

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)

e- HL Electron (442)
Electron;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Li+	EMF	mixed	25°C	10%	U	I		K(Li+e=Li(s))=-51.40(-3041mV)	1974DKb (627)	1
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		K(Li+e+Li(s))=-50.73(3001mV)	1972C0a (628)	2
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)										
Li+		oth none	25°C	0.0	U	I		K(Li+e=Li(s))=-50.73(3001mV)	1972C0a (629)	3
Method: Estimated. MeCN: -56.05(-3.316V).HCOOH: -59.72(-3.533V) Also NH3 and N2H4										
Li+		con non-aq	-71°C	100%	U			K(Li + e(solv))=2.72 K(2Li=Li2)=1.95	1972DBa (630)	4
Medium: NH3(liquid). Method:conductivity and magnetic susceptibility										
Li+	EMF	mixed	25°C	30%	U	I		K(Li+e=Li(s))=-51.32(-3036mV)	1972KRb (631)	5
Med.:30% w/w ethylene glycol/H2O; K=-51.18(-3.028V,50%), -50.95(-3.014V,70%) -51.15(-3.026V,90%), -52.35(-3.097V,100%)										
Li+	EMF	non-aq	25°C	100%	U	I		K(Li+e=Li(s))=-52.08(-3081mV)	1972KRc (632)	6
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)										
Li+	EMF	none	25°C	0.0	M			K(Li+e=Li(s))=-51.39,-3040.1mV	1968HBb (633)	7
Li+	EMF	none	25°C	0.0	U			K(Li+e=LiHg)=-36.99, -2188 mV	1967BHc (634)	8

Li+ EMF none 25°C 0.0 M 1967BHc (635) 9
K(Li+e=LiHg)=-37.13, -2196.3 mV

Li+ EMF non-aq 25°C 100% U 1966LCa (636) 10
K'=-52.806, -3123.7 mV
Medium: CH3NHCHO. K': Li + Cl + Ag(s) = Li(s) + AgCl(s)

Li+ oth none 25°C 0.0 U 1952LAB (637) 11
K(Li+e)=-51.47(-3045 mV)

Li+ EMF none 25°C 0.0 U 1923LRa (638) 12
K(Li+e=Li(s))=-50.02(-2957.8mV)

AsF6- L (8856)
Tetrafluoroarsenate;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
Li+ con non-aq 25°C 100% C K1=1.716 2002DDa (1040) 13
Medium: N,N-dimethylacetamide, 0.005-0.015 M LiAsF6.

BF4- HL (2497)
Tetrafluoroborate;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
Li+ con non-aq 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

B04H4- HL Borate CAS 10043-35-3 (991)
Borate; B(OH)4-

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

Li+ 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

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo	
Li+	con	non-aq	25°C	100%	C		K1=1.520	2002DDa	(2083)	21
Medium: N,N-dimethylacetamide, 0.005-0.015 M LiBr.										
Li+	con	non-aq	25°C	100%	C		K1=10.53 B(Li2Br)=13.33 K(2LiBr=Li2Br2)=1.70	1997CHb	(2084)	22
Medium: THF. By conductivity, species M2L and L2M are equivalent.										
Li+	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)										
Li+	con	mixed	25°C	0.10M	U I		K1=3.53	1973BHa	(2088)	26
In 99.9% w/w acetone/H2O. 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										
Li+	kin	mixed	25°C	0.00	U I		K1=3.56	1972HBa	(2091)	29
In 99.995% w/w acetone/H2O.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										
Li+	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										
Li+	con	non-aq	25°C	100%	U		K1=1.28	1969MBF	(2095)	33

Medium: propene carbonate(0 corr)

Li+ con diox/w 25°C 50% U TI K1=1.11 1969SMc (2096) 34
In 50% w/w dioxan/H2O. 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

Li+ con non-aq 40°C 100% U T K1=2.90 1967SMb (2097) 35
Medium:Me2CO. K1=2.80(25 C),2.77(30 C),2.85(35 C); also Me2CO-H2O mixtures

Li+ con non-aq 25°C 100% U K1=3.66 1966SAa (2098) 36
Medium: acetone

Li+ con alc/w 25°C 100% U K1=1.19 1966SMc (2099) 37
Medium:MeOH, also K1 values for MeOH-H2O mixtures

Li+ con non-aq 25°C 100% U K1=3.18 1965BFb (2100) 38
Medium: diaminoethane

Li+ oth non-aq 35°C 100% U K(2Li2Br2=Li4Br4)=1.3 1964TRb (2101) 39
Method:boiling point. Medium:Et2O

Li+ kin non-aq 0°C 100% U K1=0.41 1964WHa (2102) 40
Medium:DMF

Li+ con non-aq 0°C 100% U K1=4.58 1960LRb (2103) 41
Medium: liquid SO2, I=0 corr., 0.22 C

Li+ oth non-aq 16°C 100% U K(2LiBr=Li2Br2)=0.66 1959KEb (2104) 42
Method: freezing point; medium: CH3CO2H; m units.

Li+ con non-aq 30°C 100% U K1=6.14 1954JGa (2105) 43
Medium: CH3CO2H

BrO3- HL Bromate (6017)
Bromate;

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

Li+ sol NaClO4 25°C 0.15M U I K1=-0.77 1963RSe (2422) 44
Medium: LiClO4. K1=-0.82 (I=0.20)

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

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

Li+ sol oth/un 40°C var U T K(Li2L+CO2(g)=2Li+2HL)=-0.23 1958MLa (3261) 45

K=-2.63(200 C), -3.68(250 C), -4.91(290 C), m units

Li+ sol oth/un 20°C var U 1958VGa (3262) 46
Kso(Li2CO3(s))=-1.6

C6N6Fe---- H4L (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

Cl- HL Chloride 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

Li+ oth non-aq 25°C 100% U 1974GRa (5167) 54
Kd(2LiCl=Li2Cl2)=2.26
Medium: octanoic acid. Method: permittivity

Li+ 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

Li+ con non-aq 25°C 100% U K1=0.61 1972SKb (5169) 56
Medium: isopentylalcohol

Li+	con non-aq	25°C	100%	U	K1=5.55	1971BHa	(5170)	57
Medium: acetone								
Li+	con non-aq	25°C	100%	U	K1=2.2	1971ENa	(5171)	58
Medium: trifluoroethanol, K1=2.11 to 2.28								
Li+	con non-aq	25°C	100%	U	K1=2.32	1971ETa	(5172)	59
Medium: propanol, also acetone-propanol mixtures. In 100% acetone: K1=5.32								
Li+	oth non-aq	37°C	100%	U		1971HMb	(5173)	60
					Kd(2LiCl=Li2Cl2)=0.4			
Medium: ethanoic acid. Method: vapor phase osmometry								
Li+	con non-aq	25°C	100%	U	K1=0.18	1971PGa	(5174)	61
Medium: N-methylformamide								
Li+	EMF non-aq	25°C	100%	U	K1=1.70	1970SAb	(5175)	62
Medium: propene carbonate								
Li+	kin non-aq	25°C	100%	U	K1=5.55	1969BEa	(5176)	63
Medium: acetone. By conductivity: K1=5.47								
Li+	con alc/w	25°C	43%	U I	K1=0.40	1969DPa	(5177)	64
Medium: 43.5% w/w EtOH/H2O. K1=0.49(57.1%), 0.68(68.2%), 0.88(77.2%), 1.02(86.6%), 1.20(92.3%), 1.43(100%)								
Li+	con non-aq	25°C	100%	U	K1=2.75	1969MBf	(5178)	65
Medium: propene carbonate								
Li+	oth alc/w	25°C	100%	U	K1=0.5	1967MIc	(5179)	66
Method: from literature data. Medium: MeOH. K1=1.43(EtOH), 2.2(i-PrOH), 2.3(i-BuOH), 3(acetone)								
Li+	con non-aq	25°C	100%	U	K1=5.48	1966SAa	(5180)	67
Medium: acetone								
Li+	oth non-aq	18°C	100%	U	K1=0.7	1965DGa	(5181)	68
Method:freezing point. Medium: DMSO								
Li+	kin non-aq	0°C	100%	U	K1=0.74	1964WHa	(5182)	69
Medium:DMF								
Li+	con non-aq	20°C	100%	U	K1=5.3	1963MSd	(5183)	70
Medium:TBP,(BuO)3PO								
Li+	gl diox/w	25°C	70%	U	K1=2.54	1963PGb	(5184)	71
Li+	con non-aq	25°C	100%	U	K1=4.27	1962SHd	(5185)	72
Medium: CH3COOH. By EMF K1=3.98								

Li+ con mixed 25°C 90% U K1=2.3 1961AMc (5186) 73
Medium: 90% acetone/H2O

Li+ oth non-aq 16°C 100% U K(2LiCl=Li2Cl2)=0.44 1959KEb (5187) 74
Method: freezing point in CH3COOH, m units.

Li+ con alc/w 25°C 100% U K1=1.75 1957GKa (5188) 75
Medium: EtOH

Li+ EMF non-aq 25°C 100% U K1=7.08 1956BKa (5189) 76
Medium: CH3COOH

Li+ con non-aq 25°C 100% U K1=7.13 1953SEa (5190) 77
Medium: CH3COOH

Li+ con non-aq 30°C 100% U T K1=4.14 1952CSa (5191) 78
Medium: cyclohexanol. K1=4.21(35 C)

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

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

Li+ con diox/w 25°C 90% U I K1=6.42 1966CKa (6046) 79
K1=1.42(64.5% dioxan)

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

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

Li+ con non-aq 25°C 100% C K1=1.349 2002DDa (6290) 80
Medium: N,N-dimethylacetamide, 0.005-0.015 M LiClO4.

Li+ con non-aq 25°C 100% M K1=1.26 1999DSd (6291) 81
Medium: acetonitrile.

Li+ con non-aq 25°C 100% C I K1=7.34 1997CHb (6292) 82
B(Li2ClO4)=8.99

Medium: THF. By conductivity, species M2L and L2M are equivalent.
Also data for dimethoxyethane, ethyl acetate and THF/2-ethyl-1-hexanol.

Li+ gl non-aq 25°C 100% U H K1=5.11 1981TMb (6293) 83
Medium: Glacial acetic acid. Alternative method: Spectrophotometry.
DH(K1)=-52 kJ mol⁻¹

Li+ con non-aq 25°C 100% U K1=7.68 B2=9.85 1979CCa (6294) 84
Medium: THF

Li+	con non-aq	25°C	100%	U	K1=1.20	1978CAa (6295)	85
Medium: Acetonitrile							
Li+	con non-aq	25°C	100%	U	K1=5.09	1977BIb (6296)	86
Medium: - tributylphosphate							
Li+	con non-aq	25°C	100%	U	K1=0.20	1974HPb (6297)	87
Medium: hexamethylphosphotriamide. K1 by Pitt eqn. By Fuoss-Hsia: K1=1.13							
Li+	con non-aq	25°C	100%	U T	K1=7.68	1974JPa (6298)	88
KT=K(LiI+Li)=2.18							
Medium: THF. At -15 C: K1=7.18, KT=2.14; -30 C: K1=6.97, KT=2.12							
Li+	oth non-aq	25°C	100%	U T H	K1=-0.51	1974PKc (6299)	89
Medium: acetone. DH(K1)=3.68 kJ mol ⁻¹ . K1=-0.92(-90 C), -0.70(-45 C), -0.64(-25 C), -0.57(0 C), -0.39(45 C). Method: infrared spectra							
Li+	con mixed	25°C	15%	U I	K1=2.55	1974SPc (6300)	90
Medium 15% w/w THF/H ₂ O. K1=2.59(30%), 2.56(40%), 2.24(50%), 2.39(60%), 2.59(70%) 2.57(80%), 3.16(90%), 3.97(95%), 4.36(97%), 4.39(98%), 4.84(100%)							
Li+	con alc/w	25°C	100%	U	K1=1.14	1972DAa (6301)	91
Medium: MeOH							
Li+	con non-aq	25°C	100%	U	K1=0.51	1972SKb (6302)	92
Medium: isopentylalcohol							
Li+	con non-aq	25°C	100%	U	K1=3.23	1971BHa (6303)	93
Medium: acetone							
Li+	con non-aq	25°C	100%	U	K1=0.18	1971PGa (6304)	94
Medium: N-methylformamide							
Li+	con mixed	25°C	80%	U I	K1=1.75	1970ALa (6305)	95
Medium: 80% w/w t-butanol/H ₂ O. K1=2.25(85%), 3.08(90%), 3.87(95%), 4.12(97%)							
Li+	EMF mixed	25°C	0.10M	U I	K1=4.41	1970DCa (6306)	96
Medium: dimethoxy-1,2-ethane, 0.1 M H ₂ O. K1=4.2(H ₂ O conc.:0.01 M)							
Li+	EMF non-aq	rt	100%	U	K1=4.5	1969BEb (6307)	97
Medium: CF ₃ COOH							
Li+	EMF non-aq	25°C	100%	U		1968MKa (6308)	98
K1(Li+)/K1(H+)=1.12							
Method: H electrode. Medium: pyridine							
Li+	EMF non-aq	20°C	100%	U	K1=0	1967PBa (6309)	99
Method: H electrode. Medium: C ₄ H ₈ O, 0.1 M Bu ₄ NClO ₄							

Li+ con non-aq 25°C 100% U T K1=1.54 1966MWb (6310) 100
Medium: MeCN, also at 20 C, 30 C

Li+ con non-aq 25°C 100% U K1=1.83 1962Mwa (6311) 101
Medium:MeCN

Li+ oth non-aq 16°C 100% U K(2LiL=Li2L2)=0.89 1959KEb (6312) 102

Method: freezing point. Medium: CH3CO2H, m units

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

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

Li+ oth oth/un 25°C 0.0 U K1=0.7 1966MBb (6496) 103

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

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

Li+ sp oth/un 25°C 1.0M U I K1=0.34 1993MAa (6997) 104
K1 values over a range of pressures and ionic strengths

Li+ ISE NaClO4 25°C 1.0M U TI K1=-0.12 1984CTd (6998) 105

Li+ ISE NaClO4 25°C 1.00M C I K1=-0.12 1984Hca (6999) 106
Also in 1.0 M KNO3 (K1=-0.03) and 1.0 M NaNO3 (K1=-0.24).

Li+ oth oth/un 25°C ? U K1=0.25 1981ASa (7000) 107

Li+ ISE NaNO3 25°C 1.0M U K1=2.90 B2=3.67 1968SRd (7001) 108
Method: F membrane electrode

Li+ dis oth/un 25°C 0.0 U 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+ cal oth/un 25°C 0.0 U H Kso=-2.77 1964SHb (7003) 110

DH(so)=4.5 kJ mol-1

H2O L Water CAS 7732-18-5 (6115)
Water

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

Li+ oth non-aq 25°C 100% U I K1=0.81 B2=1.47 1974BLa (7596) 111

Method: partial pressure. Medium: propene carbonate. In sulfolane: K1=0.65,

K2=0.5. In DMSO, K1=-0.7 (by N.M.R.)

Li+ 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

Li+ 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- HL Iodide CAS 10034-85-2 (20)
Iodide;

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

Li+ con non-aq 25°C 100% C K1=1.478 2002DDa (8219) 115
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

Li+ 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

Li+ dis oth/un 25°C 0.0 U Kd(Li+I=Li(TBP)+I(TBP))=-0.54 1967RMe (8224) 120
In (i-amylO)2MePO: Kd=-1.03

Li+ dis oth/un 25°C 0.0 U Kd(Na+I=Na(TBP)+I(TBP))=-1.32 1967RMe (8225) 121
In (i-amylO)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%)

Li+ con non-aq 25°C 100% U K1=2.16 1966SAa (8227) 123
Medium: acetone

Li+ con non-aq 25°C 100% U K1=2.97 1965BFb (8228) 124
Medium: diaminoethane

Li+ kin non-aq 0°C 100% U K1=0.26 1964WHa (8229) 125
Medium: DMF

Li+ oth non-aq 16°C 100% U K(2LiI=Li2I2)=1.11 1959KEb (8230) 126
Method: freezing point. Medium: CH3CO2H, m units

Li+ con non-aq 25°C 100% U I K1=2.56 1957HUa (8231) 127
Medium: EtCOMe. In PhCOMe K1=2.17

MoO4-- H2L Molybdate (443)
Molybdate;

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

Li+ sp oth/un 25°C ? U M K(H2L+2Li=Li2L+2H)=-3.3 1997STa (8740) 128

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

Li+ gl diox/w 25°C 2.0M U K1=-0.01 B2=-0.06 1992MPa (9175) 129
K1=-0.28(100%H2O)
K3=-1.10(100%H2O)
K2=-0.76(100% H2O)
K4=-1.50 (100%H2O)

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

Li+ 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

Li+ cal oth/un rt dil U H 1952FYa (9177) 131
DH(B3?)=-2.1 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- HL Nitrite CAS 7782-77-6 (635)
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

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

 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 K1(Li+)/K1(H+)=0.91 1968MKa (9756) 143
 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 1959KEb (9760) 147
K(3LiL=Li3L3)=1.1

Method: Freezing point. Medium:CH3CO2H

Li+ sp oth/un 30°C 0.0 U K1=-1.45 1928HEa (9761) 148

OH- HL Hydroxide (57)
Hydroxide;

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

Li+ nmr R4N.X 25°C 3.4M C K1=-0.1 2002PLa (11701) 149
method: NMR Li-7
Medium: 3.4 M Me4NCl/Me4NOH

Li+ EMF non-aq 25°C 100% U K1=11.0 1967PBa (11702) 150
Medium: THF, 0.1 M Bu4NClO4. H electrode

Li+ EMF NaClO4 25°C 3.00M U I K1=-0.18 19640Ha (11703) 151
At I=0 corr.: K1=-0.1

Li+ EMF NaClO4 25°C 3.0M C K1=-0.2 1964PCa (11704) 152
*K1=-14.4
Method: H electrode

Li+ con none 49°C 0.0 U T K1=0.89 1961WLa (11705) 153
K1=1.13(93 C),1.51(138 C),1.42(182 C),1.59(227 C),1.76(271 C)

Li+ EMF none 25°C 0.0 C T K1=0.17 1954GMb (11706) 154
K1=0.26(5 C),0.20(15 C),0.19(35 C),0.19(45 C). Method: H electrode

Li+ con none 25°C 0.0 U K1=-0.08 1942DMa (11707) 155

PO4--- H3L Phosphate CAS 7664-38-2 (176)
Phosphate;

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

Li+ gl oth/un 37°C 0.15M C K1=0.95 1983DGa (13238) 156
K(Li+HL)=0.79
K(Li+H2L)=0.2

Li+ gl R4N.X 25°C 0.20M U T HM 1956SAc (13239) 157
K(Li+HL)=0.72
Medium: Pr4NCl, K=0.32(0 C). DH(K)=25.1 kJ mol⁻¹, DS=100 J K⁻¹ mol⁻¹

P2O6---- H4L Hypophosphate CAS 9803-60-3 (199)
Hypophosphate;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Li+	gl	R4N.X	25°C	0.50M	U			K1=0.82	1967CMc (13415)	158
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Ligand: O3POPHO2---, Medium: Me4NCl

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Li+	cal	R4N.X	5°C	1.00M	U	H			1973VAa (13615)	159
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Medium: Me4NNO3, DH(K1)=1.3 kJ mol⁻¹. 35 C, I=0, DH(K1)=4.2. DH(Li+HL)=-0.8

Li+	gl	none	25°C	0.0	U	T		K1=3.1	1959W0a (13616)	160
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K1=3.3(40 C)

Li+	gl	R4N.X	25°C	1.00M	U			K1=2.39	1957LWa (13617)	161
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K(Li+HL)=1.03

Medium: Me4NCl

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Li+	kin	NaNO3	65°C	1.0M	C				1985GGb (13692)	162
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K(Li+HP208)=0.92

Ligand is peroxydisulfate, S208----

Li+	gl	R4N.X	25°C	1.00M	U			K1=1.34	1960CEa (13693)	163
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K(Li+HL)=0.70

Medium: Me4NCl

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Li+	gl	R4N.X	25°C	1.0M	U			K1=3.61	1982CCb (13724)	164
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K(Li+HL)=3.77
K(Li+H2L)=2.0

alpha2 isomer. For alpha1 isomer, K1>3.7, K(Li+HL)=1.6, K(Li+H2L)=0.6

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Li+	gl	none	25°C	0.0	U	T		K1=3.9	1959W0a (13878)	165
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K1=3.8(40 C)

Li+ gl R4N.X 25°C 1.00M U K1=2.87 1957WLa (13879) 166
K(Li+HL)=0.88

Medium: Me4NCl

P4013----- H6L Tetrphosphate (1102)

Tetrphosphate;

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

Li+ gl R4N.X 25°C 1.0M U K1=2.64 1967WMa (14049) 167
K(Li+HL)=1.59

Medium: Me4NCl

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

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

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

Li+ gl R4N.X 25°C 1.0M U K1=1.34 1960CEa (14061) 168
K(Li+HL)=0.70

Medium: Me4NCl

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

Thiocyanate;

Metal 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

Li+ 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.

