (90393) 465
In MeOH. DH=-33.9 kJ mol-1
-----
Li+ gl alc/w 25°C 95% C K1=7.93 1981ANa (90394) 466
Medium: 95% MeOH, 0.1 M Me4NCl
______
     ISE non-ag 25°C 100% U I K1=6.99 1981CRa (90395) 467
Medium: DMF. In DMSO: K1=5.84; in EtOH: 8.47; in MeCN: >10; in NMP: 6.43
-----
Li+ cal oth/un 25°C 0.10M C
                               1981LIc (90396) 468
Medium: piperidine/HCl buffer, pH 11.4. DH(K1)=-21.8 kJ mol-1.
______
Li+ ix non-aq 25°C 100% U K1=12.87 1981SAa (90397) 469
Medium: propylene carbonate
-----
Li+ ISE non-aq 25°C 100% U K1=12.4
                              1980CRa (90398) 470
Medium: Propylene carbonate
______
Li+ EMF non-aq 25°C 100% C K1=5.3 1979BLb (90399) 471
Method: Ag electrode; competition with Ag+. Medium: MeOH, 0.05 M
Me4NClO4.
```

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ISE alc/w 25°C 100% U K1=8.04 1978CSb (90400) 472
Li+
Medium: MeOH
Li+ cal R4N.X 25°C 0.06M C H
                                  1976KLc (90401) 473
Medium: 0.057 M Me4NBr. Method: flow microcalorimetry.
DH(K1)=-21.3 \text{ kJ mol}-1, DS(K1)=34 \text{ J K}-1 \text{ mol}-1.
______
Li+ gl R4N.X 25°C 0.05M C I K1=5.5 1975LSc (90402) 474
In 95% MeOH: K1=7.58; 100%: > 6
*********************************
         L Cryptand 2,2,0 CAS 95334-31-9 (6544)
C14H28N2O4
4,7,13,16-Tetraoxa-1,10-diazabicyclo[8.8.2]eicosane;
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
-----
Li+ ISE non-aq 25°C 100% U I K1=7.8 1991ALa (90462) 475
Medium: MeCN, 0.05 M Et4NClO4. In acetone K1=8.9, MeOH K1=4.0, DMF K1=3.5,
in pyridine K1=4.0.
***********************
P-(N,N-Diethylamidocarbonyl)methyl-P,P-dibutylphosphine oxide;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
Li+ con non-aq 25°C C K1=4.0 1999ESa (90554) 476
In tetrahydrofuran; alkali metal is used as 2,4-dinitrophenolate
______
Li+ con non-aq 25°C 100% U K1=3.11 1988YKa (90555) 477
Medium: tetrahydrofuran
*******************************
P-(N,N-Diethylamidocarbonyl)methyl-P,P-dibutoxyphosphine oxide;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
     con non-aq 25°C 100% U K1=2.89 1988YKa (90558) 478
Medium: tetrahydrofuran
C14H30N2O4
                          CAS 85726-93-8 (644)
4,10-Dimethyloxyethylidene-1,7-dioxy-4,10-diazacyclododecane;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
-----
      sol non-aq 20°C 100% C K1=4.09
                                 1983SLa (90562) 479
Medium: CHCl3
**********************************
                 CAS 31255-13-7 (2448)
              L
N,N'-Dimethyl-cyclo-1,10-diaza-4,7,13,16-tetraoxaoctadecane;
______
```

Metal	Mtd Medium	Temp	Conc	Cal	Flags	Lg K values	Reference ExptNo
Medium: 9	gl alc/w 5% MeOH/H2O, *******	0.01	M Et	4NCl	04.	K1=<2	2004KVa (90581) 480
C14H30N2O	5	L				(6722	
Metal	Mtd Medium	Temp	Conc	Cal	Flags	Lg K values	Reference ExptNo
In methan	imethylforma	mide,	0.05	M E	t4NClO	4. By compet	1993RPa (90630) 481 ition with Ag+.
C14H3007 2,5,8,11,	14,17,20-Hep	L taoxal	nenei	cosa	ne; CH		2-40-8 (2499) .0)6.CH3
Metal	Mtd Medium	Temp	Conc	Cal	Flags	Lg K values	Reference ExptNo
	dis non-aq ,2-dichloroe	•		С		K1=6.75	1998KSc (90698) 482
Medium: T	HF+CHCl3 (4:	1 vol	). Al:	so da	ata fo	r other solv ******	********
	-Terpyridine	c5H	4N.C5I	H3N.	C5H4N	CAS 114	8-79-4 (488)
2,2':6'2"							8-79-4 (488)Reference ExptNo
2,2':6'2" Metal Li+ Method: 7	Mtd Medium nmr non-aq Li nmr. Med	Temp 27°C lium:	Conc 100%	Cal U	Flags	Lg K values  K1=3.24 .05 M LiClO4	Reference ExptNo 
2,2':6'2" Metal Li+ Method: 7 ********* C15H1202	Mtd Medium nmr non-aq Li nmr. Med *****	Temp 27°C ium: 1	Conc 100% nitror ****	Cal U methates	Flags  ane, 0 *****	Lg K values K1=3.24 .05 M LiClO4 ***************	Reference ExptNo 1996MAb (91159) 484
2,2':6'2" Metal Li+ Method: 7 ******** C15H12O2 1,3-Diphe	Mtd Medium nmr non-aq Li nmr. Med ********	Temp 27°C lium:   ******  HL .,3-di	Conc 100% nitror ***** Dip	Cal U meth **** ohen	Flags ane, 0 ***** ylacac nzoylm	Lg K values K1=3.24 .05 M LiClO4 ******* CAS 120 ethane; C6H5	Reference ExptNo 1996MAb (91159) 484 . **********************************
2,2':6'2" Metal Li+ Method: 7 ******** C15H12O2 1,3-Diphe Metal Li+	Mtd Medium nmr non-aq Li nmr. Med ********  nylpropane-1 Mtd Medium	Temp 27°C lium: ******  HL .,3-di Temp 25°C	Conc 100% nitror ***** Dip one, I Conc 100%	Cal U methor system Oiber Cal U	Flags ane, 0 ***** ylacac nzoylm Flags	Lg K values  K1=3.24  .05 M LiClO4  *******  CAS 120  ethane; C6H5  Lg K values  K1=4.1	Reference ExptNo  1996MAb (91159) 484  **********************************
2,2':6'2" Metal Li+ Method: 7 ******** C15H1202 1,3-Diphe Metal Li+ Medium: M Li+	Mtd Medium nmr non-aq Li nmr. Med ********  nylpropane-1 Mtd Medium gl alc/w eOH, 0.1 M L	Temp 27°C lium:     27°C   1	Conc 100% nitron ***** Dip one, I Conc 100%	Cal U metha **** cheny Ciber Cal U	Flags ane, 0 ***** ylacac nzoylm Flags	Lg K values  K1=3.24  .05 M LiClO4  *******  CAS 120  ethane; C6H5  Lg K values  K1=4.1	Reference ExptNo
2,2':6'2" Metal Li+ Method: 7 ******** C15H12O2 1,3-Diphe Metal Li+ Medium: M Li+ ************* C15H15O2P	Mtd Medium	Temp 27°C lium: HL .,3-dio Temp 25°C .iCl04	Conc 100% nitror ***** Dipone, I  Conc 100%	Cal U meth ****  chen Dibe Cal U  U  ****	Flags ane, 0 ***** ylacac nzoylm Flags	Lg K values  K1=3.24  .05 M LiC104  ********  CAS 120  ethane; C6H5  Lg K values  K1=4.1  K1=5.95  **********************************	Reference ExptNo  1996MAb (91159) 484  . **************** -46-7 (362) .CO.CH2.CO.C6H5  Reference ExptNo  1965LIa (91552) 485  1954FUa (91553) 486  ***********************************
2,2':6'2" Metal Li+ Method: 7 ******** C15H1202 1,3-Diphe Metal Li+ Medium: M Li+ ********* C15H1502P (Methylca	Mtd Medium nmr non-aq Li nmr. Med ********  nylpropane-1 Mtd Medium gl alc/w eOH, 0.1 M L gl diox/w ************************************	Temp 27°C lium: 1,3-dic 1,3-dic 25°C 1,30°C 1,30°C 1,30°C 1,30°C	Conc 100% nitron **** Dip one, I Conc 100% ******	Cal  Weth  ****  Cal  Cal  U  ****  Tosp	Flags ane, 0 ***** ylacac nzoylm Flags *****	Lg K values  K1=3.24  .05 M LiC104  ********  CAS 120  ethane; C6H5  Lg K values  K1=4.1  K1=5.95  ********  CAS 762  xide; Ph2P(0	Reference ExptNo  1996MAb (91159) 484  . **************** -46-7 (362) .CO.CH2.CO.C6H5  Reference ExptNo  1965LIa (91552) 485  1954FUa (91553) 486  ***********************************

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***********************************
              L
                           CAS 40410-38-6 (5736)
C15H17O3P
Methyl-(diphenoxymethyl)phosphine oxide; MePO(CH2.0.Ph)2
_____
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
Li+ con non-aq 25°C 100% U K1=2.05 1989TKb (91987) 488
Medium: tetrahydrofuran/CHCl3 4:1 (volume)
*************************
                      CAS 101455-18-9 (1902)
C15H18N2O8
1-Methyl-3,4-diaminobenzene-N,N,N',N'-tetraethanoic acid;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
Li+ gl R4N.X 25°C 0.10M U K1=2.31 1985MHb (92084) 489
                         K(LiL+H)=6.16
                         K(Li+HL)=1.43
Medium: 0.10 M Me4NCl.
***********************************
                        CAS 84227-47-4 (5814)
N-Benzyl-1-aza-4,7,10-Trioxacyclododecane;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
Li+ cal non-aq 25°C 100% C IH K1=4.31 1996DNa (92257) 490
Medium: CH3CN. Data for LiX where X=AsF6-,BF4-,CF3SO3-,C104-. DH(K1)=
-27.44 kJ mol-1, DS=-9.3. In PC, K1=4.59, DH(K1)=-24.70, DS(K1)=5.0.
********************************
                             (7846)
N,N-Diethylcarbamoylmethyl-(P-phenyl-P-propylphosphineoxide);
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
      con non-aq 25°C C K1=4.0 1999ESa (92329) 491
In tetrahydrofuran; alkali metal is used as 2,4-dinitrophenolate
***************************
                           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
EMF non-ag 25°C 100% U IH K1=1.99
Medium: triethylphosphate, 0.05 M Et4NClO4. DH(K1)=-34.8 kJ mol-1,
DS=91.9 J K-1 mol-1; Data also for tri-n-butylphosphate: K1=2.36
______
   gl R4N.X 25°C 0.05M U K1=2.40 1991LRc (92518) 493
______
Li+ ISE non-aq 25°C 100% U I K1=4.15 1990LAa (92519) 494
Medium: MeCN, 0.05 M Et4NClO4. In MeOH: K1=3.00; in DMF: K1=1.80;
in DEF K1=1.72, in dimethylacetamide K1=1.85
```

```
kin non-aq 25°C 100% C K1=2.80 1987ABe (92520) 495
Li+
Medium: dimethylformamide.
**********************************
                             CAS 220811-82-5 (7916)
C15H33N3O3
1,4,7-Tris((S)-2-hydroxypropyl)-1,4,7-triazacyclononane;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      EMF non-aq 25°C 100% C I K1=3.39 2001WBa (92575) 496
Medium: methanol, 0.05 M Et4NClO4. In DMF, K1=3.29. Competition with Ag+.
Also data for the 1,4,7-tris((S)-2-hydroxy-2-phenyethyl- derivative.
*****************************
                             CAS 37909-50-5 (2634)
C15H36N09P3
(N,N-Dimethylamine)methylenetris(phosphonic acid diethyl ester);
(CH3)2N.C(CH2.PO(OC2H5)2)2
-----
      Mtd Medium Temp Conc Cal Flags Lg K values
                                    Reference ExptNo
______
Li+ con non-aq 22°C 100% U K1=2.10 1981SKd (92604) 497
Medium: CH3CN
***********************************
C16H18N02P
                             CAS 32159-22-1 (2098)
P-(N-Ethylamidocarbonyl)methyl-P,P-diphenylphosphine oxide;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
-----
      con non-aq 25°C 100% U K1=3.31 1988YKa (93768) 498
Medium: tetrahydrofuran
*******************************
C16H20O3P2
                             CAS 82154-46-9 (2914)
Dimethylphosphinomethyl-diphenylphosphinomethyl-ether; Me2PO.CH2.O.CH2.PO(C6H5)2
-----
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
       con non-ag 25°C 100% U K1=3.92
                                   1982YSa (94099) 499
Medium: tetrahydrofuran+CHCl3 4:1(vol); M is 2,4-dinitrophenolate
*************************
                               (2245)
1,3-Benzo-18-crown-5, 1,3-Benzo-5,8,11,14,17-pentaoxacyclooctadecane;
-----
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
       dis non-aq 25°C 100% U H
                                    1979KLa (94344) 500
                          K(Li(picrate)+L)=2.0
Medium: CHCl3
                                    1977MTc (94345) 501
      dis non-aq 24°C 100% C
                          K(LiA+L)=2.0
Method: extraction of metal picrate (A) from H2O into CDCl3 containing L.
```

```
Data for the 5'-bromo, 5'-t-butyl, 5'-methoxy and 5'-cyanobenzo-derivs
***********************
                 AN(MOEO)2E
                           CAS 60232-72-6 (2246)
18-Methoxy-16-methyl-3,6,9,12-tetraoxabicyclo[12.3.1]octadeca-1(18),14,16-triene;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      dis non-aq 25°C 100% U H
                                   1979KLa (94354) 502
                         K(Li(picrate)+L)=3.6
Medium: CHCl3
*********************************
                         CAS 75507-20-9 (605)
Benzyloxymethyl-1,4,7,10-tetraoxacyclododecane, Benzyloxymethyl-12-crown-4;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
     dis non-ag 22°C 100% C
                                  1984CBa (94360) 503
                         K(Li+A+L(org)=LiAL(org))=<0
Extraction of metal picrate from H2O into CDCl3. HA is picric acid.
For extraction into 1,2-dichloroethane, K=<0.
**********************************
           L Benzo18-crown-6 CAS 14098-24-9 (513)
C16H2406
2,3-Benzo-1,4,7,10,13,16-hexaoxacyclooctadeca-2-ene;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
Li+ con non-aq 25°C 100% C K1=4.24 2000ICa (94422) 504
Medium: nitromethane.
-----
Li+ cal non-aq 25°C 100% C H K1=2.44 1999WBa (94423) 505
Medium: N,N-dimethylformamide. DH(K1)=-0.5 kJ mol-1.
______
Li+ sp non-aq 22°C 100% U K1=5.77 1987CCc (94424) 506
In deuterochloroform
**********************************
C16H24014
             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
Li+ gl R4N.X 25°C 0.10M M K1=3.8
                                  1991FGb (94496) 507
                        B(LiHL)=8.5
Medium: 0.10 M Et4NNO3.
*********************************
C16H26N02P
                             (2093)
P-(N,N-Diethylamidocarbonyl)methyl(P-phenyl)(P-butyl)phosphine oxide;
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
    con non-aq 25°C C K1=3.9
                                  1999ESa (94543) 508
```

```
In tetrahydrofuran; alkali metal is used as 2,4-dinitrophenolate
-----
                       K1=3.38 1988YKa (94544) 509
      con non-aq 25°C 100% U
Medium: tetrahydrofuran
***********************************
            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
______
Li+ gl R4N.X 25°C 0.10M C K1=4.32 1982DSa (94912) 510
***********************************
                          CAS 17454-53-4 (5148)
C16H3006
Cyclohexyl-18-crown-6;
-----
Metal Mtd Medium Temp Conc Cal Flags Lg K values
                                 Reference ExptNo
______
     EMF oth/un 25°C dil A
                                 1971FRa (95101) 511
                     K1<0.7
**********************************
                Cryptand 1,2,1H CAS 119017-36-6 (6587)
4,7,14,20-Tetraoxa-1,10-diazabicyclo[8.7.5]docosane;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
     gl alc/w 25°C 95% M K1=4.21 1990LNa (95118) 512
Medium: 95% MeOH, 0.05 M Bu4NBr. For the 9,13-dihydroxy- analogue: K1 < 2
********************************
                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);
______
     Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      con non-ag 25°C 100% M M K1=6.12
                                 1999DSd (95229) 513
                        K(LiL+C104)=0.94
Medium: acetonitrile.
Li+ cal non-aq 25°C 100% C H K1=3.48 1999WBa (95230) 514 Medium: N,N-dimethylformamide. DH(K1)=-15.4 kJ mol-1.
______
      gl R4N.X 25°C 0.05M C K1=3.4 1996BCh (95231) 515
Medium: 0.05 M Et4NClO4.
-----
      cal non-aq 25°C 100% M H K1=8.11
                              1994BCd (95232) 516
Medium: acetone. DH(K1)=-38.1 kJ mol-1, TDS=7.3
______
Li+ sp non-aq 20°C 100% U K1=3.96
                                 1992PSa (95233) 517
Medium: DMF, 0.01 M Me4NI
-----
    cal alc/w 25°C 100% U H K1=4.69
                               1986BUd (95234) 518
```

