SC-Database
Software version = 5.81 Data version = 4.62
Experiment list contains 1654 experiments for
 (no ligands specified)
 Metal : Na+
 (no references specified)
 (no experimental details specified)

****

e- HL Electron (442)
Electron;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	EMF	mixed	25°C	10%	U	I	K(Na+e=Na(s))=-45.69(-2.703V)	1974DKb (695)	1
Medium: 10% w/w DMSO/H2O; K=-45.56(-2.695V,20%), -44.96(-2.660V,40%), -44.32(-2.622V,60%)									
Na+	oth	none	25°C	0.0	U	I	K(Na+e+Na(s))=-45.54(-2690mV)	1972COa (696)	2
Method: Estimated. MeOH: -50.04(-2.960V).EtOH: -48.56(-2.873V).BuOH: -48.19 (-2.851V).PentOH: -45.27(-2.678V).Me2CO: -41.60(-2.461V)									
Na+	oth	none	25°C	0.0	U	I	K(Na+e=Na(s))=-45.54(-2694mV)	1972COa (697)	3
Method: Estimated. MeCN: -51.51(-3.047V).HCOOH: -56.63(-3.350V). Also NH3 and N2H4									
Na+	con	non-aq	-65°C	100%	U	T	K(Na + e(solv))=2.78 K(2Na=Na2)=1.98	1972DBa (698)	4
Medium: NH3(liquid). K=2.61, Kd=2.23(-45 C); K=2.55, Kd=2.19(-34 C)									
Na+	EMF	mixed	25°C	30%	U	I	K(Na+e=Na(s))=-45.76(-2.707V)	1972KRb (699)	5
Med. 30% w/w ethylene glycol/H2O; K=-45.64(-2.700V,50%), -45.56(-2.695V,70%) -45.93(-2.717V,90%), -47.11(-2.787V,100%)									
Na+	EMF	non-aq	25°C	100%	U	I	K(Na+e=Na(s))=-46.10(-2.727V)	1972KRc (700)	6
Medium: 30% w/w propylene glycol/MeOH; 0% PG: K=-46.13(-2.729V). 50%: -46.18 (-2.732). 70%: -46.33(-2.741V). 90%: -46.52(-2.752V). 100%: -46.65(-2.760V)									
Na+	EMF	none	25°C	0.00	U	T	K=-33.113(-1.95892V)	1971MMd (701)	7
K: Na+e=Na(Hg); x(Na(Hg)) to 0; -34.563(-1.94181V,10 C), -31.806(-1.97621V, 40 C), -30.603(-1.99255V,55 C), -29.504(-2.00878V,70 C)									
Na+	con	non-aq	-34°C	100%	U			1969DLa (702)	8

K(Na + e(solv))=2.14
K(2Na=Na2)=2.86
Medium: NH3(liquid)

Na+ con non-aq -65°C 100% U T 1968DRa (703) 9
K(Na + e(solv))=2.73
Medium: NH3(liquid); K=2.61(-45 C), 2.47(-34 C)

Na+ EMF none 25°C 0.0 U 1967BHc (704) 10
K(Na+e=Na/Hg)=-33.1, -1958 mV

Na+ EMF non-aq 25°C 100% U 1966LCa (705) 11
K'=-47.447, -2806.7 mV
Medium: CH3NHCHO. K': Na + Cl + Ag(s)=Na(s) + AgCl(s)

Na+ EMF non-aq 25°C 100% U 1966LCa (706) 12
K'=-45.871, -2713 mV
Medium: CH3NHCHO. K': Na + Br + Ag(s) = Na(s) +AgBr(s)

Na+ EMF none 25°C 0.0 U T 1940STa (707) 13
K(Na+e)=-45.88(-2713.24 mV)
K=-48.91(5 C;-2698.5 mV), -48.11(10 C;2702.1 mV), -47.34(15 C;-2705.8 mV),
-46.60(20 C;-2709.5 mV), -45.19(30 C;-2717.1 mV), -43.87(40 C;-2724.7 mV)

Na+ EMF none 25°C 0.0 U 1923LRa (708) 14
K(Na+e=Na(s))=-45.87(-2712.5mV
****
BF4- HL (2497)
Tetrafluoroborate;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ con non-aq 25°C 100% C T K1=2.40 2000VMa (1199) 15
Medium: 2-Methoxyethanol. Data for 15-35 C.

Na+ con non-aq 25°C 100% U K1=1.7 1975YKa (1200) 16
Medium: MeCN
****
BO4H4- HL Borate CAS 10043-35-3 (991)
Borate; B(OH)4-

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE oth/un 75°C 0.0 M TIH K1=0.33 1995PSc (1316) 17
Method: Na ISE. Data for various NaOH/NaCl/NaBO2 mixed media.
Data for 75-200 C. DH(K1)=-0.63 kJ mol-1. At 25 C, K1=0.28

Na+ sp oth/un 25°C 1.00M U I K1=0.48 1990RAa (1317) 18
Medium: NaCl. Data at I=0 M and at pressures to 2041 atmos.

```
Na+        sp  NaCl   25°C  0.0  C  I     K1=-0.19       1989RTa  (1318)  19
Extrapolated from data for 0.10-1.0 m NaCl.
--------------------------------------------------------------------------------
Na+        gl  NaCl   25°C 0.70M U        K1=-0.36       1988RBa  (1319)  20
--------------------------------------------------------------------------------
Na+        gl  none   25°C  0.0  M TI                    1976REa  (1320)  21
                                          K(Na+H2BO3)=0.22
Calculated from data for 0.17-0.50 M NaCl. Data for 10-50 C.
--------------------------------------------------------------------------------
Na+        EMF NaCl   25°C 0.68M U        K1=-0.24       1974BKd  (1321)  22
--------------------------------------------------------------------------------
Na+        con oth/un 20°C  var  U        K1=1.87        1963FUa  (1322)  23
********************************************************************************
Br-                    HL    Bromide          CAS 10035-10-6  (19)
Bromide;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Na+        con non-aq 25°C 100%  U T      K1=2.35        1993TAa  (2138)  24
Medium: 2-methoxyethanol, -10 to 80 C
--------------------------------------------------------------------------------
Na+        con alc/w  25°C 100%  C        K1=0.23        1992PTa  (2139)  25
Medium: methanol.
--------------------------------------------------------------------------------
Na+        con non-aq 25°C 100%  U        K1=0.94        1974HPb  (2140)  26
Medium: hexamethylphosphotriamide. K1 by Pitts eqn. K1=1.20 (Fuoss-Hsia eqn)
--------------------------------------------------------------------------------
Na+        con mixed  25°C  91%  U TI     K1=2.49        1973YKa  (2141)  27
Medium: 91% w/w butanol/H2O. K1=2.40(85%, 20 C) 0 corr
--------------------------------------------------------------------------------
Na+        con non-aq 25°C 100%  U        K1=2.50        1971BCa  (2142)  28
Medium: tetramethylurea
--------------------------------------------------------------------------------
Na+        con mixed  25°C  20%  U        K1=0.70        1970BKb  (2143)  29
Medium: 20% t-butanol/H2O
--------------------------------------------------------------------------------
Na+        con non-aq 25°C 100%  U        K1=-0.44       1970CDa  (2144)  30
Medium: DMSO
--------------------------------------------------------------------------------
Na+        con oth/un 800°C  0.0  U T                    1968QMb  (2145)  31
                                          K(Na(H2O)x+Br(H2O)y)=17.28
K=16.61(500C),16.86(600),17.09(700),n=9.85,m units
K1 given for densities 0.35 to 0.75 gm cm-3
--------------------------------------------------------------------------------
Na+        con non-aq 25°C 100%  U        K1=3.19        1965BFb  (2146)  32
Medium: diaminoethane
--------------------------------------------------------------------------------
Na+        con non-aq  0°C 100%  U        K1=4.32        1963LKc  (2147)  33
Medium: liquid SO2; I=0 corr.
--------------------------------------------------------------------------------
```

```
Na+        con non-aq 30°C 100%  U        K1=6.89        1954JGa  (2148)  34
Medium: CH3CO2H
--------------------------------------------------------------------------------
Na+        con non-aq -34°C 100%  U        K1=2.54       1949HKa  (2149)  35
Medium: liquid NH3
********************************************************************************
BrO3-                  HL    Bromate            (6017)
Bromate;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Na+        cal none   25°C  0.0  C  IH                    1992BVa  (2423)  36
DH(Kso)=26.8 kJ mol-1, measured for I=0.002-0.02 M self medium.
Also data for 0.047-0.228 mol fraction MeOH/H2O.
--------------------------------------------------------------------------------
Na+        con none   25°C  0.0  U        K1=-0.77       1971JBa  (2424)  37
--------------------------------------------------------------------------------
Na+        con none   25°C  0.0  U        K1=-0.80       1969BJa  (2425)  38
--------------------------------------------------------------------------------
Na+        oth oth/un 25?°C  0.0  M        K1=-0.1        1966MBb  (2426)  39
--------------------------------------------------------------------------------
Na+        con none   25°C  0.0  U  I     K1=-0.30       1955MKb  (2427)  40
Also data for dioxan/H2O mixtures
********************************************************************************
CO3--                  H2L    Carbonate        CAS 465-79-6  (268)
Carbonate;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Na+        ISE oth/un 25°C  0.0  C  I     K1=1.29        1998CHa  (3285)  41
Method: Na ISE.  Medium: 0.5-7.0 M CsCl. In 1.0 M Me4NCl, K1=0.397.
--------------------------------------------------------------------------------
Na+        ISE none   25°C    0  C  I                    1995RGa  (3286)  42
                                          K(Na+HL)=0.12
I=0.16 (Me4N.X) K=-0.06
--------------------------------------------------------------------------------
Na+        cal none   25°C  0.0  C   H                   1978BVa  (3287)  43
DH(Kso(NaHCO3))=18.71 kJ mol-1. DH(Kso(Na2CO3))=-26.66.
--------------------------------------------------------------------------------
Na+        EMF oth/un 25°C 0.70M U        K1=0.63        1974PHc  (3288)  44
                                          K(Na+HL)=-0.55
Medium: synthetic seawater
--------------------------------------------------------------------------------
Na+        EMF none   25°C  0.0  U T H    K1=0.55        1971NAb  (3289)  45
                                          K(Na+HL)=0.16
DH(K1)=-18.5 kJ mol-1, DS=-52 J K-1 mol-1; DH(Na+HL)=-11.7, DS=-36.
Also data from 0-50 C in 5 degree intervals
--------------------------------------------------------------------------------
Na+        ISE NaCl   25°C 0.50M U  I     K1=0.14        1970BHc  (3290)  46
                                          K(Na+HL)=-0.41
```

K1=0.27(I=1), 0.37(I=3); K(Na+HL)=-0.67(I=1). K1=ca.1.0,K(Na+HL)=ca-0.3(I=0)

Na+ oth none 25°C 0.0 U K1=-0.55 1970NAc (3291) 47
K(Na+HCO3)=-0.16
Method:Estimated data.

Na+ gl none 25°C 0.0 U 1962GTa (3292) 48
K(Na+HL)=-0.25

Na+ gl none 25°C 0.0 U K1=1.27 1961GTa (3293) 49

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	gl	NaCl	25°C	0.10M	C	TIH	K1=1.67	1986CDc (3593)	50
							B(Na2Fe(CN)6)=1.90		
							B(NaHFe(CN)6)=4.59		

Data for 10-35 C and 0.05-1.0 M NaCl. DH(K1)=3.8 kJ mol-1, DS(K1)=59
J K-1 mol-1; DH(Na2Fe(CN)6)=3.3, DS=71; DH(NaHFe(CN)6)=0.8, DS=113

Na+ EMF oth/un 25°C U K1=2.13 1969NSa (3594) 51
Assuming K(Na+Fe(CN)6)=1.30

Na+ oth none 25°C 0.0 U K1=2.08 1966NSa (3595) 52
Method: transport number

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	sol	oth/un	25°C	3.0M	U		K1=-0.3	1967RMd (3678)	53
Medium: LiNO3									
Na+	sol	oth/un	25°C	3.0M	U	H	K1=-0.77	1966MRb (3679)	54
Medium: LiCl. By calorimetry, DH=16.7 kJ mol-1, DS-71 J K-1 mol-1									

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C8N8W-- H2L (2192)
Octacyanotungstate (VI); W(VI)(CN)8--

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	con	oth/un	25°C	0.00	U		K1=1.08	1976LLa (3704)	55

****

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

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

---

Na+ ISE none 25°C 0 C I K1=-0.60 1995RGa (5251) 56
I=0.16M (Me4N.X) B1=-0.77; I=0.50M (Me4N.X) B1=-0.73.

Na+ con oth/un 25°C 0.20M U TI K1=0.03 1978BBb (5252) 57
K1=0.52 when mole fraction ethylene carbonate=0.4. At 40 C, mf 0..5: 0.81;
mf=0.6: 0.92. Further data for up to 0.8 mole fraction EC at 25 and 40 C

Na+ con non-aq 25°C 100% U K1=2.1 1974KKc (5253) 58
Medium: 50% w/w EtOH/acetone. K1=1.94 to 2.23(depending upon eqn used)

Na+ con mixed 25°C 70% U I K1=2.77 1973YKa (5254) 59
Medium: 70% w/w t-butanol/H2O. K1=2.20(55%), 1.88(40%). In 89% butanol/H2O:
K1=2.78

Na+ con diox/w 50°C 30% U I K1=-0.17 1972LDa (5255) 60
In 30% w/w dioxan/H2O. K1=0.82(44.7%),1.35(54.7%),1.59(60.2%),2.09(68.4%),
2.90(75.1%),4.13(81.1%),K(NaCl+7H2O=Na+(aq)+Cl-(aq))=-11.13, DH(K)=-70.7

Na+ con diox/w 300°C 34% U I 1972YMb (5256) 61
K=-16.0
In 34.7 to 75.0% w/w dioxan-H2O at 500-4000 bars. K: NaCl+10H2O=Na+(aq)+Cl-

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Na+ con mixed 25°C 60% U I K1=1.32 1971ALc (5257) 62
Medium: 60% w/w t-butanol/H2O. K1=1.91(70%), 2.64(80%), 3.17(85%)

Na+ con none 25°C 0.0 U K1=-1.60 1971HPa (5258) 63

Na+ con non-aq 25°C 100% U K1=-0.23 1971PGa (5259) 64
Medium: N-methylformamide

Na+ con none 25°C 0.0 U K1=-0.77 1971PJa (5260) 65

Na+ con diox/w 100°C 29% U I 1971YDa (5261) 66
K=-12.7
In 29.7 to 70.5% w/w dioxan/H2O. B: NaCl+7.8H2O=Na+(aq)+Cl-(aq). 1=4000 bars

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Na+ con non-aq 25°C 100% U K1=0.40 1970CDa (5262) 67
Medium: DMSO

Na+ oth oth/un 25°C var U T K1=-0.74 1970MIa (5263) 68
Method: dilatometry. K1=-0.46(0 C), -0.96(50 C)

Na+ oth none 150°C 0.0 U T K1=-0.97 1969HEa (5264) 69
Estimated from literature data. K1=-0.42(200 C), 0.15(250 C), 0.40(270 C),
0.82(300 C)

Na+ con none 25°C 0.0 U K1=-0.04 1968CFa (5265) 70

Na+ con mixed ? ?% U K1=4.51 1968EIa (5266) 71

Medium: pentanol(wet)

Na+ con non-aq 25°C 100% U I K1=2.02 1968PIb (5267) 72
Medium: 49.9% w/w EtOH/acetone; K1=1.76(64.2%),1.49(80.9%),1.49(89.7%),
1.58(100%)

Na+ con oth/un 800°C 0.0 U T 1968QMd (5268) 73
K(Na(H2O)x+Cl(H2O)y)=17.83
K=17.14(400C),17.32(500),17.54(600),17.70(700),M units. Reaction:
Na(H2O)x+Cl(H2O)y=NaCl(H2O)x+y-10+10H2O

Na+ sol alc/w 25°C 100% U I 1967AKa (5269) 74
Kso=-1.5
Medium: MeOH. Kso=-4.0 in (Me2N)3PO

Na+ sol oth/un 25°C 0.0 U 1967LEa (5270) 75
Kso(NaCl,halite)=1.553

Na+ con none 300°C 0.0 U T K1=1.33 1963PCb (5271) 76
I=0 corr. K1=1.82(360 C). Also other temperatures

Na+ con non-aq 25°C 100% U K1=1.35 1962SHd (5272) 77
Medium: HCOOH

Na+ con mixed 25°C 80% U K1=1.5 1961AMc (5273) 78
Medium: 80% v/v acetone/H2O

Na+ con none 281°C 0.0 U T K1=0.66 1961WLa (5274) 79
I=0 corr. K1=1.03(306 C)

Na+ con alc/w 25°C 100% U K1=1.90 1957GKa (5275) 80
Medium: MeOH

Na+ gl diox/w 25°C 70% U K1=2.27 1957PGa (5276) 81

Na+ con alc/w 25°C 100% U K1=0.9 1951EKa (5277) 82
Medium: MeOH

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

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

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Na+ cal none 25°C 0.0 C IH 1992BVa (6049) 83
DH(Kso)=21.8 kJ mol-1, measured for I=0.002-0.02 M self medium.
Also data for 0.047-0.228 mol fraction MeOH/H2O.

Na+ con none 25°C 0.0 U K1=-0.49 1972DDa (6050) 84

Na+ con mixed 25°C 60% U I K1=1.18 1971ALc (6051) 85

Medium: 60% w/w t-butanol/H2O. K1=1.79(70%), 2.51(80%), 3.67(90%)

Na+ con diox/w 25°C 90% U TI K1=6.78 1966CKa (6052) 86
K1=1.22(64.5%). At 35 C, 64.5% dioxan: K1=1.23

Na+ oth oth/un 25?°C 0.0 M K1=-0.4 1966MBb (6053) 87
K(K+L)=0.0

Na+ con oth/un 18°C 0.0 U K1=-0.54? 1931BRb (6054) 88

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Na+	dis	non-aq	25°C	100%	C		K1=1.82	2004FNa	(6330)	89
							K(Na+ClO4=NaClO4(org))=-1.06			

Method: extraction from 0.5 M NaCl into propionitrile.
For extraction from 1.0 M NaCl: K1=1.55, K(Na+ClO4=NaClO4(org))=-1.29.

Na+ con non-aq 25°C 100% M K1=1.24 1999DSd (6331) 90
Medium: acetonitrile.

Na+ gl non-aq 25°C 100% U H K1=5.37 1981TMb (6332) 91
Medium: Glacial acetic acid. Alternative method: Spectrophotometry.
DH(K1)=-41 kJ mol-1

Na+ con non-aq 25°C 100% U K1=1.26 1978CAa (6333) 92
Medium: Acetonitrile

Na+ con non-aq 25°C 100% U K1=1.2 1975YKa (6334) 93
Medium: MeCN

Na+ con non-aq 25°C 100% U K1=0.32 1974HPb (6335) 94
Medium: hexamethylphosphotriamide. K1 by Pitts eqn. By Fuoss-Hsia: 1.13

Na+ oth non-aq 25°C 100% U T H K1=-0.80 1974PKc (6336) 95
Medium: acetone. DH(K1)=2.9 kJ m-1.K1=-1.15(-90 C),-0.96(-45 C),-0.92(-25 C)
-0.85(0 C),-0.70(45 C). Method: infrared spectra

Na+ con mixed 25°C 15% U I K1=2.96 1974SPc (6337) 96
in 15% w/w THF/H2O.K1=3.00(30%),2.93(40%),2.35(50%),2.54(60%),2.70(70%),
2.83(80%),3.36(90%),4.20(95%),4.54(97%),5.23(98%),5.91(100%)

Na+ con alc/w 25°C 100% U K1=1.28 1972DAa (6338) 97
Medium: MeOH

Na+ con non-aq 25°C 100% U K1=2.81 1971BHa (6339) 98
Medium: acetone

```
Na+        con none   25°C  0.0  U        K1=-0.7        1971DAa  (6340)  99
-------------------------------------------------------------------------------
Na+        con non-aq 25°C 100%  U        K1=0.34        1971PGa  (6341) 100
Medium: N-methylformamide
-------------------------------------------------------------------------------
Na+        con mixed  25°C  70%  U  I     K1=1.38        1970ALa  (6342) 101
Medium: 70% w/w t-butanol/H2O. K1=2.09(80%), 2.55(85%), 3.25(90%)
-------------------------------------------------------------------------------
Na+        EMF mixed  25°C 0.10M U  I     K1=3.9         1970DCa  (6343) 102
Medium: dimethoxy-1,2-ethane, 0.1 M H2O. K1=4.1(H2O conc.:0.01 M)
-------------------------------------------------------------------------------
Na+        con non-aq 25°C 100%  U        K1=1.0         1967KHe  (6344) 103
Medium:MeCN
-------------------------------------------------------------------------------
Na+        oth non-aq 17°C 100%  U                       1966BPd  (6345) 104
                                        K(2NaL=Na2L2)=0.40
                                        K(3NaL=Na3L3)=1.2
                                        K(HL+NaL)=1.67
                                        K(2HL+NaL)=2.68
Method:freezing point. Medium:MeCOOH
-------------------------------------------------------------------------------
Na+        con non-aq 25°C 100%  U T      K1=1.56        1966MWb  (6346) 105
Medium: MeCN, also at 20 C, 30 C
-------------------------------------------------------------------------------
Na+        con non-aq 106°C 100%  U        K1=5.13       1962MAa  (6347) 106
                                        K(NaL+Na)=1.5
Medium: CH3CO2H
-------------------------------------------------------------------------------
Na+        con non-aq 25°C 100%  U        K1=1.85        1962MWa  (6348) 107
Medium: MeCN
-------------------------------------------------------------------------------
Na+        con mixed    ?   91%  U  I     K1=2.34        1958WEa  (6349) 108
Medium: ethanoic acid/H2O. K1=3.28 (95% HAc)
-------------------------------------------------------------------------------
Na+        EMF non-aq 25°C 100%  U        K1=5.48        1956BKa  (6350) 109
Medium: CH3CO2H
*******************************************************************************
CrO4--                H2L    Chromate         CAS 7738-94-5  (2382)
Chromate;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Na+        oth none   25?°C  0.0  M        K1=0.7         1966MBb  (6498) 110
*******************************************************************************
F-                     HL    Fluoride         CAS 7644-39-3  (201)
Fluoride;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Na+        ISE non-aq 25°C 100%  C                       1996NHa  (7031) 111
```

Kso(NaF)=-10.0
Medium: acetonitrile, 0.01 M Bu4NPF6.
Method: anion-responsive Co phthalocyanin-polymer electrode.

Na+ sp oth/un 25°C 1.0M U I K1=0.25 1993MAa (7032) 112
K1 values over a range of pressures and ionic strengths

Na+ sp NaCl 25°C 0.10M U K1=0.71 1992UAa (7033) 113
Data over pressure range 1 - 2000 atmos.

Na+ ISE NaClO4 25°C 1.0M U TI K1=-0.7 1984CTd (7034) 114

Na+ ISE KNO3 25°C 1.00M C I K1=-0.70 1984HCa (7035) 115
Also in 0.1 M KClO4 (K1=-0.33).

Na+ con none 25°C 0.0 U K1=-0.24 1972DRa (7036) 116

Na+ ISE none 25°C 0.0 U K1=-0.27 1971RDa (7037) 117

Na+ ISE NaCl 25°C 1.0M U K1=-0.79 1970BHa (7038) 118

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HPO3-- H2L Phosphite CAS 13598-36-2 (6305)
Phosphite;

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

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Na+ oth R4N.X 25°C 1.0M U K1=0.61 B2= 0.16 1983TTa (7513) 119
Method: Donnan exclusion chromatography. Medium: 1.0 M Me4NCl.

Na+ con oth/un 20°C 0.0 U K1=1.05 1964FPa (7514) 120
K(Na+HL)=0.96

****

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

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

---

Na+ oth non-aq 25°C 100% U K1=0.36 B2=0.51 1974BLa (7600) 121
Method:partial pressure. Medium:propene carbonate. By N.M.R., K1=0.26

Na+ ISE non-aq 25°C 100% U I K1=0.25 B2=0.25 1974INa (7601) 122
Medium: CH3CN, I=0.1(Et4N.picrate). Also in acetone and 0.01, 0.1 NaClO4

Na+ nmr non-aq 27°C 100% U K1=0.06 1973BBd (7602) 123
Method:N.M.R.,Medium:Me2SO

Na+ nmr non-aq 26°C 100% U 1972GEa (7603) 124
K4=0.97
Method:N.M.R.,Medium:THF: K4=0.91 to 1.02. By conductivity, 22 C, K4=1.2-1.5

Na+ nmr non-aq 36°C 100% U K1=0.15 1971CBc (7604) 125
Method:N.M.R.,Medium:propene carbonate

Na+ sol non-aq 25°C 100% U K1=0.3 B2=0.5 1967CKa (7605) 126
Medium: MeCN
****
H2PO2- HL Hypophosphite CAS 6303-21-5 (6304)
Hypophosphite;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ oth R4N.X 25°C 1.0M U K1=-0.04 1983TTa (7649) 127
Method: Donnan exclusion chromatography. Medium: 1.0 M Me4NCl.
****
I- HL Iodide CAS 10034-85-2 (20)
Iodide;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ con non-aq 25°C 100% U I K1=0.84 1982GCb (8249) 128
Medium: DMF and 1,1,3,3-Tetramethylurea. Further data for other media
available for a wide variety of mixed media

Na+ con non-aq 25°C 100% U K1=2.74 1982GRb (8250) 129
Medium: octanol

Na+ con non-aq 25°C 100% U K1=0.86 1976RMa (8251) 130
Medium: 3-methylsulfonate

Na+ con non-aq 25°C 100% U K1=0.43 1974HPb (8252) 131
Medium: hexamethylphosphotriamide. Calculated using Pitts eqn. By Fuoss-Hsia
K1=0.98

Na+ con non-aq 25°C 100% U I K1=1.10 1974LTa (8253) 132
Medium: 17% CCl4/DMF. K1=1.50(27.5%), 1.58(32,7%), 2.10(42.6%), 2.11(47.0%),
2.69(53.0%), 3.00(60.0%), 3.84(69.0%)

Na+ con alc/w 25°C 100% U TIH K1=1.28 1974SKa (8254) 133
Medium: MeOH. DH(K1)=-5.0 kJ mol-1. K1=1.31(5 C), 1.19(45 C). In EtOH:
DH(K1)=7.9. K1=1.86(5 C), 1.74(45 C). In nonyl alcohol: DH=50; K1=4.18(5 C)

Na+ con non-aq 25°C 100% U T H K1=2.65 1974SKa (8255) 134
Medium: butanol. DH(K1)=29.3 kJ mol-1. K1=2.43(5 C), 2.95(35 C), 3.10(45 C).
In heptanol: DH=21; K1=4.02(15 C), 4.41(45 C). Also all alcohols to nonanol
---
Na+ con non-aq 25°C 100% U I K1=2.16 1974SPd (8256) 135
7.15% methylpropionate/MeNO2. K1=2.13(0%), 2.35(14.8%), 2.44(22.9%), 2.80
(31.6%), 2.99(40.9%), 3.47(51.0%), 3.74(61.8%), 4.45(73.5%), 4.97(86.2%)

Na+ con non-aq 25°C 100% U T K1=2.71 1973KKa (8257) 136

Kt(Na+NaI)=1.12
Medium: i-propanol. K1=2.19(10 C), K1=2.48(20 C); K1=2.78, Kt=1.16(30 C); K1=3.07, Kt=1.26(50 C);); K1=3.37, Kt=1.42(70 C); K1=3.52, Kt=1.72(85 C)

Na+ con non-aq 25°C 100% U K1=4.08 1973TKb (8258) 137
Medium: liquid SO2

Na+ con mixed 25°C 89% U K1=2.34 1973YKa (8259) 138
Medium: 89% w/w butanol/H2O

Na+ con non-aq 25°C 100% U K1=2.14 1972IWa (8260) 139
Medium: acetone

Na+ con alc/w 25°C 93.7M U K1=1.12 1971BPa (8261) 140
Medium: 93.7% w/w EtOH/H2O

Na+ con non-aq 25°C 100% U K1=2.05 1971HNb (8262) 141
Medium: propanol

Na+ con non-aq 25°C 100% U I K1=1.46 1971LTa (8263) 142
Medium: 19.5% w/w CCl4/MeOH. K1=1.64(33.0%), 1.80(42.8%), 1.92(53.6%), 2.27 (57.9%),2.37(61.5%),2.55(64.5%),3.13(73.1%). Also CCl4/EtOH, dioxan/EtOH

Na+ con alc/w 25°C 100% U I K1=0.34 1970BWc (8264) 143
Medium: MeOH. K1=0.93 (EtOH)

Na+ EMF non-aq 25°C 100% U K1=-0.26 1970SAb (8265) 144
Medium: propene carbonate.