Li+ sp non-aq 25°C 100% U K1=-0.125 B2=0.26 1979ITa (15133) 172

Medium: N,N-Dimethylacetamide. Method: Raman spectroscopy

Li+ con non-aq 25°C 100% U K1=0.15 1971PGa (15134) 173
Medium: MeHNCHO

Li+ sp non-aq 20°C 100% U K1=2.9 1970SSa (15135) 174
Medium: MeCN

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

Sulfate;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Li+	gl	NaCl	37°C	0.10M	C	I		K1=0.77	1982DRb (16304)	175
Data for I=0.03-0.50 M NaCl. At I=0.0 M, K1=1.12										
Li+	oth	oth/un	25°C	0.50M	U	TI		K1=0.77	1980GAb (16305)	176
Method: Ultrasonic absorption. Medium: Na2SO4										
Li+	con	none	25°C	0.0	U				1978FFa (16306)	177
K(Li+LiSO4)=0.096										
Li+	oth	oth/un	25°C	.244M	U			K1=0.77	1975REa (16307)	178
Li+	oth	none	25°C	0.0	M			K1=0.7	1966MBb (16308)	179
Li+	con	oth/un	18°C	0.0	U			K1=0.64	1930RDa (16309)	180

SeCN-		HL				Selenocyanate		CAS 73102-11-2	(440)	
Selenocyanate;										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Li+	sp	non-aq	20°C	100%	U			K1=2.4	1970SSa (16991)	181
Medium: acetonitrile										

SiW11039	-----	H8L						(2464)		
alpha-Heterosilicon-polytungstate;										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Li+	gl	R4N.X	25°C	1.0M	U			K1=4.1	1982CCb (17237)	182

VO4---		H3L						CAS 15457-75-7	(1586)	
Vanadate; VO2(OH)3-- or polymers										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Li+	gl	NaClO4	25°C	1.00M	U				1975KIc (17381)	183
K(Li+H7PV12036)=1.92										
Li+	gl	R4N.X	20°C	0.10M	U				1963SGd (17382)	184
K(Li+H15L10)=0.6										
K(Li+H14L10)=1.6										
K(Li+LiH14L10)=0.6										

CH2O2		HL				Formic acid		CAS 64-18-6	(37)	
Methanoic acid; H.COOH										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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)	186
Medium: CH3CN, 0.01 M Et4NClO4									

CH4O		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)	187
Medium: CH3CN, 0.01 M Et4NClO4									

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

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									

CH6O6P2		H4L		Medronic acid			CAS 1984-15-2	(2384)	
Methanediphosphonic acid; CH2(PO3H2)2									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Li+	gl	R4N.X	25°C	0.50M	U		K1=2.48 K(Li+HL)=0.82	1967CIa (18285)	189
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	Lg K values	Reference	ExptNo
Li+	gl	R4N.X I=0.02-1 M Et4NI	25°C	0.25M	C	TI	K1=0.13	1985DRa (20031)	191

Li+	gl	R4N.X	25°C	0.16M	U	I	K1=-0.13 K1=-0.10 (I=0.04); -0.13 (0.25); -0.09 (0.49); -0.02 (1.0)	1985RSa (20032)	192
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Li+	con	alc/w in water. In 50% dioxan/H2O:	25°C	100%	U	I	K1=1.73 K1=1.65; 60%: 2.04; 70%: 2.50	1981ASa (20033)	193
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Li+	gl	non-aq Medium: Glacial acetic acid. Alternative method: Spectrophotometry. DH(K1)=-29.0 kJ mol-1	25°C	100%	U	H	K1=6.87	1981TMb (20034)	194
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Li+	con	none Also data for MeOH (K1=1.834), 50% dioxan/H2O (K1=1.788) and 70% dioxane/H2O (K1=2.874).	35°C	0.0	C	I	K1=1.295	1979ASc (20035)	195
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Li+	gl	oth/un	25°C	0.0	U		K1=0.26	1964AMa (20036)	196
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Li+	gl	non-aq Medium: ethanoic acid	25°C	100%	U		K1=6.78	1964KLa (20037)	197
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Li+	con	oth/un Medium: Li ethanoate. K1=-0.54(I=0.2), -0.52(I=0.5), -0.49(I=0.7)	18°C	0.10M	U	I	K1=-0.53	1964Sub (20038)	198
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Li+	sp	non-aq Medium: ethanoic acid	25°C	100%	U		K1=6.20	1961PSa (20039)	199
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Li+	EMF	non-aq Method: chloranil electrode. Medium: ethanoic acid	25°C	100%	U		K1=6.79	1956BKa (20040)	200
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Li+	con	non-aq Medium: ethanoic acid	30°C	100%	U		K1=6.82	1954JGa (20041)	201
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 C2H5NO L Methylformamide CAS 123-39-7 (6268)
 N-Methylformamide; HCO.NH.CH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Li+	ISE	non-aq Medium: CH3CN, 0.01 M Et4NClO4	25°C	100%	C		K1=1.4 B2=2.4	1975NAa (20675)	202
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 C2H5NO2 HL Glycine CAS 56-40-6 (85)
 2-Aminoethanoic acid; H2N.CH2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Li+	sp	oth/un	25°C	1.0M	U		K1=1.2	1987HAa (21603)	203
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C2H6OS L DMSO CAS 67-68-5 (329)
Dimethylsulfoxide; (CH3)2.S0

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Li+	ISE	non-aq	25°C	100%	M			K1=1.69 B2=2.99	1988NHa (22105)	204

Medium: MeCN, 0.01 M Et4NClO4

Li+	ISE	non-aq	25°C	100%	U T H			K1=1.70	1982NYa (22106)	205
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Medium: MeCN

Li+	ISE	non-aq	25°C	100%	C			K1=1.7 B2=3.0 B3=3.5	1975NAa (22107)	206
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Medium: CH3CN, 0.01 M Et4NClO4

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Li+	sp	alc/w	25°C	95%	U			K1=0.87	1993GSa (23186)	207

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

Li+	gl	oth/un	25°C	0.10M	C I			K1=-0.20 K(Li+HL)=-0.65	1990CDb (23187)	208
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Medium: 0.10 M LiCl. Data for I=0.25-1.0 M.

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Li+	gl	R4N.X	25°C	0.50M	U			K1=3.1 K(Li+HL)=0.99	1967CIa (23270)	209

Medium: Me4NCl

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Li+	gl	R4N.X	25°C	0.10M	U			K(Li+HL)=1.36 B(2Li+L)=4.78	1972WFa (23381)	210

Medium: (CH3)4NCl

Li+	gl	R4N.X	25°C	0.50M	U			K1=3.35 K(Li+HL)=1.08	1967CIa (23382)	211
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Medium: Me4NCl

C3H4O4 H2L Malonic acid CAS 141-82-2 (79)
Propanedioic acid; CH2(COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Li+	gl	R4N.X	37°C	0.25M	C	TI		K1=0.95 B(LiHL)=5.63	1985DRa (24488)	212

I=0.02-1 M Et4NI

Li+	gl	oth/un	37°C	0.15M	C	I		K1=0.67 B2= 1.15	1983DRb (24489)	213
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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=1.05.

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Li+	EMF	oth/un	25°C	->0	U			K1=0.20	1954DMb (25475)	214

Method: H electrode

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Li+	ISE non-aq		25°C	100%	M			K1=1.14 B2= 2.20 B3=1.66 B4=1.75	1999NMa (25659)	215

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

Li+	ISE non-aq		25°C	100%	M			K1=1.20 B2=3.04	1988NHa (25660)	216
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Medium: MeCN, 0.01 M Et4NClO4

Li+	ISE non-aq		25°C	100%	U	T H		K1=1.37	1982NYa (25661)	217
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Medium: MeCN

Li+	ISE non-aq		25°C	100%	C			K1=1.2 B2=2.0 B3=1.8	1975NAa (25662)	218
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Medium: CH3CN, 0.01 M Et4NClO4

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Li+	gl	R4N.X	25°C	0.50M	U			K1=3.8 K(Li+HL)=1.38	1967CIa (28401)	219

Medium: Me4NCl

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

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

Li+ gl R4N.X 37°C 0.25M C TI K1=0.91 1985DRa (29099) 220
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.

C4H6O3 L 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

Li+ ISE non-aq 25°C 100% C K1=0.5 1975NAa (29752) 222

Medium: CH3CN, 0.01 M Et4NClO4

C4H6O4 H2L Succinic acid CAS 110-15-6 (112)

1,4-Butanedioic acid; HOOC.CH2.CH2.COOH

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

Li+ 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.

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

2-Hydroxybutane-1,4-dioic acid, Hydroxy-succinic acid; HOOC.CH2.CH(OH).COOH

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

Li+ ISE oth/un 25°C 0.10M U K1=0.38 1964RZa (30669) 225

Li+ gl R4N.X ? 0.28M U K1=0.45 1963EDa (30670) 226

Medium: Me4NBr

C4H6O5 H2L Diglycolic acid CAS 110-99-6 (243)

Di(carboxy)methyl ether, 2,2'-Oxydiethanoic acid; HOOC.CH2.O.CH2.COOH

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

Li+ gl R4N.X 25°C 0.25M C TIH K1=0.70 1985DRa (30892) 227
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

Li+ oth oth/un 30°C 1.00M U K1=-0.62 19730Ea (30893) 228
Method: Raman spectroscopy. medium: LiCl

C4H8O L THF CAS 109-99-9 (2537)
Tetrahydrofuran; cyclo(-CH2.CH2.O.CH2.CH2-)

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

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

C4H9NO L CAS 127-19-5 (477)
N,N-Dimethylacetamide; CH3.CO.N(CH3)2

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

Li+ ISE non-aq 25°C 100% U T H K1=1.76 1982NYa (33762) 230
Medium: MeCN

Li+ 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

Li+ ISE non-aq 25°C 100% C K1=1.8 B2=2.9 1975NAa (33764) 232
B3=3.3

Medium: CH3CN, 0.01 M Et4NClO4

C4H10O HL t-Butanol CAS 75-65-0 (1740)
tert-Butanol, (CH3)3C.OH

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

Li+ con non-aq 25°C 100% U K1=8.0 1974ESa (34659) 233
Medium: DMSO

C4H10O3 L CAS 111-46-6 (3579)
2,2'-Oxydiethanol; (HO.CH2.CH2)2.O (Diethylene glycol)

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

Li+ con non-aq 25°C 100% C K1=2.7 1992MSe (34702) 234
Medium: 100% MeOH. Anion: picrate. Also data for nitrophenolate anions.

 C4H11N L (6678)
 Dimethylethylamine; (CH3)2NCH2CH3

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

 Li+ 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.

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

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

 Li+ 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

 C5H5N L Pyridine CAS 110-86-1 (31)
 Pyridine, Azine;

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

 Li+ ISE non-aq 25°C 100% C K1=0.72 B2=0.43 1975NAa (36648) 237
 Medium: CH3CN, 0.01 M Et4NClO4

 C5H6N2 L 2-Aminopyridine CAS 504-29-0 (1478)
 2-Aminoazine, 2-Pyridylamine; C5H4N.NH2

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

 Li+ 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

 C5H8O2 HL Acetylacetone CAS 123-54-6 (164)
 Pentane-2,4-dione; CH3.CO.CH2.CO.CH3

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

 Li+ 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

 Li+ gl alc/w 25°C 100% U K1=2.8 1965LIa (38014) 241
 Medium: MeOH, 0.1 M LiClO4. In EtOH: K1=4.6

 C6H3N3O7 HL Picric acid CAS 88-89-1 (593)

2,4,6-Trinitrophenol; HO.C6H2(NO2)3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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			K(LiA+L)=2.53	1998TKa (42123)	243
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Self medium, I<0.03 M. Method: Extraction of LiAL into dichloromethane. A is 18-crown-6.

Li+	con	non-aq	25°C	100%	C	I		K1=8.07 B(Li2L)=10.03	1997CHb (42124)	244
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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
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Medium: acetonitrile. Also data for benzonitrile and DMF.

Li+	sp	non-aq	25°C	100%	U			K1=3.97	1980GRa (42126)	246
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Medium: 2-butanol

Li+	con	alc/w	30°C	100%	U	I	M	K1=2.72	1979PSa (42127)	247
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Medium: isoPrOH. K(LiL+diethyleneglycol)=2.51; K(LiL+triethyleneglycol)=2.41. In H2O: K1=1.11

Li+	dis	none	25°C	0.00	U			K1=1.13	1972Iwc (42128)	248
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Li+	dis	oth/un	25°C	var	U			K1=2.2	1970SSb (42129)	249
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Method: paper chromatography

 C6H4N2O5 HL CAS 50-28-5 (505)
 2,4-Dinitrophenol; HO.C6H3(NO2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Li+	con	non-aq	25°C	100%	C	I		K1=4.29 B(Li2L)=6.71	1996HHc (42232)	250

Medium: acetonitrile. By conductivity, species M2L and L2M are equivalent. Also data for benzonitrile and DMF.

Li+	con	non-aq	25°C	100%	U			K1=3.54	1973FGa (42233)	251
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Medium: tetrahydrofuran

 C6H4N2O5 HL CAS 329-71-5 (507)
 2,5-Dinitrophenol; HO.C6H3(NO2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Li+ con non-aq 25°C 100% C I K1=5.33 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.

C6H5NO3 HL 2-Nitrophenol CAS 88-75-5 (510)
2-Nitrohydroxybenzene; HO.C6H4.NO2

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

Li+ con non-aq 25°C 100% C 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.

C6H5NO3 HL 4-Nitrophenol CAS 100-02-7 (454)
4-Nitrohydroxybenzene; HO.C6H4.NO2

Metal 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.

Li+ con non-aq 25°C 100% U K1=6.99 1991AMa (42811) 255

Medium: THF

C6H5OCl HL 4-Chlorophenol CAS 106-48-9 (1631)
4-Chlorophenol; HO.C6H4.Cl

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

Li+ con non-aq 25°C 100% U K1=9.13 1991AMa (43054) 256

Medium: THF

C6H6O HL Phenol CAS 108-95-2 (457)
Hydroxybenzene, phenol; C6H5.OH

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

Li+ con non-aq 25°C 100% U K1=10.16 1991AMa (43542) 257

Medium: THF

C6H6O2 H2L Catechol CAS 120-80-9 (534)
1,2-Dihydroxybenzene, pyrocatechol; HO.C6H4.OH

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

 Li+ sp alc/w 25°C 95% U K1=1.31 1993GSa (43783) 258
 Medium: 95% w/w EtOH/H2O, 0.05 M Et4NClO4, by competitive spectrophotometry

 C6H8N2 L CAS 95-54-5 (2899)
 1,2-Diaminobenzene, 1,2-Phenylenediamine; C6H4(NH2)2

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

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

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

C6H8O7 H3L Citric acid CAS 77-92-9 (95)
 2-Hydroxypropane-1,2,3-tricarboxylic acid; HOOCCH2.CH(OH)(COOH).CH2COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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 Li+ gl oth/un 25°C 0.50M U H K1=1.10 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.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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 Li+ ISE oth/un 25°C 0.10M U K1=0.83 1964RZa (46160) 263

 C6H9NO6 H3L NTA CAS 139-13-9 (191)
 Nitritotriethanoic acid; N(CH2.COOH)3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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 Li+ 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.)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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 Li+ sp R4N.X 25°C 0.10M C K1=2.35 1985HAd (46895) 265

Li+ gl R4N.X 20°C 0.10M U T K1=2.51 1963IFb (46896) 266
Medium: Me4HNO3

Li+ EMF oth/un 20°C 0.0 U K1=3.28 1945SKb (46897) 267
Method: H electrode

C6H10O2 HL CAS 815-57-6 (2261)
3-Methyl-pent-2,4-dione; CH3.CO.CH(CH3).CO.CH3

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

Li+ nmr alc/w -60°C 100% U K1=1.1 1979RHa (47948) 268
Medium: CD3OD

C6H14O3 L Diglyme CAS 111-96-6 (6769)
bis-2-Methoxyethyl ether, 2,5,8-Trioxanonane; CH3.O.CH2CH2.O.CH2CH2.O.CH3

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

Li+ con non-aq 25°C 100% C K1=3.2 1992MSe (51051) 269
Medium: 100% MeOH. Anion: picrate. Also data for nitrophenolate anions.

C6H15NO3 Triethanolamine CAS 102-71-6 (447)
Tris-(2-hydroxyethyl)amine; L

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

Li+ gl R4N.X 25°C 1.00M C I K1=-0.48 1982SSf (51297) 270
In 90 % (v/v) DMSO/water mixture: K1=0.49 (I=0.25 M)

Li+ con non-aq 25°C 100% U M K1=4.70 1976FGb (51298) 271
K(LiA+L)=2.34

A=Tetra-n-butylammonium-2,4-dinitrophenolate. Medium: Tetrahydrofuran

C6H15O15P3 H6L Ins(1,2,6)P3 CAS 28841-62-5 (6479)
D-myo-Inositol 1,2,6-trisphosphoric acid;

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

Li+ gl R4N.X 25°C 0.10M U K1=2.38 1991BSa (51537) 272
B(LiHL)=11.24
B(LiH2L)=17.83
B(Li2L)=3.60

C6H16N2 L Tetrameen CAS 110-18-9 (124)
N,N,N',N'-Tetramethyl-1,2-diaminoethane; (CH3)2N.CH2.CH2.N(CH3)2

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

Li+ kin non-aq 0°C 100% U M 1993BCd (51648) 273

$$K(\text{Li}_2\text{A}_2\text{B}_2+2\text{L}=\text{Li}_2\text{B}_2\text{L}_2+2\text{A})=0.204$$

Metal:Li(0). Medium:Hexane. A:di(iso-propyl)amine. B:Tetrahydrofuran.