```
In MeOH. DH=-10.3 kJ mol-1
------
     nmr non-aq 25°C 100% U K1=7.33
                                1986CHc (95235) 519
In CDCl3 saturated with D20
_____
  ISE non-aq 25°C 100% C I K1=2.63
                                1985CKa (95236) 520
Medium: DMSO. In propylenecarbonate K1=9.67
______
Li+ gl alc/w 25°C 95% C K1=4.46
                               1981ANa (95237) 521
Medium: 95% MeOH, 0.1 M Me4NCl
                ISE non-aq 25°C 100% U I K1=10.33 1981CRa (95238) 522
Medium: MeCN. In DMF: K1=3.58; in EtOH: 5.34; in DMSO: 2.77; in NMP: 3.48
______
      ISE non-aq 25°C 100% U K1=9.6 1980CRa (95239) 523
Medium: Propylene carbonate
______
      ISE alc/w 25°C 100% U K1=5.38
                                1978CSb (95240) 524
Medium: MeOH
-----
     cal R4N.X 25°C 0.06M C H
                                1976KLc (95241) 525
Medium: 0.057 M Me4NBr. Method: flow microcalorimetry.
DH(K1)=0 kJ mol-1, DS(K1)=48 J K-1 mol-1.
______
Li+
      gl R4N.X 25°C 0.05M C I K1=2.50
                                1975LSc (95242) 526
In 95% MeOH: K1=4.18: 100%: > 5
***********************************
                           (6794)
C16H32N4O4
4,10-Bis(N,N-dimethylethanamido)-1,7-dioxa-4,10-diazacyclododecane;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
Li+ cal alc/w 25°C 100% U H K1=5.38 1990KMb (95320) 527
Medium: MeOH. DH=-12.7 kJ mol-1
*******************************
                           (6411)
15-(2,5-Dioxahexyl)-15-methyl-1,4,7,10,13-pentaoxacyclohexadecane;
-----
   Mtd Medium Temp Conc Cal Flags Lg K values
                                  Reference ExptNo
_____
      con non-aq 25°C 100% C I
                        K1=4.45
                                1992TFa (95387) 528
Medium: acetonitrile. In propylene carbonate, K1=3.06.
***************
                              ********
C16H34N2O5
                           (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
- - - '
      EMF alc/w 25°C 100% U I K1=3.01 1994LLa (95416) 529
Medium: MeOH, 0.05M Et4NClO4. Also data for acetonitrile: K=9.13, PC: K=7.0
```

```
DMF: K=2.23, H20: K<2 and pyridine: K=5.08. Method: by competition with Ag+.
*************************
                            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
      ISE non-ag 25°C 100% U K1=2.29
                                   1993RPa (95451) 530
Medium: dimethylformamide, 0.05 M Et4NClO4. By competition with Ag+.
*******************************
                            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
______
Li+ gl R4N.X 25°C 0.10M U K1=3.8 1978LMa (95471) 531
In CH30H, K1>4.0. In 95 vol% CH30H, K1>3.8.
******************************
                            CAS 1191-91-9 (2500)
2,5,8,11,14,17,20,23-Octaoxatetracosane; CH3.0.(CH2.CH2.0)7.CH3
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      con non-aq 25°C 100% U K1=3.6
                                    1993EVa (95492) 532
Medium: THF+CHCl3 (4:1 vol). Also data for other solvents
***********************************
C16H36N4
                             CAS 54622-44-5 (147)
5,5,7,12,12,14-Hexamethyl-1,4,8,11-tetraazacyclotetradecane;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
Li+ gl non-aq 25°C 100% U K1=3.8 1986STb (95540) 533
Medium: THF:CHCl3 4:1 v/v. Metal ions as 2,4-dinitrophenolates
*********************************
                    (6703)
C16H36N4O4
1,4,7,10-Tetrakis(2-hydroxyethyl)-1,4,7,10-tetraazacyclododecane;
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
      EMF non-ag 25°C 100% U I K1=8.07
Medium: acetonitrile, 0.05 M NEt4ClO4. In propylene carbonate K1=8.90
______
       gl alc/w 25°C 100% C I K1=3.09 1993TCa (95575) 535
Li+
Medium: MeOH, 0.05 M Et4NClO4. In DMF, K1=2.99
*****************************
                            CAS 90163-26-1 (5212)
C17H13N505
1-(4'-(5'-Hydroxy-3'-methyl-1'-phenyl)pyrazolylazo)4-nitrobenzoic acid;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
```

```
sp mixed ? 77% U K1=4.24
Li+
                                   1968DZa (95776) 536
Medium: 77% acetone
**********************************
                 Riboflavin
             HL
                           CAS 83-88-5 (1438)
7,8-Dimethyl-10(D-1'-ribityl)isoalloxazine, Vitamin B2, Vitamin H
______
     Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      sol oth/un 22°C U K1=-0.2
                                  1980LDa (96339) 537
Medium: variable LiClO4 content 0.1-2.5 M
The same constant measured spectrophotometrically: K1=-1.2
********************************
Methyldi(2-methoxyphenoxymethyl)phosphine oxide; Me.PO(CH2.O.C6H4.OMe)2
-----
    Mtd Medium Temp Conc Cal Flags Lg K values
                                   Reference ExptNo
______
                         K1=2.65
      con non-aq 25°C 100% U
                                  1989TKb (96392) 538
Medium: tetrahydrofuran/CHCl3 4:1 (volume)
**********************************
                            CAS 217972-81-1 (8163)
9-(2-Hydroxy-3,5-dinitrophenoxy)methyl-1,4,8,11-tetraoxacyclotetradecane;
______
                                  Reference ExptNo
Metal Mtd Medium Temp Conc Cal Flags Lg K values
-----
      dis non-aq 25°C 100% C
                                   1990SSe (96433) 539
                         K(Li+HL(org)=LiL(org)+H)=-6.1
Method: extraction from aqueous phase (0.10 M MOPS, pH 7.3) into
1,2-dichloroethane. Data for 1,2-dialkyl- derivatives.
CAS 94616-60-1 (1039)
2,4,6-Trinitrophenylaminomethyl-15-crown-5
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      sp mixed 25°C 16% U
                         K1=2.28
                                   1984BPa (96464) 540
                        K(Li+HL)=1.09
CAS 92818-18-3 (8987)
12-[(Phenylmethoxy)methyl]-1,4,7,10-tetraoxacyclotridecane;
-----
Metal Mtd Medium Temp Conc Cal Flags Lg K values
-----
      dis non-aq 22°C 100% C
                                   1984CBa (96509) 541
                         K(Li+A+L(org)=LiAL(org))=0.9
Extraction of metal picrate from H2O into CDC13. HA is picric acid.
For extraction into 1,2-dichloroethane, K=1.84. In H2O, K(LiA+L)=3.80.
***********************************
                            CAS 92818-15-0 (8986)
5-[(Phenylmethoxy)methyl]-1,4,7,10-tetraoxacyclotridecane;
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Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
     dis non-aq 22°C 100% C
                                   1984CBa (96511) 542
                         K(Li+A+L(org)=LiAL(org))=1.59
Extraction of metal picrate from H2O into CDC13. HA is picric acid.
For extraction into 1,2-dichloroethane, K=2.94. In H2O, K(LiA+L)=4.43.
**************************
                           CAS 99159-90-7 (688)
2,3-Benzo-1,4,7,10,13,16-hexaoxacyclononadeca-2-ene;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
·-----
Li+ sp non-aq 22°C 100% U K1=5.33 1987CCc (96522) 543
In deuterochloroform
*********************************
C17H27N05
                           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
Li+ sp alc/w RT 50% C I K1=1.5
                                   2002GNe (96544) 544
Medium: 50% v/v MeOH/H2O, pH 7.4 (0.01 M Tris buffer), 0.1 M Me4NCl.
In 10% MeOH/H2O, K1=1.1.
CAS 142565-14-8 (6562)
4,7,13,16-Tetraoxa-1,10-diazabicyclo[8.8.5]tricosane;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
Li+ EMF non-aq 25°C 100% C K1=5.36 1993DLb (96745) 545
Medium: propylene carbonate, 0.05 M Et4NClO4.
______
Li+ gl R4N.X 25°C 0.05M C I K1=2.08 1992CGb (96746) 546
Medium: Et4NCl04. In MeOH: K1=2.30;in DMF K1=2.21; in MeCN: K1=6.07
*****************************
                            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
Li+ gl alc/w 25°C 95% C K1=1.23 2004KVa (96759) 547 Medium: 95% MeOH/H2O, 0.01 M Et4NClO4.
*************************
12,17-Dimethyl-1,9,12,17-tetraazabicyclo[7.5.5]nonadecane;
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
- - -
Li+ gl NaCl 25°C 0.15M C K1=2.6 1996BFc (96773) 548
```

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************************************
             L CAS 122874-65-1 (5903)
C17H37N5
5,12,17-Trimethyl-1,5,9,12,17-pentaazabicyclo[7.5.5]nonadecane;
_____
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
Li+ gl mixed 25°C 80% C K1=5.0 Medium: 80% v/v DMSO/H2O, 0.15 M NaCl.
                               1996BFc (96790) 549
______
     gl NaCl 25°C 0.15M C H
                              1989BBe (96791) 550
DH(K1)=-2.1 kJ mol-1, DS(K1)=54.3 J K-1 mol-1
************************************
                         CAS 21245-67-8 (2100)
C17H3802P2
Methylenebis(dibutylphosphine oxide); Bu2P(0)CH2P(0)Bu2
-----
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
     con non-aq 25°C C K1=5.0 1999ESa (96813) 551
In tetrahydrofuran; alkali metal is used as 2,4-dinitrophenolate
_____
   con non-aq 25°C 100% U K1=3.92 1988YKa (96814) 552
Medium: tetrahydrofuran
****************************
                         CAS 791-28-6 (32)
Triphenylphosphine oxide; (C6H5)3P0
______
     Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
Li+ con non-aq 25°C 100% C M K1=4.873 1990SAb (97095) 553
                       K(LiClO4+L)=4.53
                       K(LiL+C104)=-0.265
Medium: propylene carbonate.
______
Li+ con non-aq 25°C 100% U K1=1.95 1988YSb (97096) 554
Medium: acetonitrile
______
     con non-aq 25°C 100% U
                                1982GJb (97097) 555
                       Kout(LiL+A)=3.9
Medium: 1,2-dichloroethane. A=tetraphenylborate
______
     con non-aq 25°C 100% U
Li+
                                1969SSi (97098) 556
                      K(LiI+L)=2.6
Medium: CH3CN
*********************************
                         CAS 14262-60-3 (5616)
2,3:11,12-Dibenzo-1,4,7,10,13-pentaoxacyclopentadeca-2,11-diene;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
     sp non-aq 25°C 100% C K1=3.003 2002YEa (97478) 557
```

```
Method: fluorescence spectroscopy. Medium: acetonitrile.
*****************************
(N,N-Diethylamidocarbonyl)methyldiphenylphosphine oxide;
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
      con non-aq 25°C C K1=4.1 1999ESa (97507) 558
In tetrahydrofuran; alkali metal is used as 2,4-dinitrophenolate
_____
   con non-aq 25°C 100% U K1=3.69 1988YKa (97508) 559
Medium: tetrahydrofuran
***********************************
1,7-Di(2-methoxyphenyl)-1,4,7-trioxaheptane; MeO.C6H4.O.C2H4.O.C2H4.O.C6H4.OMe
-----
      Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      con non-aq 25°C 100% U K1=1.65 1989TKb (97566) 560
Medium: tetrahydrofuran/CHCl3 4:1 (volume)
********************************
                 CAS 173417-90-8 (6571)
C18H27N2O3F
23-Fluoro-4,7,20-trioxa-1,10-diazatricyclo[8.7.5.1,12,16]tricosa-12,14,16(23)triene
      Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      EMF non-aq 25°C 100% C H K1=4.34 1999BHa (97748) 561
Medium: MeOH, 0.05 M Et4NClO4. By calorimetry DH(K1)=-5.5 kJ mol-1.
Method: by competition with Ag+, using Ag/Ag+ electrode.
**********************
                             CAS 154148-31-9 (6510)
4,7,20-Trioxa-1,10-diazatricyclo[8.7.5.1,12,16]tricosa-12,14,16(23)-triene;
_____
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
       EMF non-aq 25°C 100% C H K1=0.81
                                    1999BHa (97771) 562
Medium: MeOH, 0.05 M Et4NClO4. By calorimetry DH(K1)=-2.1 kJ mol-1.
Method: by competition with Ag+, using Ag/Ag+ electrode.
*************************
                             CAS 92818-19-4 (8988)
C18H2805
2-[(Phenylmethoxy)methyl]-1,4,8,11-tetraoxacyclotetradecane;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      dis non-aq 22°C 100% C
                                    1984CBa (97819) 563
                         K(Li+A+L(org)=LiAL(org))=2.08
Extraction of metal picrate from H2O into CDC13. HA is picric acid.
For extraction into 1,2-dichloroethane, K=3.29. In H2O, K(LiA+L)=4.91.
*******************************
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C18H28O5
                             CAS 92818-28-05 (8989)
6-[(Phenylmethoxy)methyl]-1,4,8,11-tetraoxacyclotetradecane;
______
      Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
Li+ dis non-aq 22°C 100% C
                                      1984CBa (97821) 564
                           K(Li+A+L(org)=LiAL(org))=2.30
Extraction of metal picrate from H2O into CDC13. HA is picric acid.
For extraction into 1,2-dichloroethane, K=2.69. In H20, K(LiA+L)=5.15.
*******************************
                   Benzo20-crown-6 (6354)
2,3-Benzo-1,5,8,11,14,18-Hexaoxacosa-2-ene;
-----
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
      sp non-aq 22°C 100% U K1=5.48 1987CCc (97836) 565
In deuterochloroform
**********************************
              L AN(MOEOE)20
                             CAS 60232-73-7 (2247)
21-Methoxy-19-methyl-3,6,9,12,15-pentaoxabicyclo[15.3.1]heneicos-1(21),17,19-triene
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
Li+ dis non-aq 25°C 100% U H
                                      1979KLa (97847) 566
                           K(Li(picrate)+L)=4.00
Medium: CHCl3
**********************************
                              CAS 100433-53-6 (607)
Benzyloxymethyl-1,4,7,10,13-pentaoxacyclopentadecane, Benzyloxymethyl-15-crown-5;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
      Mtd Medium Temp Conc Cal Flags Lg K values
Li+ dis non-aq 22°C 100% C
                                      1984CBa (97852) 567
                           K(Li+A+L(org)=LiAL(org))=2.09
Extraction of metal picrate from H2O into CDCl3. HA is picric acid.
In H2O, K(LiA+L)=4.94
*******************************
          L Benzo21-crown-7
2,3-Benzo-1,4,7,10,13,16,19-Heptaoxaheneicosa-2-ene;
-----
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
       sp non-aq 22°C 100% U K1=5.60 1987CCc (97857) 568
In deuterochloroform
**********************************
                             CAS 24951-52-8 (2560)
Cryptand-2,2,2-dilactam
-----
      Mtd Medium Temp Conc Cal Flags Lg K values
                                     Reference ExptNo
```

```
Li+ nmr non-aq 33°C 100% U I K1=2.64 1977HPa (98133) 569
Medium: pyridine. In THF: K1=3.12; in MeCN: 3.13
***********************************
      L Cryptand 3,2,1 (7303)
1,10-Diaza-4,7,13,16,19,24-hexaoxabicyclo[8,11,5]hexacosane;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
Li+ cal alc/w 25°C 95% U H K1=3.14
                               1997ZIa (98421) 570
Medium: 95% v/v MeOH/H2O, 0.1 M. DH(K1)=-11.7 kJ mol-1, DS=20.8 J K-1 mol-1
**********************************
                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
______
Li+ con non-aq 25°C 100% M M K1=6.21 1999DSd (98629) 571
                  K(LiL+ClO4)=0.72
Medium: acetonitrile.
_____
Li+ cal R4N.X 25°C 0.10M C H
                               1996BCh (98630) 572
Medium: 0.10 M Et4NClO4. DH(K1)=-6.4 kJ mol-1.
______
Li+ EMF non-aq 25°C 100% C I K1=6.98
                               1995DGa (98631) 573
Medium: acetonitrile, 0.05 M Et4NCl04. In benzonitrile, K1=8.18.
Competitive method with Ag/Ag+ electrode.
______
Li+ cal non-aq 25°C 100% M H K1=4.62 1994BCd (98632) 574
Medium: acetone. DH(K1)=-23.9 kJ mol-1, TDS=2.4
______
Li+ sp non-aq 20°C 100% U K1=2.3
                               1992PSa (98633) 575
Medium: DMF, 0.01 M Me4NI
______
Li+ cal alc/w 25°C 100% U H K1=2.46 1986BUd (98634) 576
In MeOH. DH=-3.7 kJ mol-1
______
Li+ cal non-aq 25°C 100% U H
                             1986DGa (98635) 577
DH1 = -59.1 kJ mol-1. Medium: nitromethane
______
     cal non-aq 25°C 100% U H
                                1985DGa (98636) 578
Medium: propylene carbonate. DH1 = -36.4 kJ mol-1
______
Li+ cal non-aq 25°C 100% U H
                               1985DGa (98637) 579
Medium: acetonitrile. DH1 = -29.8 kJ mol-1
-----
Li+ ISE non-aq 25°C 100% M K1=11.49 1985DGb (98638) 580
Medium: nitromethane
-----
    gl alc/w 25°C 95% C K1=1
                               1981ANa (98639) 581
```

```
Medium: 95% MeOH, 0.1 M Me4NCl
-----
      ISE non-ag 25°C 100% U I K1=6.97 1981CRa (98640) 582
Medium: MeCN. In DMSO: < 1.0; in EtOH: < 2.3; in N-methylpropionamide: 2.97
______
Li+ ISE non-aq 25°C 100% U K1=6.9 1980CRa (98641) 583
Medium: Propylene carbonate
______
Li+ EMF non-aq 25°C 100% C I K1=4.3 1979BLb (98642) 584
Method: Ag electrode; competition with Ag+. Medium: MeOH, 0.05 M
Me4NCl04. Also K1=2 (H2O), <2.0 (DMSO), 6.7 (CH3CN).
______
      EMF oth/un 25°C 0.05M C I K1=<1.4 1978YTa (98643) 585
Method: competition with Tl+, using Tl amalgam electrode.
Electrolyte not stated. In DMSO, 0.10 M: K1<1
______
Li+ nmr non-aq 30°C 100% U I K1=2.94 1975CDa (98644) 586
Medium: pyridine. In aqueous soln: K1=0.99
______
Li+ gl R4N.X 25°C 0.05M C I K1=<2.0 1975LSc (98645) 587
In 95% MeOH: K1=1.8; 100%: 2.6
*************************
C18H36N4O4
                           (6795)
4,10-Bis(N,N-dimethylpropanamido)-1,7-dioxa-4,10-diazacyclododecane;
-----
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
     cal alc/w 25°C 100% U H K1=2.99 1990KMb (98782) 588
Medium: MeOH. DH=-23.8 kJ mol-1
************************************
1,4,7-Tris(N,N-dimethylethanamido)-1,4,7-triazacyclononane;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
   gl R4N.X 25°C 0.10M M K1=3.91 1990KMb (98799) 589
Medium: 0.10 M Me4NNO3
*******************************
                         CAS 85726-94-9 (645)
4,10-Dimethoxyethoxyethylidene-1,7-dioxo-4,10-diazacyclododecane;
-----
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      sol non-ag 20°C 100% C K1=3.98 1983SLa (98822) 590
Medium: CHCl3
**********************
                         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
```

```
sol non-aq 20°C 100% C K1=3.89
Li+
                                    1983SLa (98840) 591
Medium: CHCl3
************************************
                   Glvme-9
                             CAS 25990-94-7 (7806)
2,5,8,11,14,17,20,23,26-Nonaoxaheptacosane;
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      dis non-aq 25°C 100% C K1=7.53
                                     1998KSc (98875) 592
Medium: 1,2-dichloroethane.
************************************
                               (5731)
1,2:8,9-Dibenzo-5-methylphosphinyl-3,7,10,13,16-pentaoxacyclohexadeca-1,8-diene;
-----
      Mtd Medium Temp Conc Cal Flags Lg K values
                                     Reference ExptNo
______
                           K1=3.26
       con non-aq 25°C 100% U
                                    1989TKb (99346) 593
Medium: tetrahydrofuran/CHCl3 4:1 (volume)
**********************************
P-(N,N-Diethylamidocarbonyl)methyl,P,P-diphenylphosphine oxide;
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      con non-aq 25°C 100% U K1=4.12 1988YKa (99348) 594
Medium: tetrahydrofuran
*******************************
                              CAS 92818-26-3 (8991)
10-[(Phenylmethoxy)methyl]-1,4,8,12-tetraoxacyclopentadecane;
-----
                                     Reference ExptNo
      Mtd Medium Temp Conc Cal Flags Lg K values
dis non-aq 22°C 100% C
                                     1984CBa (99431) 595
                           K(Li+A+L(org)=LiAL(org))=1.04
Extraction of metal picrate from H2O into CDCl3. HA is picric acid.
For extraction into 1,2-dichloroethane, K=1.91. In H2O, K(LiA+L)=3.89.
**************************
                              CAS 92818-23-0 (8990)
2-[(Phenylmethoxy)methyl]-1,4,8,12-tetraoxacyclopentadecane;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
-----
      dis non-aq 22°C 100% C
                                     1984CBa (99433) 596
                          K(Li+A+L(org)=LiAL(org))=0.78
Extraction of metal picrate from H2O into CDC13. HA is picric acid.
For extraction into 1,2-dichloroethane, K=1.36. In H2O, K(LiA+L)=3.65.
***********************************
                              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
-----
      gl R4N.X 25°C 0.10M U K1=1.5
                                 1978LMa (99493) 597
In 95 vol% MeOH, K1=4.0.
********************************
C20H22O4
       L
                      CAS 82645-28-1 (8945)
o,o'-(Triethyleneglycoldiyl)-(Z)-stilbene;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
     con non-aq 25°C 100% C K1=5.47 2000ICa (99928) 598
Medium: nitromethane.
**********************************
C20H22O6
                            (6834)
1,8-Bis(2-Formyphenoxy)-3,6-dioxaoctane; (CH2.0.CH2.CH2.0.C6H4.CH0)2
-----
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
Li+ con non-aq 25°C 100% U K1=3.3 1993EVa (99932) 599
Medium: THF+CHCl3 (4:1 vol)
C20H24N2O5
                           CAS 165815-06-5 (8936)
N-(2-Pyridylmethylene)-4-aminobenzo-15-crown-5;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
Li+ sp non-aq 25°C 100% C I M
                                 2002YPc (99952) 600
                        K(ZnA2L+Li)=4.13
Medium: MeCN, 0.10 M n-Bu4NPF6. By 1H nmr in CDCl3, K(ZnA2L+Li)=4.06.
A is p-thiocresol.
*********************************
           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
______
Li+ nmr non-aq 25°C 100% C I K1=<0.3 2001KZb (100160) 601
Method: 7Li nmr. Medium: acetonitrile.
Data for 20-80% w/w nitrobenzene/acetonitrile.
-----
     con non-aq 25°C 100% C K1=4.79 2000ICa (100161) 602
Medium: nitromethane.
-----
      oth oth/un 25°C 0.04M C
                        K1 = -0.3
                                 1998TIa (100162) 603
Method: capillary electrophoresis.
Medium: 0.005 M phosphate buffer, pH 7.1, 0.04 M MCl.
_____
     nmr non-ag 27°C 1.0M C I K1=0.86 1996KAb (100163) 604
Method: 7Li nmr. Medium: acetonitrile. Also data for nitromethane and
```

```
20-80% w/w acetonitrile/nitromethane.
______
      vlt non-ag 25°C 100% U K1=11.3
                                 1990SPa (100164) 605
Medium: 1,2-dichloroethane
______
Li+ con non-aq 25°C 100% U K1=4.06
                                1986STb (100165) 606
Medium: THF:CHCl3 4:1 v/v. M as 2,4-dinitrophenolate
______
Li+ con non-ag 25°C 100% U K1=3.48
                               1985YKa (100166) 607
Medium: EtOH+CHCl3 1:1; M is used in nitrophenolate form
______
     con non-aq 25°C 100% U M
                             1982GJb (100167) 608
                        Kout(LiL+A)=3.2
Medium: 1,2-dichloroethane. A=tetraphenylborate
*******************************
                   CAS 84884-14-0 (2236)
2,3-Naphtho-18-crown-6, 2,3-Naphtho-1,4,7,10,13,16-hexaoxacyclooctadeca-2-ene;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
·
      dis non-aq 25°C 100% U H
                                  1979KLa (100347) 609
                       K(M(picrate)+L)=4.35
Medium: CHCl3
***********************************
                 AN(MOEOEO)2E
                            (2248)
24-Methoxy-22-methyl-3,6,9,12,15,18-hexaoxabicyclo[18.3.1]-tetracosa-1(24),20,22-tr
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
      dis non-aq 25°C 100% U H
                                  1979KLa (100492) 610
                       K(Li(picrate)+L)=3.5
Medium: CHCl3
***********************************
                 Benzo24-crown-8 (6356)
2,3-Benzo-1,4,7,10,13,16,19,22-Octaoxatetracosa-2-ene;
-----
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
Li+ sp non-aq 22°C 100% U K1=5.52
                                 1987CCc (100497) 611
In deuterochloroform
**********************************
                            (7763)
C20H34N40
14,19-Dimethyl-1,11,14,19-tetraazatricyclo[9.5.5.14,8]docosa-4,6,8(22)-trien-22-ol;
-----
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
Li+ gl R4N.X 25°C 0.15M C
                                  2000MFa (100513) 612
                       K(Li+L=LiH-1L+H)=-9.1
Medium: 0.10 M NMe4Cl.
```

```
************************************
C20H3606
              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
______
Li+ nmr non-aq 27°C 100% C I K1=5.60 2001KZa (100663) 613
Method: 7Li nmr. Medium: nitromethane. In acetonitrile, K1=3.41
______
Li+ nmr non-aq 25°C 100% C I K1=2.51 2001KZb (100664) 614
Method: 7Li nmr. Medium: acetonitrile.
Data for 20-80% w/w nitrobenzene/acetonitrile.
______
Li+ dis non-aq 25°C 100% U K1=9.26 2000KSa (100665) 615
Medium: 1,2-dichloroethane
-----
Li+ nmr non-aq 27°C 1.0M C I K1=3.14 1996KAb (100666) 616
Method: 7Li nmr. Medium: acetonitrile. Also data for nitromethane and
20-80% w/w acetonitrile/nitromethane.
      dis non-aq 25°C 100% U H
                                   1979KLa (100667) 617
                         K(Li(picrate)+L)=2.28
Medium: CHCl3
Li+ ISE oth/un 25°C dil A K1=0.6
                                  1971FRa (100668) 618
Data for isomer A
******************************
                             (6625)
C20H40N2O4
1,10-Diaza-4,7,13,16-tetraoxabicyclo[8.8.8]hexacosane;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
Li+ gl non-aq 25°C 100% C I K1=3.7 1992LSc (100776) 619
Medium: MeCN, 0.05 M Et4NClO4. In MeOH K1=2.2; in DMF K1=1.9; in H2O K1<2
********************************
                 Cryptand 3,2,2 CAS 31255-22-8 (1763)
C20H40N2O7
Cryptand 3,2,2
           -----
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      gl R4N.X 25°C 0.05M C I K1=<2.0 1975LSc (100815) 620
In 95% MeOH: K1 < 2; 100%: 2.3
***********************************
C20H42N404
                           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
_____
Li+ gl R4N.X 25°C 0.10M U I K1=2.4 1978LMa (100889) 621
In CH30H, K1>4.0, in 95 vol% CH30H, K1=3.8.
```