Na+ con oth/un 400°C 0.0 U T H 1969DMc (8266) 145
K(NaI+9.67H2O=Naaq+Iaq)=-15.87
Up to 4 kbars. DH(K)=-29.3 kJ mol-1; K=-16.12(500 C), -16.32(600 C), -16.52(700 C), -16.71(800 C) also 450, 550, 650, 750 C

Na+ con diox/w 25°C 10% U I K1=0.96 1969SLa (8267) 146
Medium: w/w dioxan/DMF. K1=1.36(20%), 1.65(30%), 1.78(40%), 1.97(45%), 2.18 (50%), 2.43(55%), 2.68(60%), 3.11(65%), 3.51(70%), 4.06(75%), 4.81(80%)

Na+ con non-aq 25°C 100% U K1=0.79 1969TAa (8268) 147
Medium: MeCN

Na+ con alc/w 25°C 100% U I K1=1.28 1968SLa (8269) 148
Medium:MeOH. K1=2.39(EtOH). Also K1 values for mixed dioxan/MeOH,dioxan/EtOH

Na+ con non-aq 25°C 100% U I K1=0.91 1967JTa (8270) 149
Medium: MeCN. K1=2.57(EtCOMe),2.08(PhCOMe),3.31(pyridine),0.97(HOC2H4NH2), 1.88(C6H5CN),1.90(acetone),2.03(PrOH),2.75(diaminoethane)

Na+ con non-aq 25°C 100% U K1=3.00 1965BFb (8271) 150
Medium: diaminoethane

Na+ con non-aq 25°C 100% U K1=2.34 1957HUa (8272) 151
Medium: PhCOMe. Alternative values K1=2.64, 2.23. In EtCOMe K1=2.61
****
IO3- HL Iodate CAS 7782-68-5 (1257)
Iodate;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ con none 25°C 0.0 U K1=-0.30 1971JBa (8535) 152

Na+ con none 25°C 0.0 U K1=-0.31 1969BJa (8536) 153

Na+ con none 18°C 0.0 U K1=-0.47 1927DAb (8537) 154
****
IO4- HL Periodate CAS 13444-71-8 (6063)
Periodate;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ cal none 25°C 0.0 C IH 1992BVa (8610) 155
DH(Kso)=32.9 kJ mol-1, measured for I=0.002-0.02 M self medium.
Also data for 0.047-0.228 mol fraction MeOH/H2O.
****
MnO4- HL Permanganate CAS 13456-41-3 (5678)
Manganate(VII), Permanganate;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE none 25°C 0.0 C 2003KUa (8634) 156
K(NaA+L)=2.36
K(Na+A(org)+L=NaAL(org))=2.58
Distribution from water into 1,2-dichloroethane. Na ISE in aqueous phase.
Calc. from data for self-medium, I < 0.004 M. A is 18-crown-6.
****
MoO4-- H2L Molybdate (443)
Molybdate;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp oth/un 25°C ? U M 1997STa (8741) 157
K(2Na+H2L=Na2L+2H)=-2.6
Ligand: nano-Molibdenomanganate, MnMo9O32------
****
NO2- HL Nitrite CAS 7782-77-6 (635)
Nitrite;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ cal none 25°C 0.0 C IH 1992BVa (9389) 158

DH(Kso)=13.8 kJ mol-1, measured for I=0.002-0.02 M self medium.
Also data for 0.047-0.228 mol fraction MeOH/H2O.

Na+ sp non-aq 25°C 100% U K1=1.13 1979ITa (9390) 159
Medium: N,N-Dimethylacetamide. Method: Raman spectroscopy

Na+ con oth/un 25°C 0.0 U K1=-0.42 1964PSh (9391) 160

****

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

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

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Na+ con non-aq 25°C 100% C T K1=1.66 2001SSa (9781) 161
Medium: N,N-dimethylformamide. Data for -40 to 25 C.

Na+ sp non-aq 25°C 100% U K1=0.415 1979ITa (9782) 162
Medium: N,N-Dimethylacetamide. Method: Raman spectroscopy

Na+ con non-aq 25°C 100% U K1=1.31 1974HPb (9783) 163
Medium: Hexamethylphosphotriamide. K=1.44 using Fuoss-Hsia equation.

Na+ con mixed 25°C 50% U K1=2.2 1974KKc (9784) 164
Medium:1:1 EtOH-Me2CO. K1=2.07 to 2.32 depending upon equation

---

Na+ oth NaNO3 25°C var U K1=-0.85 1974SOa (9785) 165
K(2NaL(H2O)3=(NaL)2+6H2O]=9
Method: dilatometry,densimetry

Na+ con mixed 20°C 89% U K1=2.26 1973YKa (9786) 166
Medium: 89% BuOH/H2O

Na+ con diox/w 25°C 60% U I K1=1.10 1972KAc (9787) 167
In 70% dioxan K1=2.03; 80%: 3.30

Na+ sp oth/un 25°C 0.0 U K1=-1.22 1972RLa (9788) 168
Medium: D2O. Method: Raman spectra

Na+ con diox/w 25°C 60% U I K1=1.58 1972RYa (9789) 169
In 0% dioxan K1=-0.70; 20.4%: 0.72; 39.8%: 0.93; 49.8%: 1.08;
70%: 1.55; 79.1%: 2.59

Na+ con non-aq 25°C 100% U K1=3.05 1971BCa (9790) 170
Medium: Tetramethylurea

Na+ con oth/un 25°C 0.0 U K1=-0.55 1971JBa (9791) 171

Na+ con oth/un 25°C 0.0 U K1=-0.57 1969BJa (9792) 172

Na+ con diox/w 25°C 79% U I K1=3.04 1969SBe (9793) 173

In 65.7% dioxan K1=1.04; 70.3%: 1.85; 72.8%: 2.17

Na+ con mixed 25°C 70% U I K1=1.92 1969SBe (9794) 174
Medium: MeOH-dioxan mixtures. 46.8% MeOH: K1=3.20; 49.8%: 2.99; 54.8%: 2.62; 100%: 0.70

Na+ oth oth/un 25?°C 0.0 U K1=-0.2 1966MBb (9795) 175

Na+ con oth/un 18°C 0.0 U K1=-0.59 1927DAb (9796) 176

****

N3- HL Azide CAS 7782-79-8 (441)
Azide;

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

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Na+ sol alc/w 0°C 100% U T 1967AKa (10244) 177
Kso=-0.9
Kso=-1.9 in Me2NCHO(25 C), Kso=-0.64 in DMSO(25 C)

****

OH- HL Hydroxide (57)
Hydroxide;

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

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Na+ nmr R4N.X 25°C 3.4M C K1=-1.0 2002PLa (11769) 178
NMR Na-23 under assumption that substitution of Cl for OH does not affect chemical shift, which is a rough approximation;Medium: 3.4 M Me4NCl/Me4NOH

Na+ cal oth/un 325°C 0.10M C TIH K1=0.68 1992CGe (11770) 179
Medium: 0.5-9.8 m NaOH. Data for 250-325 C. DH(K1)=145.0 kJ mol-1, DS(K1)=255 J K-1 mol-1.

Na+ con mixed 25°C 80% M K1=0.85 1971KKd (11771) 180
Medium: 80% w/w propanol/H2O

Na+ EMF non-aq 20?°C 100% U K1=8.0 1967PBa (11772) 181
Medium: THF, 0.1 M Bu4NClO4. H electrode

Na+ con none 218°C 0.0 U K1=0.26 1961WLa (11773) 182

Na+ EMF diox/w 25°C 45% C I K1=0.46 1959NMb (11774) 183
In 70% w/w dioxan K1=2.1. Method: H electrode

Na+ EMF none 25°C 0.0 C T K1=-0.57 1954GMb (11775) 184
K1=-0.45(5 C),-0.46(15 C),-0.72(35 C),-0.62(45 C). Method: H electrode

---

Na+ kin none 25°C 0.0 U K1=-0.70 1949BPb (11776) 185

****

O2 L Oxygen CAS 7782-44-7 (83)
Dioxygen, also oxide; O--, and superoxide, O2-

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--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Na+        kin oth/un 27°C  var  U                        1969LHa (12631) 186
                                          K(Na+O3-)=0.35
Ligand: ozonide.  Medium: NaOH
********************************************************************************
PF6-                   HL                        (2404)
Hexafluorophosphate;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Na+        con non-aq 25°C 100%  U        K1=1.1          1975YKa (12766) 187
Medium: MeCN
********************************************************************************
PO4---                 H3L    Phosphate        CAS 7664-38-2  (176)
Phosphate;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Na+        gl  none   25°C  0.0  C TI     K1=1.43         1991DDa (13257) 188
                                          B(NaHL)=13.40
                                          B(NaH2L)=19.81
                                          B(Na2L)=2.59
                                          B(Na2HL)=13.32
Data also for 10-50 C and 0.04-1.0 M NaCl, KCl or Et4NI
--------------------------------------------------------------------------------
Na+        gl  NaNO3  25°C 0.70M C                       1988MFa (13258) 189
                                          K(Na+H2L)=-0.31
                                          K(Na+HL)=0.11
--------------------------------------------------------------------------------
Na+        gl  NaNO3  37°C 0.15M C        K1=0.75         1983DGa (13259) 190
                                          K(Na+HL)=0.65
                                          K(Na+H2L)=0.1
--------------------------------------------------------------------------------
Na+        oth R4N.X  25°C  1.0M U        K1=0.86   B2= 0.24  1983TTa (13260) 191
Method: Donnan exclusion chromatography. Medium: 1.0 M Me4NCl.
--------------------------------------------------------------------------------
Na+        gl  oth/un 25°C 0.68M C        K1=0.52         1976ACc (13261) 192
                                          K(Na+HPO4)=0.05
                                          K(Na+H2PO4)=-0.54
Medium: NaCl/MCl2 mixtures.
--------------------------------------------------------------------------------
Na+        sol none   25°C  0.0  U                       1974PGa (13262) 193
                                          K(Na+HPO4)]=0.85
--------------------------------------------------------------------------------
Na+        gl  R4N.X  25°C 0.20M U T HM                  1956SAc (13263) 194
                                          K(Na+HL)=0.60
Medium: Pr4NCl. K=0.08(0 C); DH(K)=25 kJ mol-1, DS=100 J K-1 mol-1
********************************************************************************
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P2O6---- H4L Hypophosphate CAS 9803-60-3 (199)
Hypophosphate;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	gl	R4N.X	25°C	0.50M	U		K1=0.50	1967CMc (13416)	195

Ligand: O3POPHO2---, Medium: Me4NCl

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	con	oth/un	25°C	0.0	U		K1=2.31 K(Na+HL)=1.32	1967NSa (13417)	196

****

P2O7---- H4L Pyrophosphate CAS 2466-09-3 (198)
Diphosphate; from (HO)2PO.O.PO(OH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	gl	NaCl	25°C	0.25M	U	I	K1=1.5 B(NaHL)=9.8 B(NaH2L)=15.3 B(Na2L)=2.6 B(Na2HL)=9.7	1994SFb (13625)	197

Medium: Me4NCl. At I=0 corr. K1=2.4, B(NaHL)=11.3, B(NaH2L)=17.2, B(Na2L)=4.1, B(Na2HL)=11.5

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	gl	NaNO3	25°C	0.10M	C	TIH	K1=1.33 B(NaHL)=9.86 B(NaH2L)=15.4 B(Na2L)=2.67 B(Na2HL)=9.75	1985DRb (13626)	198

Data at 10-45 C and I=0.02-1.0 M. DH(K1)=-1 kJ mol-1; DS=20. DH(NaHL)=-6; DS=165. DH(Na2L)=-3; DS=38. DH(Na2HL)=-2; DS=177 (by T coeff).

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	gl	KCl	25°C	0.50M	U		K1=1.94 K(Na+HL)=0.69	1982DNa (13627)	199
Na+	gl	R4N.X	25°C	0.50M	C		K1=1.94 K(Na+HL)=0.68 K(NaL+H)=7.2 K(Na+H2L=NaHL+H)=5.3	1979DHa (13628)	200

Medium: 0.50 M Me4NCl.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	cal	R4N.X	5°C	1.00M	U	H		1973VAa (13629)	201

Medium: Me4NNO3, DH(K1)=1.9 kJ mol-1. 35 C, I=0, DH(K1)=5.7

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	gl	KNO3	25°C	2.00M	U	I	K1=0.21 K(NaL+Na)=-0.78 K(Na+HL)=-0.51	1964PCa (13630)	202

At I=0 corr. K1=2.22, K(NaL+Na)=2.40, K(Na+HL)=1.52

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	gl	none	25°C	0.0	U	T	K1=2.3	1959WOa (13631)	203

K1=2.3(40 C)

Na+ gl R4N.X 25°C 1.00M U K1=1.00 1957LWa (13632) 204
Medium:Me4NCl

Na+ con none 25°C 0.0 U K1=2.35 1949MOa (13633) 205
K(NaL+Na)=1.3
K(Na+HL)=1.3

****

P2O8---- H4L CAS 13825-81-5 (2402)
Peroxodiphosphate, also cyclic metaposphates, thiophosphates etc.;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	kin	NaNO3	65°C	1.0M	C		K(Na+HP2O8)=0.70	1985GGb (13694)	206

Ligand is peroxydisulfate, S2O8----

Na+ con none 25°C 0.0 U K1=4.3 1972KOb (13695) 207
Ligand:metaphosphates,cyclic;(PO3)6 6-, Additional Method:activity coefficient, K1=9.7,K2=6.0,K3=3.7(act)

Na+ con none 25°C 0.0 U K1=4.6 1972KOb (13696) 208
Ligand:metaphosphates,cyclic;(PO3)8 8-, Additional Method:activity coefficient, K1=15,K2=11,K3=7,K4=4(act)

Na+ gl R4N.X 25°C 1.00M U K1=1.02 1960CEa (13697) 209
K(Na+HL)=0.25
Medium: Me4NCl

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	gl	R4N.X	25°C	1.0M	U		K1=2.55	1982CCb (13726)	210
							K(Na+HL)=0.6		
							K(Na+H2L)=-0.6		

alpha2 isomer. For alpha1 isomer, K1=0.7, K(Na+HL)=-0.3

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	gl	NaCl	25°C	0.25M	U	I	K1=1.5	1994SFb (13884)	211
							B(NaHL)=10.0		
							B(NaH2L)=14.9		
							B(NaH3L)=15.7		
							B(Na2L)=3.7		

Medium: Me4NCl. B(Na2HL)=10.2. At I=0 corr. K1=2.5, B(NaHL)=11.7, B(NaH2L)=17.2, B(NaH3L)=18.3, B(Na2L)=5.2, B(Na2HL)=12.5

Na+ gl NaNO3 25°C 0.10M C TIH K1=1.43 1985DRb (13885) 212
B(NaHL)=9.81
B(Na2L)=3.16

Data at 10-45 C and I=0.02-1.0 M. DH(K1)=-18 kJ mol-1; DS(K1)=-35. DH(NaHL)=-10; DS(NaHL)=151. DH(Na2L)=-19; DS(Na2L)=-7. (by T coeff)

Na+ gl none 25°C 0.0 U T K1=2.8 1959WOa (13886) 213
K1=2.8(40 C)

Na+ gl R4N.X 25°C 1.00M U K1=1.64 1957WLa (13887) 214
K(Na+HL)=0.77

Medium: Me4NCl

Na+ con oth/un 25°C var U 1954WDb (13888) 215
B(Na2L)=3.8

Medium: Na5L

Na+ con none 25°C 0.0 U K1=2.57 1949MOa (13889) 216

****

P3O9--- H3L CAS 13566-25-1 (235)
Cyclotrimetaphosphate;

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

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Na+ ISE none 25°C 0.0 U K1=1.40 1969GNa (13964) 217

Na+ EMF R4N.X 25?°C 0.6?M U K1=-0.1 1958INa (13965) 218
B(Na2L)=0.0

Na+ con none 25°C 0.0 U K1=1.17 1949DMa (13966) 219

****

P4O12---- H4L CAS 13598-74-8 (234)
Cyclotetrametaphosphate;

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

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Na+ gl R4N.X 25°C 0.10M U K1=1.82 1976KOb (14013) 220

Na+ con none 25°C 0.0 U K1=2.15 1972KOb (14014) 221

Na+ ISE none 25°C 0.0 U K1=2.12 1969GNa (14015) 222

Na+ EMF R4N.X 30°C 1.00M U K1=0.81 1955GGa (14016) 223

Medium: Me4NNO3

Na+ con none 25°C 0.0 U K1=2.05 1949DMa (14017) 224

****

P4O13------ H6L Tetraphosphate (1102)
Tetraphosphate;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ gl R4N.X 25°C 1.0M U K1=1.79 1967WMa (14050) 225
K(Na+HL)=1.10
Medium: Me4NCl
****
P6O12------ H6L CAS 25268-83-1 (6590)
Dodecaoxohexaphosphate(III); anion of (PO.OH)6

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ gl R4N.X 25°C 1.0M U K1=1.02 1960CEa (14062) 226
K(Na+HL)=0.25
Medium: Me4NCl
****
P6O18------ H6L (233)
Cyclohexametaphosphate;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ gl R4N.X 25°C 0.10M U K1=2.40 B2=4.70 1976KOb (14072) 227
****
P8O24-------- H8L (232)
Cyclooctametaphosphate;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ gl R4N.X 25°C 0.10M U K1=2.70 B2=5.30 1976KOb (14084) 228
****
SCN- HL Thiocyanate CAS 463-56-9 (106)
Thiocyanate;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ cal none 25°C 0.0 C IH 1992BVa (15173) 229
DH(Kso)=6.7 kJ mol-1, measured for I=0.002-0.02 M self medium.
Also data for 0.047-0.228 mol fraction MeOH/H2O.

Na+ cal NaClO4 25°C 0.50M U H K1=0.97 B2=1.17 1988ISb (15174) 230
B4=3.41
Solution contained 10% w/w Triton X-100. DH(K1)=-11.6 kJ mol-1, DH(B2)=-24,
DH(B4)=-41.6. DS(K1)=-20 J K-1 mol-1, DS(B2)=-58, DS(B4)=-74.

Na+ sp non-aq 25°C 100% U K1=-0.319 1979ITa (15175) 231
Medium: N,N-Dimethylacetamide. Method: Raman spectroscopy

Na+ con non-aq 25°C 100% U 1976DCa (15176) 232

K(NaA+NCS)=3.15
In nitrobenzene. In 70% C6H5NO2/30% toluene, K=4.22, in 50%/50%, K=5.30
A=Dinitro-18-crown-6.

Na+ con non-aq 25°C 100% U K1=2.40 1976RMa (15177) 233
Medium: 3-methylsulfonate

Na+ con non-aq 25°C 100% U I K1=1.08 1976RMb (15178) 234
Medium: 1,3-Dimethylethyleneurea. In 1,3-Dimethylpropyleneurea K=0.67

Na+ con non-aq 25°C 100% U K1=1.92 1973GKb (15179) 235
Medium: MeCN, I=0 corr

Na+ con non-aq 25°C 100% U K1=5.07 1973TKb (15180) 236
Medium: Liquid SO2, I=0 corr

Na+ con non-aq 25°C 100% U K1=1.83 1971BCa (15181) 237
Medium: tetramethylurea, I=0 corr

Na+ con non-aq 25°C 100% U K1=0.02 1971PGa (15182) 238
Medium: MeHNCHO

Na+ con non-aq 25°C 100% U K1=1.94 1971SKa (15183) 239
Medium: MeCN, I=0 corr

Na+ dis none 20°C 0.0 U TI 1962ACa (15184) 240
Kd=-0.47
Kd: K(Na+L+nH2O=NaL(H2O)n(in TBP)); Kd=-0.70(30 C), -0.91(40 C)(n varies)
In TBP, K1=ca.4

Na+ con non-aq 30°C 100% U K1=4.08 1959CAa (15185) 241
Medium: TBP(moist)

****

SO3-- H2L Sulfite CAS 7782-99-2 (801)
Sulfite;

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

---

Na+ gl R4N.X 25°C 1.0M C I K1=0.47 1997CHa (15468) 242
Medium: 1.0 M Me4NCl. For I=1.0 M KCl: K1=-0.31.

****

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

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

---

Na+ sp oth/un 25°C 0.50M C TIH K1=0.76 2000KHc (16362) 243
Method: Raman spectroscopy. Medium: 0.50 M CsCl. Data for 0.5-4.0 M CsCl.

Na+ sp oth/un 25°C 0.0 C I K1=0.83 1999BCd (16363) 244

Method: dielectric relaxation spectroscopy. Data for 0.025-1.603 M Na2SO4.

Na+ ISE oth/un 25°C 0.0 C K1=0.834 1999CHa (16364) 245
Method: Na ISE. Media 0.50-7.00 M CsCl and 1.0 M Me4NCl
In 1.0 M Me4NCL, K1=0.093. In 1.0 M CsCl, K1=-0.150.

Na+ ISE oth/un 50°C 0.0 M TIH K1=0.72 1995PSc (16365) 246
Method: Na ISE. Data for 0.1 M NaCl/0.05 M Na2SO4 and 0.25 M NaCl/
0.125 M Na2SO4. Data for 50-200 C. DH(K1)=-2.7 kJ mol-1. At 25 C, K1=0.92.

Na+ ISE NaClO4 25°C 1.0M U K1=0.61 1992LVa (16366) 247

Na+ cal NaCl 150°C 0.0 C T H K1=0.95 1988OIa (16367) 248
Method: flow calorimetry. DH(K1)=24.68 kJ mol-1, DS(K1)=77 J K-1 mol-1.
Data for 150-320 C.

Na+ gl NaClO4 25°C 0.10M U TI K1=0.62 1988SRa (16368) 249
I=0, 40 C: K1=0.82; I=1.0, 40 C: 0.66; I=0, 10 C: 0.72; I=0.5, 10 C: 0.35;
I=0.5, 25 C: 0.44

Na+ ISE NaClO4 25°C 0.10M U I K1=0.58 1983ILa (16369) 250

Na+ gl NaCl 37°C 0.10M C I K1=0.40 1982DRb (16370) 251
Data for I=0.03-0.50 M NaCl. At I=0.0 M, K1=0.72

Na+ oth oth/un 25°C 0.30M U TI K1=0.82 1980GAb (16371) 252
Method: Ultrasonic absorption. In 0.5 M Na2SO4, 15 C: K1=0.69; 5 C: 0.66

Na+ ISE oth/un 25°C 0.21M C K1=0.57 1979EFa (16372) 253
Method: Na ion selective electrode. Medium: 0.12-0.22 M NaCl/Na2SO4.
At I=0.12 M, K1=0.73

Na+ gl NaCl 25°C 0.70M U K1=0.26 1978EWa (16373) 254

Na+ con none 25°C 0.0 U 1978FFa (16374) 255
K(Na+NaSO4)=0.100

Na+ con none 25°C 0.0 C K1=1.03 1977FFa (16375) 256
P=1 atm. Also data for P=250-2000 atm.

Na+ sol oth/un 25°C 0.70M C K1=0.086 1975EWa (16376) 257
Mixed medium of NaCl, KCl, MgCl2, NaClO4, Mg(ClO4)2, Na2SO4.
Method: solubility of gypsum.

Na+ con oth/un 25°C dil C K1=1.013 1975FFd (16377) 258
Self medium, 0.005-0.06 M.

Na+ oth oth/un 25°C 0.0 C K1=1.14 1975FIa (16378) 259
Method: ultrasonic sound absorption. Value at I=0.0 M from data for
0.017 M MgSO4 + 0.017 M NaCl.