C6H16O3P2 L (2075)
Di(dimethylphosphinylmethyl) ether; Me2P(O)CH2.O.CH2.P(O)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-aq 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

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

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

Li+ ISE non-aq 25°C 100% M K1=3.32 B2=5.51 1988NHa (51981) 277
Medium: MeCN, 0.01 M Et4NClO4

Li+ con non-aq 25°C 100% U M Kout(LiL+A)=5.8 1982GJb (51982) 278
Medium: 1,2-dichloroethane. A=tetraphenylborate

Li+ ISE non-aq 25°C 100% U T H K1=3.31 1982NYa (51983) 279
Medium: MeCN

Li+ ISE non-aq 25°C 100% C K1=3.3 B2=5.5 1975NAa (51984) 280
Medium: CH3CN, 0.01 M Et4NClO4

C7H5NO HL CAS 767-00-0 (1632)
4-Cyanophenol; HO.C6H4.CN

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

Li+ con non-aq 25°C 100% U K1=8.04 1991AMa (52582) 281
Medium: THF

C7H6O4 H3L CAS 303-38-8 (1398)
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 from I=0.04 to I=0.81

C7H8O2 HL CAS 150-76-5 (6738)
 4-Methoxyphenol; CH3O.C6H4.OH

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

Li+ con non-aq 25°C 100% U K1=11.07 1991AMa (56095) 283
 Medium: THF. With 4-t-butylphenol K=10.87, 2-t-butylphenol K=10.13

C7H8O8P2 H4L (6892)
 1,2-((Phenylenedioxy)methylene)diphosphonic acid); C6H4O2C(P03H2)2

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

Li+ gl R4N.X 25°C 0.50M U K1=2.42 1985Gmb (56169) 284
 Medium: 0.5 M Me4NCl

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

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

Li+ sp non-aq 25°C 100% U TIH K1=5.34 1995KSa (58518) 285
 Medium: 10% w/w DMF/MeCN. DH(K1)=-5.0 kJ mol-1, DS=86 J K-1 mol-1
 Data also for 20 30, 40 w/w% DMF

 Li+ sp alc/w 25°C 95% U K1=2.44 1993GSa (58519) 286
 Medium: 95% w/w EtOH/H2O, 0.05 M Et4NClO4

 Li+ sp non-aq 20°C 100% U K1=2.45 1992PSa (58520) 287
 Medium: DMF, 0.01 M Me4NI

C8H5O2F3S HL TTA CAS 326-91-0 (165)
 4,4,4-Trifluoro-1-(2-thienyl)butane-1,3-dione; F3C.CO.CH2.CO.C4H3S

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

Li+ dis non-aq 25°C 100% C M K(LiL+phen)=6.74 2002IIa (58639) 288

Medium: chlorobenzene. For extraction from 0.10 M KCl:
 K(Li+HL(o)=LiL(o)+H)=-10.34; K(Li+HL(o)+phen(o)=LiL(phen)(o)+H)=-3.60.

 Li+ gl alc/w 25°C 0.10M U I K1=3.2 1965LIa (58640) 289
 Medium: MeOH, 0.1 M LiClO4. In EtOH: K1=5.3

C8H6O4 H2L Phthalic acid CAS 88-99-3 (113)

Benzene-1,2-dicarboxylic acid; C6H4(COOH)2

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

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.

C8H8O3 HL Phenoxyacetic CAS 122-59-8 (1153)
Phenoxyethanoic acid; C6H5.O.CH2.COOH

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

Li+ gl none 25°C 0.0 C TIH K1=0.07 1985CDb (60038) 292
Calculated from protonation data for I=0.04-0.9 M LiCl. Data for 10-45 C.
DH(K1)=7.7 kJ mol⁻¹, DS(K1)=28 J K⁻¹ mol⁻¹.

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

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

Li+ cal R4N.X 20°C 0.1M C DH1= -7.61 kJ/mol
1976ANb (60637) 293

in Me4NCl

Li+ 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)

Li+ ISE oth/un 20°C 0.0 U K1=5.40 1948SBa (60639) 295

C8H10O HL CAS 576-26-1 (1498)
2,6-Dimethylphenol; HO.C6H3(CH3)2

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

Li+ nmr non-aq 22°C 100% U T H 1991JRa (60826) 296
Medium: dioxolane. 90-22 C. DH(Li2L+2LiClO4=2Li2LC1O4)=0 kJ mol⁻¹, DS=58
In THF: DH=0, DS=28. In dioxalane DH(LiL2+2LiBPh4=2Li2LBPh4)=-5, DS=-5

C8H11O2F3 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

C8H12O2 HL Dimedone CAS 126-81-8 (1137)
5,5-Dimethyl-1,3-cyclohexanedione;

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

Li+ 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

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

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

Li+ 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-, ClO4-. DH(K1)=
-21.35 kJ mol-1, DS=-4.6. In PC, K1=2.84, DH(K1)=-17.05, DS(K1)=-2.8.

Li+ 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.

Li+ 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

Li+ 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
Medium: MeCN

Li+ vlt non-aq 25°C 100% U K1=2.93 1980MDa (62693) 309
Medium: propylene carbonate

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.

C8H17NO3 L CAS 41775-76-2 (6751)
10-Aza-1,4,7-trioxacyclododecane;

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

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 L CAS 294-92-8 (654)
1,7-Dioxo-4,10-diazacyclododecane;

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

Li+ vlt non-aq 25°C 100% C K1=5.3 2000HHa (62844) 313
Medium: acetonitrile, 0.1 M Et4NClO4. Method: dc polarography.

Li+ sol non-aq 20°C 100% C K1=4.03 1983SLa (62845) 314
Medium: CHCl3

C8H18O4 L Triglyme CAS 112-49-2 (2358)
1,2-Bis(methoxyethoxy)ethane; CH3O.C2H4O.CH2.CH2.O.C2H4.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)

Li+ con non-aq 25°C 100% U M 1982GJb (62989) 316
Kout(LiL+A)=7.0

Medium: 1,2-dichloroethane. A=picrate

C8H18O5 L Tetra-Et-Glycol CAS 112-60-7 (5664)
2,2'-(Oxybis(2,2-ethanedioxy))-bis-ethanol; O(CH2.CH2.O.CH2.CH2.OH)2

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

Li+ con non-aq 25°C 100% C K1=3.3 1992MSe (63004) 317
Medium: 100% MeOH. Anion: picrate. Also data for nitrophenolate anions.

C8H19NO5 L Bis-tris CAS 6976-37-0 (2827)
Bis-(2-hydroxyethyl)imino-tris(hydroxymethyl)methane;


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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Li+        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-)
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Li+        EMF non-aq 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
*****
C8H20O4P2  L              CAS 86536-56-3 (2076)
1,2-Bis(2-dimethylphosphinylmethoxy)ethane; Me2P(O)CH2.O.CH2.CH2.O.CH2.P(O)Me2
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Li+        con non-aq 25°C 100% U      K1=4.38      1989KSa (63311) 320
Medium: tetrahydrofuran/CHCl3 4:1 (vol)
*****
C9H5NOBr2  HL              CAS 521-74-4 (3279)
5,7-Dibromo-8-hydroxyquinoline;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Li+        sp  alc/w   ?  100% U      K1=5.54      1970PMc (63520) 321
*****
C9H7NO     HL      Oxine          CAS 148-24-3 (504)
8-Hydroxyquinoline (8-quinolinol);
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Li+        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).
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Li+        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
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Li+        sp  non-aq 25°C 100% U I      K1=2.82  B2=4.54  1992GSa (64304) 324
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;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
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Li+ gl R4N.X 20°C 0.10M U K1=4.86 1963IFb (66526) 325
Medium: Me4NNO3

C9H1102F5 HL CAS 2145-68-8 (1251)

1,1,1,2,2-Pentafluoro-6,6-dimethyl-3,5-heptanedione;

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) 326

C9H1602 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) 327

C9H2006Cl2P2 L CAS 19928-93-7 (2633)

Dichloromethylenedi(phosphonic acid diethyl ester); Cl2C(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=1.11 1981SKd (68123) 328

Medium: CH3CN

C9H2206P2 L CAS 1660-94-2 (2632)

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

C10H6N2O5 HL (9002)

2,4-Dinitronaphthol;

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

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.

C10H6O8 H4L Pyromellitic Ac CAS 89-05-4 (519)

Benzene-1,2,4,5-tetracarboxylic acid; C6H2.(COOH)4

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

Li+ gl R4N.X 25°C 1.0M C K1=1.70 1991DDb (68520) 331

B(LiHL)=6.85

B(LiH2L)=10.76

B(LiH3L)=13.00

B(Li2L)=2.50

Medium: 1.0 M Et4NI. B(Li2HL)=6.87.

Li+ gl R4N.X 25°C 0.25M C I K1=1.44 1990DDb (68521) 332

B(LiHL)=6.33

B(LiH2L)=10.04

B(LiH3L)=12.12

B(Li2HL)=6.15

Medium: 0.25 M Et4NI. Data for 0.08-0.99 M. B(Li2L)=1.97

C10H8N2 L 2,2'-Bipyridyl CAS 366-18-7 (25)

2,2'-Bipyridine; (C5H4N)2

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

Li+ nmr non-aq 27°C 100% U I K1=2.11 B2= 2.97 1996MAb (69596) 333

Method: 7Li nmr. Medium: acetonitrile, 0.05 M LiClO4. Data for acetone (K1<0.5) and nitromethane (K1=2.44, K2=2.29).

Li+ sp alc/w 25°C 95% U K1=1.61 1993GSa (69597) 334

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

Li+ sp non-aq 25°C 100% U I K1=1.87 1992GSa (69598) 335

Medium: MeCN. In acetone:K1=1.85; in MeOH:K1=0.45. By fluorimetry

C10H10O2 HL Benzoylacetone CAS 93-91-4 (197)

1-Phenylbutane-1,3-dione; C6H5.CO.CH2.CO.CH3

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

Li+ con non-aq 25°C 100% U K1=0.54 1988YSb (70745) 336

Medium: acetonitrile

Li+ gl alc/w 25°C 100% U I K1=3.1 1965LIa (70746) 337

Medium: MeOH, 0.1 M LiClO4. In EtOH: K1=3.2

C10H11NO5 H3L CAS 100844-86-8 (2108)

N-(2-Hydroxyphenyl)iminodiethanoic acid; HO.C6H4.N(CH2.COOH)2

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

Li+ gl KNO3 20°C 0.10M U K1=2.20 1963IFb (71042) 338

C10H11NO7S H3L (3335)

N-(2-Sulfophenyl)iminodiethanoic acid; H03S.C6H4.N(CH2.COOH)2

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

Li+ EMF KCl 20°C 0.10M C K1=2.26 1947SWa (71067) 339

 C10H1102F7 HL 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

 Li+ oth diox/w 25°C 75% U K1=4.75 B2=8.32 1979MMa (71111) 340

C10H12N2O4 H2L CAS 16598-05-3 (967)
 2-Pyridylmethyliminodiethanoic acid; C5H4N.CH2.N(CH2.COOH)2

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

 Li+ gl KNO3 20°C 0.10M U K1=1.71 1963IFc (71264) 341

C10H13N3O7 H3L (3912)
 1,3-Dimethyluramil-N,N-diethanoic acid;

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

 Li+ gl R4N.X 20°C 0.10M U K1=4.91 1963IFb (71806) 342
 Medium: Me4NNO3

C10H13N5O4 L Adenosine CAS 58-61-7 (2154)
 Adenosine, Adenine-9-beta-D-ribofuranoside;

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

 Li+ nmr non-aq 25°C 100% U M K(LiCl+L)=0.8 1976PSc (71945) 343
 Medium: DMSO

C10H14N5O7P H2L AMP-5 CAS 18422-05-4 (842)
 Adenosine-5'-monophosphoric acid, 5-Adenylic acid;

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

 Li+ gl R4N.X 25°C 0.10M C T K1=1.22 1991SMa (72459) 344
 IUPAC evaluation

C10H14O HL CAS 98-54-4 (458)
 4-(t-Butyl)-1-hydroxybenzene; C4H9.C6H4.OH

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

 Li+ con non-aq 25°C 100% U K1=10.87 1991AMa (72610) 345
 Medium: THF. With 2-t-butylphenol K=10.13

C10H15N5O10P2 H3L ADP CAS 20398-34-9 (2181)
 Adenosine-5'-diphosphoric acid;

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

Li+ gl R4N.X 25°C 0.10M C T K1=1.32 1991SMa (72988) 346
IUPAC evaluation

C10H16N2O8 H4L EDTA CAS 60-00-4 (120)
1,2-Diaminoethane-N,N,N',N'-tetraethanoic acid, Sequestric acid;

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

Li+ gl oth/un 25°C 0.10M C TIH K1=2.90 1985DRb (73927) 347
B(LiHL)=10.85
B(Li2L)=3.05
Data at 10-45 C and I=0.02-1.0 M in LiNO3. DH(K1)=2 kJ mol⁻¹; DS=60.
DH(LiHL)=-2; DS=198; DH(Li2L)=3; DS=65.

Li+ cal R4N.X 20°C 1.0M C K1=2.66 1976ANb (73928) 348
DH1= 3.26 kJ/mol
in Me4NCl; for 0.1 M Me4NClK1=2.97; DH1=0.84 kJ/mol;

Li+ sp R4N.X 25°C 0.50M U K1=2.43 1973CSa (73929) 349
Medium: (CH3)4NCl

Li+ vlt R4N.X 20°C 0.10M U K1=3.15 1972BZc (73930) 350
Medium: (CH3)4NOH

Li+ gl oth/un 25°C 0.32M U K1=2.85 B2=3.68 1965BCa (73931) 351
K(Li+HL)=0.86
Medium: CsCl

Li+ cal oth/un 25°C 0.05M U H 1954CHa (73932) 352
Medium: LiCl. DH(K1)=-0.42 kJ mol⁻¹, DS=54.3 J K⁻¹ mol⁻¹

Li+ EMF KCl 20°C 0.10M U T K1=2.79 1947SAa (73933) 353
Method: H electrode

C10H16N5O13P3 H4L ATP CAS 56-65-5 (403)
Adenosine-5'-triphosphoric acid;

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

Li+ gl R4N.X 25°C 0.10M C IH R K1=1.78 1991SMa (74755) 354
IUPAC evaluation. DH(K1)=-4 kJ mol⁻¹ (tentative)

Li+ gl oth/un 25°C 0.25M U H 1986RSa (74756) 355
K(Li+LiHL)=1.35
B(LiHL)=6.79

Li+ gl oth/un 25°C 0.32M U K1=1.7 B2=2.23 1965BCa (74757) 356

K(Li+HL)=0.8

Medium: CsCl

C10H17N04 H2L CAS 2848-06-8 (3916)

N-(Cyclohexyl)iminodiethanoic acid; C6H11.N(CH2.COOH)2

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

Li+ gl KNO3 20°C 0.10M U K1=1.74 1963IFb (74975) 357

C10H17N05 H2L CAS 6243-06-7 (3326)

N-(2-Hydroxycyclohexyl)iminodiethanoic acid; HO.C6H10.N(CH2.COOH)2

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

Li+ gl KNO3 20°C 0.10M U K1=2.19 1963IFb (74989) 358

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 H5L AQP CAS 1062-98-2 (3341)

Adenosine-5'-tetrphosphoric 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 H2L (5608)

1-Oxa-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

C10H20O5 L 15-Crown-5 CAS 33100-27-5 (576)

1,4,7,10,13-Pentaoxacyclopentadecane; cyclo(-(O.CH2.CH2)5-)

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

Li+ 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

Li+ vlt non-aq 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

Li+ 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

C10H21NO4 L CAS 66943-05-3 (5818)

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

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

Li+ vlt non-aq 25°C 100% C K1=5.2 2000HNa (76185) 376
Medium: acetonitrile, 0.1 M Et4NClO4. Method: dc polarography.

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

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

 Li+ vlt non-aq 25°C 100% C K1=5.4 2000HHa (76323) 377
 Medium: acetonitrile, 0.1 M Et4NC104. 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

 Li+ sp non-aq 20°C 100% U K1=2.3 1992PSa (76325) 379
 Medium: DMF, 0.01 M Me4NI

 C10H22O5 L Tetraglyme CAS 143-24-8 (121)
 2,5,8,11,14-Pentaoxapentadecane; (CH3.O.CH2.CH2.O.CH2.CH2.)20

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

 Li+ dis non-aq 25°C 100% C K1=4.69 1998KSc (76456) 380
 Medium: 1,2-dichloroethane.

 Li+ 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 Kout(LiL+A)=5.7 1982GJb (76458) 382
 Medium: 1,2-dichloroethane. A=tetraphenylborate

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

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

 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

 C11H18N2O8 H4L PDTA CAS 4408-81-5 (1655)
 1,2-Diaminopropane-N,N,N',N'-tetraethanoic acid;

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

 Li+ oth R4N.X 25°C 0.50M U K1=4.01 1971CSb (79306) 385
 Method: polarimetry. Medium: Me4NOH

 C11H20O2 HL Dipivaloylmeth. CAS 1118-71-4 (363)
 2,2,6,6-Tetramethyl-3,5-heptanedione; (CH3)3C.CO.CH2.CO.C(CH3)3

Metal 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

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

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

Li+ con none 25°C 0.0 C K1=1.05 2001KMb (79859) 387

Li+ 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

C12H5N7O12 L Dipicrylamine CAS 131-73-7 (1942)
Di(2,4,6-trinitrophenyl)amine; HN(C6H2(NO2)3)2

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

Li+ dis non-aq 25°C 100% C K1=3.9 1998KSc (80078) 390
Medium: 1,2-dichloroethane.

Li+ dis oth/un 25°C var U K1=1.7 1970SSb (80079) 391
Method: paper chromatography

C12H6O12 H6L Mellitic acid (7400)
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, B(Li2H3L)=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

Li+ 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.