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************************************
      L CAS 9002-92-0 (8207)
1-Hydroxy-11-oxydodecane-3,6,9-trioxaundecane;
-----
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
Li+ dis non-aq 25°C 100% C K1=1.61 1999KKb (100902) 622
Medium: MIBK. Method: distribution of metal picrates in H2O/MIBK(ligand)
system. Also data for L= HO(CH2.CH2.0)n.(CH2)11.CH3, n=6 and 8.
******************************
                           CAS 102202-74-4 (6041)
1,4,7,10-Tetra-(2-hydroxypropyl)-1,4,7,10-tetraazacyclododecane;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
   EMF non-aq 25°C 100% C I K1=7.65 1997DMd (100928) 623
Method: Ag electrode; competitive titration. Medium: acetonitrile, 0.05 M
Et4NClO4. Also data for PC (K1=6.7), MeOH (4.0), DMF (3.24), H2O (<2).
*******************************
                         (6730)
C20H44N4O4
1,4,7,10-Tetra-(2-methoxyethyl)-1,4,7,10-tetrazacyclododecane;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
Li+ gl non-aq 25°C 100% U I K1=9.34 1996SDa (100942) 624
Medium: MeCN, 0.05 M Et4NClO4. In MeOH: K1=4.1, DMF: 3.61, DMSO: 2.82,
propylene carbonate: 8.0
_____
Li+ gl R4N.X 25°C 0.10M C K1=<2.0 1993SFb (100943) 625
Medium: 0.1 M Et4NClO4.
************************
                           CAS 29942-64-1 (2087)
C-Methylcarbonylmethylenetriphenylphosphorane; Ph3P:CHC(0)CH3
_____
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
Li+ con non-aq 25°C 100% U K1=2.75 1988YSb (101145) 626
Medium: acetonitrile
*********************************
          L CAS 78708-41-5 (799)
2,3:9,10-Dibenzo-1,4,8,11,14-pentaoxacyclohexadeca-2,9-diene-6-oxyethanoic acid;
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      gl alc/w 25°C 80% M H K1=3.27
Medium: 80% w/w MeOH/H2O, pH=11.By calorimetry: DH(K1)=-24.8 kJ mol-1,
DS(K1) = -20.4 \ J \ K-1 \ mol-1.
CAS 71817-08-8 (6905)
1,2:10,11-Dibenzo-16-methylphosphonyl)-3,6,9,12,15,17,20-heptaoxacycloeicosane;
```