Na+ oth oth/un 25°C .242M U K1=0.94 1975REa (16379) 260

Na+ ISE oth/un 25°C 0.50M U K1=0.40 1975SCb (16380) 261

Na+ oth none 20°C 0.0 U T K1=0.69 1974MVa (16381) 262
Method: chemical analysis. K1=0.79(40 C), 0.90(60 C), 0.99(80 C),
1.11(98 C)(m units)

Na+ ISE NaCl 2.4°C 0.60M U H K1=0.53 1970KPa (16382) 263
DH(K1)=-15.9 kJ mol-1. Pressure 1-1000 atm: Dv1=15.8 cm3

Na+ cal none 25°C 0.0 U H K1=0.65 1969IEa (16383) 264
DH(K1)=-2.0 kJ mol-1, DS=5.4 J K-1 mol-1

Na+ ISE oth/un 25°C var U K1=0.31 1969PKa (16384) 265
Medium:seawater (0.3 < I < 1)
K1(not logK1) = 2.73-2.58I+2.28I^2

Na+ sol oth/un 25°C 6.0M U 1969YMb (16385) 266
K1 < -4.15
Medium: 6 M Na2SO4

Na+ oth none 25°C 0.0 M K1=0.9 1966MBb (16386) 267
Estimated values also K1=1.0(K), 0.8(Rb), 0.8(Cs), 1.1(NH4)

Na+ cal oth/un 25°C 0.0 U H 1962AMe (16387) 268
DH(K1)=4.6 kJ mol-1

Na+ sol non-aq 25°C 100% U 1962KCa (16388) 269
K(NaHL(s)=Na+HL)=-6.5
Medium: MeCN

Na+ gl oth/un 25°C 1.50M U K1=<-0.9 1961PEa (16389) 270
Medium: Na2SO4

Na+ oth KNO3 -3°C sat U K1=0.14 1960SFb (16390) 271
Method: freezing point

Na+ oth oth/un 0°C 0.0 U K1=1.38 1959KEb (16391) 272
Method: freezing point

Na+ sp alc/w 25°C 20% U K1=0.9 1957BDb (16392) 273
Medium: 20% EtOH

Na+ con oth/un 25°C 0.0 U K1=0.72 1950JMa (16393) 274

Na+ con oth/un 18°C 0.0 U K1=0.70 1930RDa (16394) 275
****
S2O3-- H2L Thiosulfate CAS 73686-28-7 (177)

Thiosulfate;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	cal	R4N.X	25°C	0.50M	U		K1=0.035	1997MKa (16875)	276
DH(K1)=4.5 kJ mol-1									
Na+	ISE	NaClO4	25°C	1.00M	U		K1=0.15	1977PGa (16876)	277
Na+	ISE	NaCl	25°C	1.00M	U		K1=0.17	1975SPa (16877)	278
Using UV: K1=0.10									
Na+	cal	oth/un	25°C	0.50M	U	H	K1=0.04	1974ARa (16878)	279
DH=4.60 kJ mol-1.									
Na+	oth	oth/un	25?°C	0.0	U		K1=0.8	1966MBb (16879)	280
Na+	con	alc/w	25°C	44%	U		K1=1.84	1956BMa (16880)	281
Medium: 44% EtOH, also for MeOH/H2O									
Na+	sp	alc/w	25°C	50%	U		K1=2.15	1956TMa (16881)	282
Medium: 50% EtOH									
Na+	sp	none	25°C	0.0	U	T	K1=0.58	1955GMa (16882)	283
K1=0.55(15 C), 0.60(35 C)									
Na+	sol	none	25°C	0.0	U		K1=0.68	1951DMb (16883)	284

****

SiO3-- H2L Silicate CAS 7699-41-4 (747)

Silicate; SiO2(OH)2--

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	sol	oth/un	135°C	0.0	U	T	K(Na+HL)=1.18	1974SEb (17216)	285
K(Na+HL)=1.15(179 C), 1.11(217 C), 1.29(269 C), 1.40(301 C)									
Na+	oth	none	150°C	0.0	U	T	*Ks(NaAlSi3O8+4H)=0.31	1969HEa (17217)	286
Low albite. Method:estimated data.*Ks=0.75(high albite),4.18(NaAlSi2O6H2O), 7.62(NaAlSiO4),-2.34(montmorillonite),also other data for Temp.range 60-300C									

****

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

alpha-Heterosilicon-polytungstate;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	gl	R4N.X	25°C	1.0M	U		K1=2.75	1982CCb (17239)	287

****

TcO4- HL CAS 13568-38-2 (1418)

Pertechnetiate;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	dis	NaNO3	25°C	1.0M	U			1960BLa (17250)	288

Kd(Na+L)=-0.56(in cyclohexanol). Kd(H+L)=1.66

****

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
Na+	gl	NaClO4	25°C	1.00M	U			1975KIc (17385)	289
							K(Na+H7PV12O36)=2.29		
Na+	gl	R4N.X	20°C	1.0M	U	I	K1=0.3	1963SGd (17386)	290

Medium: Me4NCl. In 0.1 M Me4NCl: K(Na+H15L10)=0.7, K(Na+H14L10)=1.6, K(Na+NaH14L10 5-)=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
Na+	con	non-aq	30°C	100%	U		K1=7.19	1954JGa (17626)	291

Medium: ethanoic acid

****

CH4O L Methyl alcohol CAS 67-56-1 (597)

Methanol; CH3.OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	nmr	mixed	25°C	?	U	M		1976DLa (17888)	292
							K(NaA4+4L=NaL4+4A)=1.15		

Medium: tetrahydrofuran/MeOH. A=tetrahydrofuran

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	kin	alc/w	25°C	?	U	T	K1=1.6	1975LSd (17889)	293

At 0 C: K1=2.1; 5 C: 2.2; 15 C: 1.8; 29 C: 1.6; 30C: 1.4; 35 C: 1.5

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	ISE	non-aq	25°C	100%	U		K1=0.04 B2=-0.40	1974INa (17890)	294

Medium: CH3CN, I=0.1(Et4N.picrate)

****

CH4O6Cl2P2 H4L CAS 10596-23-3 (2370)

Dichloromethanediphosphonic acid; Cl2.C(PO3H2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	ISE	oth/un	25°C	0.10M	M	I	K1=1.28	1983FBa (17953)	295

For 0.1 M NH4Cl medium

****

CH4O6F2P2 H4L CAS 10596-32-4 (7848)
Difluoromethylenediphosphonic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	ISE	oth/un	25°C	0.10M	M		K1=1.29	1983FBa (17957)	296

For 0.1 M NH4Cl medium

****

CH5O3P H2L CAS 13590-71-1 (1752)
Methylphosphonic acid; CH3.PO3H2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	gl	NaClO4	25°C	0.50M	C		K1=0.54 K(Na+HL)=-0.05	1999AVa (18131)	297

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	gl	R4N.X	25°C	0.10M	U		K1=0.61	1972WFa (18150)	298

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
Na+	gl	NaClO4	25°C	0.50M	C		K1=2.13 K(Na+HL)=0.95 K(Na+H2L)=0.42	1999AVa (18287)	299
Na+	gl	R4N.X	25°C	0.50M	U		K1=1.13 K(Na+HL)=0.39	1967CIa (18288)	300

Medium: Me4NCl

****

C2H2 L Acetylene CAS 74-85-1 (703)
Ethyne; HCCH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	con	non-aq	-40°C	100%	U		K1=3.42	1963BTb (18357)	301

Medium: Liquid NH3

****

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

Na+ gl NaCl 25°C 0.0 C K1=0.92 2004CDc (18976) 302
K(Na+HL)=0.02
Method: calculated from apparent ligand protonation constants in 0.10-4.50 M NaCl.

Na+ gl NaCl 25°C 0.04M C TIH K1=0.60 1992DDb (18977) 303
B(NaHL)=3.74
DH(K1)=5 kJ mol-1, DS(K1)=27 J K-1 mol-1; DH(NaHL)=7, DS(NaHL)=96.
Data for 0.04-1.0 M NaCl and 10-45 C. At I=0.0 M, K1=0.88, DH(K1)=1.

Na+ gl NaNO3 37°C 0.15M C IH K1=0.46 1983DRb (18978) 304
Method: determination of protonation constant in NaNO3 and [Et4N]NO3 media
Data for I=0.0-1.0 M NaNO3. At I=0.0, K1=0.87; DH(K1)=5.02 kJ mol-1, DS=33

Na+ gl none 37°C 0.0 C I K1=0.91 1981DRa (18979) 305
Calculated from protonation data for I=0.03-0.3 M NaNO3
At I=0.10 M NaNO3, K1=0.53
****
C2H3O2I HL Iodoacetic acid CAS 64-69-7 (1312)
Iodoethanoic acid; ICH2.COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ con none 25°C 0.0 C T K1=0.564 1979KAa (19416) 306
At 35 C, K1=0.956
****
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
---
Na+ ISE none 25°C 0 C I K1=-0.07 1995RGa (20054) 307
I=0.16 (Me4N.X) K1=-0.25; I=0.25 (Me4N.X) K1=-0.24; I=0.49 (Me4N.X) K1=-0.21

Na+ con alc/w 25°C 10% C TIH K1=0.38 1993WZa (20055) 308
Medium: 10% MeOH/H2O. Data for 5-45 C. DH(K1)=14.1 kJ mol-1, DS(K1)=54.6
J K-1 mol-1. Data for 10-100% MeOH. For 100%, at 25 C, K1=2.01, DH=7.3

Na+ cal NaCl 275°C 0.0 C TIH K1=0.033 1988OGa (20056) 309
Method: flow calorimetry. Data for 275-320 C. Data for 0.25-1.0 m NaCl.
DH(K1)=59 kJ mol-1, DS(K1)=108 J K-1 mol-1.

Na+ gl R4N.X 25°C 0.25M C TIH K1=-0.27 1985DRa (20057) 310
I=0.02-1 M Et4NI. 10-45 C. DH = 9 kJ mol-1

Na+ gl R4N.X 25°C 0.16M U TI K1=-0.28 1985RSa (20058) 311
At 10 C: K1=-0.34 (I=0.04); 35 C: -0.21 (I=0.25); 45 C: -0.11 (I=0.49)

Na+ gl non-aq 25°C 100% U H K1=6.58 1981TMb (20059) 312
Medium: Glacial acetic acid. Alternative method: Spectrophotometry.

DH(K1)=-26 kJ mol-1

Na+ con oth/un 25°C 0.20M U TI K1=0.64 1978BBb (20060) 313
K1=1.15 in 0.5 mole fraction ethylene carbonate. Data also for 25 and 40 C and m.f. 0.2 to 0.6

Na+ gl mixed 25°C 100% U I K1=4.77 1965KLa (20061) 314
Medium: 97% ethanoic acid. K1=3.90(97.5%), 4.35(99%), 4.56(99.4%) 4.63(95%+5% anhydride), 4.49(90%+10% anhydride).

Na+ gl oth/un 25°C 0.0 U K1=-0.18 1964AMa (20062) 315

Na+ con non-aq 106°C 100% U K1=5.88 1962MAa (20063) 316
Medium: ethanoic acid

Na+ EMF non-aq 25°C 100% U K1=6.58 1956BKa (20064) 317
Method: chloranil electrode. Medium: aethanoic acid

Na+ con non-aq 30°C 100% U K1=6.68 1954JGa (20065) 318
Medium: ethanoic acid

****

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

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

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Na+ ISE oth/un 25°C 0.10M C K1=0.85 1983FBa (20670) 319
Method: Na ion selective electrode. Medium: 0.10 M NH4Cl.

****

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

---

Na+ gl NaClO4 25°C 0.50M C K1=-0.4 1995CDc (21633) 320
B(NaHL)=9.1

****

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

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

---

Na+ gl NaClO4 25°C 0.50M C K1=0.99 1999AVa (21893) 321
K(Na+HL)=0.06

****

C2H6O L Ethanol CAS 64-17-5 (1913)
Ethanol; CH3.CH2.OH

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

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Na+ kin alc/w 25°C ? U T K1=2.1 1975LSd (22029) 322
****
C2H6OS L DMSO CAS 67-68-5 (329)
Dimethylsulfoxide; (CH3)2.SO

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE non-aq 25°C 100% C K1=0.77 B2= 0.92 1997NMa (22113) 323
B3=0.93
Method: polyacrylamide/15-crown-5 sensor. Medium: acetonitrile
---
Na+ ISE non-aq 25°C 100% U K1=0.74 B2=0.92 1976CWc (22114) 324
B3=0.9
B4=0.8
Medium: propylene carbonate

Na+ ISE non-aq 25°C 100% U K1=0.78 B2=1.04 1974INa (22115) 325
B3=0.81
Medium: CH3CN, I=0.1(Et4N.picrate)
****
C2H6O2 L Ethyleneglycol CAS 107-21-1 (924)
1,2-Dihydroxyethane (Ethane-1,2-diol); HO.CH2.CH2.OH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ nmr mixed 25°C ? U M 1976DLa (22151) 326
K(NaA4+L=NaA2L+2A)=2.76
K(NaA2L+L)=2.06
Medium: tetrahydrofuran/ethyleneglycol. A=tetrahydrofuran
****
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
---
Na+ sp alc/w 25°C 95% U K1=0.9 1993GSa (23203) 327
Medium: 95% w/w EtOH/H2O, 0.05 M Et4NClO4, by competitive spectrophotometry
****
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
---
Na+ gl R4N.X 25°C 0.50M U K1=1.51 1967CIa (23271) 328
K(Na+HL)=0.50
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
Na+	gl	NaCl	25°C	0.15M	M	I	K1=1.82 K(Na+HL)=1.17 K(Na+H2L)=0.82	1987MKb (23386)	329

for 0.3 M NaCl K1=1.68;K(Na+HL)=1.08; K(Na+H2L)=0.75
for 0.5 NaCl K1=1.52; K(Na+HL)=1.04; K(Na+H2L)=0.73

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	cal	R4N.X	25°C	0.50M	U	H	K1=2.07	1986VKb (23387)	330

Medium: Et4N.Cl. DH1=6.9 kJ mol-1, DS1=63 J K-1 mol-1

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	ISE	oth/un	25°C	0.10M	M	I	K(Na+HL)=1.28	1983FBa (23388)	331

For 0.1 M NH4Cl medium

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	cal	NaCl	25°C	0.25M	U	TIH	DH(H2L+Na)=13.3 kJ mol-1	1983VKd (23389)	332

also for 35 C DH=16.6 kJmol-1

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	gl	R4N.X	25°C	0.10M	U		K(Na+HL)=0.81 B(2Na+L)=2.66	1972WFa (23390)	333

Medium: (CH3)4NCl

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	gl	R4N.X	25°C	0.50M	U		K1=2.07 K(Na+HL)=0.54	1967CIa (23391)	334

Medium: Me4NCl

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	nmr	R4N.X	25°C	1.0M	C		K1=3.2	2003PPa (23458)	335

Method: NMR Na-23; in 1 M Me4NCl/Me4NOH

****

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
Na+	gl	NaCl	25°C	0.0	C		K1=0.93 K(Na+HL)=-0.10	2004CDc (24502)	336

Method: calculated from apparent ligand protonation constants in 0.11-4.51 M NaCl.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	gl	NaNO3	20°C	1.89M	M	I	K1=0.54 B(NaHL)=5.82 B(Na2L)=0.04 B(NaKL)=0.12	1999JDa (24503)	337

Also data for I=1.64 and 1.52 M.

Na+ ISE none 25°C 0 C I K1=0.90 1995RGa (24504) 338
I=0.16 (Me4N.X) K1=0.54; I=0.25 (Me4N.X) K1=0.53.

Na+ gl R4N.X 25°C 0.25M C TIH K1=0.57 1985DRa (24505) 339
B(NaHL)=5.15
I=0.02-1 M Et4NI.T=10-45. DH(K1)=3;DH(NaHL)=9 kJ mol-1. DS1=28; DS(NaHL)=139

Na+ gl NaNO3 25°C 0.25M C K1=0.60 1985DRd (24506) 340
B(NaHL)=5.2

Na+ gl NaNO3 37°C 0.15M C IH K1=0.40 B2= 0.68 1983DRb (24507) 341
Method: determination of protonation constant in NaNO3 and [Et4N]NO3 media
Data for I=0.0-1.0 M NaNO3. At I=0.0, K1=0.81; DH(K1)=3.3 kJ mol-1, DS=26

Na+ gl oth/un 25°C 0.0 U K1=0.74 1965AEa (24508) 342

****

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

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Na+ ISE non-aq 25°C 100% C K1=0.42 B2= 0.48 1997NMa (25664) 343
B3=0.02
Method: polyacrylamide/15-crown-5 sensor. Medium: acetonitrile.

Na+ ISE non-aq 25°C 100% U K1=0.38 B2=0.32 1974INa (25665) 344
Medium: CH3CN, I=0.1(Et4N.picrate)

****

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

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

---

Na+ gl none 25°C 0.0 C TIH K1=0.3 1989CDc (26216) 345
B(NaHL)=9.61
Calculated from data for protonation of alanine in 0.04-1.0 M NaCl. Data
for 10-50 C. DH(K1)=7 kJ mol-1, DS=29 J K-1 mol-1. DH(B(NaHL))=0, DS=-5

****

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

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

---

Na+ gl R4N.X 25°C 0.50M C K1=1.28 1999VCa (27313) 346
K(Na+HL)=0.79
Medium: 0.50 M Me4NCl/NaClO4.

****

C3H8NO5P H3L Glyphosate CAS 1071-83-6 (1617)

N-(Phosphonomethyl)glycine; H2O3P.CH2.NH.CH2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	gl	R4N.X	25°C	0	C	I	K1=1.39 B(NaHL)=11.73 B(NaH2L)=16.79 B(Na2L)=2.00	1996AMa (27409)	347

****

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
Na+	gl	R4N.X	25°C	0.50M	U		K1=2.08 K(Na+HL)=0.57	1967CIa (28402)	348

Medium: Me4NCl

****

C4H2O3 L CAS 108-31-6 (4246)
Maleic anhydride;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	sp	non-aq	?	100%	U		K(MSCN+L)=-0.55 K(2MSCN+L=(MSCN)2L)=0.86	1971TGa (28622)	349

Medium: CHCl3

****

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
Na+	gl	R4N.X	37°C	0.25M	C	I	K1=0.86 B(NaHL)=6.0	1985DRa (29104)	350

I=0.02-1 M Et4NI

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	gl	NaNO3	37°C	0.15M	C	IH	K1=0.61	1983DRb (29105)	351

Method: determination of protonation constant in NaNO3 and [Et4N]NO3 media
Data for I=0.0-1.0 M NaNO3. At I=0.0, K1=0.98; DH(K1)=4.2 kJ mol-1, DS=30

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	gl	oth/un	25°C	0.0	U		K1=0.7	1965AEa (29106)	352

****

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
Na+	gl	NaCl	25°C	0.0	C		K1=0.82 K(Na+HL)=-0.01	2004CDc (30000)	353

Method: calculated from apparent ligand protonation constants in 0.11-4.54 M NaCl.

Na+ gl R4N.X 25°C 0.25M C TIH K1=0.47 1985DRa (30001) 354
B(NaHL)=5.26
I=0.02-1M Et4NI.T=15-45 C. DH(K1)=4; DH(NaHL)=4 kJ m-1. DS1=30; DS(NaHL)=124

Na+ gl NaNO3 37°C 0.15M C IH K1=0.06 B2= 0.06 1983DRb (30002) 355
Method: determination of protonation constant in NaNO3 and [Et4N]NO3 media
Data for I=0.0-1.0 M NaNO3. At I=0.0, K1=0.46; DH(K1)=5.4 kJ mol-1, DS=26

Na+ gl oth/un 25°C 0.0 U K1=0.3 1965AEa (30003) 356

****

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

---

Na+ gl R4N.X 25°C 0.25M C TIH K1=0.30 1985DRa (30678) 357
B(NaHL)=4.7
0.02-1 M NEt4I. 10-37 C. DH1=0; DH(NaHL)=1 kJ mol-1. DS1=13; DS(NaHL)=104

Na+ gl NaClO4 25°C 0.10M C H 1980ACc (30679) 358
K(Na+HL=NaL+H)=-4.46
K(Na+H2L=NaHL+H)=-3.3
By calorimetry: DH(Na+HL=NaL+H)=-0.46 kJ mol-1, DS=4.2 J K-1 mol-1; DH(Na+H2L=NaHL+H)=-5.4, DS=-20.

Na+ ISE oth/un 25°C 0.10M U K1=0.28 1964RZa (30680) 359

Na+ gl R4N.X ? 0.28M U K1=0.30 1963EDa (30681) 360
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

---

Na+ gl oth/un 25°C 0.0 C I K1=0.71 1999DGa (30901) 361
B(NaHL)=4.04
Medium: artificial seawater. Extrapolated from data for 5-45% salinity.

Na+ gl R4N.X 25°C 0.25M C TIH K1=0.34 1985DRa (30902) 362
B(NaHL)=3.5
0.02-1 M NEt4I. 12.5-48 C. DH(K1)=10 kJ mol-1, DS=47; DH(NaHL)=19, DS=144

****

C4H6O6 H2L D-Tartaric acid CAS 147-71-7 (93)
D-Tartaric acid, D-2,3-Dihydroxybutanedioic acid; HOOC.CH(OH).CH(OH).COOH

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

```
--------------------------------------------------------------------------------
Na+        gl  R4N.X  25°C  0.1M U  IH    K1=1.06        2005ZZa (30978) 363
Medium: Et4NCl; L or D isomer is not specified.  For 0.3 mol/L K1=0.87
********************************************************************************
C4H6O6                H2L    DL-Tartaric acd  CAS 133-37-9  (94)
DL-Tartaric acid,DL-2,3-Dihydroxybutanedioic acid; HOOC.CH(OH).CH(OH).COOH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Na+        gl  R4N.X  25°C 0.25M C TIH    K1=0.58        1985DRa (31028) 364
                                          B(NaHL)=4.05
0.02-1 M NEt4I. 10-37 C. DH1=1; DH(NaHL)=1 kJ mol-1. DS1=22; DS(NaHL)=92
********************************************************************************
C4H6O6                H2L    L-Tartaric acid  CAS 87-69-4  (92)
L-Tartaric acid, L-2,3-Dihydroxybutanedioic acid; HOOC.CH(OH).CH(OH).COOH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Na+        gl  NaClO4 25°C 0.10M C   H                    1980ACc (31310) 365
                                          K(Na+HL=NaL+H)=-3.56
                                          K(Na+H2L=NaHL+H)=-2.8
By calorimetry: DH(Na+HL=NaL+H)=-0.75 kJ mol-1, DS=5.8 J K-1 mol-1;
DH(Na+H2L=NaHL+H)=-2.1, DS=-5.4.
--------------------------------------------------------------------------------
Na+        ISE R4N.X  25°C 0.20M U        K1=0.28        1972DMc (31311) 366
                                          K(Na+HL)=-0.05
At I=0: K1=0.81, K(Na+HL)=0.20
--------------------------------------------------------------------------------
Na+        ISE R4N.X  25°C 0.20M U        K1=0.41        1971DMa (31312) 367
Medium: Me4NCl
--------------------------------------------------------------------------------
Na+        gl  oth/un 20°C  0.0  U        K1=1.98        1965FRa (31313) 368
                                          K(Na+HL)=1.47
********************************************************************************
C4H7NO4               H2L    Aspartic acid    CAS 56-84-8  (21)
Aminobutanedioic acid; H2N.CH(CH2.COOH).COOH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Na+        gl  NaCl   25°C  0.0  C TIH    K1=0.42        1991DDc (31897) 369
                                          B(NaHL)=9.73
DH(K1)=14 kJ mol-1, DS(K1)=54 J K-1 mol-1; DH(NaHL)=-17,
DS(NaHL)=130. Data for 10-45 C, 0.1-1.0 M NaCl, CaCl2, EtNI
********************************************************************************
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
--------------------------------------------------------------------------------
Na+        ISE non-aq 25°C 100%  U        K1=0.57   B2=0.86   1976CWc (33765) 370
```

B3=0.6
B4=0.3
Medium: propylene carbonate

Na+ ISE non-aq 25°C 100% U K1=0.72 B2=1.04 1974INa (33766) 371
Medium: CH3CN, I=0.1(Et4N.picrate)
****
C4H10N3O5P H3L Phosphocreatine (3594)
Phosphocreatine, N-(Imino(phosphonoamino)methyl)-N-methylglycine;
H2O3P.HN.C(:NH)N(CH3)CH2COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ nmr R4N.X 37°C 0.25M C 2002CFb (34639) 372
K(Na+HL)=-0.5
Method: 31P nmr. Medium: 20% v/v D2O/H2O, 0.25 M Me4NCl, pH 7.0.
****
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
---
Na+ con non-aq 25°C 100% U K1=6.0 1974ESa (34660) 373
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
---
Na+ con non-aq 25°C 100% C K1=3.0 1992MSe (34703) 374
Medium: 100% MeOH. Anion: picrate. Also data for nitrophenolate anions.
****
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
---
Na+ gl R4N.X 25°C 1.00M C I K1=-0.72 1982SSf (35060) 375
In 90 % (v/v) DMSO/water mixture: K1=0.29 (I=0.25 M)
****
C5H4N4O3 H2L Uric acid CAS 69-93-2 (5389)
2,6,8-Trihydroxypurine;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ EMF NaCl 37°C 0.15M M T H 1998WKa (36211) 376
Kso=-4.31
25 C: Kso=-4.61; 32 C: Kso=-4.43; 42 C: Kso=-4.20
****

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

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE non-aq 25°C 100% U K1=-0.15 1974INa (36660) 377
Medium: CH3CN, I=0.1(Et4N.picrate)
****
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
---
Na+ sp alc/w 25°C 95% U K1=0.8 1993GSa (37131) 378
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
---
Na+ sp non-aq 25°C 100% U K1=2.57 1984AMa (38032) 379
In Dimethyl Sulfoxide (DMSO);
Data also for other di- and triketones and esters and their alkali enolates
---
Na+ gl diox/w 30°C 75% U K1=3.56 B2=7.76 1975MMa (38033) 380

Na+ gl alc/w 25°C 100% U K1=1.6 1965LIa (38034) 381
Medium: MeOH, 0.1 M NaClO4. In EtOH: K1=2.8
****
C5H8O4 H2L Glutaric acid CAS 110-94-1 (420)
Pentanedioic acid; HOOC.CH2.CH2.CH2.COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ gl NaCl 25°C 0.0 C K1=0.78 2004CDc (38333) 382
K(Na+HL)=0.02
Method: calculated from apparent ligand protonation constants in 0.11-4.64
M NaCl.
****
C5H10O2 HL CAS 600-07-7 (1317)
2-Methyl-butanoic acid; CH3.CH2.CH(CH3)COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ con non-aq -40°C 100% U K1=4.64 ? 1963BTb (40171) 383
****
C5H15NO7P2 H4L AMOK CAS 63132-39-8 (1350)
1-Hydroxy-3-N,N-dimethylaminopropane-1,1-diphosphonic acid;
Me2N.CH2.CH2.C(OH)(PO3H2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	gl	R4N.X	25°C	0.15M	U		K1=1.81 B(NaHL)=13.7 B(NaH2L)=23.40	1988MNa (41957)	384

****

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
Na+	oth	NaCl	25°C	0.0	C		K1=0.60	2004KIa (42132)	385

Method: capillary electrophoresis.Values obtained by extrapolation of data for I=0.02-0.05 M NaCl, pH 3.3.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	dis	non-aq	25°C	100%	C		K1=3.07	1999KKb (42133)	386

Medium: MIBK. Method: distribution of metal picrates into MIBK containing HO(CH2.CH2.O)n.C12H25, n=4, 6 or 8.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	oth	oth/un	25°C	0.04M	C		K1=<0.0	1998TIa (42134)	387

Method: capillary electrophoresis.
Medium: 0.005 M phosphate buffer, pH 7.1, 0.04 M MCl.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	dis	oth/un	25°C	dil	C		K(NaA+L)=3.29	1998TKa (42135)	388

Self medium, I<0.03 M. Method: Extraction of NaAL into dichloromethane. A is 18-crown-6.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	con	non-aq	25°C	100%	C	I	K1=2.22	1996HHc (42136)	389

Medium: acetonitrile. Also data for benzonitrile and DMF.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	con	alc/w	30°C	100%	U	I M	K1=2.89	1979PSa (42137)	390

Medium: isoPrOH.K(NaL+tetraethyleneglycol)=2.37. In H2O: K1=1.33, K(NaL+triethyleneglycol)=1.55

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	sp	non-aq	20°C	100%	U		K1=4.1	1978JId (42138)	391

Medium: CH2CL2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	dis	none	25°C	0.00	U	I	K1=1.38	1972IWc (42139)	392

In nitrobenzene: K1=3.67

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	con	none	25°C	0.00	M		K1=1.38	1971YIa (42140)	393

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	dis	oth/un	25°C	var	U		K1=2.3	1970SSb (42141)	394

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
Na+	con	non-aq	25°C	100%	C	I	K1=2.93	1996HHc	(42235) 395

Medium: acetonitrile. Also data for benzonitrile and DMF.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	con	non-aq	25°C	100%	U		K1=2.40	1973FGa	(42236) 396

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
Na+	con	non-aq	25°C	100%	C	I	K1=3.55	1996HHc	(42245) 397
							K(2NaL=Na2L2)=1.65		

Medium: acetonitrile.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
Na+	con	non-aq	25°C	100%	C	I	K1=2.22	1996HHc	(42738) 398

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

****

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
Na+	con	non-aq	25°C	100%	C		K1=3.33	1996HHc	(42813) 399
							K(2NaL=Na2L2)=1.95		

Medium: acetonitrile.