Li+ 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

C12H20N2O8 H4L BDTA CAS 868-43-9 (1742)

DL-2,3-Diaminobutane-N,N,N',N'-tetraethanoic acid;
(HOOC.CH2)2N.CH(CH3).CH(CH3).N(CH2.COOH)2

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

Li+ oth R4N.X 25°C 0.50M U K1=5.26(D)
K1=2.60(meso)
K(Li+HL)=1.68
Method: polarimetry. Medium: Me4NCl

C12H20O4P2 L 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

Li+ con non-aq 25°C 100% U K1=4.31 1982YSa (82642) 401
Medium: tetrahydrofuran+CHCl3 4:1(vol); M is 2,4-dinitrophenolate

C12H22O2 HL 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

Li+ oth diox/w 25°C 75% U K1=6.85 B2=10.54 1979MMA (82859) 402

C12H23NO5 L (6793)
10-Methoxycarbonylethyl-1,4,7-trioxa-10-azacyclododecane;

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

Li+ cal alc/w 25°C 100% U H K1=2.71 1990KMb (82946) 403
Medium: MeOH. DH=-3.0 kJ mol⁻¹

C12H24N2O3 L Cryptand 1,1,1 CAS 37095-49-1 (6636)
4,10,15-Trioxa-1,7-diazabicyclo[5.5.5]heptadecane;

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

Li+ sp non-aq 20°C 100% U K1=1.7 1992PSa (83018) 404
Medium: DMF, 0.01 M Me4NI

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

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

Li+ gl oth/un 26°C 0.00 U K1=4.12 1976HYa (83113) 405
B(LiHL2)=9.06

C12H24O4 L CAS 26996-94-3 (2541)
Tetramethyl-12-crown-4

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

Li+ con non-aq 25°C 100% U K1=3.46 1980HNa (83124) 406
Medium: MeCN

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

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

Li+ nmr non-aq 27°C 100% C I K1=4.96 2001KZa (83454) 407
Method: 7Li nmr. Medium: nitromethane. In acetonitrile, K1=2.25

Li+ nmr non-aq 25°C 100% C I K1=1.92 2001KZb (83455) 408
Method: 7Li nmr. Medium: acetonitrile.
Data for 20-80% w/w nitrobenzene/acetonitrile.

Li+ dis non-aq 25°C 100% U K1=8.20 2000KSa (83456) 409
Medium: 1,2-dichloroethane

Li+ 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).

Li+	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 .									

Li+	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 kJ mol ⁻¹ , DS(K1)=-38.3 J K ⁻¹ 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.									

Li+	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			1993INa (83464)	417
							B(Li2P2L)=7.43		
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									

Li+	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

Li+	vlt	non-aq	25°C	100%	C		K1=3.2	2000HHa (83707)	421
Medium: acetonitrile, 0.1 M Et4NClO4. Method: dc polarography.									

C12H26N02P L (7849)									
N,N-Diethylcarbamoymethyl-(dipropylphosphineoxide);									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Li+	con	non-aq	25°C		C		K1=4.0	1999ESa (83720)	422
In tetrahydrofuran; alkali metal is used as 2,4-dinitrophenolate									

		L			Cryptand 2,2		CAS 23978-55-4	(925)	
C12H26N2O4 4,7,13,16-Tetraoxa-1,10-diazacyclooctadecane;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Li+	sp	alc/w	25°C	100%	C		K1=3.50	2002NFa (83860)	423
Medium: 100% MeOH. Method: electrospray ionization mass spectrometry.									
Li+	cal	non-aq	25°C	100%	M	H	K1=1.52	1994BCd (83861)	424
Medium: acetone. DH(K1) < 0 kJ mol ⁻¹									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Li+	sp	non-aq	20°C	100%	U		K1=1.2	1992PSa (83862)	425
Medium: DMF, 0.01 M Me4NI									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Li+	ISE	non-aq	25°C	100%	U	I	K1=6.98	1983CFa (83863)	426
Medium: MeNO2									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Li+	sol	non-aq	20°C	100%	C		K1=4.08	1983SLa (83864)	427
Medium: CHCl3									

		L			Pentaglyme		CAS 1191-87-3	(2498)	
C12H26O6 2,5,8,11,14,17-Hexaoxaoctadecane; (CH3.O.CH2.CH2.O.CH2.CH2.O.CH2.)2									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Li+	con	non-aq	25°C	100%	U		K1=3.2	1993EVa (84007)	428
Medium: THF+CHCl3 (4:1 vol). Also data for other solvents									

		L			THETAC		(7199)		
C12H27N3O3 1,4,7-Tris(hydroxyethyl)-1,4,7-triazacyclononane									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Li+	EMF	non-aq	25°C	100%	C		K1=3.13	1997WWa (84088)	429
Medium: MeOH, 0.05M Et4NClO4. Method: Ag/Ag+ electrode; by competition with Ag+.									

		H8L			DOTPH		CAS 91987-74-5	(229)	
C12H32N4O12P4 1,4,7,10-Tetraazacyclododecane-N,N',N'',N'''-tetramethylenephosphonic acid;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Li+	nmr	none	25°C	0	U	M		1996RSa (84414)	430
B(LiTmDOTP)=1.58 B(Li2TmDOTP)=3.03									

B(Li3TmDOTP)=4.31

B(LiTmDOTPH)=9.16

B(LiTmDOTPH2)=16.0, B(Li2TmDOTPH)=10.57, B(Li3TmDOTPH)=11.79

mixed-metal complexes in the Li(I)-Tm(III)-DOTP ternary system

C13H10O6 HL CAS 156426-82-3 (8800)

3-Acetoacetyl-7-methyl-2H,5H-pyrano(4,3-b)pyran-2,5-dione;

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

Li+ sp non-aq 20°C 100% C 1998FLb (85005) 431

K(Li+HL=LiL+H)=-3.01

Method: absorption and fluorescence spectroscopy. Medium: acetonitrile.

C13H18O4 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

Li+ 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

C13H26O5 L (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

Li+ con non-aq 25°C 100% C I K1=4.1 1992TFa (86478) 435

Medium: acetonitrile. In propylene carbonate, K1=3.13.

C13H26O6 L 19-Crown-6 CAS 55471-27-7 (8943)

1,4,7,10,13,16-Hexaoxacyclononadecane;

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

Li+ 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).

Li+ con oth/un 25°C dil C K1=0.79 1999TMa (86499) 437

Self medium (LiCl). For LiNO3, K1=0.72; for LiClO4, K1=0.77.

C14H8O2 L Anthraquinone CAS 84-65-1 (2781)

Anthraquinone;

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

Li+ vlt R4N.X 25°C 0.20M U K1=1.06 1975PTc (86623) 438

 C14H8O3 HL CAS 129-43-1 (2778)
 1-Hydroxyanthraquinone;

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

Li+ vlt R4N.X 25°C 0.20M U K1=2.94 B2=5.49 1975PTc (86629) 439

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

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

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.

 Li+ gl R4N.X 25°C 0.10M U K1=2.39 1985MHb (87957) 441
 K(LiL+H)=6.34
 K(Li+HL)=1.81
 K(LiHL+H)=4.44

Medium: 0.10 M Me4NCl.

 C14H20O5 L Benzo15-crown-5 CAS 14098-44-3 (608)
 2,3-Benzo-1,4,7,10,13-pentaoxacyclopentadeca-2-ene;

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

Li+ 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.

 Li+ 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.

 Li+ con non-aq 25°C 100% C K1=5.60 2000ICa (88297) 445
 Medium: nitromethane.

 Li+ 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 deuteriochloroform

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; HOOC.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

C14H24N2O10 EGTA CAS 67-42-5 (349)
Ethyleneglycol-0,0'-bis(2-aminoethyl ether)-N,N,N',N'-tetraethanoic acid; H4L

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

Li+ kin KCl 25°C 1.50M U K1=1.17 1968TFb (89891) 456

C14H26N2O7 H2L (1567)
1,4,10-Trioxa-7,13-diazacyclopentadecane-N,N'-diethanoic acid;

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

Li+ gl R4N.X 25°C 0.10M C K1=2.139 1987DDb (90195) 457

C14H26O5 L CAS 17454-48-7 (5039)

Li+ ISE alc/w 25°C 100% U K1=8.04 1978CSb (90400) 472
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 kJ mol⁻¹, DS(K1)=34 J K⁻¹ 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

C14H28N2O4 L Cryptand 2,2,0 CAS 95334-31-9 (6544)
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.

C14H30N2P L (2094)
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

C14H30N4P L (2096)
P-(N,N-Diethylamidocarbonyl)methyl-P,P-dibutoxyphosphine oxide;

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

Li+ con non-aq 25°C 100% U K1=2.89 1988YKa (90558) 478
Medium: tetrahydrofuran

C14H30N2O4 L 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

Li+ sol non-aq 20°C 100% C K1=4.09 1983SLa (90562) 479
Medium: CHCl3

C14H30N2O4 L CAS 31255-13-7 (2448)
N,N'-Dimethyl-cyclo-1,10-diaza-4,7,13,16-tetraoxaocetadecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Li+	gl	alc/w	25°C	95%	C		K1=<2	2004KVa (90581)	480
Medium: 95% MeOH/H2O, 0.01 M Et4NClO4. *****									
C14H30N2O5 L (6722) 7,13-Bis(2-hydroxyethyl)-1,4,10-trioxa-7,13-diazacyclopentadecane									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Li+	ISE	non-aq	25°C	100%	U I		K1=2.36	1993RPa (90630)	481
Medium: dimethylformamide, 0.05 M Et4NClO4. By competition with Ag+. In methanol, K=2.85. *****									
C14H30O7 L CAS 1072-40-8 (2499) 2,5,8,11,14,17,20-Heptaioxaheneicosane; CH3.O.(CH2.CH2.O)6.CH3									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Li+	dis	non-aq	25°C	100%	C		K1=6.75	1998KSc (90698)	482
Medium: 1,2-dichloroethane.									
Li+	con	non-aq	25°C	100%	U		K1=3.3	1993EVa (90699)	483
Medium: THF+CHCl3 (4:1 vol). Also data for other solvents *****									
C15H11N3 L CAS 1148-79-4 (488) 2,2':6'2''-Terpyridine; C5H4N.C5H3N.C5H4N									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Li+	nmr	non-aq	27°C	100%	U		K1=3.24	1996MAb (91159)	484
Method: 7Li nmr. Medium: nitromethane, 0.05 M LiClO4. *****									
C15H12O2 HL Diphenylacac CAS 120-46-7 (362) 1,3-Diphenylpropane-1,3-dione, Dibenzoylmethane; C6H5.CO.CH2.CO.C6H5									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Li+	gl	alc/w	25°C	100%	U		K1=4.1	1965LIa (91552)	485
Medium: MeOH, 0.1 M LiClO4									
Li+	gl	diox/w	30°C	75%	U		K1=5.95	1954FUa (91553)	486

C15H15O2P L CAS 76229-99-7 (2091) (Methylcarbonyl)methyldiphenylphosphine oxide; Ph2P(O)CH2C(O)Me									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Li+	con	non-aq	25°C	100%	U		K1=2.24	1988YSb (91913)	487
Medium: acetonitrile									

 C15H17O3P L CAS 40410-38-6 (5736)
 Methyl-(diphenoxymethyl)phosphine oxide; MePO(CH2.O.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)

 C15H18N2O8 H4L CAS 101455-18-9 (1902)
 1-Methyl-3,4-diaminobenzene-N,N,N',N'-tetraethanoic acid;

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

 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.

 C15H23NO3 L 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-,ClO4-. DH(K1)=
 -27.44 kJ mol-1, DS=-9.3. In PC, K1=4.59, DH(K1)=-24.70, DS(K1)=5.0.

 C15H24NO2P L (7846)
 N,N-Diethylcarbamoylmethyl-(P-phenyl-P-propylphosphineoxide);

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

 Li+ con non-aq 25°C C K1=4.0 1999ESa (92329) 491
 In tetrahydrofuran; alkali metal is used as 2,4-dinitrophenolate

 C15H30N2O3 L CAS 72640-82-5 (6040)
 4,7,13-Trioxa-1,10-diazabicyclo[8.5.5]eicosane;

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

 Li+ EMF non-aq 25°C 100% U IH K1=1.99 1993LRa (92517) 492
 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

 Li+ 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

Li+ kin non-aq 25°C 100% C K1=2.80 1987ABe (92520) 495
Medium: dimethylformamide.

C15H33N3O3 L CAS 220811-82-5 (7916)
1,4,7-Tris((S)-2-hydroxypropyl)-1,4,7-triazacyclononane;

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

Li+ 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-phenylethyl- derivative.

C15H36N09P3 L CAS 37909-50-5 (2634)
(N,N-Dimethylamine)methylenetris(phosphonic acid diethyl ester);
(CH3)2N.C(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=2.10 1981SKd (92604) 497
Medium: CH3CN

C16H18NO2P L 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

Li+ con non-aq 25°C 100% U K1=3.31 1988YKa (93768) 498
Medium: tetrahydrofuran

C16H20O3P2 L 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

Li+ con non-aq 25°C 100% U K1=3.92 1982Ysa (94099) 499
Medium: tetrahydrofuran+CHCl3 4:1(vol); M is 2,4-dinitrophenolate

C16H24O5 L (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

Li+ dis non-aq 25°C 100% U H K(Li(picrate)+L)=2.0 1979KLa (94344) 500
Medium: CHCl3

Li+ dis non-aq 24°C 100% C K(LiA+L)=2.0 1977MTc (94345) 501

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

 C16H24O5 L 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

 Li+ dis non-aq 25°C 100% U H 1979KLa (94354) 502
 K(Li(picrate)+L)=3.6

Medium: CHCl3

 C16H24O5 L 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

 Li+ dis non-aq 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.

 C16H24O6 L Benzo18-crown-6 CAS 14098-24-9 (513)
 2,3-Benzo-1,4,7,10,13,16-hexaoxacyclooctadeca-2-ene;

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

 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 deuteriochloroform

 C16H24O14 H4L CAS 61696-54-6 (6104)
 1,4,7,10,13,16-Hexaoxacyclooctadeca-2,3,11,12-tetracarboxylic acid;

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

 Li+ gl R4N.X 25°C 0.10M M K1=3.8 1991FGb (94496) 507
 B(LiHL)=8.5

Medium: 0.10 M Et4NNO3.

 C16H26NO2P L (2093)
 P-(N,N-Diethylamidocarbonyl)methyl(P-phenyl)(P-butyl)phosphine oxide;

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

 Li+ con non-aq 25°C C K1=3.9 1999ESa (94543) 508

In tetrahydrofuran; alkali metal is used as 2,4-dinitrophenolate

Li+ con non-aq 25°C 100% U K1=3.38 1988YKa (94544) 509
Medium: tetrahydrofuran

C16H28N4O8 H4L DOTA CAS 60239-18-1 (1017)
1,4,7,10-Tetraazacyclododecane-1,4,7,10-tetraethanoic acid;

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

Li+ gl R4N.X 25°C 0.10M C K1=4.32 1982DSa (94912) 510

C16H30O6 L CAS 17454-53-4 (5148)
Cyclohexyl-18-crown-6;

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

Li+ EMF oth/un 25°C dil A 1971FRa (95101) 511

K1<0.7

C16H32N2O4 L Cryptand 1,2,1H CAS 119017-36-6 (6587)
4,7,14,20-Tetraoxa-1,10-diazabicyclo[8.7.5]docosane;

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

Li+ 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

C16H32N2O5 L Cryptand 2,2,1 CAS 31364-42-8 (837)
1,10-Diaza-4,7,13,16,21-pentaoxabicyclo[8,8,5]tricosane (2,2,1);

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

Li+ con non-aq 25°C 100% M M K1=6.12 1999DSd (95229) 513

K(LiL+ClO4)=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.

Li+ gl R4N.X 25°C 0.05M C K1=3.4 1996BCh (95231) 515

Medium: 0.05 M Et4NClO4.

Li+ 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

Li+ cal alc/w 25°C 100% U H K1=4.69 1986BUd (95234) 518

In MeOH. DH=-10.3 kJ mol⁻¹

Li+ nmr non-aq 25°C 100% U K1=7.33 1986CHc (95235) 519
In CDCl₃ saturated with D₂O

Li+ 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

Li+ 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

Li+ ISE non-aq 25°C 100% U K1=9.6 1980CRa (95239) 523
Medium: Propylene carbonate

Li+ ISE alc/w 25°C 100% U K1=5.38 1978CSb (95240) 524
Medium: MeOH

Li+ 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

C16H32N4O4 L (6794)
4,10-Bis(N,N-dimethylethanamido)-1,7-dioxa-4,10-diazacyclododecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Li+ cal alc/w 25°C 100% U H K1=5.38 1990KMb (95320) 527
Medium: MeOH. DH=-12.7 kJ mol⁻¹

C16H32O7 L (6411)
15-(2,5-Dioxaheptyl)-15-methyl-1,4,7,10,13-pentaoxacyclohexadecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Li+ con non-aq 25°C 100% C I K1=4.45 1992TFa (95387) 528
Medium: acetonitrile. In propylene carbonate, K1=3.06.

C16H34N2O5 L (6953)
7,13-Bis(2-methoxyethyl)-1,4,10-trioxa-7,13-diazacyclopentadecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Li+ 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, H2O: K<2 and pyridine: K=5.08. Method: by competition with Ag+.

C16H34N2O6 L CAS 69930-74-1 (1321)
N,N'-Bis(2-hydroxyethyl)-1,7,10,16-tetraoxa-4,13-diazacyclooctadecane;

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

Li+ ISE non-aq 25°C 100% U K1=2.29 1993RPa (95451) 530
Medium: dimethylformamide, 0.05 M Et4NClO4. By competition with Ag+.

C16H34N4O2 L CAS 60598-04-1 (1530)
4,7-Dimethyl-1,4,7,10-tetraaza-13,18-dioxabicyclo[8,5,5]eicosane;

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

Li+ gl R4N.X 25°C 0.10M U K1=3.8 1978LMa (95471) 531
In CH3OH, K1>4.0. In 95 vol% CH3OH, K1>3.8.

C16H34O8 L 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

Li+ 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 L 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

C16H36N4O4 L (6703)
1,4,7,10-Tetrakis(2-hydroxyethyl)-1,4,7,10-tetraazacyclododecane;

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

Li+ EMF non-aq 25°C 100% U I K1=8.07 1996WPa (95574) 534
Medium: acetonitrile, 0.05 M NEt4ClO4. In propylene carbonate K1=8.90

Li+ gl alc/w 25°C 100% C I K1=3.09 1993TCa (95575) 535
Medium: MeOH, 0.05 M Et4NClO4. In DMF, K1=2.99

C17H13N5O5 HL CAS 90163-26-1 (5212)
1-(4'-(5'-Hydroxy-3'-methyl-1'-phenyl)pyrazolylazo)4-nitrobenzoic acid;

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

Li+ sp mixed ? 77% U K1=4.24 1968DZa (95776) 536
Medium: 77% acetone

C17H20N4O6 HL Riboflavin CAS 83-88-5 (1438)
7,8-Dimethyl-10(D-1'-ribityl)isoalloxazine, Vitamin B2, Vitamin H

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

Li+ 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

C17H21O5P L (5732)
Methyldi(2-methoxyphenoxy)methylphosphine oxide; Me.PO(CH2.O.C6H4.OMe)2

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

Li+ con non-aq 25°C 100% U K1=2.65 1989TKb (96392) 538

Medium: tetrahydrofuran/CHCl3 4:1 (volume)

C17H24N2O10 HL CAS 217972-81-1 (8163)
9-(2-Hydroxy-3,5-dinitrophenoxy)methyl-1,4,8,11-tetraoxacyclotetradecane;

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

Li+ 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.