```
Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
-----
      nmr non-aq 20°C 100% U
                      K1=2.3
                                  1982BGe (101300) 628
Medium: Acetone-D6; Method - 1H NMR
***********************************
          H4L NADPH CAS 2646-71-1 (7185)
C21H30N7017P3
Nicotinamide adenine dinucleotide phosphate reduced;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
-----
             RT
                 0 U
      nmr none
                                  1995MMf (101374) 629
                         K1eff=1.70
                         Keff(2Li+L)=0.58
Medium: D2O, pH 8.5-9.5. Coordination site is the adenine or nicotinamide
phosphate
***********************************
C21H3002P2
                             (7851)
P'P'-Diphenyl-P,P-dibutylmethylenediphosphinedioxide;
  .....
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
                         K1=5.1 1999ESa (101385) 630
      con non-aq 25°C
                 С
In tetrahydrofuran; alkali metal is used as 2,4-dinitrophenolate
*******************************
                           CAS 82154-48-1 (2916)
Methyldi((2-dimethylphosphinylmethoxy)phenoxymethyl)phosphineoxide;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
      con non-aq 25°C 100% U K1=4.54 1982YSa (101420) 631
Medium: tetrahydrofuran+CHCl3 4:1(vol); M is 2,4-dinitrophenolate
L=CH3P(0)[CH2OC6H4OCH2P(0)(CH3)2]2
************************
C21H42N406S
                           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
______
      gl alc/w 25°C 95% C K1=1.30
                                  2004KVa (101464) 632
Medium: 95% MeOH/H2O, 0.01 M Et4NClO4.
*********************************
C21H42N603
                             (6791)
1,5,9-Tris(N,N-dimethylethanamido)-1,5,9-triazacyclododecane;
-----
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
-----
      gl R4N.X 25°C 0.10M M K1=4.21
                                  1990KMb (101475) 633
Medium: 0.10 M Me4NNO3
*********************************
```

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C22H20N2O4
                           CAS 207461-96-9 (8955)
(5Z)-12,13,20,21-Tetrahydrotribenzo[b,f,l][1,8,11,14,4,5]tetraoxadiazacyclohexadeci
           -----
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
-----
Li+ sp non-aq RT 100% C K1=3.42
                                 2000GDa (101696) 634
Medium: acetonitrile.
**********************************
C22H25O3P
                          CAS 97745-35-2 (2069)
Adamantyl(diphenoxy)phosphonyl
 .-----
     Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
     sol non-aq 25°C 100% U K1=3.01 1987TCa (101924) 635
Medium: CH2Cl2, 2% MeCN. Metal as picrate
*******************************
C22H2605
                           CAS 160978-39-2 (8944)
o,o'-(Tetraethyleneglycoldiyl)-(Z)-stilbene;
_____
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      con non-aq 25°C 100% C K1=6.0 2000ICa (101998) 636
Medium: nitromethane.
************************************
                           CAS 449740-17-4 (8937)
N-(2-Pyridylmethylene)-4-aminobenzo-18-crown-6;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
     sp non-aq 25°C 100% C M
                                  2002YPc (102017) 637
                        K(ZnA2L+Li)=1.86
Medium: MeCN, 0.10 M n-Bu4NPF6. A is p-thiocresol.
************
         L Dibenzo-21-Cr-7 CAS 14098-41-0 (2876)
C22H2807
2,3:11,12-Dibenzo-1,4,7,10,13,16,19-heptaoxacycloheneicosane-2,11-diene;
_____
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      con non-aq 25°C 100% U K1=4.3
                                 1993EVa (102050) 638
Medium: THF+CHCl3 (4:1 vol)
*********************************
C22H30N02P
                           CAS 97937-88-7 (2097)
P-(N,N-Dibutylamidocarbonyl)methyl,P,P-diphenylphosphine oxide;
-----
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      con non-aq 25°C 100% U K1=3.58
                                  1988YKa (102099) 639
Medium: tetrahydrofuran
*******************************
```

```
C22H32O7P2
                            (2078)
1,5-Bis(2-(dimethylphosphinylmethoxy)phenoxy)-3-oxapentane;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
Li+ con non-aq 25°C 100% U K1=4.02 1989KSa (102207) 640
Medium: tetrahydrofuran/CHCl3 4:1 (vol)
L Bz-Cryptand 222 CAS 31250-18-7 (2269)
C22H36N2O6
5,6-Benzo-4,7,13,16,21,24-hexaoxa-1,10-diazabicylo[8:8:8]hexacosa-5-ene;
------
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
Li+ gl R4N.X 25°C 0.05M U H K1=1.7 1998DBa (102276) 641
Medium: 0.05 M Et4NClO4. By calorimetry: DH(K1)=-5.7 kJ mol-1,
-----
Li+ gl oth/un 25°C 0.02M U H K1=2.19 1980CKa (102277) 642
DH=-12.5 kJ mol-1. Alternative method: calorimetry
********************************
             L Benzo-27-Crown9 CAS 63144-76-3 (2842)
C22H3609
2,3-Benzo-1,4,7,10,13,16,19,22,25-nonanoxacycloheptacosa-2-ene;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
      sp non-aq 22°C 100% U K1=5.47
                                 1987CCc (102300) 643
In deuterochloroform
*********************************
                          CAS 76993-47-0 (2340)
C22H4006
2,5,8,11,14,17-Hexaoxatricyclo[22.4.0.0(18,23)]octacosane (trans-cis-trans isomer)
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
Li+ nmr non-aq 24°C 100% U M
                                1981BEb (102371) 644
                       K(Li(picrate)+L)=5.5
Medium: CDCl3
*********************************
             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
-----
Li+ gl R4N.X 25°C 0.05M C K1=<2 1975LSc (102429) 645
**************************
                          CAS 503465-08-5 (9241)
9,20,23,28,31-Pentaoxa-1,4,6,12,14,17-hexaazabicyclo[15.8.8]tritriacontane-5,13-dit
hione;
       Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
   gl alc/w 25°C 95% C K1=<2
                                2004KVa (102439) 646
```

```
Medium: 95% MeOH/H2O, 0.01 M Et4NClO4.
***********************************
                            CAS 85726-96-1 (647)
4,10-Dimethyloxyethoxyethoxyethylidene-1,7-dioxo-4,10-diazacyclododecane;
-----
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      sol non-aq 20°C 100% C K1=4.19
                                  1983SLa (102455) 647
Medium: CHCl3
************************************
                            CAS 85726-97-2 (650)
4,13-Dimethyloxyethoxyethylidene-1,7,10,16-tetraoxo-4,13-diazaoctadecane;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      sol non-ag 20°C 100% C K1=3.88 1983SLa (102458) 648
Medium: CHCl3
*********************************
                            CAS 39678-22-3 (1542)
4,7,13,16-Tetramethyl-1,4,7,10,13,16-hexaaza-21,24-dioxabicyclohexacosane;
_____
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
Li+ gl alc/w 25°C 95% U K1=3.5 1978LMa (102488) 649
********************
                            CAS 1474-32-4 (2089)
C,C-Di(methylcarbonyl)methylenetriphenylphosphorane; Ph3P:C(C(0)Me)2
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
_____
      con non-aq 25°C 100% U K1=2.13 1988YSb (102643) 650
Medium: acetonitrile
************************************
                            CAS 207800-89-3 (8966)
19,20,22,23-Tetrahydro-9-methyl-11,7-metheno-7H-dibenzotrioxatetraazacycloeicosin-2
5-ol:
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
Li+ sp diox/w 25°C 50% C I K1=1.70
Medium: 50% v/v dioxane/H2O, 3% v/v triethylamine; pH 12. In 50%
v/v dioxane/H2O with Et4NOH, K1=2.94.
*************************
C23H30N2O4
                           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
Li+ sp non-aq RT 100% C
                         K1=2.77 2001AVa (102751) 652
Method: spectrophotometric titration. Medium: acetonitrile.
```

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***********************************
C23H30N4O7
                           CAS 356535-57-4 (8845)
13-[2-Methoxy-4-[(4-nitrophenyl)azo]phenyl]-1,4,7,10-tetraoxa-13-azacyclopentadecan
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
   sp alc/w RT 50% C K1=ca.0.5 2002GNe (102768) 653
Medium: 50% v/v MeOH/H2O, pH 7.4 (0.1M Tris buffer), 0.1 M Me4NCl.
********************************
                            (5741)
1,10-Di(8-quinolyl)-1,4,7,10-tetraoxadecane; C9H6N.O.C2H4.O.C2H4.O.C2H4.O.C9H6N
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
Li+ con non-aq 25°C 100% U K1=4.9 1989BEa (102938) 654
Medium: tetrahydrofuran/CHCl3 4:1 (volume)
**************************
Phenylphosphonyldibenzo-17-crown-6
_____
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
      sol non-aq 25°C 100% U K1=2.38 1987TCa (102965) 655
Medium: CH2Cl2, 2% MeCN
**********************************
       L
                 ANAN(MOEO)2E
                          (2242)
2,3:4,5-Di(1,3-(2-methoxy-5-methylbenzo))-9,12,15,18-tetraoxacyclooctadeca-2,4-dien
     Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
Li+ dis non-aq 25°C 100% U H
                                 1979KLa (103071) 656
                      K(Li(picrate)+L)=4.76
Medium: CHCl3
***********************************
             L
                 AN(MOEOM)2AN (2244)
23,24-Dimethoxy-10,21-dimethyl-3,6,14,17-tetraoxatricyclo-tetracosa-1(23),8(24),9,1
1,19,21hexaene
         -----
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
-----
Li+ dis non-ag 25°C 100% U H 1979KLa (103077) 657
                       K(Li(picrate)+L)=2.95
Medium: CHCl3
***********************************
      L DP(0E0E0)2E CAS 60985-77-5 (2237)
3,4:5,6-Bis(2-methylbenzo)-2,7,10,13,16,19-hexaoxacyclodocosa-3,5-diene;
______
     Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
```

```
dis non-aq 25°C 100% U H
                                     1979KLa (103083) 658
                           K(Li(picrate)+L)=4.34
Medium: CHCl3
**********************************
C24H3208 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
Li+ nmr non-aq 27°C 100% C I K1=5.08 1998KZa (103142) 659
                           K(LiL+Li)=3.38
Method: 7Li nmr. Medium: nitromethane. Also data for 20-100% acetonitrile/
nitromethane. In 100% acetonitrile, K1=1.91, K(LiL+Li)<1
______
       sp non-aq 25°C 100% U TIH K1=3.29 1995KSa (103143) 660
Medium: 10% w/w DMF/MeCN. DH(K1)=-23 kJ mol-1, DS=14 J K-1 mol-1.
Data also for 20 30, 40 w/w% DMF
______
Li+ con non-aq 25°C 100% U K1=4.0 1993EVa (103144) 661
Medium: THF+CHCl3 (4:1 vol)
_____
      vlt non-aq 25°C 100% U K1=13.2 1990SPa (103145) 662
Medium: 1,2-dichloroethane
*******************************
                             CAS 182926-58-5 (8848)
7,13-Bis(2-methoxyphenyl)-1,4,10-trioxa-7,13-diazacyclopentadecane;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
      sp alc/w RT 50% C K1=2.5 2002GLb (103210) 663
Medium: 50% MeOH/H2O, pH 7.4 (0.1 M Tris buffer), 0.1 M Me4NCl.
******************************
                              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
Li+ sp mixed 25°C 10% C K1=3.35 2001LWa (103243) 664
Method: fluorimetry. Medium: 10%v/v acetonitrile/H2O.
*********************************
                  CAS 145519-34-2 (6831)
C24H36N2O4Fe L
1,1'-(1,4,10,13-Tetraoxa-7,16-diazacyclooctadeca-7,16-diyldimethylferrocene;
_____
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
Li+ nmr non-aq 25°C 100% U K1=3.74 1992MGa (103256) 665
Method:NMR. Medium: MeCN, 0.1 M Bu4NPF6. Data also for other ferrocene[2.2]
cryptands
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***********************************
C24H36O10P2
              L
                             (5726)
1,4-Bis(2-(diethoxyphosphinylmethoxy)phenyl)-1,4-dioxabutane;
2(Et0)2P0.CH20.C6H4.0.CH2)2
Metal Mtd Medium Temp Conc Cal Flags Lg K values
-----
      con non-ag 25°C 100% U K1=3.7
                                 1989EVa (103296) 666
Medium: tetrahydrofuran/CHCl3 4:1 (volume)
*******************************
2,5,8,11,14,17,20,23,26,29-Decaoxa-15,16-benzo-triconta-15-ene;
-----
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
-----
      sp non-ag 22°C 100% U K1=5.46
                                 1987CCc (103397) 667
In deuterochloroform
***********************************
                             (2341)
16,18,23,25-Tetramethyl-2,5,8,11,14-pentaoxatricyclo(22.4.0.0(15,20))pentacosane;
______
     Mtd Medium Temp Conc Cal Flags Lg K values
                                   Reference ExptNo
______
     nmr non-aq 24°C 100% U M
                                  1981BEb (103410) 668
                         K(Li(picrate)+L)=4.0
Medium: CDCl3
*******************************
C24H48N2O9
                 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
-----
Li+ gl R4N.X 25°C 0.05M C K1=<2 1975LSc (103465) 669
*****************************
C24H48N606S2 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-d
    Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      gl alc/w 25°C 95% C
                         K1=<2
                                 2004KVa (103506) 670
Medium: 95% MeOH/H2O, 0.01 M Et4NClO4.
*********************************
C24H48N8O4
                             (6789)
1,4,7,10-Tetrakis(N,N-dimethylethanamido)-1,4,7,10-tetraazacyclododecane;
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
Li+ gl R4N.X 25°C 0.10M M K1=5.23
                                 1990KMb (103516) 671
Medium: 0.10 M Me4NNO3
```

```
C24H50N2O6 L
                CAS 85726-95-0 (646)
4,10-Dibutoxyethoxyethylidene-1,7-dioxo-4,10-diazacyclododecane;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      sol non-aq 20°C 100% C K1=4.05
                                1983SLa (103529) 672
Medium: CHCl3
***********************************
                          CAS 207-21-8 (2099)
Methylenebis(diphenylphosphine oxide); Ph2P(0)CH2P(0)Ph2
______
    Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
Li+ con non-aq 25°C C K1=5.6 1999ESa (103631) 673
In tetrahydrofuran; alkali metal is used as 2,4-dinitrophenolate
_____
      con non-aq 25°C 100% U K1=4.73
                                1988YKa (103632) 674
Medium: tetrahydrofuran
______
      con non-aq 25°C 100% U K1=4.9
Medium: tetrahydrofuran + CHCl3 4:1, Li as 2,4-dinitrophenolate
______
Li+ oth non-aq 22°C 100% U K1=2.5 1978YSa (103634) 676
Medium: 1:1 v/v CH3CN:CHCl3 1:1 v/v. Li as LiCl; for LiI K1=2.3
______
      con non-aq 25°C 100% U
                                 1969SSi (103635) 677
                        K(LiI+L)=3.3
Medium: CH3CN
*******************************
                          CAS 207800-93-9 (8967)
19,20,22,23,25,26-Hexahydro-9-methyl-11,7-metheno-7H-dibenzotetraoxatetraazacyclotr
icosin-28-ol
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values
______
      sp diox/w 25°C 50% C K1=2.36
                                 2001INa (103652) 678
Medium: 50% v/v dioxane/H2O, 3% v/v triethylamine, pH 12.
*********************************
                     CAS 423763-92-2 (8996)
C25H28N04S+
3-Ethyl-2-[4-(2,3,5,6,8,9-hexahydro-1,4,7,10-benzotetraoxacyclododecin-12-yl)buta-1
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
-----
Li+ sp non-aq 25°C 100% C K1=1.50 2002GVc (103660) 679 Medium: acetonitrile, 0.1 M Et4NClO4.
**********************************
                 FQC
                          CAS 215095-38-8 (8804)
4'-(Dimethylamino)-2,7-(3,6,9-trioxaundecane-1,11-dioxy)flavone;
```

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Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      sp non-aq ns 100% C K1=1.51
                                  2000LXa (103680) 680
Medium: acetonitrile. By fluorescence, K1=1.68.
********************************
         L CAS 202407-79-2 (8035)
C25H37N2O7P
26,27-Dimethoxy-3,7,24-triMe-11,14,17,20-tetraoxa-2,4-diaza-phosphatricycloheptacos
ahexaeneoxide:
             Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
_____
Li+ dis non-aq 20°C 100% C
                                   1998DDc (103758) 681
                        K(LiP+L)=3.48
Medium: CHCl3. P is picrate.
******************************
C25H50N2O4
N,N'-Diheptyl-N,N',5,5'-tetramethyl-3,7-dioxanonanediamide;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
-----
     nmr non-aq 25°C 100% U I M
                                  19800Ea (103827) 682
                         K(Li(C104)+L)=6.0
                         K(Li(C104)L+L)=2.3
Medium CH2Cl2. In CH3CN: K(Li(Cl04)+L)=3.0, K(Li(Cl04)L+L)=1.0. In pyridine:
K(Li(ClO4)+L)=0.04. In MeCN: K(Li(ClO4)L+L)=1.23
********************************
                       CAS 503465-06-3 (9249)
C25H50N408S
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
Li+ gl alc/w 25°C 95% C K1=2.84 2004KVa (103845) 683
Medium: 95% MeOH/H2O, 0.01 M Et4NClO4.
*********************************
                           CAS 2039-68-1 (1741)
Tetraphenylethylene; (C6H5)2C:C(C6H5)2
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      con non-aq 20°C 100% U T K1=4.27 1975LLa (103853) 684
Medium: THF. K1=4.24 (10 C); 4.20 (0 C); 4.18(-10 C); 4.10 (-30 C);
4.05 (-40 C); 4.02 (-50 C); 4.00 (-70 C)
*****************************
                            CAS 33078-07-8 (2088)
C26H210P
C-Phenylcarbonylmethylenetriphenylphosphorane; Ph3P:CHC(0)Ph
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
```

```
con non-aq 25°C 100% U K1=2.42 1988YSb (103856) 685
Li+
Medium: acetonitrile
**********************************
                             CAS 188838-26-8 (7359)
Dipyrido[3,2-a:2',3'-c]-phenazo-(1,4,7,10,13-pentaoxacyclopentadecane);
______
      Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      sp non-aq 25°C 100% C I
                                     2002YPb (103900) 686
                          K(CuLA2+Li)=3.37
Medium: MeCN, 0.10 M Bu4NPF6. By nmr, K=3.07. Also data for acetone/
0.01 M Bu4NPF6: K=1.97 (1.75 by nmr). A is triphenylphosphine.
______
    sp non-ag 25°C 100% C I
                                     2002YPb (103901) 687
                          K(ZnLA2+Li)=3.76
Medium: MeCN, 0.10 M Bu4NPF6. A is CH3.C6H4.SH
______
       sp non-aq 25°C 100% U I M
                                     1997YLa (103902) 688
                          K(Ru(II)(bpy)2L+Li)=3.45
Medium: CH3CN; 0.1M NBu4PF6. In (CH3)2CO: K=1.64. Data also for
bis(4,4'-di-tert-butylbipyridyl) and bis(phenanthroline) RuL complexes.
***************************
C26H24O2P2
                               (6648)
Bis(diphenylphosphinyl)ethane; (C6H5)2PO.CH2CH2.PO(C6H5)2
______
      Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
-----
      con non-aq 25°C 100% U K1=4.3
                                     1990EAb (103912) 689
Medium: THF+CHCl3 4:1(vol). Metal as 2,4-dinitrophenolate
***********************************
C26H24O3P2
                               (7158)
1,3-Bis(diphenylphosphinyl)-2-oxopropane;
______
     Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
-----
      con non-aq 25°C
                          K1=4.2
                                    1999TEa (103919) 690
In: tetrahydrofurane/CHCl3 4:1 v/v
______
       oth non-aq 25°C 100% U
                           K1=4.2 1995TEa (103920) 691
Medium: tetrahydrofurane: CHCl3 4:1 (v/v).
Metal ion is used as 2.4-dinitrophenolate.
*****************************
C26H28N2O5
                               (2155)
1,13-Di-(8-quinoly1)-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
                           K1=4.3
      sp non-aq 27°C 100% C IH
                                     1996TJa (103979) 692
                          K(LiL+Li)=2.45
Method: 7Li nmr. Medium: acetonitrile. Data for 27-67 C. DH(K1)=-16 kJ
```

```
mol-1, DS=30 J K-1 mol-1; DH(LiL+Li)=10, DS=81. Also data in nitromethane.
**************************
                            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
______
     sp non-aq 25°C 100% C
                         K1=4.72
                                   2003GHa (104075) 693
                         K(LiL+Li)=2.74
Method: fluorescence spectroscopy. Medium: acetonitrile, 0.05 M Et4NCl04.
*******************************
                 DiBzCryptand222
                            (746)
5,6,14,15-Dibenzo-4,7,13,16,21,24-hexaoxa-1,10-diazabicyclo[8.8.8]hexacosan-5,14-di
       Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      cal non-aq 25°C 100% U IH
                                  1988DSa (104137) 694
Medium: MeCN. DH(K1)=-33.0 k J mol-1. Also data in propylene carbonate.
______
      ISE non-aq 25°C 100% U M K1=6.06 1987DSa (104138) 695
Medium: acetonitrile
**********************
                             (5727)
1,7-Bis(2-(diethoxyphosphinylmethoxy)phenyl)-1,4,7-trioxaheptane;2(EtO)2PO.CH2OC6H4
C2H40C2H4)20
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      con non-aq 25°C 100% U K1=3.7 1989EVa (104244) 696
Medium: tetrahydrofuran/CHCl3 4:1 (volume)
***********************
                    CAS 111928-04-2 (8968)
C26H45N306
7-Phenyl-4,10,16,19,24,27-hexaoxa-1,7,13-triazabicyclo[11.8.8]nonacosane;
-----
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
    dis none 25°C dil C K1=5.96 1987BBf (104280) 697
li+
                         K(Li+A+L(org)=LiAL(org))=3.10
Method: extraction of metal picrate from H2O into CHCl3.
**********************************
                             (2342)
19,21,26,28-Tetramethyl-2,5,8,11,14,17-hexaoxatricyclo[22.4.0.0(18,23)]octacosane;
-----
     Mtd Medium Temp Conc Cal Flags Lg K values
                                    Reference ExptNo
______
      nmr non-aq 24°C 100% U
                                   1981BEb (104310) 698
                         K(Li(picrate)+L)=5.1
Medium: CDCl3
```