****

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
Na+	sp	alc/w	25°C	95%	U		K1=1.0	1993GSa	(43796) 400

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
Na+	sp	alc/w	25°C	95%	U		K1=0.98	1993GSa	(45272) 401

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

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	ISE	none	25°C	0	C	I	K1=1.30 B(Na2L)=2.00	1995RGa (45569)	402
I=0.16 (Me4N.X) K1=0.75, B(Na2L)=1.05; I=0.25 (Me4N.X) K1=0.74, B(Na2L)=0.74									
Na+	gl	oth/un	25°C	0.0	C	I	K1=1.398 B(NaHL)=7.308 B(NaH2L)=11.558 B(Na2L)=1.981 B(Na2HL)=6.959	1994DFc (45570)	403
Values at I=0 calculated from data for 0.04-1.0 M NaCl.									

****

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
Na+	gl	R4N.X	25°C	0.1M	U	IH	K1=0.89 K(2Na+L)=1.50	2005ZZa (46186)	404
Medium: Et4NCl. For 0.3 mol/L K1=0.71; K(2Na+L)=1.05									
Na+	gl	oth/un	25°C	0.0	C	I	K1=1.54 B(NaHL)=7.33 B(NaH2L)=11.4 B(Na2HL)=7.0 B(Na2L)=2.38	1999DGa (46187)	405
Medium: artificial seawater. Extrapolated from data for 5-45% salinity. B(NaKL)=2.47, B(NaKHL)=7.3.									
Na+	ISE	none	25°C	0	C	I	K1=1.43 B(Na2L)=2.31	1995RGa (46188)	406
I=0.1 (Me4N.X) K1=0.93, B(Na2L)=1.47; I=0.16 (Me4N.X) K1=0.88, B(Na2L)=1.39.									
Na+	gl	oth/un	25°C	0.50M	U	H	K1=1.03 B(NaHL)=6.45 B(Na2L)=1.50	1990DRa (46189)	407
DH(K1)=-2.8, DH(NaHL)=-3.6 and DH(Na2L)=-5.1 kJ mol-1.									
Na+	gl	NaNO3	25°C	0.25M	C		K1=0.68 B(NaHL)=5.87	1985DRd (46190)	408
Na+	gl	KCl	37°C	0.15M	C		K1=0.68 B2=0.78	1981CDb (46191)	409
Na+	gl	NaClO4	25°C	0.10M	C	H	K(Na+HL=NaL+H)=-4.99	1980ACc (46192)	410

K(Na+H2L=NaHL+H)=-4.2
K(Na+H3L=NaH2L+H)=-2.9
By calorimetry: DH(Na+HL=NaL+H)=1.7 kJ mol-1, DS=21 J K-1 mol-1;
DH(Na+H2L=NaHL+H)=0.8, DS=5.4; DH(Na+H3L=NaH2L+H)=-2.1, DS=-5.4

Na+ ISE oth/un 25°C 0.10M U K1=0.70 1964RZa (46193) 411

Na+ sp R4N.X 25°C 0.10M C K1=0.70 1961WAa (46194) 412
Medium: 0.16 M Me4NCl.

****

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

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

---

Na+ gl NaNO3 25°C 0.10M C TIH K1=1.35 1985DRb (46928) 413
B(NaHL)=9.88
Data at 10-45 C and I=0.02-1.0 M in NaNO3. DH(K1)=8 kJ mol-1; DS=(K1)=51.
DH(NaHL)=-14; DS(NaHL)=140 (by T coeff.)

Na+ sp R4N.X 25°C 0.10M C K1=1.08 1985HAd (46929) 414

Na+ gl R4N.X 20°C 0.10M U T K1=1.22 1963IFb (46930) 415
Medium: Me4NNO3

Na+ oth oth/un 20°C 0.0 U K1=2.15 1945SKb (46931) 416

****

C6H9N3O2 HL Histidine CAS 71-00-1 (1)
2-Amino-3-(4'-imidazolyl)propanoic acid; H2N.CH(CH2.C3H3N2)COOH

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

---

Na+ gl NaCl 25°C 0.0 C TI K1=-0.5 1991DDc (47589) 417
Extrapolated from data for 0.1-1.0 M NaCl, CaCl2 and EtN4I.
Data for 10-45 C.

****

C6H10N4 L Metrazole CAS 54-95-5 (2046)
1,5-Pentamethylenetetrazole, 6,7,8,9-Tetrahydro-5H-tetrazoloazepine;

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

---

Na+ nmr non-aq 25°C 100% U K1=-0.14 1972BGd (47880) 418
Medium: nitromethane

****

C6H10O4 H2L Adipic acid CAS 124-04-9 (401)
1,6-Hexanedioic acid; HOOC.(CH2)4.COOH

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

---

Na+ gl NaCl 25°C 0.0 C K1=0.86 2004CDc (48078) 419

K(Na+HL)=0.06
Method: calculated from apparent ligand protonation constants in 0.11-4.93 M NaCl.

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	gl	R4N.X	25°C	0	M	I	K1=-0.09	1996GMb (48421)	420

At I=0.16 M: K1=-0.25

****

C6H12O5 L CAS 52485-92-4 (8236)
Methyl-alpha-D-ribofuranoside;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	kin	non-aq	25°C	100%	C		K1=0.85	1980LVc (49516)	421

Medium: methanol.

****

C6H12O6 L D-Fructose CAS 57-48-7 (1561)
D-Fructose

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	nmr	non-aq	27°C	100%	U		K1=0.79	1976DGa (49551)	422

Medium: acetone

****

C6H12O6 L D-Galactose CAS 59-23-4 (1559)
D-Galactose

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	nmr	non-aq	27°C	100%	U		K1=0.70	1976DGa (49567)	423

Medium: acetone

****

C6H12O6 L D-Glucose CAS 492-62-6 (1560)
D-Glucose

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	nmr	non-aq	27°C	100%	U		K1=0.41	1976DGa (49592)	424

Medium: acetone

****

C6H12O6 L Sorbose CAS 87-79-6 (930)
L(-)-Sorbose;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	nmr	non-aq	17°C	100%	U		K1=0.86	1977GLa (49615)	425

Medium: pyridine

Na+ nmr non-aq -23°C 100% U K1=1.10 1976DGa (49616) 426
Medium: acetone. At -3 C: K1=0.87; 7 C: 0.92; 13 C: 0.91; 17 C: 0.86
****
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
---
Na+ con non-aq 25°C 100% C K1=3.1 1992MSe (51052) 427
Medium: 100% MeOH. Anion: picrate. Also data for nitrophenolate anions.
****
C6H14O4 L CAS 112-27-6 (5663)
2,2'-(1,2-Ethanediylbis(oxy))bisethanol;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ con non-aq 25°C 100% C K1=3.3 1992MSe (51055) 428
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
---
Na+ gl R4N.X 25°C 1.00M C I K1=-1.05 1982SSf (51300) 429
In 90 % (v/v) DMSO/water mixture: K1=0.47 (I=0.25 M)

Na+ con non-aq 25°C 100% U M K1=3.68 1976FGb (51301) 430
K(NaA+L)=1.90
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
---
Na+ gl R4N.X 25°C 0.10M U K1=2.32 1991BSa (51538) 431
B(NaHL)=11.29
B(NaH2L)=17.93
B(Na2L)=3.49
****
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
---
Na+ con non-aq 25°C 100% U K1=2.81 1989KSa (51776) 432
Medium: tetrahydrofuran/CHCl3 4:1 (vol)

Na+ con non-aq 25°C 100% U K1=2.81 1982YSa (51777) 433
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
---
Na+ con non-aq 25°C 100% U M 1982GJb (51985) 434
Kout(NaL+A)=4.6
Medium: 1,2-dichloroethane. A=picrate

Na+ ISE non-aq 25°C 100% U K1=1.46 B2=2.50 1974INa (51986) 435
B3=3.11
Medium: CH3CN, I=0.1(Et4N.picrate)
****
C6H18O3Si3 L CAS 541-05-9 (1283)
Hexamethyl cyclotrisiloxane; ((CH3)2SiO)3

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ con alc/w 25°C 100% U K1=0.12 1980OPa (52216) 436
Medium: MeOH, 0.1 M Me4NBr
****
C6H18O24P6 HnL Phytic acid CAS 83-86-3 (745)
Cyclohexane-1,2,3,4,5,6-hexol-hexaphosphoric acid, Myo-inositol hexaphosphoric acid; H12L

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ EMF NaClO4 25°C 0.00 C I 1989LWd (52227) 437
K(Na7HL=Na7L+H)=-8.85
K(Na5H2L+2Na=Na7HL+H)=-8.65
K(Na4H3L+Na=Na5H2L+H)=-8.20
K(Na3H4L+Na=Na4H3L+H)=-7.00
Method: Pt/H2 electrode. Derived from data for 0.15-3.0 M NaClO4. K(Na2H5L +Na=Na3H4L+H)=-5.30, K(NaH6L+Na=Na2H5L+H)=-4.05, K(H7L+Na=NaH6L+H)=-1.65.
****
C7H6O3 H2L Salicylic acid CAS 69-72-7 (14)
2-Hydroxybenzoic acid, Salicylic acid; HO.C6H4.COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ gl R4N.X 25°C 0.25M C TI K1=-0.5 1985DRa (54265) 438
I=0.02-1 M Et4NI. 10-45 C
****
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
Na+	gl	NaClO4	25°C	0	C	I	K1=1.31 K(Na+NaL)=0.30 K(Na+HL)=0.63 K(Na+H2L)=-0.9	1992CRa	(54470) 439

Extrapolated to I=0 form I=0.04 to I=0.81

****

C7H6O5 H4L Gallic acid CAS 149-91-7 (446)
3,4,5-Trihydroxybenzoic acid; C6H2(OH)3.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	ISE	R4N.X	25°C	0.20M	C	TI	K1=0.56	1986EFa	(54757) 440

Method: Na glass electrode. Data for 25-45 C and 0.15-0.30 M Me4NCl.
At I=0.0 M, K1=0.76

****

C7H6O6S H3L CAS 5965-83-3 (399)
5-Sulfosalicylic acid, 2-Hydroxy-5-sulfobenzoic; HO3S.C6H3(OH).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	gl	NaClO4	25°C	0.0	C		K1=1.0 K(Na+HL) <0 K(Na+H2L)=0.95	1979CPc	(55028) 441

Method: effect of [Na] (0.01-0.13 M) on ligand protonation constants.

****

C7H9N L CAS 100-71-0 (721)
2-Ethylpyridine; C5H4N.C2H5

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	con	non-aq	25°C	100%		U	K=9.9	1981EJa	(56228) 442

Medium: THF. K: Na+L ion pair

****

C7H12O4 H2L Pimelic acid CAS 111-16-0 (985)
1,7-Heptanedioic acid; HOOC.(CH2)5.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	gl	NaCl	25°C	0.0	C		K1=0.76 K(Na+HL)=0.03	2004CDc	(57308) 443

Method: calculated from apparent ligand protonation constants in 0.11-4.78
M NaCl.

****

C8H4O3 L CAS 85-44-9 (4473)
Phthalic anhydride;

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

---
Na+ sp non-aq ? 100% U 1971TGa (58397) 444
K(NaSCN+L=(NaSCN)L)=-0.72
K(2NaSCN+L=(NaSCN)2L)=0.82
Medium: CH3CN
****
C8H5N5O6 H3L Murexide (453)
Purpuric acid (Murexide is ammonium salt);

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp non-aq 25°C 100% U TIH K1=4.97 1995KSa (58522) 445
Medium: 10% w/w DMF/MeCN. DH(K1)=-7.6 kJ mol-1, DS=71 J K-1 mol-1
Data also for 20 30, 40 w/w% DMF

Na+ sp alc/w 25°C 95% U K1=3.42 1993GSa (58523) 446
Medium: 95% w/w EtOH/H2O, 0.05 M Et4NClO4

Na+ sp non-aq 20°C 100% U K1=2.98 1992PSa (58524) 447
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
---
Na+ dis non-aq 25°C 100% C M 2002IIa (58649) 448
K(NaL+phen)=4.77
K(NaL+2(phen))=7.32
Medium: chlorobenzene. For extraction from 0.10 M KCl:
K(Na+HL(o)=NaL(o)+H)=-11.49; K(Na+HL(o)+phen(o)=NaL(phen)(o)+H)=-6.72.

Na+ gl alc/w 25°C 100% U K1=2.4 1965LIa (58650) 449
Medium: MeOH, 0.1 M NaClO4. In EtOH: K1=4.2
****
C8H6O3Cl2 HL CAS 94-75-7 (8292)
2,4-Dichlorophenoxyethanoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ gl NaCl 25°C 0.0 C TIH K1=-0.10 1988CDb (58813) 450
Derived from ligand protonation data in 0.06-0.98 M NaCl. Data for 10-45 C
DH(K1)=-2.4 kJ mol-1.
****
C8H6O4 H2L Phthalic acid CAS 88-99-3 (113)
Benzene-1,2-dicarboxylic acid; C6H4(COOH)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE R4N.X 25°C 0.20M C TI K1=1.19 1986EFa (58989) 451

Method: Na glass electrode. Data for 25-45 C and 0.15-0.30 M Me4NCl.
At I=0.0 M, K1=1.63

Na+ gl R4N.X 25°C 0.25M C TIH K1=0.73 1985DRa (58990) 452
B(NaHL)=4.96
0.02-1 M NEt4I. 10-37 C. DH(K1)=1 kJ mol-1, DS=23; DH(NaHL)=2, DS=111

Na+ gl NaNO3 37°C 0.15M C IH K1=0.50 B2= 0.40 1983DRb (58991) 453
Method: determination of protonation constant in NaNO3 and [Et4N]NO3 media
Data for I=0.0-1.0 M NaNO3. At I=0.0, K1=0.87; DH(K1)=4.2 kJ mol-1, DS=31

Na+ gl oth/un 25°C 0.0 U K1=0.7 1965AEa (58992) 454

****

C8H6O4 H2L Terephthalic Ac CAS 199-21-0 (518)
Benzene-1,4-dicarboxylic acid; C6H4(COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	ISE	R4N.X	25°C	0.20M	C	TI	K1=1.08	1986EFa (59073)	455

Method: Na glass electrode. Data for 25-45 C and 0.15-0.30 M Me4NCl.
At I=0.0 M, K1=1.52

****

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
Na+	gl	none	25°C	0.0	C	TIH	K1=0.00	1985CDb (60039)	456

Calculated from protonation data for I=0.04-0.9 M NaCl. Data for 10-45 C.
DH(K1)=4.1 kJ mol-1, DS(K1)=14 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
Na+	cal	R4N.X	20°C	0.1M	C			1976ANb (60644)	457

DH1= -4.39 kJ/mol
in Me4NCl

Na+	vlt	oth/un	20°C	0.10M	U		K1=3.11	1972BZc (60645)	458

Na+ gl NaNO3 34°C 0.10M U TIH K1=2.42 1963IFb (60646) 459
K1=2.72(20 C),2.54(27 C); DH(K1)=-36.4 kJ mol-1, DS=-75 J K-1 mol-1
At I=0 corr:K1=3.33(20 C)

Na+ ISE oth/un 20°C 0.0 U K1=3.32 1946SKa (60647) 460

****

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
Na+	oth	diox/w	25°C	75%	U		K1=3.61	B2=7.62	1979MMa (61305)	461

****

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
Na+	gl	alc/w	25°C	100%	U	I	K1=1.5		1965LIa (61688)	462

Medium: MeOH, 0.1 M NaClO4. In EtOH: K1=2.2

****

C8H14O4 H2L Suberic acid CAS 505-48-6 (517)
Octanedioic acid; HOOC.(CH2)6.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Na+	gl	NaCl	25°C	0.0	C		K1=0.78	K(Na+HL)=0.05	2004CDc (62097)	463

Method: calculated from apparent ligand protonation constants in 0.10-4.85 M NaCl.

****

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
Na+	ISE	alc/w	25°C	100%	C	IH T	K1=1.5	B2= 3.70	2003ADa (62697)	464

IUPAC Tentative. DH(K1)=-11 kJ mol-1, DH(B2)=-30
Medium: 0-0.1 M, various. Calorimetry also used.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Na+	nmr	alc/w	25°C	100%	C		B2=4.01		2000ABc (62698)	465

Medium: CH3OD. Method: 13C nmr.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Na+	oth	oth/un	25°C		U		K1=-0.16		2000MTa (62699)	466

Method: capillary zone electrophoresis.
Medium: 0.005 M H3BO3/Me4NOH, pH 9.2.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Na+	nmr	non-aq	27°C	100%	U	I	K1=2.30	B2= 4.00	1996KAa (62700)	467

Method: 23Na nmr. Medium: acetonitrile. Also data for 20, 40, 60, 80 wt% DMSO in AN. For DMSO: K1<0.5. For 20% DMSO, K1=1.01, K2<0.5.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Na+	cal	non-aq	25°C	100%	C	H	K1=0.43	B2= 2.13	1996OKa (62701)	468

Medium: DMF, 0.10 M Et4NCl. DH(K1)=-15.4 kJ mol-1, DS(K1)=-43 J K-1 mol-1; DH(K2)=-30, DS(K2)=-66.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Na+	con	alc/w	25°C	100%	U	I	K1=1.087		1995DSb (62702)	469

Medium : MeOH. In MeCN K1=4.416

Na+ cal non-aq 25°C 100% C H K1=1.99 B2= 5.27 1995OOa (62703) 470
Medium: 0.10 M Et4NClO4 in pyridine. DH(K1)=-19 kJ mol-1, DS(K1)=-27
J K-1 mol-1; DH(B2)=-49.2, DS(B2)=-64.3.

Na+ con non-aq 25°C 100% U K1=4.1 1993EVa (62704) 471
Medium: THF+CHCl3 (4:1 vol)

Na+ ISE alc/w 25°C 100% C H T K1=1.75 B2=3.64 1987BUa (62705) 472
Medium: MeOH. DH(K1)=-8.4 kJ mol-1; DS=5.0 J K-1 mol-1; DH(B2)=-39.9; DS=64

Na+ con non-aq 25°C 100% C K1=2.05 B2= 3.78 1987ZBb (62706) 473
Medium: MeOH.

Na+ nmr alc/w 30°C 100% U K1=2.1 B2=3.8 1983AAa (62707) 474

Na+ ISE alc/w 25°C 100% U K1=1.7 1983GGa (62708) 475
Medium: MeOH

Na+ gl alc/w 25°C 100% M H T K1=1.43 B2=3.75 1982MRa (62709) 476
Medium: MeOH. DH(K1)=-12.5 kJ mol-1, DH(K2)=-28.0

Na+ ISE alc/w 25°C 100% U T K1=1.41 B2=3.61 1982MYc (62710) 477
Medium: MeOH

Na+ con non-aq 25°C 100% U K1=3.32 1980HNa (62711) 478
Medium: MeCN

Na+ vlt non-aq 25°C 100% U K1=3.5 B2=6.31 1980MDa (62712) 479
Medium: propylene carbonate
****
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
---
Na+ vlt non-aq 25°C 100% C K1=2.7 2000HHa (62766) 480
Medium: acetonitrile, 0.1 M Et4NClO4. Method: dc polarography.
****
C8H18N2O2 L CAS 294-92-8 (654)
1,7-Dioxo-4,10-diazacyclododecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ vlt non-aq 25°C 100% C K1=3.3 2000HHa (62846) 481
Medium: acetonitrile, 0.1 M Et4NClO4. Method: dc polarography.

Na+ sol non-aq 20°C 100% C K1=2.76 1983SLa (62847) 482
Medium: CHCl3
****
C8H18O4 L Triglyme CAS 112-49-2 (2358)

1,2-Bis(methoxyethoxy)ethane; CH3O.C2H4O.CH2.CH2.OC2H4.OCH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	con	non-aq	25°C	100%	U	I	K1=2.7	1993EVa (62991)	483

Medium: THF+CHCl3 4:1(vol). In 100% THF: K1=2.5

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	con	non-aq	25°C	100%	C		K1=3.1	1992MSe (62992)	484

Medium: 100% MeOH. Anion: picrate. Also data for nitrophenolate anions.

****

C8H18O5 L Tetra-Et-Glycol CAS 112-60-7 (5664)

2,2'-(Oxybis(2,2-ethanediyloxy))-bis-ethanol; O(CH2.CH2.O.CH2.CH2.OH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	con	non-aq	25°C	100%	C		K1=2.3	1992MSe (63005)	485

Medium: 100% MeOH. Anion: picrate. Also data for nitrophenolate anions.

****

C8H19NO5 L Bis-tris CAS 6976-37-0 (2827)

Bis-(2-hydroxyethyl)imino-tris(hydroxymethyl)methane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	gl	R4N.X	25°C	1.00M	C	I	K1=-0.82	1982SSf (63065)	486

In 90 % (v/v) DMSO/water mixture: K1=0.54 (I=0.25 M)

****

C8H20N4 L Cyclen CAS 294-90-6 (10)

1,4,7,10-Tetraazacyclododecane; cyclo(-(NH.CH2.CH2.)4-)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	EMF	non-aq	25°C	100%	U	I	K1=3.60	1996WPa (63295)	487

Medium: acetonitrile, 0.05 M NEt4ClO4. In propylene carbonate K1=5.5; in dimethylformamide K1<2

****

C8H20O4P2 L CAS 86536-56-3 (2076)

1,2-Bis(2-dimethylphosphinylmethoxy)ethane; Me2P(O)CH2.O.CH2.CH2.O.CH2.P(O)Me2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	con	non-aq	25°C	100%	U		K1=3.60	1989KSa (63312)	488

Medium: tetrahydrofuran/CHCl3 4:1 (vol)

****

C9H6O6 H3L Hemimellitic ac CAS 569-51-7 (1621)

1,2,3-Benzenetricarboxylic acid; C6H3.(COOH)3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	gl	NaCl	25°C	0.0	C		K1=1.53 B(NaHL)=7.04	1995DGb (63973)	489

B(NaH2L)=10.70
B(Na2L)=2.45
B(Na2HL)=7.04
Calculated from data for 0.1-0.75 M NaCl.
****
C9H6O6 H3L Trimellitic aci CAS 528-44-9 (1622)
1,2,4-Benzenetricarboxylic acid; C6H3.(COOH)3

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ gl NaCl 25°C 0.0 C K1=1.49 2003CDb (63993) 490
B(NaHL)=6.43
B(NaH2L)=9.74
B(Na2L)=1.88
Extrapolated from values for 0.1-1.0 M Et4NI or NaCl.
****
C9H6O6 H3L CAS 554-95-0 (1623)
1,3,5-Benzenetricarboxylic acid; C6H3.(COOH)3

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ gl NaCl 25°C 0.0 C K1=0.99 2003CDb (64001) 491
B(NaHL)=5.41
B(NaH2L)=9.03
B(Na2L)=1.24
Extrapolated from values for 0.1-1.0 M Et4NI or NaCl.
****
C9H7NO HL Oxine CAS 148-24-3 (504)
8-Hydroxyquinoline (8-quinolinol);

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ nmr non-aq 27°C 100% U I K1=1.10 B2= 1.42 1996MAb (64322) 492
Method: 23Na nmr. Medium: acetonitrile, 0.05 M NaClO4. Data for acetone
(K1=1.50, K2=0.52) and nitromethane (K1=2.18, K2=0.37).

Na+ sp alc/w 25°C 95% U K1=1.42 1993GSa (64323) 493
Medium: 95% w/w EtOH/H2O, 0.05 M Et4NClO4, by competitive spectrophotometry
---
Na+ sp non-aq 25°C 100% U I K1=2.60 B2=4.32 1992GSa (64324) 494
Medium: MeCN. In acetone:K1=1.40; in MeOH:K1=0.77. By fluorimetry
****
C9H11N3O7 H3L (3877)
N-(1-Methyl-2,4,6-trioxo-perhydropyrimidinyl)iminodiethanoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ gl R4N.X 20°C 0.10M U K1=2.67 1963IFb (66527) 495
Medium: Me4NNO3
****

C9H11O2F5 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
---
Na+ oth diox/w 25°C 75% U K1=3.93 B2=7.73 1979MMa (66537) 496
****
C9H16O2 HL CAS 18362-64-6 (1134)
2,6-Dimethyl-3,5-heptanedione; (CH3)2.CH.CO.CH2.CO.CH(CH3)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ gl diox/w 30°C 75% U K1=4.47 B2=8.35 1975MMa (67747) 497
****
C9H16O4 H2L Azelaic acid CAS 123-99-9 (3255)
Nonanedioic acid; HOOC.(CH2)7.COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ gl NaCl 25°C 0.0 C K1=0.81 2004CDc (67794) 498
K(Na+HL)=0.12
Method: calculated from apparent ligand protonation constants in 0.09-4.64
M NaCl.
****
C9H18O3Si3 L CAS 3091-77-7 (1284)
Trimethyl-triethenyl-cyclotrisiloxane; ((CH3)(CH2:CH)SiO)3

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ con alc/w 25°C 100% U K1=0.04 1980OPa (67968) 499
Medium: MeOH, 0.1 M Me4NBr
****
C9H20O6Cl2P2 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
---
Na+ con non-aq 22°C 100% U K1=0.90 1981SKd (68124) 500
Medium: CH3CN
****
C9H22O6P2 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
---
Na+ con non-aq 22°C 100% U K1=1.37 1981SKd (68261) 501
Medium: CH3CN
****
C10H2O6 L CAS 3308-42-7 (4698)
1,2,4,5-Benzenetetracarboxylic dianhydride;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	sp	non-aq	?	100%	U			1971TGa (68420)	502
							K(2NaSCN+L)=0.77		

Medium: CH3CN

****

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
Na+	gl	none	25°C	0.0	C			1990CDc (68523)	503
							B(NaH3L)=14.22		
							B(Na2L)=3.5		
							B(Na2HL)=8.7		
							B(Na2H2L)=12.6		

Additional technique: spectrophotometry. Kso(Na2H2L)=-15.84.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	gl	R4N.X	25°C	0.25M	C	I	K1=1.28	1990DDb (68524)	504
							B(NaHL)=6.15		
							B(NaH2L)=9.91		
							B(NaH3L)=12.10		
							B(Na2HL)=5.9		

Medium: 0.25 M Et4NI. Data for 0.08-0.99 M. B(Na2L)=1.5

****

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
Na+	nmr	non-aq	27°C	100%	U	I	K1=1.31 B2= 2.07	1996MAb (69624)	505

Method: 23Na nmr. Medium: acetonitrile, 0.05 M NaClO4. Data for acetone (K1=1.22, K2=0.43), nitrobenzene (K1=3.2), nitromethane (K1=2.39, K2=0.90)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	sp	alc/w	25°C	95%	U		K1=1.30	1993GSa (69625)	506

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

---

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	sp	non-aq	25°C	100%	U	I	K1=1.67	1992GSa (69626)	507

Medium: MeCN. In acetone:K1=1.19; in MeOH:K1=0.31. 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
Na+	gl	alc/w	25°C	100%	U	I	K1=1.8	1965LIa (70753)	508

Medium: MeOH, 0.1 M NaClO4. 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
Na+	gl	KNO3	20°C	0.10M	U		K1=1.0	1963IFb (71044)	509

****

C10H11NO7S H3L (3335)

N-(2-Sulfophenyl)iminodiethanoic acid; HO3S.C6H4.N(CH2.COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	EMF	KCl	20°C	0.10M	C		K1=0.98	1947SWa (71068)	510

****

C10H11O2F7 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
Na+	oth	diox/w	25°C	75%	U		K1=3.93 B2=7.76	1979MMa (71112)	511

****

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
Na+	gl	KNO3	20°C	0.10M	U		K1=0.85	1963IFc (71268)	512

****

C10H13N3O7 H3L (3912)

1,3-Dimethyluramil-N,N-diethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	gl	R4N.X	20°C	0.10M	U		K1=2.53	1963IFb (71807)	513

Medium: Me4NNO3

****

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
Na+	gl	R4N.X	25°C	0.10M	C	TI R	K1=0.88	1991SMa (72479)	514

IUPAC evaluation

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	ISE	oth/un	25°C	0.0	C		K1=1.94	1976KRb (72480)	515

Method: Na ion selective electrode. Self medium, pH 9.1.