C17H24N4O11 L CAS 94616-60-1 (1039)
2,4,6-Trinitrophenylaminomethyl-15-crown-5

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

Li+ sp mixed 25°C 16% U K1=2.28 1984BPa (96464) 540

K(Li+HL)=1.09

C17H26O5 L CAS 92818-18-3 (8987)
12-[(Phenylmethoxy)methyl]-1,4,7,10-tetraoxacyclotridecane;

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

Li+ 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 CDCl3. HA is picric acid.
For extraction into 1,2-dichloroethane, K=1.84. In H2O, K(LiA+L)=3.80.

C17H26O5 L 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
-----
Li+        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 CDCl3. HA is picric acid.
For extraction into 1,2-dichloroethane, K=2.94. In H2O, K(LiA+L)=4.43.
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C17H26O6      L                                CAS 99159-90-7 (688)
2,3-Benzo-1,4,7,10,13,16-hexaoxacyclononadeca-2-ene;
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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 deuteriochloroform
*****
C17H27NO5      L                                CAS 98269-22-8 (8844)
13-(2-Methoxyphenyl)-1,4,7,10-tetraoxa-13-azacyclopentadecane;
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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.
*****
C17H34N2O4      L                                CAS 142565-14-8 (6562)
4,7,13,16-Tetraoxa-1,10-diazabicyclo[8.8.5]tricosane;
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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 Et4NC1O4.
-----
Li+        gl  R4N.X  25°C 0.05M C I      K1=2.08      1992CGb (96746) 546
Medium: Et4NC1O4. In MeOH: K1=2.30;in DMF K1=2.21; in MeCN: K1=6.07
*****
C17H34N4O4S      L                                CAS 503465-04-1 (9247)
4,7,13,16-Tetraoxa-1,10,21,23-tetraazabicyclo[8.8.7]pentacosane-22-thione;
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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 Et4NC1O4.
*****
C17H36N4      L                                (6788)
12,17-Dimethyl-1,9,12,17-tetraazabicyclo[7.5.5]nonadecane;
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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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 C17H37N5 L CAS 122874-65-1 (5903)
 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 1996BFc (96790) 549
 Medium: 80% v/v DMSO/H2O, 0.15 M NaCl.

 Li+ 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

C17H38O2P2 L CAS 21245-67-8 (2100)
 Methylenebis(dibutylphosphine oxide); Bu2P(O)CH2P(O)Bu2

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

 Li+ con non-aq 25°C C K1=5.0 1999ESa (96813) 551
 In tetrahydrofuran; alkali metal is used as 2,4-dinitrophenolate

 Li+ con non-aq 25°C 100% U K1=3.92 1988YKa (96814) 552
 Medium: tetrahydrofuran

C18H15OP L CAS 791-28-6 (32)
 Triphenylphosphine oxide; (C6H5)3PO

 Metal 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(LiI+ClO4)=-0.265

Medium: propylene carbonate.

 Li+ con non-aq 25°C 100% U K1=1.95 1988YSb (97096) 554
 Medium: acetonitrile

 Li+ con non-aq 25°C 100% U Kout(LiI+A)=3.9 1982GJb (97097) 555
 Medium: 1,2-dichloroethane. A=tetraphenylborate

 Li+ con non-aq 25°C 100% U K(LiI+L)=2.6 1969SSi (97098) 556

Medium: CH3CN

C18H20O5 L 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

 Li+ sp non-aq 25°C 100% C K1=3.003 2002YEa (97478) 557

Method: fluorescence spectroscopy. Medium: acetonitrile.

C18H22N02P L (2092)
(N,N-Diethylamidocarbonyl)methyldiphenylphosphine oxide;

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

Li+ con non-aq 25°C C K1=4.1 1999ESa (97507) 558
In tetrahydrofuran; alkali metal is used as 2,4-dinitrophenolate

Li+ con non-aq 25°C 100% U K1=3.69 1988YKa (97508) 559
Medium: tetrahydrofuran

C18H22O5 L (5737)
1,7-Di(2-methoxyphenyl)-1,4,7-trioxaheptane; MeO.C6H4.O.C2H4.O.C2H4.O.C6H4.OMe

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

Li+ con non-aq 25°C 100% U K1=1.65 1989TKb (97566) 560
Medium: tetrahydrofuran/CHCl3 4:1 (volume)

C18H27N2O3F L CAS 173417-90-8 (6571)
23-Fluoro-4,7,20-trioxa-1,10-diazatricyclo[8.7.5.1,12,16]tricoso-12,14,16(23)triene
;

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

Li+ 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.

C18H28N2O3 L CAS 154148-31-9 (6510)
4,7,20-Trioxa-1,10-diazatricyclo[8.7.5.1,12,16]tricoso-12,14,16(23)-triene;

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

Li+ 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.

C18H28O5 L CAS 92818-19-4 (8988)
2-[(Phenylmethoxy)methyl]-1,4,8,11-tetraoxacyclotetradecane;

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

Li+ 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 CDCl3. HA is picric acid.
For extraction into 1,2-dichloroethane, K=3.29. In H2O, K(LiA+L)=4.91.

C18H2805 L CAS 92818-28-05 (8989)
6-[(Phenylmethoxy)methyl]-1,4,8,11-tetraoxacyclotetradecane;

Metal 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 CDCl3. HA is picric acid.
For extraction into 1,2-dichloroethane, K=2.69. In H2O, K(LiA+L)=5.15.

C18H2806 L Benzo20-crown-6 (6354)
2,3-Benzo-1,5,8,11,14,18-Hexaoxacos-2-ene;

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

Li+ sp non-aq 22°C 100% U K1=5.48 1987CCc (97836) 565
In deuteriochloroform

C18H2806 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

C18H2806 L 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

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

C18H2807 L Benzo21-crown-7 (6355)
2,3-Benzo-1,4,7,10,13,16,19-Heptaoxaheneicos-2-ene;

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

Li+ sp non-aq 22°C 100% U K1=5.60 1987CCc (97857) 568
In deuteriochloroform

C18H32N2O8 L CAS 24951-52-8 (2560)
Cryptand-2,2,2-dilactam

Metal 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

C18H36N2O6 L Cryptand 3,2,1 (7303)
1,10-Diaza-4,7,13,16,19,24-hexaoxabicyclo[8,11,5]hexacosane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Li+	cal	alc/w	25°C	95%	U	H		K1=3.14	1997ZiA (98421)	570
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Medium: 95% v/v MeOH/H2O, 0.1 M. DH(K1)=-11.7 kJ mol⁻¹, DS=20.8 J K⁻¹ mol⁻¹

C18H36N2O6 L Cryptand 2,2,2 CAS 23978-09-8 (514)
1,10-Diaza-4,7,13,16,21,24-hexaoxabicyclo[8.8.8]hexacosane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Li+	con	non-aq	25°C	100%	M	M		K1=6.21 K(LiI+ClO4)=0.72	1999DSd (98629)	571
-----	-----	--------	------	------	---	---	--	-----------------------------	-----------------	-----

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 Et4NClO4. 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
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Medium: DMF, 0.01 M Me4NI

Li+	cal	alc/w	25°C	100%	U	H		K1=2.46	1986BUd (98634)	576
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In MeOH. DH=-3.7 kJ mol⁻¹

Li+	cal	non-aq	25°C	100%	U	H			1986DGa (98635)	577
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DH1 = -59.1 kJ mol⁻¹. Medium: nitromethane

Li+	cal	non-aq	25°C	100%	U	H			1985DGa (98636)	578
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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

Li+	gl	alc/w	25°C	95%	C			K1=1	1981ANa (98639)	581
-----	----	-------	------	-----	---	--	--	------	-----------------	-----

Medium: 95% MeOH, 0.1 M Me4NCl

Li+ ISE non-aq 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
Me4NClO4. Also K1=2 (H2O), <2.0 (DMSO), 6.7 (CH3CN).

Li+ 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 L (6795)
4,10-Bis(N,N-dimethylpropanamido)-1,7-dioxa-4,10-diazacyclododecane;

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

Li+ cal alc/w 25°C 100% U H K1=2.99 1990KMb (98782) 588
Medium: MeOH. DH=-23.8 kJ mol-1

C18H36N6O3 L (6790)
1,4,7-Tris(N,N-dimethylethanamido)-1,4,7-triazacyclononane;

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

Li+ gl R4N.X 25°C 0.10M M K1=3.91 1990KMb (98799) 589
Medium: 0.10 M Me4NNO3

C18H38N2O6 L 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

Li+ sol non-aq 20°C 100% C K1=3.98 1983SLa (98822) 590
Medium: CHCl3

C18H38N2O6 L CAS 72911-99-0 (649)
4,13-Bis(2-methoxyethyl)-1,7,10,16-tetraoxo-4,13-diazacyclooctadecane;

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

Li+ sol non-aq 20°C 100% C K1=3.89 1983SLa (98840) 591
Medium: CHCl3

C18H3809 L Glyme-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

Li+ dis non-aq 25°C 100% C K1=7.53 1998KSc (98875) 592
Medium: 1,2-dichloroethane.

C19H2306P L (5731)
1,2:8,9-Dibenzo-5-methylphosphinyl-3,7,10,13,16-pentaoxacyclohexadeca-1,8-diene;

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

Li+ con non-aq 25°C 100% U K1=3.26 1989TKb (99346) 593
Medium: tetrahydrofuran/CHCl3 4:1 (volume)

C19H24N02P L (2095)
P-(N,N-Diethylamidocarbonyl)methyl,P,P-diphenylphosphine oxide;

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

Li+ con non-aq 25°C 100% U K1=4.12 1988YKa (99348) 594
Medium: tetrahydrofuran

C19H3005 L CAS 92818-26-3 (8991)
10-[(Phenylmethoxy)methyl]-1,4,8,12-tetraoxacyclopentadecane;

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

Li+ 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.

C19H3005 L 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

Li+ 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 CDCl3. HA is picric acid.
For extraction into 1,2-dichloroethane, K=1.36. In H2O, K(LiA+L)=3.65.

C19H39N305 L CAS 60598-00-7 (1537)
4-Methyl-1,4,10-triaza-7,13,16,21,24-pentaoxa-bicyclo[8,8,8]hexacosane;

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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Li+        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;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Li+        con non-aq 25°C 100% C          K1=5.47       2000ICa (99928) 598
Medium: nitromethane.
*****
C20H22O6          L          (6834)
1,8-Bis(2-Formyphenoxy)-3,6-dioxaoctane; (CH2.O.CH2.CH2.O.C6H4.CH0)2
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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        L          CAS 165815-06-5 (8936)
N-(2-Pyridylmethylene)-4-aminobenzo-15-crown-5;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Li+        sp  non-aq 25°C 100% C  I  M          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.
*****
C20H24O6          L  DiBz-18-Crown-6 CAS 14187-32-7 (604)
2,3:11,12-Dibenzo-1,4,7,10,13,16-hexaoxacyclooctadeca-2,11-diene
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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.
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Li+        con non-aq 25°C 100% C          K1=4.79       2000ICa (100161) 602
Medium: nitromethane.
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Li+        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.
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Li+        nmr non-aq 27°C 1.0M C  I          K1=0.86       1996KAb (100163) 604
Method: 7Li nmr. Medium: acetonitrile. Also data for nitromethane and
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20-80% w/w acetonitrile/nitromethane.

Li+ vlt non-aq 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-aq 25°C 100% U K1=3.48 1985YKa (100166) 607
Medium: EtOH+CHCl3 1:1; M is used in nitrophenolate form

Li+ con non-aq 25°C 100% U M 1982GJb (100167) 608
Kout(LiL+A)=3.2
Medium: 1,2-dichloroethane. A=tetraphenylborate

C20H26O6 L 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

Li+ dis non-aq 25°C 100% U H 1979KLa (100347) 609
K(M(picrate)+L)=4.35
Medium: CHCl3

C20H32O7 L AN(MOEEO)2E (2248)
24-Methoxy-22-methyl-3,6,9,12,15,18-hexaoxabicyclo[18.3.1]-tetracos-1(24),20,22-triene;

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

Li+ dis non-aq 25°C 100% U H 1979KLa (100492) 610
K(Li(picrate)+L)=3.5
Medium: CHCl3

C20H32O8 L Benzo24-crown-8 (6356)
2,3-Benzo-1,4,7,10,13,16,19,22-Octaoxatetracos-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 deuteriochloroform

C20H34N4O HL (7763)
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.

C20H36O6 L DiCy-18-crown-6 CAS 16069-36-6 (1653)
2,3:11,12-Dicyclohexyl-1,4,7,10,13,16-hexaoxacyclooctadecane;

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

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.

Li+ dis non-aq 25°C 100% U H K(Li(picrate)+L)=2.28 1979KLa (100667) 617
Medium: CHCl3

Li+ ISE oth/un 25°C dil A K1=0.6 1971FRa (100668) 618
Data for isomer A

C20H40N2O4 L (6625)
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

C20H40N2O7 L Cryptand 3,2,2 CAS 31255-22-8 (1763)
Cryptand 3,2,2

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

Li+ gl R4N.X 25°C 0.05M C I K1=<2.0 1975LSc (100815) 620
In 95% MeOH: K1 < 2; 100%: 2.3

C20H42N4O4 L CAS 39678-14-3 (1543)
4,7-Dimethyl-1,4,7,10-tetraaza-13,16,21,24-tetraoxa-bicyclohexacosane;

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

Li+ gl R4N.X 25°C 0.10M U I K1=2.4 1978LMa (100889) 621
In CH3OH, K1>4.0, in 95 vol% CH3OH, K1=3.8.

 C20H42O5 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.O)n.(CH2)11.CH3, n=6 and 8.

 C20H44N4O4 L CAS 102202-74-4 (6041)
 1,4,7,10-Tetra-(2-hydroxypropyl)-1,4,7,10-tetraazacyclododecane;

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

 Li+ 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).

 C20H44N4O4 L (6730)
 1,4,7,10-Tetra-(2-methoxyethyl)-1,4,7,10-tetrazacyclododecane;

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

 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.

 C21H19OP L CAS 29942-64-1 (2087)
 C-Methylcarbonylmethylenetriphenylphosphorane; Ph3P:CHC(O)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

 C21H24O8 L CAS 78708-41-5 (799)
 2,3:9,10-Dibenzo-1,4,8,11,14-pentaoxacyclohexadeca-2,9-diene-6-oxyethanoic acid;

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

 Li+ gl alc/w 25°C 80% M H K1=3.27 1985AEb (101267) 627
 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.

 C21H27O8P L CAS 71817-08-8 (6905)
 1,2:10,11-Dibenzo-16-methylphosphonyl)-3,6,9,12,15,17,20-heptaoxacycloeicosane;

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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
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Li+        nmr non-aq 20°C 100% U          K1=2.3          1982BGe (101300) 628
Medium: Acetone-D6; Method - 1H NMR
*****
C21H30N7O17P3      H4L      NADPH          CAS 2646-71-1 (7185)
Nicotinamide adenine dinucleotide phosphate reduced;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
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Li+        nmr none    RT      0 U          K1eff=1.70
                                     Keff(2Li+L)=0.58
Medium: D2O, pH 8.5-9.5. Coordination site is the adenine or nicotinamide
phosphate
*****
C21H30O2P2          L          (7851)
P'P'-Diphenyl-P,P-dibutylmethylenediphosphinedioxide;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Li+        con non-aq 25°C          C          K1=5.1          1999ESa (101385) 630
In tetrahydrofuran; alkali metal is used as 2,4-dinitrophenolate
*****
C21H31O7P3          L          CAS 82154-48-1 (2916)
Methyl di((2-dimethylphosphinylmethoxy)phenoxy)methyl)phosphineoxide;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Li+        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(O)[CH2OC6H4OCH2P(O)(CH3)2]2
*****
C21H42N4O6S          L          CAS 503465-05-2 (9248)
4,12,18,21,26,29-Hexaoxa-1,7,9,15-tetraazabicyclo[13.8.8]hentriacontane-8-thione;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
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Li+        gl alc/w 25°C 95% C          K1=1.30          2004KVa (101464) 632
Medium: 95% MeOH/H2O, 0.01 M Et4NClO4.
*****
C21H42N6O3          L          (6791)
1,5,9-Tris(N,N-dimethylethanamido)-1,5,9-triazacyclododecane;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Li+        gl R4N.X 25°C 0.10M M          K1=4.21          1990KMb (101475) 633
Medium: 0.10 M Me4NNO3
*****

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C22H20N2O4 L CAS 207461-96-9 (8955)
(5Z)-12,13,20,21-Tetrahydrotribenzo[b,f,l][1,8,11,14,4,5]tetraoxadiazacyclohexadecine;

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 L CAS 97745-35-2 (2069)
Adamantyl(diphenoxy)phosphonyl

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

Li+ sol non-aq 25°C 100% U K1=3.01 1987TCa (101924) 635
Medium: CH2Cl2, 2% MeCN. Metal as picrate

C22H26O5 L CAS 160978-39-2 (8944)
o,o'-(Tetraethyleneglycoldiyl)-(Z)-stilbene;

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

Li+ con non-aq 25°C 100% C K1=6.0 2000ICa (101998) 636
Medium: nitromethane.

C22H28N2O6 L CAS 449740-17-4 (8937)
N-(2-Pyridylmethylene)-4-aminobenzo-18-crown-6;

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

Li+ sp non-aq 25°C 100% C M K(ZnA2L+Li)=1.86 2002YPc (102017) 637
Medium: MeCN, 0.10 M n-Bu4NPF6. A is p-thiocresol.

C22H28O7 L Dibenzo-21-Cr-7 CAS 14098-41-0 (2876)
2,3:11,12-Dibenzo-1,4,7,10,13,16,19-heptaoxacycloheptacosane-2,11-diene;

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

Li+ con non-aq 25°C 100% U K1=4.3 1993EVa (102050) 638
Medium: THF+CHCl3 (4:1 vol)

C22H30N2O2P L 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

Li+ con non-aq 25°C 100% U K1=3.58 1988YKa (102099) 639
Medium: tetrahydrofuran

C22H3207P2 L (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)

C22H36N206 L Bz-Cryptand 222 CAS 31250-18-7 (2269)
5,6-Benzo-4,7,13,16,21,24-hexaoxa-1,10-diazabicyclo[8:8:8]hexacosane-5-ene;

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

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

C22H36O9 L Benzo-27-Crown9 CAS 63144-76-3 (2842)
2,3-Benzo-1,4,7,10,13,16,19,22,25-nonanoxacycloheptacosane-2-ene;

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

Li+ sp non-aq 22°C 100% U K1=5.47 1987CCc (102300) 643
In deuteriochloroform

C22H40O6 L CAS 76993-47-0 (2340)
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 K(Li(picrate)+L)=5.5 1981BEb (102371) 644

Medium: CDCl3

C22H44N208 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

C22H44N6O5S2 L CAS 503465-08-5 (9241)
9,20,23,28,31-Pentaoxa-1,4,6,12,14,17-hexaazabicyclo[15.8.8]tritiacontane-5,13-dithione;

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

Li+ gl alc/w 25°C 95% C K1=<2 2004KVa (102439) 646

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

C22H46N2O8 L CAS 85726-96-1 (647)
4,10-Dimethyloxyethoxyethylidene-1,7-dioxo-4,10-diazacyclododecane;

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

Li+ sol non-aq 20°C 100% C K1=4.19 1983SLa (102455) 647
Medium: CHCl3

C22H46N2O8 L 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

Li+ sol non-aq 20°C 100% C K1=3.88 1983SLa (102458) 648
Medium: CHCl3

C22H48N6O2 L CAS 39678-22-3 (1542)
4,7,13,16-Tetramethyl-1,4,7,10,13,16-hexaaza-21,24-dioxabicyclohexacosane;

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

Li+ gl alc/w 25°C 95% U K1=3.5 1978LMa (102488) 649

C23H21O2P L CAS 1474-32-4 (2089)
C,C-Di(methylcarbonyl)methylenetriphenylphosphorane; Ph3P:C(C(O)Me)2

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

Li+ con non-aq 25°C 100% U K1=2.13 1988YSb (102643) 650
Medium: acetonitrile

C23H22N4O4 HL 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 2001INa (102645) 651
Medium: 50% v/v dioxane/H2O, 3% v/v triethylamine; pH 12. In 50%
v/v dioxane/H2O with Et4NOH, K1=2.94.