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L
                  Cryptand 221D CAS 62002-40-8 (8956)
C26H52N2O5
5-Decyl-4,7,13,16,21-pentaoxa-1,10-diazabicyclo[8.8.5]tricosane;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
Li+ con non-aq 25°C 100% M M K1=5.91 1999DSd (104322) 699
                          K(LiL+ClO4)=1.14
Medium: acetonitrile.
**********************************
                            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
Li+ gl alc/w 25°C 95% C K1=<2 2004KVa (104340) 700
Medium: 95% MeOH/H2O, 0.01 M Et4NClO4.
**********************************
                              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
       gl alc/w 25°C 95% C K1=<2 2004KVa (104350) 701
Medium: 95% MeOH/H2O, 0.01 M Et4NClO4.
*********************
                             CAS 85726-99-4 (652)
C26H54N2O10
4,13-Dimethyloxyethoxyethoxyethylidene-1,7,10,16-tetraoxy-4,13-diazaoctadecane;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      sol non-aq 20°C 100% C K1=4.03 1983SLa (104361) 702
Medium: CHCl3
***********************************
C27H2602P2
                               (6811)
1,2-Bis(2-Diphenylphosphinyl)-1-methylethane;
-----
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
con non-aq 25°C 100% U K1=4.0 1990EAb (104397) 703
Medium: THF+CHCl3 4:1(vol). Metal as 2,4-dinitrophenolate. Data also for
1,1-dimethyl, 1-hexyl, 1-heptyl, 1-octyl and 1-decyl analogues
*************************
C27H26O3P2
                               (6812)
1,2-Bis(2-Diphenylphosphinyl)-1-hydroxymethylethane;
(C6H5)2PO.CH(CH2OH)CH2.PO(C6H5)2
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
```

```
con non-aq 25°C 100% U K1=4.2 1990EAb (104402) 704
Li+
Medium: THF+CHCl3 4:1(vol). Metal as 2,4-dinitrophenolate. Data also for
3-hydroxypropyl analogue
***********************************
                               (7159)
C27H26O3P2
1,4-Bis(diphenylphosphinyl)-2-oxobutane;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
Li+ oth non-aq 25°C 100% U K1=4.9 1995TEa (104407) 705
Medium: tetrahydrofurane: CHCl3 4:1 (v/v).
Metal ion is used as 2,4-dinitrophenolate.
**********************************
C27H32N05S+
                             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-vl)butadien
         ______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
Li+ sp non-aq 25°C 100% C K1=4.16 2002GVc (104517) 706
Medium: acetonitrile, 0.1 M Et4NClO4.
*******************************
C27H33N07
               L FLC
                             CAS 223390-37-2 (8805)
2-[4-Dimethylaminophenyl]-6-methyl-3-(1,4,7,10-tetraoxacyclododec-2-ylmethoxy)-4H-1
-Benzopyran-4;
______
      Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
       sp non-aq ns 100% C K1=3.02 2000LXa (104525) 707
Medium: acetonitrile. Method: fluorescence spectroscopy.
**********************************
C27H47N306
Tripodal ionophore 3;
______
      Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      sp non-aq 25°C 100% C
                                     2001LFa (104625) 708
                          K(LiP+L=LiPL)=5.11
Method: Analyses by spectrophotometry. Medium: chloroform. P is picrate.
******************************
C28H24N2O4
                               (5742)
5,6-Benzo-1,10-di(8-quinolyl)-1,4,7,10-tetraoxadecane;
C9H6N.O.C2H4.O.C6H4.O.C2H4.O.C9H6N
-----
      Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      con non-aq 25°C 100% U K1=4.4 1989BEa (104676) 709
Medium: tetrahydrofuran/CHCl3 4:1 (volume)
********************************
C28H28O3P2
                               (6815)
```

```
1,5-Bis(diphenylphosphinyl)-3-oxapentane; O(CH2.CH2.PO(C6H5)2)2
  _____
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
Li+ con non-aq 25°C 100% U K1=5.15 1993EBa (104712) 710
Medium: CH3CN
_____
Li+ con non-aq 25°C 100% U K1=5.6 1993EVa (104713) 711
Medium: THF+CHCl3 (4:1 vol). Also data for other solvents
______
Li+ con non-aq 25°C 100% U K1=5.3 1992BEa (104714) 712
Medium: THF+CHCl3 (4:1 vol)
C28H28O4P2
1,6-Bis(diphenylphosphinyl)-2,5-dioxohexane;
-----
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
-----
Li+ con non-aq 25°C C K1=5.7 1999TEa (104722) 713 In: tetrahydrofurane/CHCl3 4:1 v/v
C28H30N2O2P2
                        CAS 68745-29-9 (5707)
N,N'-Bis(diphenylphosphinylmethyl)-1,2-diaminoethane; ((C6H5)2PO.CH2.NH.CH2-)2
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
con non-ag 25°C 100% U K1=4.4 1984YKa (104727) 714
Medium: therahydrofuran + CHCl3 4:1, Li as 2,4-dinitrophenolate
*******************************
               (5743)
C28H32N2O6 L
1,16-Di(8-quinolyl)-1,4,7,10,13,16-hexaoxahexadecane; C9H6N.O.(C2H4O)5.C9H6N
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
Li+ con non-aq 25°C 100% U K1=4.4 1989BEa (104750) 715
Medium: tetrahydrofuran/CHCl3 4:1 (volume)
********************************
C28H3507P L CAS 90275-27-7 (2068)
Adamantylphosphonyldibenzo-17-crown-6
_____
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
------
Li+ sol non-aq 25°C 100% U K1=3.86 1987TCa (104768) 716
Medium: CH2Cl2, 2% MeCN. Metal as picrate
********************************
                         CAS 150196-54-6 (7735)
C28H36N2O7S2
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
```

```
sp non-aq 18°C 100% C K1=2.2
Li+
                                 1997LHa (104784) 717
Medium: acetonitrile.
***********************************
                   AN(MOEOEOM)2AN
                               (2243)
C28H4008
29,30-Dimethoxy-13,27-dimethyl-3,6,9,17,20,23-hexaoxatricyclo-triconta-1,11,13,15,2
5,27-hexaene;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
     Mtd Medium Temp Conc Cal Flags Lg K values
       dis non-aq 25°C 100% U H
                                     1979KLa (104857) 718
                          K(Li(picrate)+L)=2.75
Medium: CHCl3
**********************************
C28H40010
          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
      con non-aq 25°C 100% U I K1=4.68 1991ASb (104892) 719
Medium: 1,2-dichlorethane. In nitromethane: K1=4.49
______
       vlt non-aq 25°C 100% U K1=14.2 1990SPa (104893) 720
Medium: 1,2-dichloroethane
*******************************
1,10-Bis(2-(diethoxyphosphinylmethoxy)phenyl)-1,4,7,10-tetraoxadecane;
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
-----
       con non-aq 25°C 100% U K1=4.0 1989EVa (104946) 721
Medium: tetrahydrofuran/CHCl3 4:1 (volume)
****************************
16,16,18,18,23,23,25,25-Octamethyl-2,5,8,11,14-pentaoxatricyclo(22.4.0.0(15,20))pen
tacosane;
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
-----
       nmr non-aq 24°C 100% U M
                                     1981BEb (105010) 722
                          K(Li(picrate)+L)=3.9
Medium: CDCl3
*******************************
C28H5206
                               (5352)
Di(t-butylcyclohexyl)-18-crown-6
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
Li+ oth oth/un 25°C dil U K1=<0.9 1970MSa (105016) 723
*******************************
```

```
C28H56N2O6
                  Cryptand 222D CAS 69878-46-2 (8957)
              L
5-Decyl-4,7,13,16,21,24-hexaoxa-1,10-diazabicyclo[8.8.8]hexacosane:
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
Li+ con non-aq 25°C 100% M M K1=5.28 1999DSd (105030) 724
                          K(LiL+ClO4)=1.20
Medium: acetonitrile.
************************************
                             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
Li+ gl alc/w 25°C 95% C K1=<2 2004KVa (105041) 725
Medium: 95% MeOH/H2O, 0.01 M Et4NClO4.
**********************************
C28H56N6O8S2
                             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
______
Li+ gl alc/w 25°C 95% C K1=<2 B2= 6.03 2004KVa (105051) 726 Medium: 95% MeOH/H2O, 0.01 M Et4NClO4.
*********************
                            CAS 176849-77-7 (7160)
C29H30O3P2
1,6-Bis(diphenylphosphinyl)-2-oxohexane;
-----
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
Li+ oth non-aq 25°C 100% U K1=4.8 1995TEa (105080) 727
Medium: tetrahydrofurane:CHCl3 4:1 (v/v).
Metal ion is used as 2,4-dinitrophenolate.
*******************************
C29H30O3P2
                            CAS 176849-78-8 (7161)
1,6-Bis(diphenylphosphinyl)-3-oxohexane;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      oth non-aq 25°C 100% U K1=4.8 1995TEa (105085) 728
Medium: tetrahydrofurane: CHCl3 4:1 (v/v).
Metal ion is used as 2,4-dinitrophenolate.
**************************
                               (7897)
C29H3004P2
1,7-Bis(diphenylphosphinyl)-2,6-dioxoheptane;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
```

```
con non-aq 25°C C K1=5.8 1999TEa (105090) 729
Li+
In: tetrahvdrofurane/CHCl3 4:1 v/v
**********************************
                          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
______
Li+ sp mixed 25°C 90% C
                                 1997KKa (105101) 730
                       K(LiSCN+L)=1.68
Method: fluorescence emission. Medium: MeOH/CHCl3 (9:1 v/v).
**********************************
                          CAS 423763-96-6 (8998)
2-[4-(2,3,5,6,8,9,11,12,14,15-Decahydro-1,4,7,10,13,16-benzohexaoxacyclooctadecin-1
8-vl)butadien
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
     sp non-aq 25°C 100% C K1=1.98 2002GVc (105106) 731
Medium: acetonitrile, 0.1 M Et4NClO4.
*******************************
C30H32O4P2
                           (6816)
1,8-Bis(diphenylphosphinyl)-3,6-dioxaoctane;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
Li+ con non-aq 25°C 100% U K1=5.50 1993EBa (105229) 732
Medium: CH3CN. Data also for 3,5,8-trioxa, 3,5,8,11-tetraoxa and 3,5,8,11-pe
ntaoxa analogues
-----
    con non-aq 25°C 100% U K1=5.1 1992BEa (105230) 733
Medium: THF+CHCl3 (4:1 vol)
***********************************
                            (7892)
1,9-Bis(diphenylphosphinyl)-2,5,8-trioxononane;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      con non-aq 25°C C K1=5.1 1999TEa (105236) 734
In: tetrahydrofurane/CHCl3 4:1 v/v
CAS 68743-31-3 (2066)
Diaminoethane-N,N'-di-2-ethyldiphenylphosphine oxide; (CH2.NH.C2H4.P(0)(C6H5)2)2
-----
     Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      con non-aq 25°C 100% U K1=4.77 1986STb (105241) 735
Medium: THF:CHCl3 4:1 v/v. M as 2,4-dinitrophenolate
*******************************
                 Furan-cryptand CAS 121954-37-8 (7451)
C30H36N8O3
```

```
39,40,41-Trioxa-1,4,11,14,17,24,29,36-octaazapentacyclo[12.12.12.1.1.1]henLetetraco
ntadodecane:
______
                                      Reference ExptNo
     Mtd Medium Temp Conc Cal Flags Lg K values
- - - '
Li+ sp non-aq 25°C 100% U K1=3.91 1996AAb (105255) 736
Medium: MeCN. L = 39,40,41-Trioxa-1,,4,11,14,17,24,29,36-octaazapen
tacyclo[12.12.12.1(6,9).1(19,22).1(31,34]hentetetraconta-4,6,8.....dodecaene
*************************
                   ANANAN(MOE)20 (2239)
2,3,4,5,6,7,8,9,10-Tri(1,3-(2-methoxy-5-methylbenzo))-12,15,18-trioxacyclooctadeca-
2,5,8-triene;
        ______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
Li+ dis non-aq 25°C 100% U H
                                       1979KLa (105261) 737
                           K(Li(picrate)+L)=5.25
Medium: CHCl3
*********************************
                               CAS 552856-74-3 (8846)
7-[2-Methoxy-4-[(4-nitrophenyl)azo]phenyl]-13-(2-methoxyphenyl)-1,4,10-trioxa-7,13-
diazacyclopen;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
Li+ sp alc/w RT 50% C K1=1.8 2002GLb (105267) 738
Medium: 50% MeOH/H2O, pH 7.4 (0.1 M Tris buffer), 0.1 M Me4NCl.
********************************
C30H38N2O4
                                (5828)
Trimethoxyphenylcryptand 3,1.
25,26,27-Trimethoxy-5,10,15-trimethyl-22-oxa-1,19-diazatetra-
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
Li+ nmr non-aq 25°C 100% U K1=<4.94 1986CHc (105273) 739
In CDCl3. L=25,26,27-Trimethoxy-5,10,15-trimethyl-22-oxa-1,19-diazatetracycl
o[24.1(3,7).1(8,12).1(13,17)] heptacosa-3,5,7,8,10,12,13,15,17-nonaene
********************************
                          CAS 137571-97-2 (6821)
C30H38N2O8
Anthraquinone[2.2]cryptand;
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
Li+ nmr non-aq 21°C 100% U K1=4.61 B2=6.83 1992CSc (105278) 740
Method:NMR. Medium:CD3CN
**********************************
                               CAS 97910-31-1 (2083)
Tris-((2-(dimethylphosphinylmethoxy)phenoxy)methyl)phosphine oxide;
-----
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
```