****

C10H15N5O10P2 H3L ADP CAS 20398-34-9 (2181)

Adenosine-5'-diphosphoric acid;

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

```
--------------------------------------------------------------------------------
Na+        gl  R4N.X  25°C 0.10M C TI   R K1=1.12        1991SMa (73007) 516
IUPAC evaluation. 37 C, 0.15 NaCl: K1=0.71
--------------------------------------------------------------------------------
Na+        nmr R4N.X  22°C 0.10M U                      1985PHb (73008) 517
                                        K(Na+H5L)=-0.28
--------------------------------------------------------------------------------
Na+        ISE oth/un 25°C 0.20M U        K1=0.65        1954MEa (73009) 518
********************************************************************************
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
--------------------------------------------------------------------------------
Na+        gl  R4N.X  25°C 0.15M M        K1=2.35        1993CRa (73977) 519
                                        K(NaL+H)=10.09
                                        K(NaHL+H)=6.01
Medium: 0.15 M Me4NCl.
--------------------------------------------------------------------------------
Na+        gl  NaNO3  25°C 0.10M C TIH    K1=1.84        1985DRb (73978) 520
                                        B(NaHL)=9.94
Data at 10-45 C and I=0.02-1.0 M in NaNO3. DH(K1)=-3.2 kJ mol-1; DS=23.
DH(NaHL)=0; DS=187.
--------------------------------------------------------------------------------
Na+        cal KNO3   25°C  0.3M C TI     K1=1.34        1976VBd (73979) 521
                                        DH(K1)=-9.5 kJ mol-1
For 0.3 M Me4NNO3 medium K1=1.34; DH1=-9.7 kJ/mol
For 1.0 M KNO3 medium K1=1.21; DH1=-6.9 kJ/mol
--------------------------------------------------------------------------------
Na+        sp  R4N.X  25°C 0.50M U        K1=1.43        1973CSa (73980) 522
Medium: (CH3)4NCl
--------------------------------------------------------------------------------
Na+        gl  R4N.X  25°C 0.10M U      T K1=1.82        1968WSa (73981) 523
Medium: (CH3)4NCl
--------------------------------------------------------------------------------
Na+        gl  oth/un 25°C 0.32M U        K1=1.79   B2=2.47   1965BCa (73982) 524
                                        K(Na+HL)=0.49
Medium: CsCl
--------------------------------------------------------------------------------
Na+        ISE NaCl     ?  0.01M U        K1=2.61        1963PAa (73983) 525
                                        K(Na+HL)=-0.03
Method: sodium-sensitive glass electrode. Medium: 0.01 M NaCl, Me4NOH var
--------------------------------------------------------------------------------
Na+        cal NaCl   25°C 0.05M U   H                  1954CHa (73984) 526
DH(K1)=-5.9 kJ mol-1, DS=13 J K-1 mol-1
--------------------------------------------------------------------------------
Na+        ISE KCl    20°C 0.10M U      T K1=1.66        1947SAa (73985) 527
********************************************************************************
C10H16N5O13P3         H4L    ATP              CAS 56-65-5  (403)
Adenosine-5'-triphosphoric acid;
```

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Na+	gl	R4N.X	25°C	0.10M	C	IH R	K1=1.31		1991SMa (74794)	528

IUPAC evaluation. DH(K1)=-0.8 kJ mol-1 (tentatitive). 37 C, I=0.15 M: 0.83

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Na+	gl	oth/un	25°C	0.25M	U	H	K1=1.31		1986RSa (74795)	529
							B(NaHL)=6.56			

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Na+	gl	R4N.X	25°C	0.10M	U	H	K1=1.57		1981CMd (74796)	530

Method: effect of Na on ligand protonation.
By calorimetry, DH(K1)=-0.84 kJ mol-1, DS(K1)=29 J K-1 mol-1.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Na+	kin	oth/un	20°C	0.17M	U				1973LJa (74797)	531
							K(MgL+Na)=-1.52			

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Na+	sp	oth/un	25°C	var	U		K1=1.41		1971HRa (74798)	532

Method: Raman spectra

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Na+	ISE	oth/un	25°C	0.0	U		K1=2.36		1970MRb (74799)	533

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Na+	gl	oth/un	25°C	0.32M	U		K1=1.2	B2=2.13	1965BCa (74800)	534
							K(Na+HL)=0.7			

Medium: CsCl

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Na+	ISE	oth/un	25°C	0.20M	U		K1=0.98		1954MEa (74801)	535

****

C10H17NO4 H2L CAS 2848-06-8 (3916)
N-(Cyclohexyl)iminodiethanoic acid; C6H11.N(CH2.COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Na+	gl	KNO3	20°C	0.10M	U		K1=0.90		1963IFb (74976)	536

****

C10H17NO5 H2L CAS 6243-06-7 (3326)
N-(2-Hydroxycyclohexyl)iminodiethanoic acid; HO.C6H10.N(CH2.COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Na+	gl	KNO3	20°C	0.10M	U		K1=0.76		1963IFb (74990)	537

****

C10H17NO5 H2L (3917)
N-(Tetrahydropyran-2-ylmethyl)iminodiethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Na+	gl	KNO3	20°C	0.10M	U		K1=0.85		1963IFa (75004)	538

****

C10H17N5O16P4 H5L AQP CAS 1062-98-2 (3341)
Adenosine-5'-tetraphosphoric acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ gl R4N.X 25°C 0.10M C T K1=1.71 1991SMa (75160) 539
IUPAC evaluation
****
C10H18O6 L 2-Oxo15-crown-5 CAS 73349-22-1 (609)
1,4,7,10,13-Pentaoxacyclopentadecan-2-one;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE alc/w 25°C 100% U K1=1.98 1982MKa (75610) 540
Medium: MeOH
****
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
---
Na+ con non-aq 25°C 100% C IH K1=1.837 2004JOa (76060) 541
Medium: 100% N,N-dimethylacetamide. Data for H2O and 0.1-0.9 mol fraction
DMA/H2O. By calorimetry, DH(K1)=-15.67 kJ mol-1, DS(K1)=-17.4 J K-1 mol-1.

Na+ con mixed 25°C 20% C H K1=1.06 2004JOb (76061) 542
Medium: 20% mole fracion hexamethylphosphortriamide/H2O.
DH(K1)=-39.64 kJ mol-1, DS(K1)=-112.8 J K-1 mol-1.

Na+ ISE alc/w 25°C 100% C IH T K1=3.32 B2= 5.82 2003ADa (76062) 543
IUPAC Tentative. Medium: 0-0.1 M. DH(K1)=-22.5 kJ mol-1, DH(K2)=-10.
In H2O: K1=0.8, DH(K1)=-6.3

Na+ con none 25°C dil C IH K1=4.95 2002JOa (76063) 544
Medium: 0-0.9 mol fraction acetonitrile/H2O. By calorimetry: DH(K1)=-30.90
kJ mol-1, DS=-8.86 J K-1 mol-1. For x=0.5, K1=2.52, DH(K1)=-10.38, DS=13.5

Na+ sp non-aq 25°C 100% C K1=3.64 2002NMa (76064) 545
Medium: THF, using metal picrate salt.

Na+ cal none 25°C 0.03M C T H K1=0.58 2001VGa (76065) 546
DH(K1)=-6.9 kJ mol-1
Ionic strength is provided by Na-salt used: 0.01-0.04 M. For 15 C K1=0.62
for 35 C K1=0.54; DH(K1)=-6.8l; for 45 C K1=0.51, DH(K1)=-6.4

Na+ nmr alc/w 25°C 100% C K1=3.42 2000ABc (76066) 547
Medium: CH3OD. Method: 13C nmr.

Na+ sp non-aq 25°C 100% C K1=3.7 2000KBb (76067) 548
Medium: MeCN. Method: electrospray ionization mass spectrometry.

Na+ oth oth/un 25°C U K1=0.48 2000MTa (76068) 549

Method: capillary zone electrophoresis.
Medium: 0.005 M H3BO3/Me4NOH, pH 9.2.

Na+ con non-aq 25°C 100% C H K1=2.75 B2= 3.96 1999WBa (76069) 550
Medium: N,N-dimethylformamide. By calorimetry: DH(K1)=-18.0 kJ mol-1, DH(K2)=-3.9 kJ mol-1.

Na+ vlt non-aq 25°C 100% C I K1=4.9 1999WKb (76070) 551
Medium: acetonitrile, 0.10 M Et4NClO4. Also data for TMS, propylene carbonate, acetone, formamide, DMF, DMA, DMSO, MeOH, EtOH.

Na+ ISE alc/w 25°C 100% U H K1=3.25 B2= 5.18 1998SSf (76071) 552
Medium: 100% MeOH, 0,05 M Et4NI

Na+ nmr non-aq 27°C 100% U I K1=4.96 1996KAa (76072) 553
Method: 23Na nmr. Medium: acetonitrile. Also data for 20, 40, 60, 80 wt% DMSO in AN. For DMSO: K1=1.17. For 20% DMSO, K1=2.80.

Na+ con alc/w 25°C 100% U I K1=3.513 1995DSb (76073) 554
Medium : MeOH. In MeCN K1=4.436

Na+ cal non-aq 25°C 100% M H K1=4.26 1994BCd (76074) 555
Medium: acetone. DH(K1)=-27.3 kJ mol-1, TDS=-3.1

Na+ ISE none 25°C 0.0 C K1=5.81 B2=12.57 1993GEb (76075) 556
B(Na2L)=13.42
B(Na2L2)=19.89
Method: Na-selective glass electrode. Self medium.

Na+ nmr oth/un 25°C ? U K1=3.68 B2=5.51 1989LFa (76076) 557
Medium: acetone, 0.03-0.05 M NaI

Na+ cal non-aq 25°C 100% C H K1=4.91 1988BUb (76077) 558
Medium: acetonitrile. DH(K1)=-29.2 kJ mol-1, DS(K1)=-44.6 J K-1 mol-1.

Na+ con non-aq 25°C 100% C T K1=5.4 1988TKa (76078) 559
Medium: MeCN

Na+ ISE alc/w 25°C 90% U K1=2.95 1987KHa (76079) 560
Medium: 90% w/w MeOH/H2O

Na+ con non-aq 25°C 70% C I K1=2.32 1987ZBb (76080) 561
Medium: 70% w/w MeOH/H2O.

Na+ gl R4N.X 25°C 0.10M U K1=1.08 1985BFa (76081) 562

Na+ ISE non-aq 25°C 100% M K1=3.31 1984NMb (76082) 563
Medium: MeOH.

Na+ ISE alc/w 25°C 100% U K1=3.24 1983GGa (76083) 564

Medium: MeOH

Na+ ISE alc/w 25°C 100% C I T K1=3.25 1982DGa (76084) 565
Method: Na ion selective electrode. Data for 0-100% MeOH/H2O.
K1=0.79 (0%), 1.49 (20%), 1.71 (40%), 2.21 (60%), 2.65 (80%), 2.97 (90%).

Na+ gl alc/w 25°C 100% M H T K1=3.14 B2=5.74 1982MRa (76085) 566
Medium: MeOH. DH(K1)=-23.0 kJ mol-1

Na+ ISE alc/w 25°C 100% U T K1=3.30 B2=4.74 1982MYc (76086) 567
Medium: MeOH

Na+ ISE non-aq 25°C 100% U T H K1=4.9 1982NYa (76087) 568
Medium: MeCN

Na+ nmr non-aq 25°C 100% U I K1=2.68 1981LPb (76088) 569
Medium: pyridine. In MeCN: K1 > 4.0; in DMSO: 1.31; in THF: > 4;
in aqueous: 0.44; in DMF: 1.97; in nitromethane: K1 > 4, K2=1.6

Na+ con non-aq 25°C 100% U K1=5.28 1980HNa (76089) 570
Medium: MeCN

Na+ cal alc/w 25°C 100% U H T K1=3.48 1980LIa (76090) 571
Medium: MeOH. DH=-20.9 kJ mol-1.

Na+ dis non-aq 25°C 100% U K1=3.7 1980TYa (76091) 572
Medium: propylene carbonate

Na+ EMF oth/un 25°C var C T K1=0.67 1979HRa (76092) 573
Method: ISE based on cation exchange membrane. Medium: aqueous,
containing 0.06-0.25 m ligand.

Na+ oth oth/un 25°C ? U K1=0.67 1977RLa (76093) 574
Method: ultrasound absorption

Na+ cal oth/un 25°C 0.10M U H T K1=0.70 1976ITb (76094) 575
DH=-6.28 kJ mol-1.
****
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
---
Na+ vlt non-aq 25°C 100% C K1=4.6 2000HHa (76187) 576
Medium: acetonitrile, 0.1 M Et4NClO4. Method: dc polarography.

Na+ ISE alc/w 25°C 100% U K1=1.70 1985SWa (76188) 577
****
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
--------------------------------------------------------------------------------
Na+        vlt non-aq 25°C 100%  C        K1=4.1         2000HHa (76327) 578
Medium: acetonitrile, 0.1 M Et4NClO4. Method: dc polarography.
--------------------------------------------------------------------------------
Na+        cal non-aq 25°C 100%  M   H    K1=3.35        1994BCd (76328) 579
Medium: acetone. DH(K1)=-11.7 kJ mol-1, TDS=7.3
--------------------------------------------------------------------------------
Na+        sp  non-aq 20°C 100%  U        K1=3.11        1992PSa (76329) 580
Medium: DMF, 0.01 M Me4NI
--------------------------------------------------------------------------------
Na+        ISE non-aq 25°C 100%  U  I     K1=2.10        1988CAa (76330) 581
In dimethylformamide; medium: 0.05M Et4NClO4. In diethylformamide, K=3.19,
in dimethylacetamide, K=2.88
********************************************************************************
C10H22O5                L    Tetraglyme       CAS 143-24-8  (121)
2,5,8,11,14-Pentaoxapentadecane; (CH3.O.CH2.CH2.O.CH2.CH2.)2O
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Na+        dis non-aq 25°C 100%  C        K1=6.06        1998KSc (76460) 582
Medium: 1,2-dichloroethane.
--------------------------------------------------------------------------------
Na+        con non-aq 25°C 100%  U  I     K1=3.4         1993EVa (76461) 583
Medium: THF+CHCl3 4:1(vol). In 100% THF: K1=3.2
--------------------------------------------------------------------------------
Na+        con non-aq 25°C 100%  C        K1=3.1         1992MSe (76462) 584
Medium: 100% MeOH. Anion: picrate. Also data for nitrophenolate anions.
--------------------------------------------------------------------------------
Na+        cal non-aq 25°C 100%  U        K1=1.11        1991TNa (76463) 585
Medium: MeOH
--------------------------------------------------------------------------------
Na+        con non-aq 25°C 100%  U    M                  1982GJb (76464) 586
                                           Kout(NaL+A)=5.9
Medium: 1,2-dichloroethane. A=picrate
--------------------------------------------------------------------------------
Na+        ISE alc/w  25°C 100%  U        K1=1.28        1975CJa (76465) 587
Medium: MeOH
********************************************************************************
C11H6O10             H5L                      (6712)
Benzenepentacarboxylic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Na+        gl  KCl    25°C 0.30M U         K1=3.48        1991RSa (76886) 588
                                          B(Na2L)=5.54
                                          K(Na+HL)=2.83
                                          K(Na+H2L)=2.24
                                          K(Na+H3L)=1.37
```

K(Na+H4L)=0.56, K(2Na+HL)=4.04

****

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
Na+	gl	R4N.X	20°C	0.10M	U		K1=0.89	1963IFb (77833)	589

Medium: Me4NNO3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	EMF	KCl	20°C	0.10M	U		K1=0.98	1950WIa (77834)	590

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
Na+	oth	R4N.X	25°C	0.50M	U		K1=2.55	1971CSb (79316)	591

Method: polarimetry. Medium: Me4NOH

****

C11H19N3O6 HL CAS 264130-48-5 (8946)

alpha-Methylurazolyl-12-crown-4;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	nmr	alc/w	25°C	100%	C		K(Na+HL)=0.71	2000ABc (79689)	592

Medium: CH3OD. Method: 13C nmr.

****

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
Na+	gl	diox/w	30°C	75%	U		K1=4.08	1975MMa (79751)	593

****

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
Na+	dis	none	25°C	0.0	U		Keff=4.54	1991IOa (79862)	594

By solvent extraction of the metal picrate into dichloromethane.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	ISE	none	25°C	0.0	C		K1=0.78	1991TKa (79863)	595

Self medium (ca. 0.008M). Method: Na ion-selective electrode.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	dis	none	25°C	0.0	C	M		1989TKc (79864)	596

K(NaL+A=NaAL(org))=2.68
Method: extraction of metal picrate/L from H2O into benzene.
K(Na+HA(org)+L(org)=NaAL(org)+H)=1.474. HA is picric acid.

Na+ con non-aq 25°C 100% C I K1=5.4 1988TKa (79865) 597
Medium: MeCN. In propylene carbonate K1=5.7; in MeOH 4.10
****
C11H22O6 L CAS 69496-26-0 (1663)
1,4,7,10,14-Pentaoxacyclohexadecan-12-ol, Hydroxy-16-crown-5

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE alc/w 25°C 100% U K1=3.03 1983IKa (79879) 598
****
C11H23NO4 L CAS 69978-46-7 (5819)
N-Methyl-1-aza-4,7,10,13-tetraoxacyclopentadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE alc/w 25°C 100% U T K1=3.39 1985SWa (79885) 599
Medium: MeOH. Data for many other N-substituted 1-aza-4,7,10,13-tetraaza-
cyclopentadecanes with Na+ and NH4+
****
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
---
Na+ dis non-aq 25°C 100% C K1=4.1 1998KSc (80080) 600
Medium: 1,2-dichloroethane.

Na+ sp non-aq 20°C 100% U K1=4.8 1978JId (80081) 601
Medium: CH2Cl2

Na+ ISE oth/un 25°C var C K1=1.7 1970SSb (80082) 602
By paper chromatography, K1=1.9
****
C12H6O3 L CAS 81-84-8 (4892)
1,8-Naphthalenedicarboxylic anhydride;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp non-aq ? 100% U 1971TGa (80102) 603
K(2NaSCN+L)=0.68
Medium: CH3CN
****
C12H6O12 H6L Mellitic acid (7400)
Benzenehexacarboxylic acid; (C(COOH))6

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

---
Na+ ISE R4N.X 25°C 0 C I K1=3.06 1996RSb (80114) 604
B(NaHL)=10.23
B(NaH2L)=16.18
B(NaH3L)=20.79
B(NaH4L)=23.52
B(Na2L)=4.75, B(Na2HL)=11.94, B(Na2H2L)=17.56, B(Na2H3L)=21.06
B(Na3L)=7.02,B(Na3HL)=13.27, B(Na4L)=7.97. I=0-3 M Et4NI
****
C12H8N2 L Phenanthroline CAS 66-71-7 (144)
1,10-Phenanthroline;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ nmr non-aq 27°C 100% U I K1=1.55 B2= 2.99 1996MAb (80497) 605
Method: 23Na nmr. Medium: acetonitrile, 0.05 M NaClO4.
Also data for acetone: K1=1.61, K2=0.80.

Na+ sp alc/w 25°C 95% U K1=2.10 1993GSa (80498) 606
Medium: 95% w/w EtOH/H2O, 0.05 M Et4NClO4, by competitive spectrophotometry
---
Na+ sp non-aq 25°C 100% U I K1=2.64 B2=4.63 1992GSa (80499) 607
Medium: MeCN. In acetone:K1=3.04, K2=1.00; in MeOH:K1=0.81. 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
---
Na+ sp non-aq 25°C 100% U K1=6.56 2000EGa (81681) 608
Method: fluorescence emission spectroscopy. Medium: acetonitrile.

Na+ vlt non-aq 25°C 100% C K1=5.1 1995KTb (81682) 609
Method: ion transfer polarography. Medium: nitrobenzene, 0.05 M
tetrabutylammonium tetraphenylborate.

Na+ cal non-aq 25°C 100% U H K1=1.88 1989SSd (81683) 610
Medium: CH3CN

Na+ cal non-aq 25°C 100% U H K1=1.88 B2=4.50 1988SSc (81684) 611
Medium: MeCN
****
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
---
Na+ oth R4N.X 25°C 0.50M U 1973CSa (82320) 612
K1=3.93(D)

K1=0.48(meso)
K(Na+HL)=0.78

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
Na+	con	non-aq	25°C	100%	U		K1=3.28	1982YSa (82643)	613

Medium: tetrahydrofuran+CHCl3 4:1(vol); M is 2,4-dinitrophenolate

****

C12H20O8 L CAS 62796-84-3 (2141)

1,4,7,10,13,16-Hexaoxacyclooctadecane-2,6-dione;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	cal	alc/w	25°C	100%	U	H	K1=2.50	1980BMa (82655)	614

Medium: MeOH. DH=-9.50 kJ mol-1.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	cal	alc/w	25°C	100%	U	H	K1=2.5	1980LIb (82656)	615

Medium: MeOH. DH=-9.50 kJ mol-1.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	cal	alc/w	25°C	100%	U	H	K1=2.5	1977ILa (82657)	616

Medium: MeOH. DH(K1)=-9.50 kJ mol-1

****

C12H20O8 L CAS 62796-83-4 (611)

2,11-Dione-18-crown-6, 1,4,7,10,13,16-hexaoxacyclooctadecan-2,6-dione;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	ISE	alc/w	25°C	100%	U		K1=2.29	1982MKa (82661)	617

Medium: MeOH

****

C12H22N2O6 H2L (6394)

1,7-Dioxa-4,10-diazacyclododecan-4,10-diethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	gl	R4N.X	25°C	0.10M	C		K1=2.16	1992ADa (82794)	618

Medium: 0.1 M Me4NNO3

****

C12H22N2O6 H2L (6641)

7,10-Diaza-1,4-Dioxacyclododecane-7,10-diethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	gl	R4N.X	25°C	0.10M	C		K1=2.51	1992ADa (82808)	619

Medium: 0.1 M Me4NNO3

****

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
---
Na+ oth diox/w 25°C 75% U K1=3.28 B2=7.33 1979MMa (82860) 620
****
C12H22O7 L 2-Oxa18-crown-6 CAS 73349-23-2 (610)
1,4,7,10,13,16-Hexaoxacyclooctadecan-2-one;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE alc/w 25°C 100% U K1=3.27 1982MKa (82863) 621
Medium: MeOH
****
C12H23NO5 L (6793)
10-Methoxycarbonylethyl-1,4,7-trioxa-10-azacyclododecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ cal alc/w 25°C 100% U H 1990KMb (82947) 622
Medium: MeOH. DH=-20.8 kJ mol-1
****
C12H23N3O5 H2L (6393)
1-Oxa-4,7,10-triazacyclododecan-4,10-diethanoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ gl R4N.X 25°C 0.10M C K1=1.14 1992ADa (82975) 623
Medium: 0.1 M Me4NNO3
****
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
---
Na+ sp non-aq 20°C 100% U K1=0.8 1992PSa (83019) 624
Medium: DMF, 0.01 M Me4NI
****
C12H24N2O6 L CAS 57721-99-0 (2508)
1,14-Diacetamido-3,6,9,12-tetraoxatetradecane; (CH2.O.CH2.CH2.O.CH2.CH2.CO.NH2)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE alc/w 25°C 100% U K1=1.03 1975CJa (83053) 625
Medium: MeOH
****
C12H24O4 L CAS 26996-94-3 (2541)
Tetramethyl-12-crown-4

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	ISE	alc/w	25°C	100%	A		K1=1.41	1971FRa (83125)	626

Medium: MeOH

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	nmr	non-aq	25°C	100%	U	M	K(NaB(Ph)4+L)=3.25	1981RPa (83139)	627

Medium: MeNO2. K(NaB(Ph)4+L)=0 in DMSO; 1.52 in DMF; 2.42 in acetone; 1.82 in MeCN; 1.87 in propylene carbonate

****

C12H24O5S L Thia-18-crown-6 CAS 52559-79-2 (2263)
1-Thia-4,7,10,13,16-pentaoxacyclooctadecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	cal	alc/w	25°C	100%	U	H	K1=2.57	1980LIa (83156)	628

Medium: MeOH. DH=-20.9 kJ mol-1.

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	ISE	mixed	25°C	50%	C		K1=2.56 B2= 5.75	2004YYb (83490)	629

Method: Na ion specific electrode. Medium: 50% THF/H2O.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	EMF	alc/w	25°C	100%	C		K1=4.25	2004ZTa (83491)	630

Medium: 100% methanol, 0.05 M Bu4NClO4. Method: Ag electrode, competition with Ag+ ion.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	ISE	alc/w	25°C	100%	C	IH R	K1=4.33	2003ADa (83492)	631

IUPAC Recommended. Medium: 0-0.1 M various. DH(K1)=-35 kJ mol-1
In H2O: K1=0.8, DH(K1)=-11. In PC K1=5.5, DH=-29

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	dis	oth/un	25°C		dil	C		2002KCa (83493)	632

NaL extracted from Li acetate buffer into benzene in the presence of bromocresol green, HA. K(Na+L(org)+A=NaLA(org))=3.74.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	cal	none	25°C	0.03M	C T	H	K1=0.53 DH(K1)=-12.6 kJ mol-1	2001VGa (83494)	633

Ionic strength is provided by Na-salt used: 0.01-0.04 M.
for 35 C K1=0.45, DH(K1=-11.6; for 45 C K1=0.39, DH(K1)=-10.9

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	gl	mixed	25°C	1.0M	U	I	K1=4.61 in 100% H2O K1=0.50	2001ZKb (83495)	634

Medium: 1.0 mass parts CH3CN;
for 0.6 m.p. CH3CN/H2O K1=1.81; for 0.2 m.p. K1=1.22

Na+ sp non-aq 25°C 100% C I K1=4.5 2000KBb (83496) 635
Medium: MeOH. Method: electrospray ionization mass spectrometry.
Comment: In H2O, K1=1.4; in MeCN, K1=4.2

Na+ dis non-aq 25°C 100% U K1=9.71 2000KSa (83497) 636
Medium: 1,2-dichloroethane

Na+ oth oth/un 25°C U K1=0.67 2000MTa (83498) 637
K(NaL+picrate)=0.90
Method: capillary zone electrophoresis.
Medium: 0.005 M H3BO3/Me4NOH, pH 9.2.

Na+ cal non-aq 25°C 100% C H K1=2.67 1999WBa (83499) 638
Medium: N,N-dimethylformamide. DH(K1)=-16.4 kJ mol-1.

Na+ ISE alc/w 25°C 100% U I K1=4.36 1998SSf (83500) 639
Medium: 100% MeOH, 0,05 M Et4NI. Many other crown ethers studied

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Na+ dis non-aq 25°C 100% C I 1998TKa (83501) 640
K(Na+A+L(org)=NaAL(org))=3.90
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.

Na+ cal non-aq 25°C 100% C K1=4.89 1997DZa (83502) 641
Medium: benzonitrile. DH(K1)=-40.61 kJ mol-1, DS(K1)=-42.6 J K-1 mol-1.

Na+ oth non-aq 15°C 100% U T H K1=4.54 1997EKa (83503) 642
Medium: CH3CN. Also data for H2O/CH3CN mixtures. For 40% CH3CN w/w K1=1.60;
for 100% H2O: K1=0.60

Na+ cal alc/w 25°C 100% U 1997LKa (83504) 643
Data for H2O/MeOH mixtures. DH(K1)=-15.8 kJ mol-1 (0% MeOH); DH(K1)=-15.1
(20% MeOH); DH(K1)=-15.8 (40%); DH(K1)=-16.6 (60%); DH(K1)=-36.8 (100%)

Na+ nmr non-aq 27°C 100% U I K1=4.29 1996KAa (83505) 644
Method: 23Na nmr. Medium: acetonitrile. Also data for 20, 40, 60, 80 wt%
DMSO in AN. For DMSO: K1=1.24. For 20% DMSO, K1=3.19.

Na+ cal alc/w 25°C 80% C H K1=3.05 1995KZa (83506) 645
Medium: 80% v/v CH3OH/H2O. DH(K1)=-23.3 kJ mol-1, DS(K1)=-20 J K-1 mol-1

Na+ cal non-aq 25°C 100% U IH T K1=4.96 1995OKb (83507) 646
Medium: Acetonitrile, 0.1 M Et4NClO4. DH(K1)=1.7 kJ mol-1
In propylene carbonate K1=5.23, DH(K1)=-29

Na+ cal non-aq 25°C 100% C H K1=5.45 1995OOa (83508) 647
Medium: 0.10 M Et4NClO4 in pyridine. DH(K1)=-42.3 kJ mol-1,

DS(K1)=-38 J K-1 mol-1.

Na+ cal non-aq 25°C 100% M H K1=4.46 1994BCd (83509) 648
Medium: acetone. DH(K1)=-34.0 kJ mol-1, TDS=-8.7

Na+ cal non-aq 25°C 100% U H T K1=2.43 1994OOa (83510) 649
Medium: DMF, 0.1 M Et4NClO4. DH(K1)=-22.2 kJ mol-1, DS=-28 J K-1 mol-1

Na+ ISE none 25°C 0.0 C K1=6.23 B2=13.92 1993GEb (83511) 650
B(Na2L)=14.72
B(Na2L2)=22.33
Method: Na-selective glass electrode. Self medium.

Na+ dis non-aq 25°C 100% U 1993INa (83512) 651
B(NaPL)=3.89
K is the equilibrium constant for extraction of the metal picrate (P) into CH2Cl2. For extraction from D2O, B=3.83

Na+ con oth/un 25°C 0.05M M K1=4.42 1992BUb (83513) 652
K1=4.32 (by calorimetry), K1=4.35 (by potentiometry)

Na+ cal R4N.X 25°C 0.10M C H K1=0.57 1992OIa (83514) 653
DH(K1)=-13.8 kJ mol-1, DS=-35 J K-1 mol-1

Na+ ix none 25°C 0.0 U I K1=2.5 1991BMb (83515) 654
Ligand bound to silica gel. In EtOH, K=3.1, in acetone, K=3.4

Na+ nmr oth/un 30°C dil C K1=1.182 B2= 4.04 1991ERa (83516) 655
B(Na2L)=3.571
B(Na2L2)=6.685
B(Na2L3)=9.836
B(Na3L3)=12.643.
Medium: D2O. Method: 13C nmr.

Na+ ISE alc/w 25°C 70% C K1=2.60 1991GTa (83517) 656
Medium: 70% v/v MeOH/H2O, 0.10 M Bu4NI. Method of corresponding solutions.

Na+ ix alc/w RT 50% C K1=2.37 1990MBb (83518) 657
Medium: 50% v/v MeOH/H2O. In 25% v/v MeOH/H2O K1=1.15.

Na+ con non-aq 25°C 100% C K1=5.649 1990SAb (83519) 658
Medium: propylene carbonate.

Na+ oth non-aq 25°C 100% C K1=2.32 1989BBh (83520) 659
Method: FABMS. Medium: glycerol.

Na+ cal non-aq 25°C 100% C H K1=4.71 1988BUb (83521) 660
Medium: acetonitrile. DH(K1)=2.3 kJ mol-1, DS(K1)=97.7 J K-1 mol-1.

Na+ ISE alc/w 25°C 90% U K1=3.46 1987KHa (83522) 661

Medium: 90% w/w MeOH/H2O

Na+ ISE alc/w 25°C 100% C K1=4.65 1986XJa (83523) 662

Na+ gl R4N.X 25°C 0.10M U K1=1.09 1985BFa (83524) 663

Na+ nmr non-aq 25°C 100% U I K1=2.10 1985BPa (83525) 664
Medium: DMF. In MeCN: K1=4.21

Na+ vlt alc/w 25°C 100% U K1=4.43 1985ZBa (83526) 665
Medium: MeOH

Na+ ISE NaCl 25°C 0.10M C I K1=0.90 1985ZPa (83527) 666
Na ion selective electrode. At I=0.01 M NaCl, K1=1.38. Data for 0.01-1.0 M NaCl, NaOH and NaSCN media. K1 is anion-dependent. Also by 23Na NMR.

Na+ ISE non-aq 25°C 100% C K1=5.60 1984FLa (83528) 667
In propylenecarbonate; electrolyte Et4NClO4

Na+ ISE non-aq 25°C 100% M K1=4.30 1984NMb (83529) 668
Medium: MeOH.

Na+ oth oth/un RT 0.01M C K1=0.52 1984STb (83530) 669
Method: isotachophoresis. Medium: 0.01 M Bu4NCl or 0.01 M Tris.

Na+ ISE alc/w 25°C 100% U K1=4.35 1983GGa (83531) 670
Medium: MeOH

Na+ ISE alc/w 25°C ? U K1=5.98 1983KTa (83532) 671

Na+ con alc/w 25°C 100% U K1=4.46 1983LSa (83533) 672

Na+ sol non-aq 20°C 100% C K1=5.57 1983SLa (83534) 673
Medium: CHCl3

Na+ ISE alc/w 25°C 100% C I T K1=4.35 1982DGa (83535) 674
Method: Na ion selective electrode. Data for 0-100% MeOH/H2O.
K1=1.80 (0%), 2.18 (20%), 2.47 (40%), 2.81 (60%), 3.25 (80%), 3.73 (90%).

Na+ cal alc/w 25°C 90% U IH K1=3.66 1982HLa (83536) 675
Medium: 90% MeOH. DH=-27.80 kJ mol-1, DS=-6.91 J K-1 mol-1

Na+ ISE alc/w 25°C 100% U K1=4.30 1982MKa (83537) 676
Medium: MeOH

Na+ gl alc/w 25°C 100% M H T K1=4.38 1982MRa (83538) 677
Medium: MeOH. DH(K1)=-31.4 kJ mol-1

Na+ ISE non-aq 25°C 100% U T H K1=4.7 1982NYa (83539) 678
Medium: MeCN

Na+ nmr non-aq 25°C 100% U I K1=3.8 1981LPb (83540) 679
Medium: DMSO. In MeCN: 3.8; in pyridine: K1 > 3.0; in acetone: > 4.0;
in DMF: 2.31; in PC: > 4.0; in aqueous: 0.82; in THF and in MeNO2: > 4

Na+ cal alc/w 25°C 100% U H K1=4.36 1980BMa (83541) 680
Medium: MeOH. DH=-35.0 kJ mol-1.

Na+ cal alc/w 25°C 100% U H T K1=4.36 1980LIa (83542) 681
Medium: MeOH. DH=-35.1 kJ mol-1.

Na+ ISE alc/w 25°C 90% C K1=3.51 1980LVb (83543) 682
Method: Na ion selective glass electrode. Medium: 90% v/v MeOH/H2O, 0.10 M
Me4NBr.

Na+ dis non-aq 25°C 100% U K1=5.6 1980TYa (83544) 683
Medium: propylene carbonate

Na+ oth alc/w 25°C 100% U K1=4.32 1980WJa (83545) 684
Method: fluorimetry in CH3OH

Na+ EMF oth/un 25°C var C T K1=0.82 1979HRa (83546) 685
Method: ISE based on cation exchange membrane. Medium: aqueous,
containing 0.06-0.25 m ligand.

Na+ ISE non-aq 25°C 100% C K1=4.28 1979SPf (83547) 686
Medium: MeOH, 0.10 M NaClO4. Method: Na ion selective electrode. Data for
I=0.005-0.50 M NaClO4. At I=0, K1=4.34.

Na+ gl alc/w 20°C 100% U H K1=4.70 1978CLa (83548) 687
Medium: MeOH. Temperature: 20 to 25 C

Na+ cal alc/w 25°C 100% U H K1=4.36 1977ILa (83549) 688
Medium: MeOH. DH(K1)=-35.0 kJ mol-1

Na+ cal alc/w 25°C 70% U H K1=2.76 1976ITa (83550) 689
Medium: 70% w/w MeOH/H2O. DH(K1)=-20.5 kJ mol-1.

Na+ cal oth/un 25°C 100% U H T K1=0.80 1976ITb (83551) 690
Medium: MeOH. DH=-9.14 kJ mol-1.

Na+ ISE alc/w 25°C 100% A K1=4.32 1971FRa (83552) 691
Medium: MeOH. In H2O: K1<0.3
****
C12H25NO5 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
---
Na+ vlt non-aq 25°C 100% C K1=4.6 2000HHa (83708) 692

Medium: acetonitrile, 0.1 M Et4NClO4. Method: dc polarography.

Na+ ISE alc/w 25°C 100% U IH K1=1.96 1998SSf (83709) 693
Medium: 100% MeOH, 0,05 M Et4NI. DH(K1)=-19.5 kJ mol-1

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C12H26NO2P L (7849)
N,N-Diethylcarbamoylmethyl-(dipropylphosphineoxide;

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

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Na+ con non-aq 25°C C K1=3.6 1999ESa (83721) 694
In tetrahydrofuran; alkali metal is used as 2,4-dinitrophenolate

****

C12H26N2O4 L (6933)
1,4-Diaza-7,10,13,16-tetraoxacyclooctadecane;

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

---

Na+ cal alc/w 25°C 100% U H K1=1.92 1994IZa (83732) 695
Medium: MeOH. DH(K1)=-18.1 kJ mol-1, DS(K1)=-24.1 J K-1 mol-1

****

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

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

---

Na+ ISE alc/w 25°C 100% U I K1=1.63 1998SSf (83866) 696
Medium: 100% MeOH, 0,05 M Et4NI. Many other crown ethers studied

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Na+ EMF non-aq 25°C 100% C K1=5.66 1995DGa (83867) 697
Medium: benzonitrile, 0.05 M Et4NClO4.
Competitive method with Ag/Ag+ electrode.

Na+ cal non-aq 25°C 100% M H K1=3.61 1994BCd (83868) 698
Medium: acetone. DH(K1)=-5.8 kJ mol-1, TDS=14.7

Na+ sp non-aq 20°C 100% U K1=2.2 1992PSa (83869) 699
Medium: DMF, 0.01 M Me4NI

Na+ cal non-aq 25°C 100% U H K1=3.92 1986BUb (83870) 700
In CH3CN. DH=-3.6 kJ mol-1

Na+ sol non-aq 20°C 100% C K1=5.47 1983SLa (83871) 701
Medium: CHCl3

Na+ con non-aq 25°C 100% U K1=4.30 1980KMb (83872) 702
Medium: MeCN

****

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