C23H30N2O4 L CAS 361454-16-2 (8960)
N-(Phenylmethylene)-4-(1,4,7,10-tetraoxa-13-azacyclopentadec-13-yl)benzamine;

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

Li+ sp non-aq RT 100% C K1=2.77 2001AVa (102751) 652
Method: spectrophotometric titration. Medium: acetonitrile.

 C23H30N4O7 L CAS 356535-57-4 (8845)
 13-[2-Methoxy-4-[(4-nitrophenyl)azo]phenyl]-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			K1=ca.0.5	2002GNe (102768)	653

Medium: 50% v/v MeOH/H2O, pH 7.4 (0.1M Tris buffer), 0.1 M Me4NCl.

C24H24N2O4 L (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)

C24H25O7P L (2067)
 Phenylphosphonyldibenzo-17-crown-6

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Li+	sol	non-aq	25°C	100%	U			K1=2.38	1987TCa (102965)	655

Medium: CH2Cl2, 2% MeCN

C24H32O6 L ANAN(MOE0)2E (2242)
 2,3:4,5-Di(1,3-(2-methoxy-5-methylbenzo))-9,12,15,18-tetraoxacyclooctadeca-2,4-diene;

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

C24H32O6 L AN(MOE0M)2AN (2244)
 23,24-Dimethoxy-10,21-dimethyl-3,6,14,17-tetraoxatricyclo-tetracos-1(23),8(24),9,11,19,21hexaene

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Li+	dis	non-aq	25°C	100%	U	H			1979KLa (103077)	657

K(Li(picrate)+L)=2.95
 Medium: CHCl3

C24H32O6 L DP(OE0E0)2E CAS 60985-77-5 (2237)
 3,4:5,6-Bis(2-methylbenzo)-2,7,10,13,16,19-hexaoxacyclodocosa-3,5-diene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Li+ dis non-aq 25°C 100% U H 1979KLa (103083) 658
K(Li(picrate)+L)=4.34

Medium: CHCl3

C24H32O8 L DiBz-24-Crown-8 CAS 14174-09-5 (580)
2,3:14,15-Dibenzo-1,4,7,10,13,16,19,22-octaoxacyclotetracos-2,14-diene;

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

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

Li+ 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)

Li+ vlt non-aq 25°C 100% U K1=13.2 1990SPa (103145) 662
Medium: 1,2-dichloroethane

C24H34N2O5 L CAS 182926-58-5 (8848)
7,13-Bis(2-methoxyphenyl)-1,4,10-trioxa-7,13-diazacyclpentadecane;

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

Li+ 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.

C24H35NO9 L CAS 330462-64-1 (8032)
6,7-Dimethoxy-4-(1,4,7,10,13-pentaoxa-16-azacyclooctadec-16-ylmethyl)-2H-1-benzopyr
an-2-one;

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

Li+ sp mixed 25°C 10% C K1=3.35 2001LWa (103243) 664
Method: fluorimetry. Medium: 10%v/v acetonitrile/H2O.

C24H36N2O4Fe L CAS 145519-34-2 (6831)
1,1'-(1,4,10,13-Tetraoxa-7,16-diazacyclooctadeca-7,16-diyl)dimethylferrocene;

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

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

C24H36O10P2 L (5726)
1,4-Bis(2-(diethoxyphosphinylmethoxy)phenyl)-1,4-dioxabutane;
2(EtO)2PO.CH2O.C6H4.O.CH2)2

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

Li+ con non-aq 25°C 100% U K1=3.7 1989EVa (103296) 666
Medium: tetrahydrofuran/CHCl3 4:1 (volume)

C24H42O10 L (2505)
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

Li+ sp non-aq 22°C 100% U K1=5.46 1987CCc (103397) 667
In deuteriochloroform

C24H44O5 L (2341)
16,18,23,25-Tetramethyl-2,5,8,11,14-pentaoxatricyclo(22.4.0.0(15,20))pentacosane;

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

Li+ nmr non-aq 24°C 100% U M K(Li(picrate)+L)=4.0 1981BEb (103410) 668
Medium: CDCl3

C24H48N2O9 L Cryptand 3,3,3 CAS 132162-61-9 (1761)
Cryptand 3,3,3

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

Li+ gl R4N.X 25°C 0.05M C K1=<2 1975LSc (103465) 669

C24H48N6O6S2 L CAS 503465-10-9 (9242)
9,12,23,26,31,34-Hexaoxa-1,4,6,15,17,20-hexaazabicyclo[18.8.8]hexatricontane-5,16-dithione;

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

Li+ gl alc/w 25°C 95% C K1=<2 2004KVa (103506) 670
Medium: 95% MeOH/H2O, 0.01 M Et4NClO4.

C24H48N8O4 L (6789)
1,4,7,10-Tetrakis(N,N-dimethylethanamido)-1,4,7,10-tetraazacyclododecane;

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

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
Li+	sol	non-aq	20°C	100%	C		K1=4.05	1983SLa (103529)	672

Medium: CHCl3

C25H22O2P2 L CAS 207-21-8 (2099)
Methylenebis(diphenylphosphine oxide); Ph2P(O)CH2P(O)Ph2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Li+	con	non-aq	25°C		C		K1=5.6	1999ESa (103631)	673

In tetrahydrofuran; alkali metal is used as 2,4-dinitrophenolate

Li+	con	non-aq	25°C	100%	U		K1=4.73	1988YKa (103632)	674
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Medium: tetrahydrofuran

Li+	con	non-aq	25°C	100%	U		K1=4.9	1984YKa (103633)	675
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Medium: tetrahydrofuran + CHCl3 4:1, Li as 2,4-dinitrophenolate

Li+	oth	non-aq	22°C	100%	U		K1=2.5	1978YSa (103634)	676
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Medium: 1:1 v/v CH3CN:CHCl3 1:1 v/v. Li as LiCl; for LiI K1=2.3

Li+	con	non-aq	25°C	100%	U		K(LiI+L)=3.3	1969SSi (103635)	677
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Medium: CH3CN

C25H26N4O5 HL 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	Reference	ExptNo
Li+	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.

C25H28N04S+ L CAS 423763-92-2 (8996)
3-Ethyl-2-[4-(2,3,5,6,8,9-hexahydro-1,4,7,10-benzotetraoxacyclododecin-12-yl)buta-1
,3-dienyl]benz

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.

C25H29N07 L FQC CAS 215095-38-8 (8804)
4'-(Dimethylamino)-2,7-(3,6,9-trioxaundecane-1,11-dioxy)flavone;

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

Li+ sp non-aq ns 100% C K1=1.51 2000LXa (103680) 680
Medium: acetonitrile. By fluorescence, K1=1.68.

C25H37N2O7P L CAS 202407-79-2 (8035)
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 K(LiP+L)=3.48 1998DDc (103758) 681

Medium: CHCl3. P is picrate.

C25H50N2O4 L (2317)
N,N'-Diheptyl-N,N',5,5'-tetramethyl-3,7-dioxanonanediamide;

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

Li+ nmr non-aq 25°C 100% U I M K(Li(ClO4)+L)=6.0 19800Ea (103827) 682
K(Li(ClO4)L+L)=2.3

Medium CH2Cl2. In CH3CN: K(Li(ClO4)+L)=3.0, K(Li(ClO4)L+L)=1.0. In pyridine:
K(Li(ClO4)+L)=0.04. In MeCN: K(Li(ClO4)L+L)=1.23

C25H50N4O8S L CAS 503465-06-3 (9249)
4,7,15,18,24,27,32,35-Octaoxa-1,10,12,21-tetraazabicyclo[19.8.8]heptatriacontane-11
-thione;

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

Li+ gl alc/w 25°C 95% C K1=2.84 2004KVa (103845) 683
Medium: 95% MeOH/H2O, 0.01 M Et4NClO4.

C26H20 L CAS 2039-68-1 (1741)
Tetraphenylethylene; (C6H5)2C:C(C6H5)2

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

Li+ 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)

C26H21OP L CAS 33078-07-8 (2088)
C-Phenylcarbonylmethylenetriphenylphosphorane; Ph3P:CHC(O)Ph

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

Li+ con non-aq 25°C 100% U K1=2.42 1988YSb (103856) 685
Medium: acetonitrile

C26H24N4O5 L CAS 188838-26-8 (7359)
Dipyrido[3,2-a:2',3'-c]-phenazo-(1,4,7,10,13-pentaoxacyclopentadecane);

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

Li+ 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.

Li+ sp non-aq 25°C 100% C I 2002YPb (103901) 687

K(ZnLA2+Li)=3.76

Medium: MeCN, 0.10 M Bu4NPF6. A is CH3.C6H4.SH

Li+ 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 L (6648)
Bis(diphenylphosphinyl)ethane; (C6H5)2PO.CH2CH2.PO(C6H5)2

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

Li+ 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 L (7158)
1,3-Bis(diphenylphosphinyl)-2-oxopropane;

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

Li+ con non-aq 25°C C K1=4.2 1999TEa (103919) 690

In: tetrahydrofuran/CHCl3 4:1 v/v

Li+ oth non-aq 25°C 100% U K1=4.2 1995TEa (103920) 691

Medium: tetrahydrofuran:CHCl3 4:1 (v/v).

Metal ion is used as 2,4-dinitrophenolate.

C26H28N2O5 L (2155)
1,13-Di-(8-quinolyl)-1,4,7,10,13-tetraoxatridecane; C9H6N.O.(CH2.CH2.O)4.C9H6N

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

Li+ sp non-aq 27°C 100% C IH K1=4.3 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.

C26H34N4 L CAS 677034-80-9 (9063)

1-(2-{10-[2-Piperazinoethyl]-9-anthryl}ethyl)piperazine;

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

Li+ 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 Et4NC104.

C26H36N206 L DiBzCryptand222 (746)

5,6,14,15-Dibenzo-4,7,13,16,21,24-hexaoxa-1,10-diazabicyclo[8.8.8]hexacosan-5,14-diene;

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

Li+ 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.

Li+ ISE non-aq 25°C 100% U M K1=6.06 1987DSa (104138) 695
Medium: acetonitrile

C26H40O11P2 L (5727)

1,7-Bis(2-(diethoxyphosphinylmethoxy)phenyl)-1,4,7-trioxaheptane;2(EtO)2PO.CH2OC6H4C2H4OC2H4)2O

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

Li+ con non-aq 25°C 100% U K1=3.7 1989EVa (104244) 696
Medium: tetrahydrofuran/CHCl3 4:1 (volume)

C26H45N306 L CAS 111928-04-2 (8968)

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

Li+ dis none 25°C dil C K1=5.96 1987BBf (104280) 697
K(Li+A+L(org))=LiAL(org))=3.10

Method: extraction of metal picrate from H2O into CHCl3.

C26H48O6 L (2342)

19,21,26,28-Tetramethyl-2,5,8,11,14,17-hexaoxatricyclo[22.4.0.0(18,23)]octacosane;

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

Li+ nmr non-aq 24°C 100% U M 1981BEb (104310) 698
K(Li(picrate)+L)=5.1

Medium: CDC13

C26H52N2O5 L Cryptand 221D CAS 62002-40-8 (8956)
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.

C26H52N6O7S2 L CAS 503465-16-5 (9245)
4,12,20,26,29,34,37-Heptaoxa-1,7,9,15,17,23-hexaazabicyclo[21.8.8]nonatriacontane-8,
16-dithione;

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

Li+ gl alc/w 25°C 95% C K1=<2 2004KVa (104340) 700
Medium: 95% MeOH/H2O, 0.01 M Et4NClO4.

C26H52N6O7S2 L CAS 503465-12-1 (9243)
9,12,15,26,29,34,37-Heptaoxa-1,4,6,18,20,23-hexaazabicyclo[21.8.8]nonatricontane-5,
19-dithione;

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

Li+ gl alc/w 25°C 95% C K1=<2 2004KVa (104350) 701
Medium: 95% MeOH/H2O, 0.01 M Et4NClO4.

C26H54N2O10 L CAS 85726-99-4 (652)
4,13-Dimethyloxyethoxyethoxyethylidene-1,7,10,16-tetraoxy-4,13-diazaoctadecane;

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

Li+ sol non-aq 20°C 100% C K1=4.03 1983SLa (104361) 702
Medium: CHCl3

C27H26O2P2 L (6811)
1,2-Bis(2-Diphenylphosphinyl)-1-methylethane;

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

Li+ 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 L (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

Li+ con non-aq 25°C 100% U K1=4.2 1990EAb (104402) 704
Medium: THF+CHCl3 4:1(vol). Metal as 2,4-dinitrophenolate. Data also for
3-hydroxypropyl analogue

C27H26O3P2 L (7159)
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+ L CAS 423763-94-4 (8997)
3-Ethyl-2-[4-(2,3,5,6,8,9,11,12-octahydro-1,4,7,10,13-benzopentaoxacyclopentadecin-
15-yl)butadien

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

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;

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

Li+ sp non-aq ns 100% C K1=3.02 2000LXa (104525) 707
Medium: acetonitrile. Method: fluorescence spectroscopy.

C27H47N3O6 L (8029)
Tripodal ionophore 3;

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

Li+ 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 L (5742)
5,6-Benzo-1,10-di(8-quinolyl)-1,4,7,10-tetraoxadecane;
C9H6N.O.C2H4.O.C6H4.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=4.4 1989BEa (104676) 709
Medium: tetrahydrofuran/CHCl3 4:1 (volume)

C28H28O3P2 L (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
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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
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Medium: THF+CHCl3 (4:1 vol)

 C28H28O4P2 L (7891)
 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: tetrahydrofuran/CHCl3 4:1 v/v

 C28H30N2O2P2 L CAS 68745-29-9 (5707)
 N,N'-Bis(diphenylphosphinylmethyl)-1,2-diaminoethane; ((C6H5)2PO.CH2.NH.CH2-)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Li+	con	non-aq	25°C	100%	U			K1=4.4	1984YKa (104727)	714

Medium: tetrahydrofuran + CHCl3 4:1, Li as 2,4-dinitrophenolate

 C28H32N2O6 L (5743)
 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)

 C28H35O7P 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

 C28H36N2O7S2 HL CAS 150196-54-6 (7735)
 3-(3-Sulfopropyl)-2-[4-[N-(1,4,7,10,13-pentaoxa-16-azacyclooctadeca)]]styryl-benzot
 hiazolium;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Li+ sp non-aq 18°C 100% C K1=2.2 1997LHa (104784) 717
Medium: acetonitrile.

C28H4008 L AN(MOEOEOM)2AN (2243)
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

Li+ dis non-aq 25°C 100% U H K(Li(picrate)+L)=2.75 1979KLa (104857) 718

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

Li+ con non-aq 25°C 100% U I K1=4.68 1991ASb (104892) 719
Medium: 1,2-dichloroethane. In nitromethane: K1=4.49

Li+ vlt non-aq 25°C 100% U K1=14.2 1990SPa (104893) 720
Medium: 1,2-dichloroethane

C28H44012P2 L (5728)
1,10-Bis(2-(diethoxyphosphinylmethoxy)phenyl)-1,4,7,10-tetraoxadecane;

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

Li+ con non-aq 25°C 100% U K1=4.0 1989EVa (104946) 721
Medium: tetrahydrofuran/CHCl3 4:1 (volume)

C28H5205 L (2339)
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

Li+ nmr non-aq 24°C 100% U M K(Li(picrate)+L)=3.9 1981BEb (105010) 722

Medium: CDCl3

C28H5206 L (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 L Cryptand 222D CAS 69878-46-2 (8957)
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.

C28H56N6O8S2 L CAS 503465-18-7 (9246)
4,12,15,23,29,32,37,40-Octaoxa-1,7,9,18,20,26-hexaazabicyclo[24.8.8]dotetracontane-
8,19-dithione;

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

Li+ gl alc/w 25°C 95% C K1=<2 2004KVa (105041) 725
Medium: 95% MeOH/H2O, 0.01 M Et4NClO4.

C28H56N6O8S2 L CAS 503465-14-3 (9244)
9,12,15,18,29,32,37,40-Octaoxa-1,4,6,21,23,26-hexaazabicyclo[24.8.8]dotetradecatriacontane-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.

C29H30O3P2 L CAS 176849-77-7 (7160)
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: tetrahydrofuran:CHCl3 4:1 (v/v).
Metal ion is used as 2,4-dinitrophenolate.

C29H30O3P2 L CAS 176849-78-8 (7161)
1,6-Bis(diphenylphosphinyl)-3-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 (105085) 728
Medium: tetrahydrofuran:CHCl3 4:1 (v/v).
Metal ion is used as 2,4-dinitrophenolate.

C29H30O4P2 L (7897)
1,7-Bis(diphenylphosphinyl)-2,6-dioxoheptane;

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

Li+ con non-aq 25°C C K1=5.8 1999TEa (105090) 729
In: tetrahydrofurane/CHCl3 4:1 v/v

C29H35N05 L CAS 201154-06-5 (7825)

N-(1-Pyrenylmethyl)-1,4,7,10,13-pentaoxa-16-azacyclooctadecane;

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

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).

C29H36N06S+ L 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-yl)butadien

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

Li+ sp non-aq 25°C 100% C K1=1.98 2002GVc (105106) 731

Medium: acetonitrile, 0.1 M Et4NClO4.