```
con non-aq 25°C 100% U
                         K1=4.49 1989KSa (105302) 741
Li+
Medium: tetrahydrofuran/CHCl3 4:1 (vol)
*********************************
                           CAS 112120-14-6 (5729)
C30H48013P2
1,13-Bis(2-(diethoxyphosphinylmethoxy)phenyl)-1,4,7,10,13-pentaoxatridecane;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
     con non-ag 25°C 100% U K1=4.0 1989EVa (105344) 742
Medium: tetrahvdrofuran/CHCl3 4:1 (volume)
*******************************
C31H34O4P2
                            (7157)
1,9-Bis(diphenylphosphinyl)-3,7-dioxononane;
    Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      oth non-aq 25°C 100% U K1=4.7 1995TEa (105526) 743
Medium: THF:CHCl3 4:1 v/v. Li as 2,4-dinitrophenolate. Also other
milar ligands
*******************************
C32H28O4P2
                           CAS 88928-04-5 (2072)
1,2-Dihydroxybenzene bis(diphenylphosphinylmethyl) ether
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
-----
      con non-aq 25°C C
                                 1999TEa (105576) 744
                        K1=4.7
In: tetrahydrofurane/CHCl3 4:1 v/v
______
Li+
      con non-aq 25°C 100% U K1=4.40 1989KSa (105577) 745
Medium: tetrahydrofuran/CHCl3 4:1 (vol)
*******************************
C32H29O3P3
                           CAS 21851-89-8 (2640)
P,P,P',P",P"-Pentaphenyldimethylenetri(phosphineoxide); (Ph2P(0)CH2)2P(0)Ph
-----
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
                        1981SPb (105583) 746
Li+ sp non-aq 25°C 100% U
                        K(LiI+L)=2.69
Medium: CH3CN
*********************************
                           CAS 137728-07-5 (6837)
1,11-Bis(diphenylphosphinyl)-3,6,9-trioxaundecane;
-----
     Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
                      K1=5.4 1992BEa (105646) 747
      con non-aq 25°C 100% U
Medium: THF+CHCl3 (4:1 vol)
***********************************
C32H3606P2
                             (7893)
```

```
1,12-Bis(diphenylphosphinyl)-2,5,8,11-tetraoxododecane;
  .__________
     Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
Li+ con non-aq 25°C C K1=4.8 1999TEa (105651) 748
In: tetrahydrofurane/CHCl3 4:1 v/v
*******************************
                          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
______
Li+ sp non-aq 18°C 100% C K1=1.9 1997LHa (105757) 749
Medium: acetonitrile.
*********************************
C32H44O12P2
                          CAS 112120-16-8 (5738)
3,4:9,10:15,16-Tribenzo-1,18-di(diethoxyphosphinyl)-2,5,8,11,14,17-hexaoxaoctadeca-
3.9.15-triene:
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
_____
     con non-aq 25°C 100% U K1=3.7 1989BEa (105777) 750
Medium: tetrahydrofuran/CHCl3 4:1 (volume)
*************************
                          CAS 170801-55-5 (8952)
1,5-Bis[2,2'-azo-4,4'-(1,1,3,3-tetramethylbutyl)phenoxy]-3-oxapentane;
-----
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
_____
     sp non-aq RT 100% C K1=3.28 2000GDa (105795) 751
Medium: acetonitrile.
*************************************
                          CAS 112120-15-7 (5730)
1,13-Bis(2-(diethoxyphosphinylmethoxy)phenyl)-1,4,7,10,13,16-hexaoxahexadecane;
______
    Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      con non-aq 25°C 100% U K1=3.7 1989EVa (105824) 752
Medium: tetrahydrofuran/CHCl3 4:1 (volume)
*******************************
                          CAS 118448-50-3 (2085)
C-Methylcarbonyl, C-diphenylphosphinylmethylenetriphenylphosphorane;
-----
     Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
_____
      con non-aq 25°C 100% U K1=2.98 1988YSb (105871) 753
Medium: acetonitrile
*********************************
                Pyr-cryptand CAS 141258-00-6 (7452)
```

C33H39N11

```
1,4,12,15,18,26,31,39,42,43,44-Undecaazapentacyclo[13.13.13.1.1.1]tetratetetraconta
pentadecane:
______
                                 Reference ExptNo
    Mtd Medium Temp Conc Cal Flags Lg K values
-----
Li+ sp non-aq 25°C 100% U K1=2.36 1996AAb (105918) 754
Medium: CH3CN. L = 11,4,12,15,18,26,31,39,42,43,44-undecazapentacyclo[13.13]
.13.1(6,10).1(20,24).1(33,37) tetratetraconta-4-6-8-10(44),11...pentadecaene
********************
C33H41N306
                            (8027)
Tripodal ionophore :
______
    Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
-----
Li+ sp non-aq 25°C 100% C
                                 2001LFa (105924) 755
                       K(LiP+L=LiPL)=5.37
Method: Analyses by spectrophotometry. Medium: chloroform. P is picrate.
*******************************
C34H36N4O10
N,N'-Bis(2-hydroxy-5-nitrobenzyl)4,13-diazadibenzo-18-crown-6;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
sp alc/w 25°C 70% U
                      K1=9.75 B2=17.90 1995VZa (106008) 756
                        K3=6.20
                        K4 = 3.60
Medium: 70% MeOH
*********************************
                            (6906)
1,2:10,11:15,16:24,25-Tetrabenzo-13,27-di(methylphospha)-3,6,9,12,14,17,20,23,27,28
-10-crown-28
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
_____
Li+ oth non-aq 22°C 100% U K1=1.9 1978YSa (106040) 757
Medium: 1:1 v/v EtOH+CHCl3. Li as acetate salt
************************
                  CAS 137728-08-6 (6838)
C34H4006P2
1,14-Bis(diphenylphosphinyl)-3,5,8,11-tetraoxatetradecane;
-----
    Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
Li+ con non-aq 25°C 100% U K1=5.6 1992BEa (106044) 758
Medium: THF+CHCl3 (4:1 vol)
***********************************
                            (7894)
C34H4007P2
1,15-Bis(diphenylphosphinyl)-2,5,8,11,14-pentaoxopentadecane;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
```

```
con non-aq 25°C C K1=4.7 1999TEa (106051) 759
Li+
In: tetrahvdrofurane/CHCl3 4:1 v/v
***********************************
C34H44N2O5
                             CAS 101671-92-5 (5825)
Trimethoxyphenylcryptand 3,1,1.
30,31,32-Trimethoxy-5,10,15-trimethyl-22,27-dioxo-1,9-diaza....
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
Li+ nmr non-aq 25°C 100% U K1=13.79 1986CHc (106069) 760
CDCl3. L=30,31,32-Trimethoxy-5,10,15-trimethyl-22,27-dioxa-1,19-diazapentacy
clo[17.5.5.1(3,7).1(8,12).1(13,17)]dotriaconta-3,5,7,8,10,12,13,15,17nonaene
*******************************
C34H5308Br
                             CAS 38784-08-6 (2336)
5-Bromolasalocid;
______
      Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
Li+ gl alc/w 25°C 100% M H
                                     1988PJa (106099) 761
                           K(Li+HL)=1.8
Medium: MeOH. DH = 8.2 \text{ kJ mol-1}; DS = 62
******************************
C34H5408
              H2L Lasalocid CAS 25999-20-6 (2335)
Lasalocid acid;
______
     Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      nmr non-aq 20°C 100% C
                                     1998MLa (106142) 762
                          K(Li+HL)=0.0
Medium: CD3OD. Method: 13C nmr.
-----
Li+ dis oth/un 25°C 0.0 U K1=2.2 1992LPb (106143) 763
  gl alc/w 25°C 100% M H
                                     1988PJa (106144) 764
                           K(Li+HL)=1.9
Medium: MeOH. DH = 4.9 \text{ kJ mol-1}; DS = 53
Li+ gl alc/w 25°C 100% U
                                     1982BDc (106145) 765
                           K(Li+2HL)=1.44
Medium: MeOH
******************************
                              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
                          K1=3.4
Li+ gl R4N.X 25°C 0.10M U
                                    2001BBa (106203) 766
                           K(LiL+H)=9.5
                           K(LiHL+H)=9.3
```

```
Medium: 0.10 M NMe4NO3.
***********************************
5,6:11,12-Dibenzo-1,16-di(8-quinolyl)-1,4,7,10,13,16-hexaoxahexadecane;
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
                                1989BEa (106220) 767
                        K1=4.1
      con non-aq 25°C 100% U
Medium: tetrahydrofuran/CHCl3 4:1 (volume)
**************************
             L Cucurbituril CAS 283175-97-3 (6744)
C36H36N24O12
Cucurbit[6]uril;
_____
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
-----
      cal mixed 25°C 50% C H K1=2.38
                                1998BJb (106263) 768
Medium: 50% (v/v) HCOOH/H2O. DH(K1)=-3.4 kJ mol-1
-----
  sp none 25°C 0 U K1=2.23 B2=2.73 1994HKa (106264) 769
**********************************
                            (2073)
3-t-Butyl-1,2-dihydroxybenzene bis(diphenylphosphinylmethyl) ether
-----
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
-----
      con non-aq 25°C 100% U
                        K1=4.25 1989KSa (106281) 770
Medium: tetrahydrofuran/CHCl3 4:1 (vol)
***************************
                          CAS 103990-64-3 (2077)
1,2-Bis(2-(diphenylphosphinylmethoxy)ethoxy)benzol;
-----
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
      con non-aq 25°C 100% U K1=4.20 1989KSa (106285) 771
Medium: tetrahydrofuran/CHCl3 4:1 (vol)
*****************************
        L
                ANAN(MSM)2ANAN CAS 1129-04-9 (2240)
Tetra(1,3-(2-methoxy-5-methylbenzo))-9,18-dithiacyclooctadeca-2,5,12,14-tetraene;
______
     Mtd Medium Temp Conc Cal Flags Lg K values
                                  Reference ExptNo
-----
      dis non-aq 25°C 100% U H
                                 1979KLa (106295) 772
                        K(Li(picrate)+L)=2.96
Medium: CHCl3
**********************************
        L
                ANANAN(MOM)2AN CAS 1129-07-2 (2238)
C36H4006
Tetra(1,3-(2-methoxy-5-methylbenzo))-12,18-dioxacyclooctadeca-2,5,8,14-tetraene;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values
______
```

```
1979KLa (106301) 773
Li+
       dis non-aq 25°C 100% U
                      Н
                          K(Li(picrate)+L)=2.91
Medium: CHCl3
*******************************
                               (5725)
C36H4407P2
1,17-Di(diphenylphosphinyl))-3,6,9,12,15-pentaoxaseptadecane;
Ph2PO.C2H4(0.C2H4)40C2H4P0Ph2
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
Li+ con non-aq 25°C 100% U K1=5.5 1992BEa (106336) 774
Medium: THF+CHCl3 (4:1 vol)
______
   cal non-aq 25°C 100% U
                          K1=3.5 1991SGa (106337) 775
                         K(Li+LiL)=2.70
***********************
C36H44O8P2
                              (7895)
1,18-Bis(diphenylphosphinyl)-hexaoxooctadecane;
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
-----
    In: tetrahydrofurane/CHCl3 4:1 v/v
C36H47N306
                              (8028)
Tripodal ionophore 2:
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
Li+ sp non-aq 25°C 100% C
                                    2001LFa (106375) 777
                          K(LiP+L=LiPL)=5.21
Method: Analyses by spectrophotometry. Medium: chloroform. P is picrate.
**************************
C36H48N2O6
                             CAS 101695-36-7 (5826)
Trimethoxyphenylcryptand 3,2,1.
33,34,35-Trimethoxy-5,10,15-trimethyl-22,25,30-trioxa-1,19-diaza-
-----
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
      nmr non-ag 25°C 100% U K1=9.79
                                    1986CHc (106379) 778
In CDCl3. L=33,34,35-trimethoxy-5,10,15-trimethyl-22,25,30-trioxa-1,19-diaza
pentacyclo[17.8.5.1(3,7).1(8,12).1(13,17)]pentatriaconta-3,5,7,8,....nonaene
                               (5739)
3,4:12,13:21,22-Tribenzo-1,24-di(diethoxyphosphinyl)-2,5,8,11,14,17,20,23-octaoxate
tracosatriene;
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      con non-aq 25°C 100% U K1=3.9
                                   1989BEa (106397) 779
```

```
Medium: tetrahydrofuran/CHCl3 4:1 (volume)
**************************
                          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
______
   gl non-aq 20°C 100% U K1=2.60 1993EAa (106442) 780
Method: circular dichroism. Medium: MeCN, ClO4-
*********************************
             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
______
Li+ con non-aq 25°C 100% C K1=4.4 1997PBb (106511) 781
Medium: acetonitrile. Additional method: potentiometry with ISE.
By calorimetry, DH(K1)=-31 kJ mol-1, DS(K1)=-21 J K-1 mol-1.
______
Li+ vlt non-aq 25°C 100% C I K1=12.1 1997WRa (106512) 782
Method: cyclic voltammetry. Medium: acetonitrile, 0.05 M Et4NCl04. In DMSO
K1=3.8; in acetone, K1=11.0; in hexamethylphosphoric triamide, K1<1.
______
Li+ vlt non-aq 23°C 100% U I K1=12.1 1994FRa (106513) 783
Medium: MeCN. In PrCN: K1=12.2; acetone: 11.0; DMF: 6.0; Me-pyrrol.: 4.7;
NN-DMA: 4.3; DMSO: 3.8; Di-Et-formamide: 3.5; Di-Et-acetamide: 2.8; PC: 11.5
______
      ISE alc/w 25°C 100% M K1=3.60 1984CTa (106514) 784
Li+
Medium: MeOH
-----
Li+ ISE non-aq 25°C 100% M K1=5.90
                                1984CTa (106515) 785
Medium: N,N-dimethylformamide. In DMSO K1=3.71
______
Li+ ISE alc/w 25°C 100% U K1=5.35 1984CTb (106516) 786
Medium: EtOH
______
     vlt alc/w 25°C 100% U K1=3.3
                                1978HPa (106517) 787
Method: Cyclic voltametry
*********************
                          CAS 118448-51-4 (2086)
C-Phenylcarbonyl, C-diphenylphosphinylmethylenetriphenylphosphorane;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
-----
      con non-aq 25°C 100% U K1=2.56
                                1988YSb (106640) 788
Medium: acetonitrile
**********************************
1,3-Bis(2-Diphenylphosphinylphenyl)-2-oxapropane; O(CH2.C6H4(PO.(C6H5)2)
______
```

```
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
-----
  con non-aq 25°C 100% U K1=5.5 1993BEb (106643) 789
Medium: THF+CHCl3 4:1(vol)
(1320)
1,4-Di(2-diphenylphosphinylphenyl)-1,4-dioxabutane;
Ph2PO.C6H4.O.CH2.CH2.O.C6H4.P(0)Ph2
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
_____
Li+ con non-aq 25°C 100% U K1=5.8 1991EBa (106649) 790
Medium: THF+CHCl3 4:1(vol)
C38H4006P2
                          (6833)
1,2-Bis(2-(2-(diphenylphosphinyl)ethoxy)ethoxy)benzene;
C6H4(OCH2CH2OCH2CH2PO(C6H5)2)2
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
_____
   con non-aq 25°C 100% U
                       K1=5.5 1993EVa (106660) 791
Medium: THF+CHCl3 (4:1 vol). Also data for other solvents
*******************
                         CAS 145864-37-5 (6839)
1,20-Bis(diphenylphosphinyl)-3,5,8,11,14,17-hexaoxaeicosane;
-----
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
_____
    con non-aq 25°C 100% U K1=5.0 1992BEa (106681) 792
Medium: THF+CHCl3 (4:1 vol)
**********************************
1,21-Bis(diphenylphosphinyl)-2,5,8,11,14,17,20-heptaoxoheneeicozane;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
     con non-aq 25°C C K1=4.6
                              1999TEa (106686) 793
In: tetrahydrofurane/CHCl3 4:1 v/v
C38H52N2O7
                         CAS 101671-93-6 (5827)
Trimethoxyphenylcryptand 3,2,2.
36,37,38-Trimethoxy-5,10,15-trimethyl-22,25,30,33-tetraoxa-1,19-
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
-----
                       K1=7.26 1986CHc (106691) 794
Li+ nmr non-aq 25°C 100% U
CDCl3. L=36,37,38-trimethoxy-5,10,15-trimethyl-22,25,30,33-tetraoxa-1,19-dia
zapentacyclo[17.8.8.1(3,7).1(8,12).1(13,17)]octatriaconta-3,5,7,8...nonaene
**************************
C40H36O4P2
                          (6805)
```