```
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Na+        con non-aq 25°C 100%  U        K1=4.0         1993EVa (84009) 703
Medium: THF+CHCl3 (4:1 vol). Also data for other solvents
--------------------------------------------------------------------------------
Na+        cal oth/un 25°C 0.05M M        K1=1.54        1992BUb (84010) 704
--------------------------------------------------------------------------------
Na+        cal alc/w  25°C  90%  U  IH    K1=1.44        1982HLa (84011) 705
Medium: 90% MeOH. DH=-16.8 kJ mol-1, DS=-8.63 J K-1 mol-1
--------------------------------------------------------------------------------
Na+        ISE alc/w  25°C 100%  U        K1=1.47        1975CJa (84012) 706
Medium: MeOH
--------------------------------------------------------------------------------
Na+        ISE alc/w  25°C 100%  A        K1=1.52        1971FRa (84013) 707
Medium: MeOH
********************************************************************************
C12H27N3O3              L    THETAC             (7199)
1,4,7-Tris(hydroxyethyl)-1,4,7-triazacyclononane
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Na+        EMF non-aq 25°C 100%  C        K1=3.52        1997WWa (84089) 708
Medium: MeOH, 0.05M Et4NClO4.
Method: Ag/Ag+ electrode; by competition with Ag+.
********************************************************************************
C12H32N4O12P4         H8L    DOTPH            CAS 91987-74-5  (229)
1,4,7,10-Tetraazacyclododecane-N,N',N",N"'-tetramethylenephosphonic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Na+        gl  R4N.X  25°C 0.10M M                         1990DSa (84417) 709
                                        B(NaHL)=16.72
                                        B(NaH2L)=27.93
                                        B(NaH3L)=36.67
                                        B(NaH4L)=44.10
Medium: Me4NNO3
********************************************************************************
C13H20O5                L                       (2511)
1-Hydroxy-2-(1,4,7,10-tetraoxaundecyl)benzene; HO.C6H4.O.(CH2.CH2.O)3.CH3
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Na+        ISE alc/w  25°C 100%  U        K1=1.35        1975CJa (86149) 710
Medium: MeOH
********************************************************************************
C13H22O8                L                     CAS 58484-46-1  (2140)
1,5,8,11,14,17-Hexaoxacyclononadecane-2,4-dione;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
```

Na+ kin alc/w ? 76% U K1=1.62 1991HHb (86380) 711
Medium: 76% w/w EtOH/H2O

Na+ cal alc/w 25°C 100% U H K1=1.80 1980LIb (86381) 712
Medium: MeOH. DH=-4.60 kJ mol-1.

Na+ cal alc/w 25°C 100% U H K1=1.8 1977ILa (86382) 713
Medium: MeOH. DH(K1)=-4.6 kJ mol-1
****
C13H23N3O7 HL CAS 264130-50-9 (8947)
alpha-Methylurazolyl-15-crown-5;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ nmr alc/w 25°C 100% C 2000ABc (86390) 714
K(Na+HL)=2.20
Medium: CH3OD. Method: 13C nmr.
****
C13H24O7 L CAS 76377-06-5 (612)
3-Methyl-11,4,7,10,13,16-hexaoxacyclooctadecan-2-one, 3-Methyl-2-one-18-crown-6;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE alc/w 25°C 100% U K1=3.07 1982MKa (86427) 715
Medium: MeOH
****
C13H26O5 L (8408)
1,4,7,10,13-Pentaoxacyclooctadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ cal non-aq 25°C 0.05M U K1=2.46 1996RSc (86465) 716
Medium: 0.05 M Et4NI in MeOH; by Na-selective electrode K1=2.48
DH(K1)=-23.5 kJ mol-1. IN 0.05 M Et4NI in H2O K1=0.79
****
C13H26O5 L (6410)
15,15-Dimethyl-1,4,7,10,13-pentaoxacyclohexadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ con none 25°C 0.0 C K1=0.60 2001KMb (86479) 717

Na+ con non-aq 25°C 100% C I K1=4.3 1992TFa (86480) 718
Medium: acetonitrile. In propylene carbonate, K1=4.0.

Na+ con alc/w 25°C 100% U K1=3.73 1991IOa (86481) 719
Medium: MeOH
****
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
---
Na+ con non-aq 25°C 100% C I K1=4.31 2000TMb (86500) 720
Medium: CH3CN. In other media, K1=4.49 (propylene carbonate), 2.83 (MeOH).

Na+ con oth/un 25°C dil C K1=0.93 1999TMa (86501) 721
Self medium (NaCl).
****
C13H26O7 L CAS 77887-91-3 (1662)
1,4,7,10,13,16-Hexaoxacyclononadecan-12-ol, Hydroxy-19-crown-6

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE alc/w 25°C 100% U K1=2.62 1983IKa (86508) 722
Medium: MeOH
****
C14H8O3 L CAS 6050-13-1 (5026)
2,2'-Biphenyldicarboxylic anhydride; (diphenic anhydride)

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp non-aq ? 100% U 1971TGa (86632) 723
K(NaSCN+L)=-0.07
K(2NaSCN+L)=0.98
Medium: CH3CN
****
C14H12N2O7S H3L CAS 5138-23-8 (5082)
4,8-Diamino-9,10-dihydro-1,5-dihydroxy-9,10-dioxo-anthracene-2-sulfonic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ con diox/w 15°C 70% U T K1=3.12 1970MHa (87298) 724
K1(25 C)=3.14, K1(35 C)=3.21. DH=8.06 kJ mol-1, DS=88.2 J K-1 mol-1

Na+ con diox/w 15°C 82% U T K1=3.94 1970MHa (87299) 725
K1(25 C)=3.99; K1(35 C)=4.11. DH=14.92 kJ mol-1, DS=127.5 J K-1 mol-1

Na+ con diox/w 25°C 60% U I K1=2.60 1969MFa (87300) 726
Medium: I near zero, 75% dioxan: K1=3.27; 85%: K1=4.54
****
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
---
Na+ gl R4N.X 25°C 0.10M C H K1=0.9 1990NNa (87961) 727
K(NaL+H)=6.6
Medium: Et4NClO4. DH(K1)=9 kJ mol-1. DS(K1)=40 J mol-1 K-1.

```
---------------------------------------------------------------------------
Na+        gl  R4N.X  25°C 0.10M U        K1=1.60        1985MHb (87962) 728
                                          K(NaL+H)=6.41
                                          K(Na+HL)=1.31
                                          K(NaHL+H)=4.50
Medium: 0.10 M Me4NCl.
***************************************************************************
C14H18N2O9              L                      CAS 99624-13-2  (1769)
2,3-(3',4'-Dinitrobenzo)-1,4,7,10,13-pentaoxacyclopentadeca-2-ene,
3',4'-Dinitrobenzo-15-crown-5
---------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
---------------------------------------------------------------------------
Na+        con non-aq 25°C 100%  U        K1=2.18        1976UHa (88086) 729
Medium: acetone
***************************************************************************
C14H19O5Br              L                      CAS 60835-72-5  (1772)
2,3-(4'-Bromobenzo)-1,4,7,10,13-pentaoxacyclopentadeca-2-ene,
4'-Bromobenzo-15-crown-5
---------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
---------------------------------------------------------------------------
Na+        con non-aq 25°C 100%  U        K1=3.31        1976UHa (88158) 730
Medium: acetone
***************************************************************************
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
---------------------------------------------------------------------------
Na+        con mixed  25°C  20%  C   H    K1=0.65        2004JOb (88312) 731
Medium: 20% mole fraction hexamethylphosphortriamide/H2O.
DH(K1)=-51.63 kJ mol-1, DS(K1)=-160.6 J K-1 mol-1.
---------------------------------------------------------------------------
Na+        con non-aq 25°C 100%  C  IH    K1=4.24        2003JOa (88313) 732
Medium: acetonitrile. Data for 0-1.0 mol fraction acetonitrile in H2O.
DH(K1)=-22.90 kJ mol-1, DS(K1)=4.36 J K-1 mol-1.
---------------------------------------------------------------------------
Na+        dis non-aq 24°C 100%  C                       2002MRd (88314) 733
                                          K(Na+A+L)=6.26
Medium: CDCl3. HA is picric acid.
---------------------------------------------------------------------------
Na+        dis none   25°C  dil  C  I M                 2002THb (88315) 734
                                          K(NaL+A)=2.66
                                          K(Na+A+L(org)=NaAL(org))=3.821
HA is picric acid. Data for several aryl and alkyl solvents.
Method: extraction of metal picrate into dichloromethane/L.
---------------------------------------------------------------------------
Na+        con none   25°C  0.0  C        K1=0.45        2002TTa (88316) 735
---------------------------------------------------------------------------
```

Na+ sp non-aq 25°C 100% U K1=9.45 2000EGa (88317) 736
Method: fluorescence emission spectroscopy. Medium: acetonitrile.

Na+ con non-aq 25°C 100% C K1=5.29 2000ICa (88318) 737
Medium: nitromethane.

Na+ vlt non-aq 20°C 100% C K1=1.6 1999OBa (88319) 738
Medium: DMF, 0.10 M Bu4N[BPh4]. Method: by competition with Tl(I).

Na+ con non-aq 25°C 100% C H K1=1.42 B2= 2.17 1999WBa (88320) 739
Medium: N,N-dimethylformamide. By calorimetry: DH(K1)=-12.4 kJ mol-1,
DH(K2)=-5.0 kJ mol-1.

Na+ vlt non-aq 25°C 100% C I K1=4.5 1999WKb (88321) 740
Medium: acetonitrile, 0.10 M Et4NClO4. Also data for TMS, propylene
carbonate, acetone, formamide, DMF, DMA, DMSO, MeOH, EtOH.

Na+ nmr non-aq 27°C 100% U I K1=4.62 1996KAa (88322) 741
Method: 23Na nmr. Medium: acetonitrile. Also data for 20, 40, 60, 80 wt%
DMSO in AN. For DMSO: K1=1.00. For 20% DMSO, K1=2.54.

Na+ dis oth/un 25°C 0 U K1=2.87 1994OUa (88323) 742

Na+ ISE none 25°C 0.0 C K1=5.08 B2=11.76 1993GEb (88324) 743
B(Na2L)=12.56
B(Na2L2)=19.00
Method: Na-selective glass electrode. Self medium.

Na+ ISE alc/w ? 100% U K1=2.78 1992CLb (88325) 744
Medium: MeOH

Na+ ISE alc/w 25°C 100% C I K1=2.94 1992PTa (88326) 745
K(NaL+Br)=1.28
Method: Na ISE. Medium: methanol, 1-5 mM NaBr. In DMF, K1=1.38.
Data for 4,5-dibromo-, 4,5-dimethoxy- and 4,5-dibutoxybenzo-15-crown-5.

Na+ ISE mixed 25°C 50% C K1=2.2 1991LMc (88327) 746
Method: Na ion selective glass electrode. Medium: 50% w/w MeOH/DMF.

Na+ nmr oth/un 25°C ? U K1=3.47 B2=5.21 1989LFa (88328) 747

Na+ cal non-aq 25°C 100% U H K1=4.02 1989SSd (88329) 748
Medium: CH3CN

Na+ cal non-aq 25°C 100% C H K1=4.47 1988BUb (88330) 749
Medium: acetonitrile. DH(K1)=-23.5 kJ mol-1, DS(K1)=6.4 J K-1 mol-1.

Na+ con non-aq 25°C 100% C I K1=4.25 1988TKb (88331) 750
Medium: MeCN. In propylene carbonate K1=4.35; in MeOH 2.99

Na+ con non-aq 25°C 100% C T H K1=4.61 1988TMb (88332) 751
Medium: acetonitrile. Data for 15-35 C. Anion: tetraphenylborate.
DH(K1)=-36 kJ mol-1, DS(K1)=-32.8 J K-1 mol-1.

Na+ sp non-aq 22°C 100% U K1=6.26 1987CCc (88333) 752
In deuterochloroform

Na+ ISE alc/w 25°C 90% U K1=2.68 1987KHa (88334) 753
Medium: 90% w/w MeOH/H2O

Na+ con non-aq 25°C 100% C I K1=2.94 1987ZBb (88335) 754
Medium: MeOH. In 70% w/w MeOH/H2O, K1=1.97.

Na+ sp mixed 25°C 20% U I K1=0.76 1986GSa (88336) 755
In 0.015 M Et4NCl, 20% CH3CN/H2O. In 40%, K1=1.18; 60%, K1=1.68;
80%, K1=2.45; 100% CH3CN, K1=3.65

Na+ cal non-aq 25°C 100% C H K1=2.89 1986ICa (88337) 756
Medium: MeOH. DH(K1)=-18.6 kJ mol-1, DS(K1)=-7.1 J K-1 mol-1.

Na+ ISE R4N.X 25°C 0.10M C K1=2.91 1986XJa (88338) 757

Na+ cal alc/w 25°C 80% U H K1=2.20 1985LWa (88339) 758

Na+ vlt alc/w 25°C 100% U K1=2.97 1985ZBa (88340) 759
Medium: MeOH

Na+ ISE alc/w 25°C 100% C K1=3.05 1985ZFa (88341) 760
Medium: MeOH, 0.001 M NaClO4

Na+ con alc/w 25°C 100% U K1=3.37 1983LSa (88342) 761

Na+ con non-aq 25°C 100% U K1=4.35 1982TAa (88343) 762
Medium: propylene carbonate

Na+ nmr non-aq 25°C 100% U I K1=2.60 1981LPb (88344) 763
Medium: pyridine. In MeCN: K1 > 4; in DMSO: 1.10; in THF > 4;
in DMF: 1.60; in nitromethane: K1 > 4, K2=0.8

Na+ ISE alc/w 25°C 100% C K1=3.05 1981PTa (88345) 764
Medium: MeOH

Na+ cal alc/w 25°C 70% U I K1=1.99 B2=4.15 1976ITa (88346) 765
Medium: 70% w/w MeOH/H2O. DH(B2)=-58.2 kJ mol-1. In 20% MeOH: K1=1.17;
60%: 1.62. In 80%: K1=2.2, B2=4.80, DH(B2)=-64.85 kJ mol-1

Na+ oth alc/w 25°C 100% U K1=2.82 1976MHa (88347) 766
Medium: MeOH. Method: circular dichroism

Na+ con non-aq 25°C 100% U K1=3.54 1976UHa (88348) 767

Medium: acetone
****
C14H21NO5 L CAS 60835-71-4 (1777)
2,3-(4'-Aminobenzo)-1,4,7,10,13-pentaoxacyclopentadeca-2-ene;
4'-Aminobenzo-15-crown-5

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	con	non-aq	25°C	100%	U	T	K1=3.91	1976UHa (88402)	768

Medium: acetone
****
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
Na+	vlt	R4N.X	20°C	0.10M	U		K1=3.79	1972BZc (88724)	769

Medium: Me4NOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	oth	R4N.X	25°C	0.50M	U		K1=4.66 K(Na+HL)=0.74	1971CSa (88725)	770

Method: polarimetry. Medium: Me4NOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	ISE	oth/un	25°C	0.10M	U		K1=4.40	1970CSa (88726)	771

Medium: CsNO3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	vlt	KNO3	30°C	0.10M	U		K1=2.70	1967SSe (88727)	772

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	kin	KCl	25°C	1.50M	U		K1=1.38	1968TFb (89898)	773

****
C14H24O8 L CAS 96813-83-1 (2271)
1,4,7,10,13,16-Hexaoxacycloeicos-17,20-dione;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	cal	alc/w	25°C	100%	U	H	K1=1.70	1980LIb (90044)	774

Medium: MeOH. DH=-4.20 kJ mol-1.
****
C14H25N3O7 H3L (5397)
1-Oxa-4,7,10-triazacyclododecane-4,7,10-triethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	gl	R4N.X	25°C	0.10M	U		K1=3.27	1988ADa (90089)	775

****

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
Na+	gl	R4N.X	25°C	0.10M	C		K1=2.72	1987DDb (90199)	776

****
C14H26N4O6 H3L DOTRA (6701)
1,4,7,10-Tetraazacyclododecane-1,4,7-triethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	gl	R4N.X	25°C	0.10M	C		K1=2.20	2000BCa (90254)	777

Medium: 0.10 M NMe4Cl.
****
C14H26O5 L CAS 17454-48-7 (5039)
Cyclohexyl-15-crown-5, 2,3-Cyclohexyl-1,4,7,10,13-pentaoxacyclopentadecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	ISE	alc/w	25°C	100%	A		K1=3.71	1971FRa (90273)	778

Medium: MeOH. In H2O: K1<0.3
****
C14H26O7 L CAS 83410-59-7 (613)
3,3-Dimethyl-1,4,7,10,13,16-hexaoxacyclooctadecan-2-one,
3,3-Dimethyl-2-one-18-crown-6;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	ISE	alc/w	25°C	100%	U		K1=2.93	1982MKa (90275)	779

Medium: MeOH
****
C14H28N2O4 L Cryptand 2,1,1 CAS 31250-06-3 (836)
1,10-Diaza-4,7,13,18-tetraoxabicyclo[8,5,5]eicosane (2,1,1);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	cal	non-aq	25°C	100%	C	H	K1=4.85	1999WBa (90405)	780

Medium: N,N-dimethylformamide. DH(K1)=-35.7 kJ mol-1.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	gl	R4N.X	25°C	0.05M	C	H	K1=3.8	1996BCh (90406)	781

Medium: 0.05 M Et4NClO4. By calorimetry: K1=3.4, DH(K1)=-22.5 kJ mol-1.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	cal	non-aq	25°C	100%	M	H	K1=7.69	1994BCd (90407)	782

Medium: acetone. DH(K1)=-48.0 kJ mol-1, TDS=-4.3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	ISE	non-aq	25°C	100%	U	IH	K1=4.72	1993LRa (90408)	783

Medium: triethylphosphate, 0.05 M Et4NClO4. DH(K1)=-67.0 kJ mol-1,
DS=2.6 J K-1 mol-1; Data also for tri-n-butylphosphate: K1=4.94