C30H32O4P2 L (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

Li+ con non-aq 25°C 100% U K1=5.1 1992BEa (105230) 733

Medium: THF+CHCl3 (4:1 vol)

C30H32O5P2 L (7892)

1,9-Bis(diphenylphosphinyl)-2,5,8-trioxononane;

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

Li+ con non-aq 25°C C K1=5.1 1999TEa (105236) 734

In: tetrahydrofurane/CHCl3 4:1 v/v

C30H34N2O2P2 L CAS 68743-31-3 (2066)

Diaminoethane-N,N'-di-2-ethylidiphenylphosphine oxide; (CH2.NH.C2H4.P(O)(C6H5)2)2

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

Li+ 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

C30H36N8O3 Furan-cryptand CAS 121954-37-8 (7451)

39,40,41-Trioxa-1,4,11,14,17,24,29,36-octaazapentacyclo[12.12.12.1.1.1]henLetetraco
ntadodecane;

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

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

C30H36O6 L 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 K(Li(picrate)+L)=5.25 1979KLa (105261) 737
Medium: CHCl3

C30H37N5O7 HL 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 L (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 CDC13. 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)]heptacos-3,5,7,8,10,12,13,15,17-nonaene

C30H38N2O8 L CAS 137571-97-2 (6821)
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

C30H42O10P4 L CAS 97910-31-1 (2083)
Tris-((2-(dimethylphosphinylmethoxy)phenoxy)methyl)phosphine oxide;

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

Li+ con non-aq 25°C 100% U K1=4.49 1989KSa (105302) 741
Medium: tetrahydrofuran/CHCl3 4:1 (vol)

C30H48O13P2 L CAS 112120-14-6 (5729)
1,13-Bis(2-(diethoxyphosphinylmethoxy)phenyl)-1,4,7,10,13-pentaoxatridecane;

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

Li+ con non-aq 25°C 100% U K1=4.0 1989EVa (105344) 742
Medium: tetrahydrofuran/CHCl3 4:1 (volume)

C31H34O4P2 L (7157)
1,9-Bis(diphenylphosphinyl)-3,7-dioxononane;

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

Li+ 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 si
milar ligands

C32H28O4P2 L CAS 88928-04-5 (2072)
1,2-Dihydroxybenzene bis(diphenylphosphinylmethyl) ether

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

Li+ con non-aq 25°C C K1=4.7 1999TEa (105576) 744
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 L CAS 21851-89-8 (2640)
P,P,P',P'',P'''-Pentaphenyldimethylenetri(phosphineoxide); (Ph2P(O)CH2)2P(O)Ph

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

Li+ sp non-aq 25°C 100% U M 1981SPb (105583) 746
K(LiI+L)=2.69

Medium: CH3CN

C32H36O5P2 L CAS 137728-07-5 (6837)
1,11-Bis(diphenylphosphinyl)-3,6,9-trioxaundecane;

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

Li+ con non-aq 25°C 100% U K1=5.4 1992BEa (105646) 747
Medium: THF+CHCl3 (4:1 vol)

C32H36O6P2 L (7893)

1,12-Bis(diphenylphosphinyl)-2,5,8,11-tetraoxododecane;

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Metal      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: tetrahydrofuran/CHCl3 4:1 v/v

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*****
C32H43N2O7S      HL      CAS 189057-31-6 (7756)
3-(4-Carboxybutyl)-2-[4-[N-(1,4,7,10,13-pentaoxa-16-azacyclooctadeca)]]styryl-benzo
thiazolium;

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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.

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*****
C32H44O12P2      L      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;

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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Li+        con non-aq 25°C 100% U      K1=3.7      1989BEa (105777) 750
Medium: tetrahydrofuran/CHCl3 4:1 (volume)

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*****
C32H48N2O3      L      CAS 170801-55-5 (8952)
1,5-Bis[2,2'-azo-4,4'-(1,1,3,3-tetramethylbutyl)phenoxy]-3-oxapentane;

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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Li+        sp non-aq RT 100% C      K1=3.28     2000GDa (105795) 751
Medium: acetonitrile.

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*****
C32H52O14P2      L      CAS 112120-15-7 (5730)
1,13-Bis(2-(diethoxyphosphinylmethoxy)phenyl)-1,4,7,10,13,16-hexaoxaohexadecane;

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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Li+        con non-aq 25°C 100% U      K1=3.7      1989EVa (105824) 752
Medium: tetrahydrofuran/CHCl3 4:1 (volume)

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*****
C33H28O2P2      L      CAS 118448-50-3 (2085)
C-Methylcarbonyl,C-diphenylphosphinylmethylenetriphenylphosphorane;

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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Li+        con non-aq 25°C 100% U      K1=2.98     1988YSb (105871) 753
Medium: acetonitrile

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*****
C33H39N11      L      Pyr-cryptand      CAS 141258-00-6 (7452)

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1,4,12,15,18,26,31,39,42,43,44-Undecazapentacyclo[13.13.13.1.1.1]tetratetraconta pentadecane;

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

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

C33H41N3O6 L (8027)
Tripodal ionophore ;

Metal 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 H4L CCE (7373)
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

Li+ 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

C34H38O12P2 L (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

C34H40O6P2 L CAS 137728-08-6 (6838)
1,14-Bis(diphenylphosphinyl)-3,5,8,11-tetraoxatetradecane;

Metal 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)

C34H40O7P2 L (7894)
1,15-Bis(diphenylphosphinyl)-2,5,8,11,14-pentaoxopentadecane;

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

Li+ con non-aq 25°C C K1=4.7 1999TEa (106051) 759
In: tetrahydrofurane/CHCl3 4:1 v/v

C34H44N2O5 L 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

C34H53O8Br H2L CAS 38784-08-6 (2336)
5-Bromolasalocid;

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

Li+ gl alc/w 25°C 100% M H K(Li+HL)=1.8 1988PJa (106099) 761
Medium: MeOH. DH = 8.2 kJ mol⁻¹; DS = 62

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

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

Li+ nmr non-aq 20°C 100% C K(Li+HL)=0.0 1998MLa (106142) 762
Medium: CD3OD. Method: 13C nmr.

Li+ dis oth/un 25°C 0.0 U K1=2.2 1992LPb (106143) 763

Li+ gl alc/w 25°C 100% M H K(Li+HL)=1.9 1988PJa (106144) 764
Medium: MeOH. DH = 4.9 kJ mol⁻¹; DS = 53

Li+ gl alc/w 25°C 100% U K(Li+2HL)=1.44 1982BDc (106145) 765
Medium: MeOH

C35H45N9 L CAS 312304-65-7 (7962)
29,32,35-TriMe-1,14,29,32,35,38,39,40,41-Nonaazahexacyclohentetraconta-3,5,7,8,10,1
2,16,18,20,21,

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

Li+ gl R4N.X 25°C 0.10M U K1=3.4 2001BBa (106203) 766
K(LiL+H)=9.5
K(LiHL+H)=9.3

Medium: 0.10 M NMe4NO3.

C36H32N2O6 L (5744)
5,6:11,12-Dibenzo-1,16-di(8-quinoly1)-1,4,7,10,13,16-hexaoxahexadecane;

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

Li+ con non-aq 25°C 100% U K1=4.1 1989BEa (106220) 767
Medium: tetrahydrofuran/CHCl3 4:1 (volume)

C36H36N24O12 L Cucurbituril CAS 283175-97-3 (6744)
Cucurbit[6]uril;

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

Li+ 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

Li+ sp none 25°C 0 U K1=2.23 B2=2.73 1994HKa (106264) 769

C36H36O4P2 L (2073)
3-t-Butyl-1,2-dihydroxybenzene bis(diphenylphosphinylmethyl) ether

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

Li+ con non-aq 25°C 100% U K1=4.25 1989KSa (106281) 770
Medium: tetrahydrofuran/CHCl3 4:1 (vol)

C36H36O6P2 L CAS 103990-64-3 (2077)
1,2-Bis(2-(diphenylphosphinylmethoxy)ethoxy)benzol;

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

Li+ con non-aq 25°C 100% U K1=4.20 1989KSa (106285) 771
Medium: tetrahydrofuran/CHCl3 4:1 (vol)

C36H40O4S2 L ANAN(MSM)2ANAN CAS 1129-04-9 (2240)
Tetra(1,3-(2-methoxy-5-methylbenzo))-9,18-dithiacyclooctadeca-2,5,12,14-tetraene;

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

Li+ dis non-aq 25°C 100% U H 1979KLa (106295) 772
K(Li(picrate)+L)=2.96

Medium: CHCl3

C36H40O6 L ANANAN(MOM)2AN CAS 1129-07-2 (2238)
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 Reference ExptNo

Li+ dis non-aq 25°C 100% U H 1979KLa (106301) 773
K(Li(picrate)+L)=2.91

Medium: CHCl3

C36H4407P2 L (5725)
1,17-Di(diphenylphosphinyl)-3,6,9,12,15-pentaoxaseptadecane;
Ph2PO.C2H4(O.C2H4)4OC2H4POPh2

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

Li+ con non-aq 25°C 100% U K1=5.5 1992BEa (106336) 774
Medium: THF+CHCl3 (4:1 vol)

Li+ cal non-aq 25°C 100% U K1=3.5 1991SGa (106337) 775
K(Li+LiL)=2.70

C36H4408P2 L (7895)
1,18-Bis(diphenylphosphinyl)-hexaoxooctadecane;

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

Li+ con non-aq 25°C C K1=4.6 1999TEa (106345) 776
In: tetrahydrofurane/CHCl3 4:1 v/v

C36H47N3O6 L (8028)
Tripodal ionophore 2;

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

Li+ sp non-aq 25°C 100% C K(LiP+L=LiPL)=5.21 2001Lfa (106375) 777

Method: Analyses by spectrophotometry. Medium: chloroform. P is picrate.

C36H48N2O6 L 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

Li+ nmr non-aq 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

C36H52O14P2 L (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

Li+ con non-aq 25°C 100% U K1=3.9 1989BEa (106397) 779

Medium: tetrahydrofuran/CHCl3 4:1 (volume)

C36H58N10O10S4 H5L CAS 136685-24-0 (6875)
(1-Cys-,1'-Cys-,4-Cys-,4'-Cys)-dithiobis(Ac-1-Cys-Pro-D-Val-4-Cys-NH2);

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

Li+ gl non-aq 20°C 100% U K1=2.60 1993EAa (106442) 780

Method: circular dichroism. Medium: MeCN, ClO4-

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

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

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 Et4NClO4. 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

Li+ ISE alc/w 25°C 100% M K1=3.60 1984CTa (106514) 784
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

Li+ vlt alc/w 25°C 100% U K1=3.3 1978HPa (106517) 787
Method: Cyclic voltametry

C38H30O2P2 L CAS 118448-51-4 (2086)
C-Phenylcarbonyl,C-diphenylphosphinylmethylenetriphenylphosphorane;

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

Li+ con non-aq 25°C 100% U K1=2.56 1988YSb (106640) 788

Medium: acetonitrile

C38H32O3P2 L (6804)
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
Li+	con	non-aq	25°C	100%	U		K1=5.5	1993BEb (106643)	789
Medium: THF+CHCl3 4:1(vol)									

C38H32O4P2			L				(1320)		
1,4-Di(2-diphenylphosphinylphenyl)-1,4-dioxabutane; Ph2PO.C6H4.O.CH2.CH2.O.C6H4.P(O)Ph2									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Li+	con	non-aq	25°C	100%	U		K1=5.8	1991EBa (106649)	790
Medium: THF+CHCl3 4:1(vol)									

C38H40O6P2			L				(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
Li+	con	non-aq	25°C	100%	U		K1=5.5	1993EVa (106660)	791
Medium: THF+CHCl3 (4:1 vol). Also data for other solvents									

C38H48O8P2			L				CAS 145864-37-5 (6839)		
1,20-Bis(diphenylphosphinyl)-3,5,8,11,14,17-hexaoxaicosane;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Li+	con	non-aq	25°C	100%	U		K1=5.0	1992BEa (106681)	792
Medium: THF+CHCl3 (4:1 vol)									

C38H48O9P2			L				(7896)		
1,21-Bis(diphenylphosphinyl)-2,5,8,11,14,17,20-heptaoheneicosane;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Li+	con	non-aq	25°C		C		K1=4.6	1999TEa (106686)	793
In: tetrahydrofurane/CHCl3 4:1 v/v									

C38H52N2O7			L				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
Li+	nmr	non-aq	25°C	100%	U		K1=7.26	1986CHc (106691)	794
CDCl3. L=36,37,38-trimethoxy-5,10,15-trimethyl-22,25,30,33-tetraoxa-1,19-diazapentacyclo[17.8.8.1(3,7).1(8,12).1(13,17)]octatriaconta-3,5,7,8...nonaene									

C40H36O4P2			L				(6805)		

1,6-Bis(2-Diphenylphosphinylphenyl)-2,5-dioxahexane; (CH2.O.CH2.C6H4(PO(6H5)2)2

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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Li+        con non-aq 25°C 100% U          K1=5.2          1993BEb (106734) 795
Medium: THF+CHCl3 4:1(vol)
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*****
C40H3605P2          L          CAS 86341-96-0 (5724)
1,7-Di(2-diphenylphosphinyl)phenyl-1,4,7-trioxaheptane;Ph2PO.C6H4.O.C2H4.O.C2H4.O.C
6H4.POPh2
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Li+        con non-aq 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
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*****
C40H4404P2          L          (2074)
3,5-Di(t-butyl)-1,2-dihydroxybenzene bis(diphenylphosphinylmethyl)ether
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Li+        con non-aq 25°C 100% U          K1=4.72         1989KSa (106765) 797
Medium: tetrahydrofuran/CHCl3 4:1 (vol)
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*****
C40H4607          L          CAS 177723-37-4 (8912)
25,27-Diethoxycalix[4]arenecrown-5, 1,3-alternate;
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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Li+        dis non-aq 22°C 100% C    M          K(LiA+L(org))=LiAL(org))=4.93
1996CPa (106772) 798
```