```
1,6-Bis(2-Diphenylphosphinylphenyl)-2,5-dioxahexane; (CH2.0.CH2.C6H4(PO(6H5)2)2
  Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      con non-aq 25°C 100% U K1=5.2 1993BEb (106734) 795
Medium: THF+CHCl3 4:1(vol)
*************************
                             CAS 86341-96-0 (5724)
1,7-Di(2-diphenylphosphinyl)phenyl-1,4,7-trioxaheptane;Ph2PO.C6H4.O.C2H4.O.C2H4.O.C
6H4.POPh2
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values
______
Li+ con non-ag 25°C 100% U K1=4.6
                                    1991EBa (106746) 796
Medium: THF+CHCl3 4:1(vol). Data also for 1,4,7,10-tetraoxa,1,4,7,10,13-pent
aoxa and 1,4,7,10,13,16-hexaoxa and 4-tributyl analogues
*******************************
C40H4404P2
                               (2074)
3,5-Di(t-butyl)-1,2-dihydroxybenzene bis(diphenylphosphinylmethyl)ether
  -----
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      con non-aq 25°C 100% U K1=4.72 1989KSa (106765) 797
Medium: tetrahydrofuran/CHCl3 4:1 (vol)
***************************
                             CAS 177723-37-4 (8912)
25,27-Diethoxycalix[4]arenecrown-5, 1,3-alternate;
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
       dis non-aq 22°C 100% C M
                                    1996CPa (106772) 798
                          K(LiA+L(org)=LiAL(org))=4.93
Medium: CHCl3 saturated with H2O. Method: extraction of LiA into CHCl3/L
solution. HA is picric acid. For the cone conformation, K=4.74.
**********************************
                             CAS 161282-95-7 (8680)
C40H4608
25,27-Dimethoxycalix[4]arene-crown-6;
-----
      Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
       sp non-aq 25°C 100% C
                        K1=<=1
                                    1995CUa (106777) 799
Medium: methanol, 0.01 M Et4NCl.
*******************************
                  AN2DP(OEOEO)2E
                              (2235)
3,4,5,6-Bis(3-methyl-5-(2-methoxy-5-methylbenzo))-2,7,10,13,16,19-hexaoxacyclodocos
a-3,5-diene;
    Mtd Medium Temp Conc Cal Flags Lg K values
-----
      dis non-aq 25°C 100% U H
                                    1979KLa (106795) 800
```

```
K(Li(picrate)+L)=5.01
```

```
Medium: CHCl3
***********************************
                            CAS 143902-45-8 (8935)
Decamethylcucurbit[5]uril;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
-----
      cal mixed 25°C 50% C H K1=1.99
                                   2000ZKb (106807) 801
Medium: 50% v/v formic acid/H20. DH(K1)=-14.4 kJ mol-1, DS(K1)=-10 J K-1
                            CAS 205066-94-0 (8760)
C40H52N4O4
Tetraphenyl-1,4,7,10-tetraazacyclododecane-1,4,7,10-tetraethanol;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
                       K1=3.13 1998WLc (106823) 802
      ISE non-aq 25°C 100% C
Medium: DMF, 0.05 M Et4NClO4.
Ligand is (all-R)-(all-alpha)-Tetraphenyl-
*******************************
C40H52O14P2
                            CAS 127832-94-4 (5740)
2,3:9,10:15,16:21-Tetrabenzo-1,24-di(diethoxyphosphinyl)-2,5,8,11,14,17,20,23-octao
xatetracosane:
     Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      con non-aq 25°C 100% U K1=3.6 1989BEa (106828) 803
Medium: tetrahydrofuran/CHCl3 4:1 (volume)
CAS 151832-07-4 (6874)
9-(Dimethylethyl)-29,30,31,32,33-pentamethoxy-23-oxahexacyclotritriacontapentadecan
e;
-----
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      dis non-aq 25°C 100% U
                                   1993HSa (106871) 804
                         K(Li(picrate)+L)=9.38
Medium: CDCl3 saturated with D20. With 23-thia- analogue K=7.96
**********************************
C42H4004P2
                              (7153)
1,2-Bis(2-(2-(diphenylphosphinyl)ethyl)phenoxy)ethane
     ______
      Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
-----
      oth non-aq 25°C 100% U
                          K1=5.2
                                   1995TEa (106912) 805
Medium: THF:CHCl3 4:1 v/v. Li as 2,4-dinitrophenolate
********************************
1,6-Bis(2-Diphenylphosphinylphenyl)-3,4-dimethyl-2,5-dioxahexane;
```

```
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      con non-aq 25°C 100% U K1=4.9
                                  1993BEb (106917) 806
Medium: THF+CHCl3 4:1(vol)
*********************
         L CAS 163172-12-6 (2080)
C42H4005P2
Bis((2-diphenylphosphinylmethyl)phenyl)diethyleneglycol ether;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
Li+ con non-aq 25°C 100% U K1=5.3 1993BEb (106927) 807
Medium: THF+CHCl3 4:1(vol)
______
Li+ con non-aq 25°C 100% U K1=4.31 1989KSa (106928) 808
Medium: tetrahydrofuran/CHCl3 4:1 (vol)
******************************
                            CAS 95651-36-8 (2079)
C42H4007P2
1,7-Di(2-(diphenylphosphinylmethoxy)phenyl)-1,4,7-trioxaheptane;
(Ph2PO.CH2.0.C6H4.0.C2H4)20
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
_____
Li+ con non-aq 25°C 100% U K1=3.65 1989KSa (106937) 809
Medium: tetrahydrofuran/CHCl3 4:1 (vol)
______
      con non-ag 25°C 100% U K1=3.65 1989TKb (106938) 810
Medium: tetrahydrofuran/CHCl3 4:1 (volume)
******************************
         L CAS 177723-38-5 (8793)
C42H5007
1,3-Diisopropoxycalix[4]arene-crown-5, 1,3-alternate;
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
-----
     dis non-aq 22°C 100% C M 1996CPa (106952) 811
                         K(LiA+L(org)=LiAL(org))=4.78
Medium: CHCl3 saturated with H2O. Method: extraction of LiA into CHCl3/L
solution. HA is picric acid. For the cone conformation, K=4.70.
********************************
                            CAS 188593-77-3 (8954)
2,17-Didodecyl-6,7,9,10,12,13-hexahydro-dibenzo[b,f][1,8,11,14,4,5]tetraoxadiazacyc
lohexadecine
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      sp non-aq RT 100% C K1=4.0 2000GDa (106974) 812
Medium: acetonitrile.
                              (7156)
C43H42O4P2
1,3-Bis((2-diphenylphosphinyl)phenoxy)propane;
```

```
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      oth non-aq 25°C 100% U K1=4.4
                                     1995TEa (107000) 813
Medium: THF:CHCl3 4:1 v/v. Li as 2,4-dinitrophenolate. Also other
milar ligands
**************************
1,7-Di((2-diphenylphosphynylmethoxy)phenyl-1,7-dioxaheptane;
(Ph2PO.CH2O.C6H4.O.C2H4)2CH2
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
Li+ con non-aq 25°C 100% U K1=3.46 1989TKb (107005) 814
Medium: tetrahydrofuran/CHCl3 4:1 (volume)
*******************************
C43H43N04P2
                               (8538)
Methyl[bis-(2-diphenylphosphorylmethyl)phenoxyethyl]amine;
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      cal non-aq 25°C 100% U H K1=4.56
                                    1998SBb (107007) 815
Medium: MeCN Calorimetric titration of LiNCS. DH(K1)=-17.5 kJ mol-1
********************************
C44H22N4O12Br8S4 H6L
                            CAS 176173-80-1 (6959)
2,3,7,8,12,13,17,18-Octabromo-5,10,15,20-tetrakis(4-sulfonatophenyl)porphyrin;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
Li+ gl NaNO3 25°C 0.1M C
                                     1996TNa (107039) 816
                         K(Li+H2L=LiL+2H)=-18.81
********************************
C44H30N8Br8
2,3,7,8,12,13.17.18-Octabromo-5,10,15,20-tetrakis(N-methylpyridinium-4-yl)porphin(+
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
                        K1=4.21
Li+ sp NaNO3 25°C 0.1M C
                                     1998TNa (107086) 817
                         K(Li+HL=LiL+H)=-8.80
_____
      sp oth/un 25°C 0.10M C
                                    1996RHb (107087) 818
                        K1eff=2.98
**********************************
C44H36O4P2
                               (6810)
1,2-Bis(2-Diphenylphosphinylphenylmethoxy)benzene; C6H4(OCH2.C6H4(PO(C6H5)2)2
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
-----
      con non-aq 25°C 100% U K1=4.3
                                   1993BEb (107091) 819
```

```
Medium: THF+CHCl3 4:1(vol)
***********************************
                          CAS 48242-70-2 (6629)
5,10,15,20-Tetrakis(1-methylpyridinium-4-yl)porphine;
-----
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
                     K1=2.58 1998IHb (107106) 820
     sp NaNO3 25°C 0.50M C
For the 2-pyridyl analogue, K1=3.28
*************************
1,12-Bis(2-Diphenylphosphinylphenyl)-2,5,8,11-tetraoxadodecane;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
_____
      con non-aq 25°C 100% U K1=5.2
                                1993BEb (107110) 821
Medium: THF+CHCl3 4:1(vol)
*************************
C44H4405P2
                            (5735)
1,7-Di((2-diphenylphosphinylmethoxy)phenyl)-4-oxaheptane; (Ph2PO.CH2O.C6H4.C3H6)20
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
-----
      con non-aq 25°C 100% U K1=3.18 1989TKb (107114) 822
Medium: tetrahydrofuran/CHCl3 4:1 (volume)
******************************
C44H4405P2
1,7-Di(2-(diphenylphosphynylethyl)phenyl)-1,4,7-trioxaheptane;
(Ph2P0.C2H2.C6H4.0C2H4)20
-----
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
     oth non-ag 25°C 100% U K1=4.6
                                1995TEa (107119) 823
Medium: THF:CHCl3 4:1 v/v. Li as 2,4-dinitrophenolate
______
      con non-aq 25°C 100% U
                        K1=4.05
                              1989TKb (107120) 824
Medium: tetrahydrofuran/CHCl3 4:1 (volume)
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
______
      cal non-aq 25°C 100% U H
                        K1=4.90 1998SBb (107128) 825
Medium: MeCN Calorimetric titration of LiNCS. DH(K1)=-25.2 kJ mol-1
**********************************
                          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
-----
Li+ gl non-aq 25°C 100% C K1=4.28 2000ABb (107144) 826
                      B(Li2L)=7.11
Medium: MeOH, 0.05 M Et4NClO4.
C44H52N4O8
                        CAS 246035-33-6 (2925)
25,27-Bis(N,N-diethylaminocarbonylmethoxy)-26,28-bis(aminocarbonylmethoxy)calix[4]a
      Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
-----
Li+ sp non-aq 25°C 100% C K1=<1 1999USa (107159) 827
Medium: MeOH, 0.10 M Et4NCl
************************************
C44H52010
                        CAS 163317-54-2 (9089)
1,3-Calix[4]-bis-crown-5;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
-----
Li+ sp non-aq 25°C 100% C I K1=1.80 1996AAe (107165) 828
Medium: acetonitrile. In 100% MeOH, K1<=1.
**************************
                         CAS 161282-98-0 (8679)
25,27-Bis(1-proplyoxy)calix[4]arene-crown-6, 1,3-alternate;
_____
     Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
     sp non-aq 25°C 100% C K1=<=1 1995CUa (107176) 829
Medium: methanol, 0.01 M Et4NCl.
**********************************
                         CAS 161282-96-8 (8678)
25,27-Bis(2-proplyoxy)calix[4]arene-crown-6, 1,3-alternate;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      sp non-aq 25°C 100% C K1=<=1 1995CUa (107182) 830
Medium: methanol, 0.01 M Et4NCl.
***********************
C44H5604
4-Tert-butyl-calix[4]arene;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
-----
                      K1=2.9
     sp non-aq 25°C 100% U
                               1996ABa (107187) 831
                      B(Li2L)=4.04
Medium: MeCN
***********************************
                        CAS 73218-92-5 (5679)
1,3,5-Tris(diphenylphosphinylmethyl)-benzene; C6H3(CH2.PO(C6H5)2)3
```

```
Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      con non-ag 25°C 100% U K1=5.1
                                    1984YKa (107213) 832
Medium: tetrahydrofuran + CHCl3 4:1, Li as 2,4-dinitrophenolate
***********************************
C45H48N06P3
                              (7953)
Tris[2-(diphenylphosphorylmethoxy)ethyl]amine;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      cal non-ag 25°C 100% U H
                          K1=4.08
Medium: MeCN Calorimetric titration of LiNCS. DH(K1)=-28.1 kJ mol-1
*********************************
C45H48N3O3P3
                            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
      con non-ag 25°C 100% U K1=5.6 1984YKa (107226) 834
Medium: tetrahydrofuran + CHCl3 4:1, Li as 2,4-dinitrophenolate
***********************************
C46H4006P2
                              (6814)
1,2-Bis((2-(2-diphenylphosphinyl)phenoxy)ethoxy)benzene;
    -----
      Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      con non-aq 25°C 100% U
                          K1=7.0 1991EBa (107241) 835
Solvent : Tetrahydrofurane + CHCl3 4:1(vol);
*********************************
                            CAS 185118-12-1 (7824)
C46H46N2O4
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
______
Li+
      sp mixed 25°C 90% C
                                    1997KKa (107250) 836
                          K(LiSCN+L)=0.48
Method: fluorescence emission. Medium: MeOH/CHCl3 (9:1 v/v).
**********************************
C46H4607P2
1,15-Bis(2-Diphenylphosphinylphenyl)-2,5,8,11,14-pentaoxapentadecane;
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
-----
      con non-aq 25°C 100% U
                         K1=4.9
                                    1993BEb (107260) 837
Medium: THF+CHCl3 4:1(vol)
*************************
C46H4806P2
1,8-Bis(2-(2-(diphenylphosphinyl)ethyl)phenoxy)-3,6-dioxyoctane
```

```
Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
-----
      oth non-ag 25°C 100% U K1=4.6 1995TEa (107271) 838
Medium: THF:CHCl3 4:1 v/v. Li as 2,4-dinitrophenolate. Also other
milar ligands
******************************
C46H4809P2
               L
                            CAS 95651-38-0 (2082)
1,5-Bis(2-(2-(diphenylphosphinylmethoxy)ethoxy)phenoxy)-3-oxapentane;
______
    Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      con non-ag 25°C 100% U K1=4.18
                                   1989KSa (107280) 839
Medium: tetrahydrofuran/CHCl3 4:1 (vol)
*******************************
C48H4408P2
                            CAS 95651-37-9 (2081)
1,2-Bis(2-(2-(diphenylphosphinylmethoxy)phenoxy)ethoxy)benzol;
-----
      Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
.
      con non-ag 25°C 100% U K1=3.75 1989KSa (107361) 840
Medium: tetrahydrofuran/CHCl3 4:1 (vol)
*********************************
C48H5008P2
                             (6808)
1,18-Bis(2-Diphenylphosphinylphenyl)-2,5,8,11,14,17-hexaoxananodecane;
-----
     Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      con non-aq 25°C 100% U K1=4.6 1993BEb (107365) 841
Medium: THF+CHCl3 4:1(vol)
*************************
                              (7975)
C48H54N06P3
Tris(3-oxa-5-(diphenylphosphoryl)pentyl]amine;
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
-----
Li+
      cal non-ag 25°C 100% U H
                          K1=4.16
                                   1998SBb (107376) 842
                         B(Li2L)=6.04
                         B(Li3L)=9.99
Medium: MeCN Calorimetric titration of LiNCS. DH(K1)=-32.8 kJ mol-1
DH(Li2L)=-68.4, DH(Li3L)=-46.7
********************************
C48H54N608
                            CAS 449738-94-7 (8791)
1,7-Dioxa-4,10-diazacyclododecane-4,10-bis[methylene-8-(1,3,3-trimethyl-6-nitro-spi
robenzopyran)]
             ------
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      sp alc/w 25°C 100% C K1=6.62
                                   2002NFa (107384) 843
Medium: 100% MeOH. Method: electrospray ionization mass spectrometry.
*******************************
```

```
C48H54O10P4
                          CAS 97910-30-0 (2084)
Tris((2-(diphenylphosphinylmethoxy)ethoxy)methyl)phosphine oxide;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
Li+ con non-aq 25°C 100% U K1=4.45 1989KSa (107388) 844
Medium: tetrahydrofuran/CHCl3 4:1 (vol)
H2L R-Bu-Calixarene CAS 147513-53-9 (6705)
C48H6008
4-tert-Butylcalix[4]arenedicarboxylic acid;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
Li+ gl alc/w 25°C 100% C K1=4.5 1993ABb (107403) 845
                       B(Li2L) = 7.6
                       B(LiHL)=12.4
Medium: MeOH, 0.01 M Et4NClO4. Data also for di-tert-butyl ester
***********************************
                       CAS 157769-14-7 (9090)
1,3-Calix[4]-bis-crown-6;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
     sp non-aq 25°C 100% C I K1=2.3 1996AAe (107411) 846
Medium: acetonitrile. In 100% MeOH, K1<=1.
*****************************
                          CAS 105880-81-7 (8677)
C48H6404
tert-Butylcalix-4-arene tetramethyl ether;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
_____
      sp non-aq 25°C 100% C K1=5.10 2004BCb (107421) 847
Medium: acetonitrile, 0.01 M Et4NClO4.
************************
        ; L CAS 190781-91-0 (8792)
C52H62N6010
1,4,10,13-Tetraoxa-7,16-diazacyclododecane-7,16-bis[methylene-8-(trimethyl-6-nitro-
spirobenzopyra
-----
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
sp alc/w 25°C 100% C K1=6.85 2002NFa (107480) 848
Medium: 100% MeOH. Method: electrospray ionization mass spectrometry.
*******************************
            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
-----
Li+ gl alc/w 25°C 100% C K1=7.89 1993ABb (107491) 849
```

B(LiHL)=18.93 B(LiH2L)=27.98 B(LiH3L)=35.68