```
Na+        sp  non-aq 20°C 100%  U        K1=5.23        1992PSa (90409) 784
Medium: DMF, 0.01 M Me4NI
--------------------------------------------------------------------------------
Na+        gl  R4N.X  25°C 0.05M U   H    K1=5.38        1991LRc (90410) 785
DH(K1)=-62.2 kJ mol-1, DS=20.3 J K-1 mol-1
--------------------------------------------------------------------------------
Na+        ISE non-aq 25°C 100%  C        K1=4.4         1989MGa (90411) 786
Medium: DMF, 0.10 M Et4NClO4
--------------------------------------------------------------------------------
Na+        ISE non-aq 25°C 100%  U  I     K1=5.10        1988CAa (90412) 787
Medium: diethylformamide, 0.05 M Et4NClO4. In dimethylacetamide, K=4.74
--------------------------------------------------------------------------------
Na+        ISE non-aq 25°C 100%  U   H    K1=8.74        1986BUb (90413) 788
In CH3CN. DH=-52.9 kJ mol-1
--------------------------------------------------------------------------------
Na+        cal alc/w  25°C 100%  U   H    K1=6.64        1986BUd (90414) 789
In MeOH. DH=-33.1 kJ mol-1
--------------------------------------------------------------------------------
Na+        ISE non-aq 25°C 100%  C  I     K1=4.52        1985CKa (90415) 790
Medium: DMSO. In propylenecarbonate K1=8.40; in DMF K1=5.17
--------------------------------------------------------------------------------
Na+        gl  alc/w  25°C  95%  C        K1=6.53        1981ANa (90416) 791
Medium: 95% MeOH, 0.1 M Me4NCl
--------------------------------------------------------------------------------
Na+        ISE non-aq 25°C 100%  U        K1=5.23        1981CRa (90417) 792
Medium: DMF. In DMSO: K1=4.63; in EtOH: 7.09, in MeCN: >9; in NMP: 5.04
--------------------------------------------------------------------------------
Na+        ISE non-aq 25°C 100%  U        K1=8.7         1980CRa (90418) 793
Medium: Propylene carbonate
--------------------------------------------------------------------------------
Na+        EMF non-aq 25°C 100%  C        K1=2.8         1979BLb (90419) 794
Method: Ag electrode; competition with Ag+. Medium: MeOH, 0.05 M
Me4NClO4.
--------------------------------------------------------------------------------
Na+        cal R4N.X  25°C 0.06M C   H                   1976KLc (90420) 795
Medium: 0.057 M Me4NBr. Method: flow microcalorimetry.
DH(K1)=-22.6 kJ mol-1, DS(K1)=-13 J K-1 mol-1.
--------------------------------------------------------------------------------
Na+        gl  R4N.X  25°C 0.05M C  I     K1=3.2         1975LSc (90421) 796
In 95% MeOH: K1=6.08; 100%: 6.1
********************************************************************************
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
--------------------------------------------------------------------------------
Na+        ISE R4N.X  25°C 0.05M U  I     K1=3.2         1991LSb (90463) 797
Medium: 0.05 M Et4NClO4. In acetonitrile, K1=9.4; CH3OH, K1=6.6;
DMF, K1=6.1; DMSO, K1=5.6l; pyridine, K1=8.4
********************************************************************************
```

C14H28N2O7 L (2509)
1,17-Diacetamido-3,6,9,12,15-pentaoxaheptadecane; O((CH2.CH2.O)2.CH2.CH2.CO.NH2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	ISE	alc/w	25°C	100%	U		K1=1.25	1975CJa (90493)	798

Medium: MeOH

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	sol	non-aq	25°C	100%	C		K1=3.54	1999KCa (90530)	799

Medium: acetonitrile.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	ISE	alc/w	25°C	100%	U		K1=2.54	1983GGa (90531)	800

Medium: MeOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	cal	alc/w	25°C	100%	U	H	K1=1.73	1980LIa (90532)	801

Medium: MeOH. DH=-43.4 kJ mol-1.

****

C14H30NO2P L (2094)
P-(N,N-Diethylamidocarbonyl)methyl-P,P-dibutylphosphine oxide;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	con	non-aq	25°C		C		K1=3.6	1999ESa (90556)	802

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	con	non-aq	25°C	100%	U		K1=3.08	1988YKa (90557)	803

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
Na+	sol	non-aq	20°C	100%	C		K1=5.49	1983SLa (90563)	804

Medium: CHCl3

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	gl	alc/w	25°C	95%	C		K1=3.33	2004KVa (90582)	805

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	ISE	alc/w	25°C	100%	U	I	K1=3.53	1998SSf (90583)	806

Medium: 100% MeOH, 0,05 M Et4NI

Na+ ISE alc/w 25°C 90% C K1=3.08 1980LVb (90584) 807
Method: Na ion selective glass electrode. Medium: 90% v/v MeOH/H2O, 0.10 M Me4NBr.

Na+ gl alc/w 25°C 93% U K1=2.55 1978WVa (90585) 808
Medium: 93% MeOH/H2O

****

C14H30N2O5 L (6722)
7,13-Bis(2-hydroxyethyl)-1,4,10-trioxa-7,13-diazacyclopentadecane

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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	ISE	non-aq	25°C	100%	U	I	K1=3.93	1993RPa	(90632) 809

Medium: dimethylformamide, 0.05 M Et4NClO4. By competition with Ag+.
In acetonitrile, K=7.00.

****

C14H30N2O5 L (6929)
N,N'-Bis(hydroxyethyl)-1,4-diaza-7,10,13-trioxacyclopentadecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	cal	alc/w	25°C	90%	U	H	K1=3.14	1994IZa	(90639) 810

Medium: 90% v/v MeOH/H2O. DH(K1)=-24.9 kJ mol-1
DS(K1)=-23.5 J K-1 mol-1

****

C14H30O7 L CAS 1072-40-8 (2499)
2,5,8,11,14,17,20-Heptaoxaheneicosane; CH3.O.(CH2.CH2.O)6.CH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	dis	non-aq	25°C	100%	C		K1=8.45	1998KSc	(90701) 811

Medium: 1,2-dichloroethane.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	con	non-aq	25°C	100%	U			1993EVa	(90702) 812

Medium: THF+CHCl3 (4:1 vol). Also data for other solvents

Na+ ISE alc/w 25°C 100% U K1=1.60 1975CJa (90703) 813
Medium: MeOH

****

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
Na+	nmr	non-aq	27°C	100%	U		K1=1.67	1996MAb	(91164) 814

Method: 23Na nmr. Medium: nitromethane, 0.05 M NaClO4.

****

C15H12O2 HL Diphenylacac CAS 120-46-7 (362)

1,3-Diphenylpropane-1,3-dione, Dibenzoylmethane; C6H5.CO.CH2.CO.C6H5

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	gl	alc/w	25°C	100%	U		K1=2.4	1965LIa (91555)	815

Medium: MeOH, 0.1 M NaClO4

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	gl	diox/w	30°C	75%	U		K1=4.18	1954FUa (91556)	816

****

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
Na+	con	non-aq	25°C	100%	U		K1=1.57	1989TKb (91988)	817

Medium: tetrahydrofuran/CHCl3 4:1 (volume)

****

C15H18NO7Cl L CAS 71022-76-9 (2322)

19-Chloro-3,6,9,12,15-pentaoxa-21-azabicyclo[15.3.1]heneicosa-1(21),17,19-teiene-2,16-dione;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	cal	alc/w	25°C	100%	U	H	K1=4.14	1980BMa (91994)	818

Medium: MeOH. DH=-25.2 kJ mol-1.

****

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
Na+	gl	R4N.X	25°C	0.10M	U		K1=1.43 K(NaL+H)=6.71 K(Na+HL)=0.95	1985MHb (92085)	819

Medium: 0.10 M Me4NCl.

****

C15H19NO7 L CAS 64397-58-4 (2170)

3,6,9,12,15-Pentaoxa-21-azabicyclo[15.3.1]heneicosa-1(21),17,19-triene-2,16-dione;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	cal	alc/w	25°C	100%	U	H	K1=4.29	1981BBb (92121)	820

Medium: MeOH. DH(K1)=-25.9 kJ mol-1

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	cal	alc/w	25°C	100%	U	H	K1=4.29	1980BMa (92122)	821

Medium: MeOH. DH=-25.9 kJ mol-1.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	cal	alc/w	25°C	100%	U	H	K1=4.29	1980LIb (92123)	822

Medium: MeOH. DH=-25.9 kJ mol-1

Na+ sp alc/w 25°C 100% U H K1=4.29 1977ILc (92124) 823
Medium: Methanol. DH(K1)= -25.9 kJ mol-1
****
C15H20O6 L (1770)
2,3-(4'-Formylbenzo)-1,4,7,10,13-pentaoxacyclopentadeca-2-ene;
4'-Formylbenzo-15-crown-5

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ con non-aq 25°C 100% U K1=3.05 1976UHa (92192) 824
Medium: acetone
****
C15H20O7 HL (1771)
2,3-(4'-Carboxybenzo)-1,4,7,10,13-pentaoxacyclopentadeca-2-ene;
4'-Carboxybenzo-15-crown-5

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ con non-aq 25°C 100% U K1=3.21 1976UHa (92193) 825
Medium: acetone
****
C15H22O5 L CAS 65112-33-6 (6058)
18-Methoxy-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
---
Na+ cal alc/w 25°C 100% U H K1=1.14 1987ZBa (92250) 826
Medium: MeOH. DH=-8.4 kJ mol-1; DS=-6.7. By ISE potentiometry; K1=1.11
****
C15H22O5 L (1773)
2,3-(4'-Methylbenzo)-1,4,7,10,13-pentaoxacyclopentadeca-2-ene;
4'-Methylbenzo-15-crown-5

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ con non-aq 25°C 100% U K1=3.60 1976UHa (92251) 827
Medium: acetone
****
C15H22O5 L CAS 32702-27-5 (681)
2,3-Benzo-6-methyl-15-crown-5;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ nmr oth/un 25°C ? U K1=3.60 B2=4.00 1989LFa (92252) 828
B(Na3L2)=1.00
****
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

---
Na+ ISE alc/w 25°C 100% U K1=2.08 1985SWa (92258) 829
Medium: MeOH
****
C15H23NO4 L CAS 90774-27-9 (5815)
N-(2-Methoxyphenyl)-1-aza-4,7,10-trioxacyclododecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE alc/w 25°C 100% U K1=2.75 1985SWa (92259) 830
Medium: MeOH. For 4-Methoxyphenyl-, K1=1.38
****
C15H23NO5 L CAS 53914-89-9 (2262)
3,6,9,12,15-Pentaoxa-21-azabicyclo[15.3.1]heneicosa-1(21),17,19-triene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ cal alc/w 25°C 100% U H K1=4.09 1980BMa (92272) 831
Medium: MeOH. DH=-22.8 kJ mol-1.

Na+ cal alc/w 25°C 100% U H K1=4.09 1980LIa (92273) 832
Medium: MeOH. DH=-22.8 kJ mol-1.

Na+ sp alc/w 25°C 100% U H K1=4.09 1977ILc (92274) 833
Medium: Methanol. DH= -22.8 kJ mol-1
****
C15H24NO2P L (7846)
N,N-Diethylcarbamoylmethyl-(P-phenyl-P-propylphosphineoxide);

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ con non-aq 25°C C K1=3.5 1999ESa (92330) 834
In tetrahydrofuran; alkali metal is used as 2,4-dinitrophenolate
****
C15H24O6 HL CAS 57722-03-9 (2353)
1-Hydroxy-2-(1,4,7,10,13-pentaoxatridecyl)benzene; HO.C6H4.O(CH2CH2O)4CH3

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp alc/w 25°C 100% U K1=2.99 1981EMb (92345) 835
Medium: MeOH

Na+ ISE alc/w 25°C 100% U K1=2.19 1975CJa (92346) 836
Medium: MeOH
****
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
---

Na+ ISE non-aq 25°C 100% U K1=1.55 1993LRa (92522) 837
Medium: tri-n-butylphosphate, 0.05 M Et4NClO4

Na+ gl R4N.X 25°C 0.05M U K1=1.90 1991LRc (92523) 838

Na+ ISE non-aq 25°C 100% U I K1=2.87 1988CAa (92524) 839
In dimethylformamide; medium: 0.05M Et4NClO4. In diethylformamide, K=2.52, in dimethylacetamide, K=2.05.

Na+ kin non-aq 25°C 100% C I K1=2.87 1987ABe (92525) 840
Medium: dimethylformamide. In MeOH, K1=3.76; in pyridine, K1=3.72, in acetonitrile, K1=5.08, in propylene carbonate, K1=5.12; in acetone K1=3.98

Na+ ISE non-aq 25°C 100% U I K1=3.72 1986LSc (92526) 841
Medium: pyridine, 0.05 M Et4NClO4. Method: competitive equilibrium plus Ag wire electrode. In MeOH K1=3.76; in DMF K1=2.87
****
C15H31NO6 L (5817)
N-1-(3,6,9-Trioxadecyl)-1-aza-4,7,10-trioxacyclododecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE alc/w 25°C 100% U K1=3.97 1985SWa (92540) 842
Medium: MeOH. For 3,6,9,12-Tetraoxatridecyl- K1=3.76;
11-Allyl-oxy-3,6,9-trioxa-undecyl- K1=3.97
****
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
---
Na+ EMF non-aq 25°C 100% C I K1=2.50 2001WBa (92576) 843
Medium: methanol, 0.05 M Et4NClO4. In DMF, K1=2.29. Competition with Ag+. Also data for the 1,4,7-tris((S)-2-hydroxy-2-phenyethyl- derivative.
****
C15H33N3O3 L CAS 75403-76-8 (8202)
4,6,10-Trimethyl-1,7,13-trioxa-4,10,16-triazacyclooctadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE alc/w 25°C 90% C K1=3.11 1980LVb (92579) 844
Method: Na ion selective glass electrode. Medium: 90% v/v MeOH/H2O, 0.10 M Me4NBr.
****
C15H36NO9P3 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
---

Na+ con non-aq 22°C 100% U K1=1.74 1981SKd (92605) 845
Medium: CH3CN
****
C16H16O6 H2L (5634)
1-(2-Hydroxyphenyl)-4-(2-carboxymethoxyphenyl)-1,4-dioxabutane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE alc/w 25°C 100% U K1=1.48 1981PTb (93716) 846
Medium: MeOH
****
C16H20N3O8F3 L (1041)
2,4-Dinitro-6-trifluoromethylphenyl-aminomethyl-12-crown-4

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp mixed 25°C 16% U K1=1.66 1984BPa (94084) 847
K(Na+HL)=1.17
****
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
---
Na+ con non-aq 25°C 100% U K1=2.90 1982YSa (94100) 848
Medium: tetrahydrofuran+CHCl3 4:1(vol); M is 2,4-dinitrophenolate
****
C16H22O6 L (6667)
2'-Acetyl-2,3-benzo-1,4,7,10,13-pentaoxacyclopentadeca-2-ene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE alc/w ? 100% U K1=2.31 1992CLb (94241) 849
Medium: MeOH. Data also for 2'-t-butyl, 2'-(1,1-dibutylethyl), 2'-(1-methyl-
1-dodecylethyl) analogues and others
****
C16H22O6 HL (6823)
3,6,9,12-Tetraoxabicyclo[12.3.1]octadeca-1(18),14,16-triene-18-ethanoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ kin alc/w 25°C 100% U K1=<0.48 1992CDc (94244) 850
Medium:MeOH. Data also for other related ligands
****
C16H22O7 HL (1774)
2,3-(4'-Methylcarboxybenzo)-1,4,7,10,13-pentaoxacyclopentadeca-2-ene;
4'-Methylcarboxy-15-crown-5

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

Na+ con non-aq 25°C 100% U K1=3.09 1976UHa (94254) 851
Medium: acetone
****
C16H23NO8 L CAS 53408-96-1 (1765)
2,3-(4'-Nitrobenzo)-1,4,7,10,13,16-hexaoxacyclooctadeca-2-ene;
4'-Nitrobenzo-18-crown-6

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE R4N.X 25°C 0.10M C K1=2.20 1986XJa (94270) 852

Na+ con non-aq 25°C 100% U K1=4.67 1976UHa (94271) 853
Medium: acetone
****
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
---
Na+ dis non-aq 25°C 100% U H 1979KLa (94348) 854
K(Na(picrate)+L)=3.23
Medium: CHCl3

Na+ dis non-aq 24°C 100% C 1977MTc (94349) 855
K(NaA+L)=3.23
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
---
Na+ dis non-aq 25°C 100% U H 1979KLa (94356) 856
K(Na(picrate)+L)=4.15
Medium: CHCl3
****
C16H24O5 L CAS 68985-72-0 (687)
2,3-Benzo-1,4,7,11,14-pentaoxacycloheptadeca-2-ene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ cal alc/w 25°C 80% U H K1=1.84 1985LWa (94357) 857
****
C16H24O5 L (682)
2,3-Benzo-8,12-dimethyl-15-crown-5;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ nmr oth/un 25°C ? U K1=3.00 B2=3.19 1989LFa (94358) 858

B(Na3L2)=0.99

****

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
Na+	cal	alc/w	25°C	80%	C	H	K1=2.23	1991LTa (94361)	859

Medium: 80% MeOH/H2O. DH(K1)=-1.63 kJ mol-1.

Na+	dis	non-aq	22°C	100%	C			1984CBa (94362)	860
							K(Na+A+L(org)=NaAL(org))=0.95		

Extraction of metal picrate from H2O into CDCl3. HA is picric acid.

Na+	ISE	alc/w	25°C	100%	U		K1=1.35 B2=3.33	1982MYc (94363)	861

Medium: MeOH

****

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
Na+	dis	NaClO4	25°C	0.1M	C	I	K1=0.81	2002TYa (94426)	862
							K(NaL+ClO4)=-1.95		

Extraction of NaClO4 with L into dichloromethane. K1 by conductivity.
K(Na+L(org)+ClO4=NaLClO4(org))=0.56. K(NaL+ClO4=NaLClO4(org)=2.27.

Na+	sp	non-aq	25°C	100%	U		K1=9.19	2000EGa (94427)	863

Method: fluorescence emission spectroscopy. Medium: acetonitrile.

Na+	con	non-aq	25°C	100%	C		K1=>6	2000ICa (94428)	864

Medium: nitromethane.

Na+	dis	non-aq	25°C	100%	U		K1=9.43	2000KSa (94429)	865

Medium: 1,2-dichloroethane

Na+	oth	alc/w	25°C	3%	U	M		2000MTa (94430)	866
							K(NaL+phenolate)=1.18		
							K(NaL+o-nitrophenolate)=1.48		
							K(NaL+m-nitrophenolate)=1.42		
							K(NaL+p-nitrophenolate)=1.49		

Method: CZE. Medium: 3% v/v EtOH/H2O. K(NaL+2,4-dinitrophenolate)=1.58,
K(NaL+picrate)=1.45, K(NaL+SCN)=1.43, K(NaL+ClO4)=1.02.

Na+	oth	alc/w	35°C	3.0%	C		K1=1.42	1999MTd (94431)	867

Method: capillary zone electrophoresis. Medium: 3% v/v EtOH/H20, 0.005 M
phosphate buffer, pH 7.0

Na+	cal	non-aq	25°C	100%	C	H	K1=2.59	1999WBa (94432)	868

Medium: N,N-dimethylformamide. DH(K1)=-24.4 kJ mol-1.