```
Medium: CHCl3 saturated with H2O. Method: extraction of LiA into CHCl3/L
solution. HA is picric acid. For the cone conformation, K=4.74.
*****
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```
C40H4608          L          CAS 161282-95-7 (8680)
25,27-Dimethoxycalix[4]arene-crown-6;
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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Li+        sp non-aq 25°C 100% C          K1=<=1          1995CUa (106777) 799
Medium: methanol, 0.01 M Et4NCl.
```

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*****
C40H4808          L          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;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Li+        dis non-aq 25°C 100% U    H          1979KLa (106795) 800
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K(Li(picrate)+L)=5.01

Medium: CHCl3

C40H50N20010 L CAS 143902-45-8 (8935)

Decamethylcucurbit[5]uril;

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

Li+ cal mixed 25°C 50% C H K1=1.99 2000ZKb (106807) 801

Medium: 50% v/v formic acid/H2O. DH(K1)=-14.4 kJ mol⁻¹, DS(K1)=-10 J K⁻¹ mol⁻¹.

C40H52N404 L CAS 205066-94-0 (8760)

Tetraphenyl-1,4,7,10-tetraazacyclododecane-1,4,7,10-tetraethanol;

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

Li+ ISE non-aq 25°C 100% C K1=3.13 1998WLC (106823) 802

Medium: DMF, 0.05 M Et4NClO4.

Ligand is (all-R)-(all-alpha)-Tetraphenyl-

C40H52O14P2 L 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-octaoxatetracosane;

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

Li+ con non-aq 25°C 100% U K1=3.6 1989BEa (106828) 803

Medium: tetrahydrofuran/CHCl3 4:1 (volume)

C41H42O6 L CAS 151832-07-4 (6874)

9-(Dimethylethyl)-29,30,31,32,33-pentamethoxy-23-oxahexacyclotritriacontapentadecane;

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

Li+ dis non-aq 25°C 100% U 1993HSa (106871) 804

K(Li(picrate)+L)=9.38

Medium: CDCl3 saturated with D2O. With 23-thia- analogue K=7.96

C42H40O4P2 L (7153)

1,2-Bis(2-(2-(diphenylphosphinyl)ethyl)phenoxy)ethane

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

Li+ 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

C42H40O4P2 L (6809)

1,6-Bis(2-Diphenylphosphinylphenyl)-3,4-dimethyl-2,5-dioxahexane;

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

Li+ con non-aq 25°C 100% U K1=4.9 1993BEb (106917) 806
Medium: THF+CHCl3 4:1(vol)

C42H40O5P2 L CAS 163172-12-6 (2080)
Bis((2-diphenylphosphinylmethyl)phenyl)diethyleneglycol ether;

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

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)

C42H40O7P2 L CAS 95651-36-8 (2079)
1,7-Di(2-(diphenylphosphinylmethoxy)phenyl)-1,4,7-trioxahseptane;
(Ph2PO.CH2.O.C6H4.O.C2H4)2O

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)

Li+ con non-aq 25°C 100% U K1=3.65 1989TKb (106938) 810
Medium: tetrahydrofuran/CHCl3 4:1 (volume)

C42H50O7 L CAS 177723-38-5 (8793)
1,3-Diisopropoxycalix[4]arene-crown-5, 1,3-alternate;

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

Li+ dis non-aq 22°C 100% C M K(LiA+L(org))=LiAL(org))=4.78 1996CPa (106952) 811

Medium: CHCl3 saturated with H2O. Method: extraction of LiA into CHCl3/L
solution. HA is picric acid. For the cone conformation, K=4.70.

C42H68N2O4 L CAS 188593-77-3 (8954)
2,17-Didodecyl-6,7,9,10,12,13-hexahydro-dibenzo[b,f][1,8,11,14,4,5]tetraoxadiazacyc
lohexadecine

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

Li+ sp non-aq RT 100% C K1=4.0 2000GDa (106974) 812
Medium: acetonitrile.

C43H42O4P2 L (7156)
1,3-Bis((2-diphenylphosphinyl)phenoxy)propane;

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

Li+ 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 similar ligands

C43H42O6P2 L (5734)
1,7-Di((2-diphenylphosphorylmethoxy)phenyl)-1,7-dioxheptane;
(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)

C43H43NO4P2 HL (8538)
Methyl[bis-(2-diphenylphosphorylmethyl)phenoxyethyl]amine;

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

Li+ 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 K(Li+H2L=LiL+2H)=-18.81 1996TNa (107039) 816

C44H30N8Br8 L (7212)
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

Li+ sp NaNO3 25°C 0.1M C K1=4.21 1998TNa (107086) 817
K(Li+HL=LiL+H)=-8.80

Li+ sp oth/un 25°C 0.10M C K1eff=2.98 1996RHb (107087) 818

C44H36O4P2 L (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

Li+ con non-aq 25°C 100% U K1=4.3 1993BEb (107091) 819

Medium: THF+CHCl3 4:1(vol)

C44H38N8 H2L 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

Li+ sp NaNO3 25°C 0.50M C K1=2.58 1998IHb (107106) 820
For the 2-pyridyl analogue, K1=3.28

C44H42O6P2 L (6806)

1,12-Bis(2-Diphenylphosphinylphenyl)-2,5,8,11-tetraoxadodecane;

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

Li+ con non-aq 25°C 100% U K1=5.2 1993BEb (107110) 821
Medium: THF+CHCl3 4:1(vol)

C44H44O5P2 L (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

Li+ con non-aq 25°C 100% U K1=3.18 1989TKb (107114) 822
Medium: tetrahydrofuran/CHCl3 4:1 (volume)

C44H44O5P2 L (5733)

1,7-Di(2-(diphenylphosphinylethyl)phenyl)-1,4,7-trioxaheptane;
(Ph2PO.C2H2.C6H4.OC2H4)20

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

Li+ oth non-aq 25°C 100% U K1=4.6 1995TEa (107119) 823
Medium: THF:CHCl3 4:1 v/v. Li as 2,4-dinitrophenolate

Li+ con non-aq 25°C 100% U K1=4.05 1989TKb (107120) 824
Medium: tetrahydrofuran/CHCl3 4:1 (volume)

C44H44O6P2 L CAS 126763-09-5 (7790)

1,8-Bis[2-(diphenylphosphinylmethyl)phenoxy]-3,6-dioxaoctane;

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

Li+ 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

C44H50N2O10 H2L CAS 329183-28-0 (8807)

25,27-Bis(carboxymethoxy)-26,28-bis[(N,N-diethylaminocarbonyl)methoxy]calix[4]arene
;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Li+	gl	non-aq	25°C	100%	C		K1=4.28 B(Li2L)=7.11	2000ABb (107144)	826

Medium: MeOH, 0.05 M Et4NClO4.

C44H52N4O8	L						CAS 246035-33-6 (2925)		
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25,27-Bis(N,N-diethylaminocarbonylmethoxy)-26,28-bis(aminocarbonylmethoxy)calix[4]arene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Li+	sp	non-aq	25°C	100%	C		K1<=1	1999USa (107159)	827

Medium: MeOH, 0.10 M Et4NCl

C44H52O10	L						CAS 163317-54-2 (9089)		
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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.

C44H54O8	L						CAS 161282-98-0 (8679)		
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25,27-Bis(1-propyloxy)calix[4]arene-crown-6, 1,3-alternate;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Li+	sp	non-aq	25°C	100%	C		K1<=1	1995CUa (107176)	829

Medium: methanol, 0.01 M Et4NCl.

C44H54O8	L						CAS 161282-96-8 (8678)		
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25,27-Bis(2-propyloxy)calix[4]arene-crown-6, 1,3-alternate;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Li+	sp	non-aq	25°C	100%	C		K1<=1	1995CUa (107182)	830

Medium: methanol, 0.01 M Et4NCl.

C44H56O4	H4L						(7294)		
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4-Tert-butyl-calix[4]arene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Li+	sp	non-aq	25°C	100%	U		K1=2.9 B(Li2L)=4.04	1996ABa (107187)	831

Medium: MeCN

C45H39O3P3	L						CAS 73218-92-5 (5679)		
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1,3,5-Tris(diphenylphosphinylmethyl)-benzene; C6H3(CH2.PO(C6H5)2)3

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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Li+        con non-aq 25°C 100% U      K1=5.1      1984YKa (107213) 832
Medium: tetrahydrofuran + CHCl3 4:1, Li as 2,4-dinitrophenolate
*****
C45H48N06P3          L                      (7953)
Tris[2-(diphenylphosphorylmethoxy)ethyl]amine;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Li+        cal non-aq 25°C 100% U  H   K1=4.08     1998SBb (107219) 833
Medium: MeCN Calorimetric titration of LiNCS. DH(K1)=-28.1 kJ mol-1
*****
C45H48N303P3          L                      CAS 90179-28-5 (5682)
N,N',N''-tris(Diphenylphosphinylmethyl)-1,4,7-triazacyclononane;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Li+        con non-aq 25°C 100% U      K1=5.6      1984YKa (107226) 834
Medium: tetrahydrofuran + CHCl3 4:1, Li as 2,4-dinitrophenolate
*****
C46H4006P2          L                      (6814)
1,2-Bis((2-(2-diphenylphosphinyl)phenoxy)ethoxy)benzene;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Li+        con non-aq 25°C 100% U      K1=7.0      1991EBa (107241) 835
Solvent : Tetrahydrofurane + CHCl3 4:1(vol);
*****
C46H46N204          L                      CAS 185118-12-1 (7824)
N,N'-Bis(1-pyrenylmethyl)-1,4,10,13-tetraoxa-7,16-diazacyclooctadecane;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Li+        sp mixed 25°C 90% C                      K(LiSCN+L)=0.48
Method: fluorescence emission. Medium: MeOH/CHCl3 (9:1 v/v).
*****
C46H4607P2          L                      (6807)
1,15-Bis(2-Diphenylphosphinylphenyl)-2,5,8,11,14-pentaoxapentadecane;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Li+        con non-aq 25°C 100% U      K1=4.9      1993BEb (107260) 837
Medium: THF+CHCl3 4:1(vol)
*****
C46H4806P2          L                      (7155)
1,8-Bis(2-(2-(diphenylphosphinyl)ethyl)phenoxy)-3,6-dioxyoctane
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Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo

Li+ oth non-aq 25°C 100% U K1=4.6 1995TEa (107271) 838
Medium: THF:CHCl3 4:1 v/v. Li as 2,4-dinitrophenolate. Also other similar ligands

C46H48O9P2 L CAS 95651-38-0 (2082)
1,5-Bis(2-(2-(diphenylphosphinylmethoxy)ethoxy)phenoxy)-3-oxapentane;

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

Li+ con non-aq 25°C 100% U K1=4.18 1989KSa (107280) 839
Medium: tetrahydrofuran/CHCl3 4:1 (vol)

C48H44O8P2 L CAS 95651-37-9 (2081)
1,2-Bis(2-(2-(diphenylphosphinylmethoxy)phenoxy)ethoxy)benzol;

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

Li+ con non-aq 25°C 100% U K1=3.75 1989KSa (107361) 840
Medium: tetrahydrofuran/CHCl3 4:1 (vol)

C48H50O8P2 L (6808)
1,18-Bis(2-Diphenylphosphinylphenyl)-2,5,8,11,14,17-hexaoxananodecane;

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

Li+ con non-aq 25°C 100% U K1=4.6 1993BEb (107365) 841
Medium: THF+CHCl3 4:1(vol)

C48H54N06P3 L (7975)
Tris(3-oxa-5-(diphenylphosphoryl)pentyl]amine;

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

Li+ cal non-aq 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

C48H54N6O8 L CAS 449738-94-7 (8791)
1,7-Dioxa-4,10-diazacyclododecane-4,10-bis[methylene-8-(1,3,3-trimethyl-6-nitro-spirobenzopyran)]

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

Li+ sp alc/w 25°C 100% C K1=6.62 2002NFa (107384) 843
Medium: 100% MeOH. Method: electrospray ionization mass spectrometry.

C48H54O10P4 L 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 1989K5a (107388) 844
Medium: tetrahydrofuran/CHCl3 4:1 (vol)

C48H60O8 H2L R-Bu-Calixarene CAS 147513-53-9 (6705)
4-tert-Butylcalix[4]arene dicarboxylic acid;

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

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

C48H60O12 L CAS 157769-14-7 (9090)
1,3-Calix[4]-bis-crown-6;

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

Li+ sp non-aq 25°C 100% C I K1=2.3 1996AAe (107411) 846
Medium: acetonitrile. In 100% MeOH, K1<=1.

C48H64O4 L CAS 105880-81-7 (8677)
tert-Butylcalix-4-arene tetramethyl ether;

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

Li+ sp non-aq 25°C 100% C K1=5.10 2004BCb (107421) 847
Medium: acetonitrile, 0.01 M Et4NClO4.

C52H62N6O10 ; L CAS 190781-91-0 (8792)
1,4,10,13-Tetraoxa-7,16-diazacyclododecane-7,16-bis[methylene-8-(trimethyl-6-nitro-
spirobenzopyra

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

Li+ sp alc/w 25°C 100% C K1=6.85 2002NFa (107480) 848
Medium: 100% MeOH. Method: electrospray ionization mass spectrometry.

C52H64O12 H4L R-Bu-Calixarene CAS 113215-72-8 (6704)
5,11,17,23-Tetra-(t-butyl)-25,26,27,28-tetrakis[(hydroxycarbonyl)methoxy]calix[4]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)4NClO4

C52H68N4O8 CAS 150588-24-2 (3074)
25,26,27,28-Tetrakis-(N,N-diethylaminocarbonylmethoxy)calix[4]arene; L

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

Li+ sp non-aq 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

C52H68N4O8 L (4823)
25,27-Bis(N,N-diethylaminocarbonylmethoxy)-26,28-bis(N-butylaminocarbonylmethoxy)calix[4]arene;

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

Li+ sp non-aq 25°C 100% C K1=<1 1999USa (107508) 851
Medium: MeOH, 0.10 M Et4NCl

C52H72O6 L (9263)
5,11,17,23-Tetra(t-butyl)-25,27-dimethoxy-26,28-dimethoxyethoxycalix[4]arene;

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

Li+ sp mixed 25°C 100% C K1=5.41 2004BCb (107526) 852
Medium: acetonitrile, 0.01 M Et4NClO4.

C54H74O7 L (7302)
25,27-Dimethoxy-4-tert-butylcalix[4]arene-crown-5;

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

Li+ dis non-aq 22°C 100% U K1=4.53 1996SCa (107542) 853
Medium: CHCl3 saturated with H2O

Data also for other substituted t-butylcalix[4]arene-crown-5 analogues

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

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

Li+ 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.

C56H60O12 L CAS 157769-17-0 (9091)

1,3-Calix[4]-bis-benzo-crown-6;

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Metal      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.
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*****
C56H64010          L          CAS 405108-40-9 (8249)
1,2-Di-O-[2-(2-benzyloxyethoxy)ethyl]-3,4,5,6-tetra-O-benzyl-myo-inositol;
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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Li+        dis non-aq 25°C 100% C          K(Li.pic+L(org))=LiL.pic)=2.19
2001SSb (107587) 856
```

Distribution of picrate salt into CHCl₃/HL.
 K: Li.pic(aq)+L(org)=LiL.pic(org). Data for series of myo-inositol ligands

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*****
C56H7208          L          CAS 123311-74-0 (6160)
Tetramethyl-t-butylcalix[4]arenetetraetone;
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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Li+        sp alc/w 25°C 100% U I      K1=2.7        1989ACb (107598) 857
Medium: MeOH. In CH3CN, K1=5.8
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*****
C56H72012          L          (8751)
Tetramethyl-4-t-Butylcalix[4]arenetetraethanoate;
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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Li+        EMF non-aq 25°C 100% C IH    K1=5.61      1995DGa (107602) 858
Medium: acetonitrile, 0.05 M Et4NClO4. In benzonitrile, K1=5.63.
```

Competitive method: Ag/Ag⁺ electrode. DH(K₁)=-37.80, DS=-19.4.

 C56H7808 L CAS 122356-76-7 (8681)
 Tetra-tert-butyl-1,3-dimethoxycalix[4]arene-crown-6;

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-----
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.
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*****
C56H8008          L          (9259)
5,11,17,23-Tetra(t-butyl)-25,26,27,28-tetramethoxyethoxycalix[4]arene;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Li+        sp non-aq 25°C 100% C H      B2=9.23      2004BCb (107614) 860
Medium: acetonitrile, 0.01 M Et4NClO4. By calorimetry: DH(B2)=-28.3
kJ mol-1, DS(B2)=81.7 J K-1 mol-1.
```

C58H78O11 HL CAS 465527-74-6 (9287)
7,13,19,25-Tetra-t-butyl-28-methoxy-27,29,30-triethylacetate-2,3-dihomo-3-oxacalix[4]arene;

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

Li+ sp alc/w 25°C 100% C K1=2.6 2001MAa (107623) 861
Medium: MeOH, 0.01 M Et4NCl.

C58H80O10 L (9264)
5,11,17,23-Tetra-t-butyl-25,27-di(2-methoxyethoxy)-26,28-di(ethylacetate)calix[4]arene;

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

Li+ sp non-aq 25°C 100% C H K1=5.99 B2=10.72 2004BCb (107632) 862
Medium: acetonitrile, 0.01 M Et4NClO4. DH(K1)=-33.8 kJ mol⁻¹,
DS(K1)=1.0 J K⁻¹ mol⁻¹; DH(B2)=-19.0, DS(B2)=141.1.

C60H54N06P3 L (8067)
Tris[2-diphenylphosphoryl]phenoxyethylamine;

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

Li+ cal non-aq 25°C 100% U H K1=4.30 1998SBb (107639) 863
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

C60H72O4 L (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

Li+ sp non-aq 25°C 100% C K1=3.54 2004BCb (107643) 864
Medium: acetonitrile, 0.01 M Et4NClO4.

C60H80O12 L CAS 97600-39-0 (6158)
Tetraethyl-4-t-butylcalix[4]arenetetraethanoate;

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

Li+ 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 Et4NClO4. 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

C60H82N2O10 L CAS 155377-20-1 (8806)
5,11,17,23-Tetra-butyl-25,27-bis(carboxymethoxy)-bis[(N,N-diethylaminocarbonyl)methoxy]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.

C60H84N4O8 L CAS 246035-32-5 (2735)
25,27-Bis(N,N-diethylaminocarbonylmethoxy)-26,28-bis(aminocarbonylmethoxy)-t-butylcalix[4]arene;

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

Li+ sp non-aq 25°C 100% C K1=<1 1999USa (107680) 869
Medium: MeOH, 0.10 M Et4NCl

C62H78N2O4S2 L (8158)
5,11,17,23-Tetrakis(1,1-dimethylethyl)-25,27-bis(2-methylthioethoxy)...calix(4)arene;

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

C62H84O14 L CAS 135581-11-2 (8630)
9,23-Dioxpentacyclo[23.3.1.13,7.111.15.117.21]dotriacontane, ethanoic acid derivative;

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

Li+ sp non-aq 25°C 100% C K1=3.2 1991ACc (107695) 871
Medium: acetonitrile, 0.01 M Et4NClO4.

C63H60N06P3 L (8437)
Tris[2-(diphenylphosphorylmethyl)phenoxyethyl]amine;

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

Li+ 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

C64H60012 L CAS 211870-40-5 (4258)

Calix[4]arene-bis(dibenzo)crown-6;

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

Li+ sp non-aq 25°C 100% C K1=2.18 1999Lda (107735) 873
Medium: acetonitrile, 0.01 M Et4NClO4.

C64H6206P4 L (6813)

1,2-Bis(4,5-di(diphenylphosphinyl)-pent-1-oxy)benzene;

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

Li+ con non-aq 25°C 100% U K1=6.0 1990EAb (107740) 874
Medium: THF+CHCl3 4:1(vol). Metal as 2,4-dinitrophenolate

C64H64012 L CAS 162898-44-4 (9092)

1,3-Calix[4]-bis-naphtho-crown-6;

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.

C64H72N404P4 L 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

Li+ 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

C64H8006 L (9262)

5,11,17,23-Tetra-t-butyl-25,27-di(phenylmethoxy)-26,28-di(2-methoxyethoxy)-calix[4]arene;

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

Li+ sp non-aq 25°C 100% C H K1=3.76 B2= 7.88 2004BCb (107762) 877
Medium: acetonitrile, 0.01 M Et4NClO4. DH(K1)=-30.5 kJ mol-1
DS(K1)=-30.6 J K-1 mol-1; DH(B2)=-20.0, DS(B2)=83.6.

C64H8607 L CAS 182684-17-9 (7455)

4-tert-Butylcalix[5]crown-4 trimethylester;

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

Li+ 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

C66H80O8 L (9261)
5,11,17,23-Tetra(t-butyl)-25,27-diethoxycarbonylmethoxy-26,28-diphenylmethoxycalix[4]arene;

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

Li+ sp non-aq 25°C 100% C K1=4.30 2004BCb (107777) 879
Medium: acetonitrile, 0.01 M Et4NClO4.

C68H76N4O4 L CAS 123207-92-1 (7812)
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

Li+ EMF non-aq 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.

C68H92N4O8 L 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.

C68H96O8 L (6161)
Tetra-t-butyl-4-t-butylcalix[4]arenetetraetone;

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

Li+ sp alc/w 25°C 100% U K1=1.8 1989ACb (107795) 882
Medium: MeOH, 0.1 M Et4NCl

C68H100N4O8 L CAS 246035-35-8 (3034)
25,27-Bis(N,N-diethylaminocarbonylmethoxy)-26,28-bis(N-butylaminocarbonylmethoxy)-t-butylcalix[4]

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

Li+ sp non-aq 25°C 100% C K1=<1 1999USa (107805) 883
Medium: MeOH, 0.10 M Et4NCl

C68H100N4O8 L CAS 114155-16-7 (7183)
4-tert-Butylcalix[4]arene tetradiethylacetamide;

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

Li+ cal alc/w 25°C 100% U IH 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.

Li+ dis non-aq 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 acid.

C69H102N4O9 L CAS 116352-85-3 (9286)
para-t-Butyldihomooxacalix[4]arene tetra(diethyl)amide;

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

Li+ sp alc/w 25°C 100% C K1=3.81 2004MFa (107835) 886
Medium: MeOH, 0.01 M Et4NCl.

C72H68O10P4 L 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

Li+ con non-aq 25°C 100% U K1=3.09 1985YKa (107847) 887
Medium: EtOH+CHCl₃ 1:1; M is used in nitrophenolate form

C75H100O15 L CAS 152495-34-6 (7033)
Penta-tert-butylpentakis(ethoxycarbonylmethoxy)calix[5]arene;

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

Li+ sp alc/w 25°C 100% U K1=1.0 1993BMa (107860) 888
Medium: MeOH, 0.1 M Et4NCl.

C76H80O8 L (6162)
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

Li+ sp non-aq 25°C 100% U K1=6.3 1989ACb (107870) 889
Medium: CH₃CN

C77H82O9 L CAS 253317-20-3 (9288)
p-Tert-butyl-dihomooxacalix[4]arene tetraphenylketone;

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

Li+ 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.

C78H90O10P2 L CAS 160638-26-6 (9130)

5,11,17,23-Tetra-*t*-butyl-bis(diethylcarbamoylmethoxy)-bis(diphenylphosphinoylmethoxy)calix[4]aren

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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
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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.
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*****
C85H120O15          L          CAS 152495-35-7 (7034)
Penta-tert-butylpentakis(tert-butoxycarbonylmethoxy)calix[5]arene;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
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Li+        sp alc/w  25°C 100% U          K1=1.5       1993BMa (107917) 892
Medium: MeOH, 0.1 M Et4NCl.
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C90H120O18          L          CAS 92003-62-8 (6159)
Hexaethyl-4-t-butylcalix[6]arenehexaethanoate;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Li+        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.
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Li+        sp non-aq 25°C 100% U I       K1=3.7       1989ACb (107943) 894
Medium: CH3CN
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C90H130O15          L          CAS 269057-78-5 (3334)
5,11,17,23,29-Penta-tert-octylcalix[5]arene-31,32,33,34,35-pentaethanoate
pentamethyl ester;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
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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.
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Polymer          H2L      X-14885A          (4547)
Antibiotic X14885A, calcium ionophore
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
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Li+        gl alc/w  25°C 100% U          K1=4.1       1989ABb (108076) 896
Medium: MeOH
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Polymer          (4181)
Phosphatidic acid;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
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Li+ 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

Polymer HL (3531)

Polyacrylic acid;

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

Li+ gl oth/un 25°C 0.20M U K'=0.28 1957GFa (108323) 899

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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