```
In methanol; 0.01 M (CH3CH2)4NCl04
***********************************
                            CAS 150588-24-2 (3074)
25,26,27,28-Tetrakis-(N,N-diethylaminocarbonylmethoxy)calix[4]arene;
-----
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
      sp non-ag 25°C 100% C H K1=3.0 1999USa (107499) 850
Medium: MeOH, 0.10 M Et4NCl. By calorimetry: DH(K1)=-1 kJ mol-1
**************************
C52H68N408
                              (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
Li+ sp non-aq 25°C 100% C K1=<1 1999USa (107508) 851
Medium: MeOH, 0.10 M Et4NCl
**********************************
                              (9263)
C52H7206
5,11,17,23-Tetra(t-butyl)-25,27-dimethoxy-26,28-dimethoxyethoxycalix[4]arene;
_____
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      sp mixed 25°C 100% C K1=5.41 2004BCb (107526) 852
Medium: acetonitrile, 0.01 M Et4NCl04.
**********************************
                              (7302)
25,27-Dimethoxy-4-tert-butylcalix[4]arene-crown-5;
-----
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      dis non-aq 22°C 100% U K1=4.53 1996SCa (107542) 853
Medium: CHCl3 saturated with H20
Data also for other substituted t-butylcalix[4]arene-crown-5 analogues
********************
C54H90N6018
              L Valinomycin CAS 2001-95-8 (2142)
Valinomycin, Potassium Ionophore
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
-----
      dis non-aq 22°C 100% C M
                                    1996CPa (107554) 854
                          K(LiA+L(org)=LiAL(org))=5.83
Medium: CHCl3 saturated with H2O. Method: extraction of LiA into CHCl3/L
solution. HA is picric acid.
**********************************
                             CAS 157769-17-0 (9091)
C56H60012
```

```
1,3-Calix[4]-bis-benzo-crown-6;
  Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
_____
Li+ sp non-aq 25°C 100% C K1=1.5 1996AAe (107578) 855
Medium: acetonitrile.
***********************************
                            CAS 405108-40-9 (8249)
1,2-Di-O-[2-(2-benzyloxyethoxy)ethyl]-3,4,5,6-tetra-O-benzyl-myo-inositol;
-----
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      dis non-aq 25°C 100% C
                                   2001SSb (107587) 856
                         K(Li.pic+L(org)=LiL.pic)=2.19
Distribution of picrate salt into CHCl3/HL.
K: Li.pic(aq)+L(org)=LiL.pic(org). Data for series of myo-inositol ligands
*******************
C56H7208
                            CAS 123311-74-0 (6160)
Tetramethyl-t-butylcalix[4]arenetetraketone;
  Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      sp alc/w 25°C 100% U I K1=2.7 1989ACb (107598) 857
Medium: MeOH. In CH3CN, K1=5.8
*************************************
                             (8751)
Tetramethyl-4-t-Butylcalix[4]arenetetraethanoate;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
      EMF non-aq 25°C 100% C IH K1=5.61 1995DGa (107602) 858
Medium: acetonitrile, 0.05 M Et4NCl04. In benzonitrile, K1=5.63.
Competitive method: Ag/Ag+ electrode. DH(K1)=-37.80, DS=-19.4.
***********************
              L CAS 122356-76-7 (8681)
C56H7808
Tetra-tert-butyl-1,3-dimethoxycalix[4]arene-crown-6;
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
-----
Li+ sp non-aq 25°C 100% C K1=<=1 1995CUa (107607) 859
Medium: methanol, 0.01 M Et4NCl.
*********************************
                              (9259)
C56H8008
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
______
      sp non-aq 25°C 100% C H B2=9.23
                                   2004BCb (107614) 860
Medium: acetonitrile, 0.01 M Et4NCl04. By calorimetry: DH(B2)=-28.3
kJ \text{ mol-1}, DS(B2)=81.7 J K-1 mol-1.
```

```
************************************
                            CAS 465527-74-6 (9287)
7,13,19,25-Tetra-t-butyl-28-methoxy-27,29,30-triethylacetate-2,3-dihomo-3-oxacalix[
4larene:
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
    sp alc/w 25°C 100% C K1=2.6 2001MAa (107623) 861
Medium: MeOH, 0.01 M Et4NCl.
*********************************
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
-----
Li+ sp non-aq 25°C 100% C H K1=5.99 B2=10.72 2004BCb (107632) 862
Medium: acetonitrile, 0.01 M Et4NCl04. DH(K1)=-33.8 kJ mol-1,
DS(K1)=1.0 \text{ J K-1 mol-1; } DH(B2)=-19.0, \ DS(B2)=141.1.
**********************************
                             (8067)
Tris[2-diphenylphosphoryl)phenoxyethyl]amine;
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
                         K1=4.30 1998SBb (107639) 863
Li+ cal non-aq 25°C 100% U H
                         B(Li2L)=6.35
                         B(Li3L)=8.22
Medium: MeCN Calorimetric titration of LiNCS. DH(K1)=-10.7 kJ mol-1
DH(Li2L)=-16.6, DH(Li3L)=-19.3
(9260)
5,11,17,23-Tetra(t-butyl)-25,27-dimethoxy-26,28-diphenylmethoxycalix[4]arene;
_____
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      sp non-aq 25°C 100% C K1=3.54 2004BCb (107643) 864
Medium: acetonitrile, 0.01 M Et4NClO4.
******************************
                   CAS 97600-39-0 (6158)
C60H80012
Tetraethyl-4-t-butylcalix[4]arenetetraethanoate;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
-----
      con non-aq 25°C 100% C H K1=6.25
                                   2002ASc (107652) 865
Medium: acetonitrile. DH(K1)=-45.83 kJ mol-1, DS(K1)=-42.36 J K-1 mol-1.
______
Li+ EMF non-aq 25°C 100% C I K1=6.20 1995DGa (107653) 866
Medium: acetonitrile, 0.05 M Et4NCl04. Competitive method: Ag/Ag+
electrode. Also data for solvent benzonitrile and for tetrabutyl deriv.
```

```
Li+ sp alc/w 25°C 100% U I K1=2.6 1989ACb (107654) 867
Medium: MeOH. In CH3CN, K1=6.4
******************************
                             CAS 155377-20-1 (8806)
C60H82N2O10
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
-----
Li+ gl non-aq 25°C 100% C K1=4.32 2000ABb (107667) 868
Medium: MeOH, 0.05 M Et4NClO4.
*********************************
C60H84N408
                             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
______
Li+ sp non-aq 25°C 100% C K1=<1 1999USa (107680) 869
Medium: MeOH, 0.10 M Et4NCl
**********************************
                              (8158)
C62H78N2O4S2
5,11,17,23-Tetrakis(1,1-dimethylethyl)-25,27-bis(2-methylthioethoxy)....calix(4)are
ne:
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
Li+ cal non-aq 25°C 100% U H K1=5.42 2002NRa (107686) 870
Method: microcalorimetry. Medium: MeCN.. DH(K1)=-26.2 kJ mol-1
In benzonitrile K1=5.88, DH=-37.6
**********************
                             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
______
      sp non-aq 25°C 100% C K1=3.2 1991ACc (107695) 871
Medium: acetonitrile, 0.01 M Et4NClO4.
**********************************
Tris[2-(diphenylphosphorylmethyl)phenoxyethyl]amine;
-----
      Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      cal non-aq 25°C 100% U H K1=3.48 1998SBb (107720) 872
                          B(Li2L)=4.56
                          B(Li3L)=7.60
Medium: MeCN Calorimetric titration of LiNCS. DH(K1)=-20.2 kJ mol-1
```

```
DH(Li2L) = -40.7, DH(Li3L) = -27.1
CAS 211870-40-5 (4258)
Calix[4]arene-bis(dibenzo)crown-6;
_____
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
   sp non-aq 25°C 100% C K1=2.18 1999LDa (107735) 873
Medium: acetonitrile, 0.01 M Et4NClO4.
**********************************
1,2-Bis(4,5-di(diphenylphosphinyl)-pent-1-oxy)benzene;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
    con non-aq 25°C 100% U K1=6.0 1990EAb (107740) 874
Medium: THF+CHCl3 4:1(vol). Metal as 2,4-dinitrophenolate
*******************************
C64H64O12 L
1,3-Calix[4]-bis-naphtho-crown-6;
                         CAS 162898-44-4 (9092)
_____
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
Li+ sp non-aq 25°C 100% C K1=1.2 1996AAe (107745) 875
Medium: acetonitrile.
*********************************
C64H72N4O4P4
                           CAS 104786-07-4 (2065)
1,4,7,10-Tetra(diphenylphosphinylethyl)-1,4,7,10-tetraazacyclododecane;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
·-----
      con non-aq 25°C 100% U K1=5.91
                               1986STb (107753) 876
Medium: THF:CHCl3 4:1 v/v. M as 2,4-dinitrophenolate
**********************************
       L (9262)
5,11,17,23-Tetra-t-butyl-25,27-di(phenylmethoxy)-26,28-di(2-methoxyethoxy)-calix[4]
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
Li+ sp non-aq 25°C 100% C H K1=3.76 B2= 7.88 2004BCb (107762) 877
Medium: acetonitrile, 0.01 M Et4NCl04. DH(K1)=-30.5 kJ mol-1
DS(K1)=-30.6 \text{ J K}-1 \text{ mol}-1; DH(B2)=-20.0, DS(B2)=83.6.
**************************
                  CAS 182684-17-9 (7455)
4-tert-Butylcalix[5]crown-4 trimethylester;
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
   sp alc/w 25°C 100% U K1=1.5
                                1996AAc (107769) 878
```

```
Medium MeOH, 0.1M Et4NCl. Data also for the crown-5 and crown-6 analogues
*************************
                              (9261)
5,11,17,23-Tetra(t-butyl)-25,27-diethoxycarbonylmethoxy-26,28-diphenylmethoxycalix[
4larene;
            Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
-----
      sp non-aq 25°C 100% C K1=4.30 2004BCb (107777) 879
Medium: acetonitrile, 0.01 M Et4NClO4.
**********************************
                            CAS 123207-92-1 (7812)
C68H76N4O4
5,11,17,23-Tetra-t-butyl-[25,26,27,28-tetrakis(2-pyridylmethyl)oxy]calix(4)arene;
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
-----
      EMF non-ag 25°C 100% C IH K1=5.95
                                   1999DCa (107785) 880
Medium: acetonitrile, 0.05 M Bu4NClO4. Method: by competition with Ag+.
By calorimetry: K1=5.95, DH(K1)=-23.91 kJ mol-1, DS(K1)=33.7 J K-1 mol-1.
CAS 133801-01-1 (7184)
4-tert-Butylcalix[4]arene tetrapyrrolidinylamide;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
Li+ cal alc/w 25°C 100% U H
                                   1995ABc (107791) 881
Medium: 100% Methanol. DH(K1)=6 kJ mol-1, DS(K1)=77 J K-1 mol-1.
********************************
                             (6161)
Tetra-t-butyl-4-t-butylcalix[4]arenetetraketone;
-----
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
      sp alc/w 25°C 100% U K1=1.8 1989ACb (107795) 882
Medium: MeOH, 0.1 M Et4NCl
*********************************
                            CAS 246035-35-8 (3034)
25,27-Bis(N,N-diethylaminocarbonylmethoxy)-26,28-bis(N-butylaminocarbonylmethoxy)-t
-butvlcalix[4]
              Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
-----
Li+ sp non-aq 25°C 100% C K1=<1 1999USa (107805) 883
Medium: MeOH, 0.10 M Et4NCl
**********************************
                            CAS 114155-16-7 (7183)
C68H100N408
4-tert-Butylcalix[4]arene tetradiethylacetamide;
  -----
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
```

```
cal alc/w 25°C 100% U IH
Li+
                                   1995ABc (107815) 884
Medium: 100% Methanol. DH(K1)=-7 kJ mol-1, DS(K1)=50 J K-1 mol-1.
In acetonitrile, K1>8.5, DH(K1)=-55 kJ mol-1, DS(K1)=-22 J K-1 mol-1.
______
      dis non-ag 20°C 100% C M
                                   1988AGa (107816) 885
                         K(Li+A+L(org)=LiAL(org))=7.11
Method: extraction of metal picrate into CHCl3/L solution. HA is picric
************************************
C69H102N409
                            CAS 116352-85-3 (9286)
para-t-Butyldihomooxacalix[4]arene tetra(diethyl)amide;
 .....
    Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
Li+ sp alc/w 25°C 100% C K1=3.81 2004MFa (107835) 886
Medium: MeOH, 0.01 M Et4NCl.
******************************
C72H68010P4
                            CAS 88928-02-3 (5680)
Tetrakis-4',5',4",5"-(diphenylphosphinylmethyl)-2,3:11,12-dibenzo-18-crown-6;
  -----
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
                          K1=3.09 1985YKa (107847) 887
      con non-aq 25°C 100% U
Medium: EtOH+CHCl3 1:1; M is used in nitrophenolate form
*******************************
                            CAS 152495-34-6 (7033)
Penta-tert-butylpentakis(ethoxycarbonylmethyloxy)calix[5]arene;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
-----
    sp alc/w 25°C 100% U K1=1.0
                                  1993BMa (107860) 888
Medium: MeOH, 0.1 M Et4NCl.
************************************
5,11,17,23-Tetra-t-butyl-25,26,27,28-tetra(benzoyl)methoxycalix[4]arene;
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
      sp non-aq 25°C 100% U K1=6.3
                                   1989ACb (107870) 889
Medium: CH3CN
**********************************
                            CAS 253317-20-3 (9288)
p-Tert-butyldihomooxacalix[4]arene tetraphenyketone;
______
      Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      sp alc/w 25°C 100% C I K1=2.3
                                  1999MAb (107894) 890
Medium: MeOH, 0.01 M Et4NCl. In acetonitrile, K1=3.6.
**********************************
                            CAS 160638-26-6 (9130)
C78H90010P2
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5,11,17,23-Tetra-t-butyl-bis(diethylcarbamoylmethoxy)-bis(diphenylphosphinoylmethox
v)calix[4]aren
Metal Mtd Medium Temp Conc Cal Flags Lg K values
                                Reference ExptNo
Li+ sp alc/w 20°C 100% C K1=2.88 2003YVa (107900) 891
Medium: 100% EtOH, 0.01 M Et4NBr. Ligand is cone isomer. For paco isomer,
K=2.64. Also data for bis(diethyl ester) analogues.
*************************
C85H120015
                         CAS 152495-35-7 (7034)
Penta-tert-butylpentakis(tert-butoxycarbonylmethoxy)calix[5]arene;
______
    Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
Li+ sp alc/w 25°C 100% U K1=1.5 1993BMa (107917) 892
Medium: MeOH, 0.1 M Et4NCl.
C90H120O18
                         CAS 92003-62-8 (6159)
Hexaethyl-4-t-butylcalix[6]arenehexaethanoate;
 Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
     cal non-aq 25°C 100% C K1=4.37 1997DZa (107942) 893
Medium: benzonitrile. DH(K1)=-21.04 kJ mol-1, DS(K1)=13.1 J K-1 mol-1.
_____
      sp non-aq 25°C 100% U I K1=3.7 1989ACb (107943) 894
Medium: CH3CN
**********************************
                          CAS 269057-78-5 (3334)
5,11,17,23,29-Penta-tert-octylcalix[5]arene-31,32,33,34,35-pentaethanoate
pentamethyl ester;
           -----
_____
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
Li+ sp non-aq 25°C 100% C I K1=2.28 2000AAa (107951) 895
Medium: methanol, 0.01 M Et4NCl. Also data for acetonitrile, 0.01 M Et4NCl
and for the pentaethyl ester.
*********************************
            H2L
                X-14885A
                           (4547)
Antibiotic X14885A, calcium ionophore
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
      gl alc/w 25°C 100% U K1=4.1 1989ABb (108076) 896
Medium: MeOH
***********************************
                           (4181)
Phosphatidic acid;
-----
```

Mtd Medium Temp Conc Cal Flags Lg K values

Reference ExptNo

```
gl oth/un 24°C 0.10M U K1=1.3 1966AKa (108271) 897
********************
Polymer
                                          (4192)
Polyacrylic acid and 7.5% divinylbenzene copolymer
______
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
Li+ gl oth/un 25°C 0.2M U K1=0.29 1957GFa (108304) 898
(3531)
Polyacrylic acid;
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
______
Li+ gl oth/un 25?°C 0.20M U
                                                  1957GFa (108323) 899
                                   K' = 0.28
Medium: LiCl. See reference for definitions
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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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**END**