```
--------------------------------------------------------------------------------
Na+        dis oth/un 25°C    0  U        K1=4.16        1994OUa (94433) 869
--------------------------------------------------------------------------------
Na+        ISE none   25°C  0.0  C        K1=4.97   B2=11.64  1993GEb (94434) 870
                                          B(Na2L)=12.43
                                          B(Na2L2)=18.86
Method: Na-selective glass electrode. Self medium.
--------------------------------------------------------------------------------
Na+        ISE none   25°C  0.0  U        K1=1.38        1989TKa (94435) 871
--------------------------------------------------------------------------------
Na+        sp  non-aq 22°C 100%  U        K1=5.65        1987CCc (94436) 872
In deuterochloroform
--------------------------------------------------------------------------------
Na+        ISE alc/w  25°C  90%  U        K1=3.62        1987KHa (94437) 873
Medium: 90% w/w MeOH/H2O
--------------------------------------------------------------------------------
Na+        cal non-aq 25°C 100%  C   H    K1=4.21        1986ICa (94438) 874
Medium: MeOH. DH(K1)=-34.6 kJ mol-1, DS(K1)=-35.6 J K-1 mol-1.
--------------------------------------------------------------------------------
Na+        sp  diox/w 25°C  0.0  U  I     K1=2.18        1983KOa (94439) 875
On PVA. In 24.4% w/w dioxan/H2O. Data given for 9.7-84.6 w/w mixtures.
--------------------------------------------------------------------------------
Na+        sp  mixed  25°C  0.0  U  I     K1=2.04        1983KOa (94440) 876
On PVA. In 21.9% w/w tetrahydrofuran/H2O. Data given for 11.1-86.4 w/w mix
--------------------------------------------------------------------------------
Na+        sp  alc/w  25°C 100%  U        K1=4.03        1981EMb (94441) 877
Medium: MeOH
--------------------------------------------------------------------------------
Na+        sp  diox/w 25°C 100%  U    M                  1981SSd (94442) 878
                                          K(K(Picrate)+L)=4.41
--------------------------------------------------------------------------------
Na+        con non-aq 25°C 100%  U        K1=4.72        1976UHa (94443) 879
Medium: acetone
********************************************************************************
C16H24O6               HL                      CAS 65112-36-9  (6060)
3,6,9,12,15-Pentaoxabicyclo[15.3.1]heneicosa-1(21),17,19-trien-21-ol;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Na+        cal alc/w  25°C 100%  U   H    K1=2.25        1987ZBa (94473) 880
Medium: MeOH. DH=-22.2 kJ mol-1; DS=-31.9. By ISE potentiometry: K1=2.23
********************************************************************************
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
--------------------------------------------------------------------------------
Na+        gl  R4N.X  25°C 0.05M C    M   K1=4.4         1998TSb (94499) 881
                                          B(NaHL)=9.2
                                          B(NaH2L)=12.7
```

Medium: 0.05 M Et4NClO4. Also ternary complexes, NaAlH-nL.

Na+	gl	R4N.X	25°C	0.10M	M	K1=3.3 B(NaHL)=7.9

1991FGb (94500) 882

Medium: 0.10 M Et4NNO3.

****

C16H25NO4 L (7444)

1-Aza-4,7,10,13-tetraoxa-1-phenyl-cyclopentadecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	nmr	alc/w	20°C	100%	C		K1=6.82	1989GSc	(94519) 883

Medium: 100% MeOH. Method: 1H pulsed gradient spin-echo nmr

****

C16H25NO4 L CAS 97004-28-0 (5816)

N-(2-Methoxybenzyl)-1-aza-4,7,10-trioxacyclododecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	ISE	alc/w	25°C	100%	U		K1=2.49	1985SWa	(94522) 884

Medium: MeOH. For 2-Nitrobenzyl- K1=1.77, 3-hydroxypropyl- K1=2.35,
3-Oxabutyl- K1=3.17, 3,6-Dioxaheptyl- K1=3.60

****

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
Na+	con	non-aq	25°C		C		K1=3.5	1999ESa	(94545) 885

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

---

Na+	con	non-aq	25°C	100%	U		K1=3.24	1988YKa	(94546) 886

Medium: tetrahydrofuran

****

C16H26N2O12 H4L (6659)

1,4,10,13-Tetraoxa-7,16-diaza-2,3,11,12-tetracarboxycyclooctadecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	gl	R4N.X	25°C	0.10M	U		K1=2.8	1990AFa	(94590) 887

****

C16H26N2O12 H4L CAS 130190-52-2 (6660)

1,4,10,13-Tetraoxa-7,16-diaza-2,3,7,16-tetracarboxycyclooctadecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	gl	R4N.X	25°C	0.10M	U		K1=3.2 B(NaHL)=12.5	1990AFa	(94604) 888

****

C16H26O6 L CAS 57721-93-4 (2502)

2,5,8,11,14,17-Hexaoxa-9,10-benzo-octadeca-9-ene; C6H4(O.(CH2.CH2.O)2.CH3)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	con	none	25°C	0.0	C		K1=0.68	1998KTb (94632)	889
Na+	ISE	alc/w	25°C	100%	U		K1=1.44	1975CJa (94633)	890

Medium: MeOH

****

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
Na+	gl	R4N.X	25°C	0.10M	C		K1=4.03	2000BCa (94918)	891

Medium: 0.10 M NMe4Cl.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	gl	R4N.X	25°C	0.10M	C		K1=4.38	1982DSa (94919)	892

****

C16H30O6 L CAS 83410-56-4 (614)
3-Hexyl-1,4,7,10,13-pentaoxacyclopentadecan-2-one, 3-Hexyl-2-one-15-crown-5;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	ISE	alc/w	25°C	100%	U		K1=1.48	1982MKa (95097)	893

Medium: MeOH

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	ISE	oth/un	25°C	dil	A	I	K1=0.8	1971FRa (95103)	894

In MeOH: K1=4.09

****

C16H30O7 L CAS 94618-63-0 (8714)
1,9-Dimethyl-2,5,8,11,14,17,20-heptaoxabicyclo[7.6.6]heneicosane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	ISE	non-aq	25°C	100%	M		K1=4.26	1984NMb (95105)	895

Medium: MeOH.

****

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
Na+	gl	alc/w	25°C	95%	M		K1=5.20	1990LNa (95119)	896

Medium: 95% MeOH, 0.05 M Bu4NBr. For the 9,13-dihydroxy- analogue: K1=3.15

****

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
Na+	con	non-aq	25°C	100%	M	M	K1=>12 K(NaL+ClO4)=1.10	1999DSd (95245)	897

Medium: acetonitrile.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	ISE	non-aq	25°C	100%	C	H	K1=7.80	1999WBa (95246)	898

Medium: N,N-dimethylformamide. Method: competitive titration against Ag+, using Ag+ ISE. By calorimetry: DH(K1)=-50.9 kJ mol-1.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	gl	R4N.X	25°C	0.05M	C	H	K1=5.4	1996BCh (95247)	899

Medium: 0.05 M Et4NClO4. By calorimetry: DH(K1)=-27.9 kJ mol-1.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	EMF	non-aq	25°C	100%	C		K1=6.91	1995CDb (95248)	900

Medium: DMSO, 0.1 M Et4NClO4.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	cal	non-aq	25°C	100%	M	H	K1=10.07	1994BCd (95249)	901

Medium: acetone. DH(K1)=-62.9 kJ mol-1, TDS=-5.7

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	sp	non-aq	20°C	100%	U		K1=7.7	1992PSa (95250)	902

Medium: DMF, 0.01 M Me4NI

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	ISE	non-aq	25°C	100%	U	H	K1=10.97	1986BUb (95251)	903

In CH3CN. DH=-65.5 kJ mol-1

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	cal	alc/w	25°C	100%	U	H	K1=9.71	1986BUd (95252)	904

In MeOH. DH=-49.8 kJ mol-1

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	nmr	non-aq	25°C	100%	U		K1=12.98	1986CHc (95253)	905

In CDCl3 saturated with D2O

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	ISE	non-aq	25°C	100%	C	I	K1=7.18	1985CKa (95254)	906

Medium: DMSO. In propylenecarbonate K1=11.61; in DMF K1=7.8

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	gl	alc/w	25°C	95%	C		K1=9.35	1981ANa (95255)	907

Medium: 95% MeOH, 0.1 M Me4NCl

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	ISE	non-aq	25°C	100%	U	I	K1=7.93	1981CRa (95256)	908

Medium: DMF: In EtOH: K1=10.20; in DMSO: 6.93; in MeCN: >11.3; in NMP: 6.55

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	ix	non-aq	25°C	100%	U		K1=7.24	1981SAa (95257)	909

Medium: DMSO, 0.1 M R4NX. In propylene carbonate: K1=12.78

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	ISE	non-aq	25°C	100%	U		K1=12.0	1980CRa (95258)	910

Medium: Propylene carbonate

Na+ ISE alc/w 25°C 100% U K1=9.65 1978CSb (95259) 911
Medium: MeOH

Na+ cal R4N.X 25°C 0.06M C H 1976KLc (95260) 912
Medium: 0.057 M Me4NBr. Method: flow microcalorimetry.
DH(K1)=-22.4 kJ mol-1, DS(K1)=26 J K-1 mol-1.

Na+ gl R4N.X 25°C 0.05M C I K1=5.40 1975LSc (95261) 913
In 95% MeOH: K1=8.84; 100%: > 8
****
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
---
Na+ cal alc/w 25°C 100% U H K1=4.72 1990KMb (95321) 914
Medium: MeOH. DH=-26.0 kJ mol-1
****
C16H32N4O6 L CAS 98608-90-3 (1322)
N,N'-Bis(carbamoylmethyl)-1,7,10,16-tetraoxa-4,13-diazacyclooctadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ gl NaClO4 25°C 0.50M U K1=<2 1981KMb (95335) 915
****
C16H32O7 L (6411)
15-(2,5-Dioxahexyl)-15-methyl-1,4,7,10,13-pentaoxacyclohexadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ con non-aq 25°C 100% C I K1=5.0 1992TFa (95388) 916
Medium: acetonitrile. In propylene carbonate, K1=5.2.

Na+ con alc/w 25°C 100% U K1=3.53 1991IOa (95389) 917
Medium: MeOH
****
C16H32O8 L 24-Crown-8 CAS 33089-37-1 (5149)
1,4,7,10.13,16,19,22-Octaoxacyclotetracosane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sol non-aq 25°C 100% C K1=3.90 1999KCa (95398) 918
Medium: acetonitrile.

Na+ cal alc/w 25°C 100% U H K1=2.02 1993ILa (95399) 919
Medium: MeOH. DH=-26.9 kJ mol-1.
****
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
Na+	EMF	alc/w	25°C	100%	U	I	K1=4.89	1994LLa (95418)	920

Medium: MeOH, 0.05M Et4NClO4. Also data for acetonitrile: K=8.17, PC: K=7.1 DMF: K=3.50, H2O: K<2 and pyridine: K=6.71. By competition with Ag+.

****

C16H34N2O6 L (6934)
N,N'-Bis(1-hydroxyethyl)-1,4-diaza-7,10,13,16-tetraoxacyclooctadecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	cal	alc/w	25°C	90%	U	H	K1=4.35	1994IZa (95432)	921

Medium: 90% v/v MeOH/H2O. DH(K1)=-41.0 kJ mol-1, DS(K1) -54.3 J K-1 mol-1
Data also for other 'lariat' analogues

****

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
Na+	ISE	non-aq	25°C	100%	U		K1=3.65	1993RPa (95453)	922

Medium: dimethylformamide, 0.05 M Et4NClO4. By competition with Ag+.

Na+	gl	NaClO4	25°C	0.50M	U		K1=<2	1981KMb (95454)	923

****

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
Na+	gl	R4N.X	25°C	0.10M	U		K1=<1.0	1978LMa (95472)	924

****

C16H34O6 L CAS 57721-92-3 (2501)
2,5,8,15,18,21-Hexaoxadocosane; CH3.O.(CH2.CH2.O)2.(CH2)6.O.(CH2.CH2.O)2.CH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	ISE	alc/w	25°C	100%	U		K1=<0.1	1975CJa (95486)	925

Medium: MeOH

****

C16H34O8 L CAS 1191-91-9 (2500)
2,5,8,11,14,17,20,23-Octaoxatetracosane; CH3.O.(CH2.CH2.O)7.CH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	con	non-aq	25°C	100%	U		K1=4.5	1993EVa (95493)	926

Medium: THF+CHCl3 (4:1 vol). Also data for other solvents

Na+	ISE	alc/w	25°C	100%	U		K1=1.67	1975CJa (95494)	927

Medium: MeOH

****
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
---
Na+ gl non-aq 25°C 100% U K1=3.6 1986STb (95541) 928
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
---
Na+ EMF non-aq 25°C 100% U I K1=6.66 1996WPa (95576) 929
Medium: acetonitrile, 0.05 M NEt4ClO4. In propylene carbonate K1=7.49

Na+ gl alc/w 25°C 100% C I K1=4.53 1993TCa (95577) 930
Medium: MeOH, 0.05 M Et4NClO4. In DMF, K1=3.37
****
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
---
Na+ sol oth/un 22°C U K1=-0.045 1980LDa (96342) 931
Medium: variable NaClO4 content 0.1-2.5 M
The same constant measured spectrophotometrically: K1=-1.3
****
C17H21O5P L (5732)
Methyldi(2-methoxyphenoxymethyl)phosphine oxide; Me.PO(CH2.O.C6H4.OMe)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ con non-aq 25°C 100% U K1=2.25 1989TKb (96393) 932
Medium: tetrahydrofuran/CHCl3 4:1 (volume)
****
C17H23NO6 L (7047)
5'-(N-Acrylamide)-benzo-15-crown-5; CH2:CH.CO.NH.C14H19O5

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp non-aq 25°C 100% U K1=6.02 1979KMb (96407) 933
Medium: CHCl3
****
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
---

Na+ dis non-aq 25°C 100% C 1990SSe (96434) 934
K(Na+HL(org)=NaL(org)+H)=-7.0
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
Na+	sp	mixed	25°C	16%	U		K1=2.05 K(Na+HL)=1.47	1984BPa (96465)	935

****

C17H24O7 L CAS 60835-74-7 (1767)
2,3-(4'-Formylbenzo)-1,4,7,10,13,16-hexaoxacyclooctadeca-2-ene; 4'-Formylbenzo-18-crown-6

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	con	non-aq	25°C	100%	U		K1=4.59	1976UHa (96469)	936

Medium: acetone

****

C17H24O7 HL CAS 55440-83-0 (9074)
2,6-Dimethylenebenzoic acid-18-crown-5;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	gl	alc/w	25°C	80%	M	IH	K1=4.11 K(Na+HL)=2.68 K(NaL+H)=5.64	1986ALb (96470)	937

Medium: 80% w/w MeOH/H2O. DH(Na+HL)=-4.6 kJ mol-1, DS(Na+HL)=35.4 J K-1 mol-1. In 99% MeOH/H2O, K1=5.0, K(Na+HL)=2.22, K(NaL+H)=7.39.

****

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
Na+	dis	non-aq	22°C	100%	C		K(Na+A+L(org)=NaAL(org))=0.48	1984CBa (96510)	938

Extraction of metal picrate from H2O into CDCl3. HA is picric acid.

****

C17H26O5 L CAS 92818-15-0 (8986)
5-[(Phenylmethoxy)methyl]-1,4,7,10-tetraoxacyclotridecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	dis	non-aq	22°C	100%	C		K(Na+A+L(org)=NaAL(org))=0.9	1984CBa (96512)	939

Extraction of metal picrate from H2O into CDCl3. HA is picric acid.

****
C17H26O6 L CAS 32702-28-6 (1768)
2,3-(4'-Methylbenzo)-1,4,7,10,13,16-hexaoxacyclooctadeca-2-ene;
4'-Methylbenzo-18-crown-6

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE none 25°C 0.0 C K1=1.43 1980WSb (96517) 940
Method: Na ion selective electrode. Also data for the4'-polyvinylbenzene-
derivative: by spectrophotometry, K1=0.38

Na+ con non-aq 25°C 100% U K1=5.09 1976UHa (96518) 941
Medium: acetone
****
C17H26O6 L CAS 99159-90-7 (688)
2,3-Benzo-1,4,7,10,13,16-hexaoxacyclononadeca-2-ene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp non-aq 22°C 100% U K1=5.10 1987CCc (96523) 942
In deuterochloroform

Na+ nmr alc/w 29°C 100% U K1=3.97 1987LLa (96524) 943
Medium: MeOH
****
C17H26O6 L CAS 65112-34-7 (6059)
21-Methoxy-3,6,9,12,15-pentaoxabicyclo[15.3.1]heneicosa-1(21),17,19-triene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ cal alc/w 25°C 100% U H K1=2.30 1987ZBa (96528) 944
Medium: MeOH. DH=-15.9 kJ mol-1; DS=-9.4. By ISE potentiometry: K1=2.28
****
C17H27NO5 L CAS 98269-22-8 (8844)
13-(2-Methoxyphenyl)-1,4,7,10-tetraoxa-13-azacyclopentadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp alc/w RT 50% C I K1=2.4 2002GNe (96545) 945
Medium: 50% v/v MeOH/H2O, pH 7.4 (0.01 M Tris buffer), 0.1 M Me4NCl.
In 10% MeOH/H2O, K1=1.8.
****
C17H30O6 H2L CAS 159029-04-6 (7605)
15-(Methoxymethoxy)-9,11-dioxo-pentadecanoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp alc/w RT 80% C K1=0.0 1994HWc (96672) 946
Medium: 80%MeOH/H2O. Also data for many analogues.
****

C17H32N4O7 H3L CAS 120041-08-9 (6702)
10-Hydroxypropyl-1,4,7,10-tetraazacyclododecane-1,4,7-triethanoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ gl R4N.X 25°C 0.10M C K1=3.19 2000BCa (96719) 947
****
C17H32N4O9 H3L CAS 124628-01-9 (2013)
1,4,7,10-Tetraazacyclododecane-1,4,7-tri(2-hydroxymethylethanoic acid);

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ gl R4N.X 25°C 0.10M C K1=2.58 2000BCa (96732) 948
Medium: 0.10 M NMe4Cl.
****
C17H34N2O4 L CAS 142565-14-8 (6562)
4,7,13,16-Tetraoxa-1,10-diazabicyclo[8.8.5]tricosane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ EMF non-aq 25°C 100% C K1=5.95 1993DLb (96747) 949
Medium: propylene carbonate, 0.05 M Et4NClO4.

Na+ gl R4N.X 25°C 0.05M C I K1=2.58 1992CGb (96748) 950
Medium: Et4NClO4. In MeCN: K1=7.55

Na+ ISE R4N.X 25°C 0.05M U I K1=1.8 1991CLa (96749) 951
Medium: 0.05 M Et4NClO4. In acetonitrile, K1>7; DMF, K1=3.66;
pyridine, K1=6.41; DMSO, K1=3.15; CH3OH, K1=5.41
****
C17H34N4O4S L CAS 503465-04-1 (9247)
4,7,13,16-Tetraoxa-1,10,21,23-tetraazabicyclo[8.8.7]pentacosane-22-thione;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ gl alc/w 25°C 95% C K1=2.19 2004KVa (96760) 952
Medium: 95% MeOH/H2O, 0.01 M Et4NClO4.
****
C17H34O5 L CAS 96047-83-5 (606)
Octyloxymethyl-1,4,7,10-Tetraoxacyclododecane, Octyloxymethyl-12-crown-4;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE alc/w 25°C 100% U K1=1.32 B2=3.29 1982MYc (96766) 953
Medium: MeOH
****
C17H35NO4 L (1694)
N-n-Heptanyl-1,4,7,10-tetraoxa-13-azacyclopentadecane;

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

---
Na+ ISE alc/w 25°C 10% U K1=2.76 1986HAa (96769) 954
Medium: 10% MeOH/H2O
****
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
---
Na+ con non-aq 25°C C K1=4.1 1999ESa (96815) 955
In tetrahydrofuran; alkali metal is used as 2,4-dinitrophenolate
---
Na+ con non-aq 25°C 100% U 1969SSg (96816) 956
K(NaI+L)=1.71
Medium: CH3CN
****
C17H38O6P2 L CAS 6997-56-4 (5225)
Tetrabutylmethylenediphosphonate; (C4H9O)2.PO.CH2.P(:O)(C4H9O)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ con non-aq 25°C 100% U 1969SSg (96817) 957
K(NaI+L)=1.46
Medium: CH3CN
****
C18H15OP L CAS 791-28-6 (32)
Triphenylphosphine oxide; (C6H5)3PO

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ con non-aq 25°C 100% U M 1982GJb (97099) 958
Kout(NaL+A)=4.6
Medium: 1,2-dichloroethane. A=picrate
****
C18H18N4 L CAS 16858-01-8 (1528)
Tris(2-pyridylmethyl)amine; (C5H4NCH2)3N

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ cal non-aq 25°C 100% U H K1=3.5 B2=4.91 1989TIa (97268) 959
Medium: acetonitrile, 0.1 M Et4NClO4. DH(K1)=-18.0 kJ mol-1 DH(B2)=-28.9,
DS(K1)=7 J K-1 mol-1, DS(B2)=-3.
****
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
---
Na+ ISE mixed 25°C 50% C K1=1.88 B2= 3.78 2004YYb (97479) 960
Method: Na ion specific electrode. Medium: 50% THF/H2O.

```
--------------------------------------------------------------------------------
Na+        sp  non-aq 25°C 100%  C        K1=>1.74       2002YEa (97480) 961
Method: fluorescence spectroscopy. Medium: acetonitrile.
--------------------------------------------------------------------------------
Na+        ISE alc/w  25°C 100%  C        K1=2.2         1981PTa (97481) 962
Medium: MeOH
********************************************************************************
C18H20O7              H2L                        (5627)
1-(2-Hydroxyphenyl)-7-(2-carboxymethoxyphenyl)-1,4,7-trioxaheptane;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Na+        ISE alc/w  25°C 100%  U        K1=1.69        1981PTb (97483) 963
Medium: MeOH
********************************************************************************
C18H22NO2P            L                          (2092)
(N,N-Diethylamidocarbonyl)methyldiphenylphosphine oxide;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Na+        con non-aq 25°C       C        K1=3.8         1999ESa (97509) 964
In tetrahydrofuran; alkali metal is used as 2,4-dinitrophenolate
--------------------------------------------------------------------------------
Na+        con non-aq 25°C 100%  U        K1=3.50        1988YKa (97510) 965
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
--------------------------------------------------------------------------------
Na+        con non-aq 25°C 100%  U        K1=2.86        1989TKb (97567) 966
Medium: tetrahydrofuran/CHCl3 4:1 (volume)
********************************************************************************
C18H22O5              L                          (6668)
2,3-Naphtho-1,4,7,10,13-pentaoxacyclopentadeca-2-ene;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Na+        ISE alc/w    ?  100%  U        K1=2.57        1992CLb (97570) 967
Medium: MeOH. Data also for 7'-t-butyl, 7'-(1,1-dibutylethyl) and
7'-(1-methyl-1-dodecylethyl) analogues
--------------------------------------------------------------------------------
Na+        dis non-aq 15°C 100%  C                       1985YIa (97571) 968
                                        K(Na+L(org)+A=NaLA(org))=3.86
                                        K(NaL(org)+A(org)=NaLA)=5.1
Media: H2O/dichloroethane. Analysis by spectrophotometry.
HA: picric acid.
********************************************************************************
C18H22O6              L                          (5633)
```

1,4-bis(2-Hydroxyethoxyphenyl)-1,4-dioxabutane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	ISE	alc/w	25°C	100%	U		K1=1.42	1981PTb (97573)	969

Medium: MeOH

****

C18H23NO8 L CAS 332843-39-7 (8209)

2,3,5,6,8,9,11,12,14,15-Decahydro-1,4,7,10,13,16-hexaoxacyclooctadecino[2,3-]isoindole18,20dione;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	sp	non-aq	25°C	100%	C		K1=3.9	2001OYa (97576)	970

Medium: methanol. For the N-propyl derivative, K1=3.8.

****

C18H26O7 L CAS 55440-80-7 (9075)

2,6-Dimethylenebenzoic acid-18-crown-5 methyl ester;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	gl	alc/w	25°C	80%	M	IH	K1=2.55	1986ALb (97731)	971

Medium: 80% w/w MeOH/H2O. DH(K1)=-18.4 kJ mol-1, DS(K1)=-13.7 J K-1 mol-1.
In 99% w/w MeOH/H2O, K1=2.80.

****

C18H26O7 L CAS 83410-62-2 (615)

3-Phenyl-1,4,7,10,13,16-hexaoxacyclooctadecan-2-one, 3-Phenyl-2-one-18-crown-6;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	ISE	alc/w	25°C	100%	U		K1=3.23	1982MKa (97733)	972

Medium: MeOH

****

C18H27N2O3F L CAS 173417-90-8 (6571)

23-Fluoro-4,7,20-trioxa-1,10-diazatricyclo[8.7.5.1,12,16]tricosa-12,14,16(23)triene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	EMF	non-aq	25°C	100%	C	H	K1=4.70	1999BHa (97749)	973

Medium: MeOH, 0.05 M Et4NClO4. By calorimetry DH(K1)=-24.8 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]tricosa-12,14,16(23)-triene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	EMF	non-aq	25°C	100%	C	H	K1=2.86	1999BHa (97772)	974

Medium: MeOH, 0.05 M Et4NClO4. By calorimetry DH(K1)=-23.6 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
---
Na+ dis non-aq 22°C 100% C 1984CBa (97820) 975
K(Na+A+L(org)=NaAL(org))=1.08
Extraction of metal picrate from H2O into CDCl3. HA is picric acid.
****
C18H28O5 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
---
Na+ dis non-aq 22°C 100% C 1984CBa (97822) 976
K(Na+A+L(org)=NaAL(org))=0.9
Extraction of metal picrate from H2O into CDCl3. HA is picric acid.
****
C18H28O6 L Benzo20-crown-6 (6354)
2,3-Benzo-1,5,8,11,14,18-Hexaoxacosa-2-ene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp non-aq 22°C 100% U K1=3.79 1987CCc (97837) 977
In deuterochloroform
****
C18H28O6 L CAS 85556-93-0 (642)
2,3-Benzo-8,15-dimethyl-1,4,7,10,13,16-hexaoxacycloocotadeca-2-ene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ nmr alc/w 29°C 100% U K1=3.74 1987LLa (97842) 978
Medium: MeOH

Na+ con alc/w 25°C 100% U K1=3.76 1983LSa (97843) 979
Medium: MeOH
****
C18H28O6 L AN(MOEOE)2O 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
---
Na+ dis non-aq 25°C 100% U H 1979KLa (97849) 980
K(Na(picrate)+L)=4.67
Medium: CHCl3
****
C18H28O6 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
---
Na+ dis non-aq 22°C 100% C 1984CBa (97853) 981
K(Na+A+L(org)=NaAL(org))=3.83
Extraction of metal picrate from H2O into CDCl3. HA is picric acid.

Na+ ISE alc/w 25°C 100% U K1=3.07 B2=5.01 1982MYc (97854) 982
Medium: MeOH
****
C18H28O7 L Benzo21-crown-7 (6355)
2,3-Benzo-1,4,7,10,13,16,19-Heptaoxaheneicosa-2-ene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp non-aq 22°C 100% U K1=5.35 1987CCc (97858) 983
In deuterochloroform
****
C18H30N4O12 H6L TTHA CAS 869-52-3 (694)
Triethylenetetraaminehexaethanoic acid;((HOOC.CH2)2N.CH2.CH2.N(CH2.COOH).CH2)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp NaClO4 25°C 0.50M U K1=1.00 1980KNa (98071) 984
****
C18H30O6 L (2503)
3,6,9,12,15,18-Hexaoxa-10,11-benzo-eicosa-10-ene; C6H4(O.(CH2.CH2.O)2.C2H5)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE alc/w 25°C 100% U K1=1.29 1975CJa (98116) 985
Medium: MeOH
****
C18H32N2O8 L CAS 24951-52-8 (2560)
Cryptand-2,2,2-dilactam

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ nmr non-aq 33°C 100% U I 1977HPa (98134) 986
K1 > 4
Medium: MeCN
****
C18H32N4O8 H4L TETA CAS 60239-22-7 (1019)
1,4,8,11-Tetraazacyclotetradecane-1,4,8,11-tetraethanoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ gl KNO3 25°C 0.10M C K1=0.4 1982DSa (98216) 987
****

C18H32O4 L (5234)
2,3:9,10-Dicyclohexyl-1,4,8,11-tetraoxacyclotetradecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE alc/w 25°C 100% A K1=2.18 1971FRa (98271) 988
Medium: MeOH
****
C18H32O8 L CAS 473704-12-0 (8708)
4-[(2-Propenyloxy)methyl]-2,5,8,11,14,17,20-heptaoxabicyclo[7.6.6]heneicosane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ cal none 25°C 0.0 C H K1=2.39 2001ZKd (98273) 989
Self-medium, ca. 0.005 M. DH(K1)=-6.5 kJ mol-1, DS(K1)=24 J K-1 mol-1.
****
C18H34N4O9 H3L DO3A-B (7301)
10-[2,3-Dihydroxy-(1-hydroxymethyl)-propyl]-1,4,7,10-tetraazacyclododecane-1,4,7-tr
iethanoic ac.;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ gl R4N.X 25°C 0.10M C K1=2.32 1996TKa (98382) 990
Medium: Me4NCl
****
C18H34O7 L (616)
3-Hexyl-1,4,7,10,13,16-hexaoxacyclooctadecan-2-one, 3-Hexyl-2-one-18-crown-6;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE alc/w 25°C 100% U K1=2.90 1982MKa (98393) 991
Medium: MeOH
****
C18H34O8 L CAS 94618-62-9 (8713)
1,11-Dimethyl-3,6,9,12,15,18,20,23-octaoxabicyclo[9.7.6]tetracosane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE non-aq 25°C 100% M K1=5.38 1984NMb (98395) 992
Medium: MeOH.
****
C18H34O9 L CAS 57721-61-7 (2510)
3,6,9,12,15-Pentaoxaheptadecane-1,17-dioic acid diethyl ester
---
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE alc/w 25°C 100% U K1=1.34 1975CJa (98398) 993
Medium: MeOH
****
C18H36N2O5 L Cryptand 1,2,2H (6605)

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	gl	alc/w	25°C	95%	M		K1=6.13	1990LNa (98407)	994

Medium: 95% MeOH, 0.05 M Bu4NBr. For the 12,16-dihydroxy- analogue: K1=4.01

****

C18H36N2O5 L Cryptand 2,2,1H CAS 119017-37-7 (6588)
5,8,15,18,23-Pentaoxa-1,12-diazabicyclo[10.8.5]pentacosane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	gl	alc/w	25°C	95%	M		K1=4.83	1990LNa (98415)	995

Medium: 95% MeOH, 0.05 M Bu4NBr. For the 9,16-dihydroxy- analogue: K1=3.07

****

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
Na+	cal	none	25°C	0	U	IH	K1=2.84	1997ZIa (98422)	996

DH(K1)=-13.0 kJ mol-1, DS=10.7. In 95% v/v MeOH/H2O: K1=6.95, DH(K1)=-37.1
DS=8.7

****

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
Na+	con	non-aq	25°C	100%	M	M	K1=7.14	1999DSd (98649)	997
							K(NaL+ClO4)=1.03		
Na+	vlt	non-aq	25°C	100%	C	I	K1=10.8	1999FKb (98650)	998
Na+	ISE	non-aq	25°C	100%	C	H	K1=5.93	1999WBa (98651)	999
Na+	gl	R4N.X	25°C	0.05M	C	H	K1=4.6	1996BCh (98652)	1000
Na+	EMF	non-aq	25°C	100%	C		K1=5.15	1995CDb (98653)	1001
Na+	EMF	non-aq	25°C	100%	C	I	K1=9.72	1995DGa (98654)	1002

Medium: acetonitrile, 0.10 M Et4NClO4. Method: cyclic voltammetry.
Also in: DMF (K1=6.1), DMSO (5.4), MeOH (7.9), acetone (9.0) etc.

Medium: N,N-dimethylformamide. Method: competitive titration against
Ag+, using Ag+ ISE. By calorimetry: DH(K1)=-43.6 kJ mol-1.

Medium: 0.05 M Et4NClO4. By calorimetry: K1=4.1, DH(K1)=-36.1 kJ mol-1.

Medium: DMSO, 0.1 M Et4NClO4.

Medium: acetonitrile, 0.05 M Et4NClO4. In benzonitrile, K1=11.20.
Competitive method with Ag/Ag+ electrode.

Na+ cal alc/w 25°C 80% C H K1=6.04 1995KZa (98655)1003
Medium: 80% v/v CH3OH/H2O. DH(K1)=-40.5 kJ mol-1, DS(K1)=-20 J K-1 mol-1

Na+ cal non-aq 25°C 100% M H K1=8.89 1994BCd (98656)1004
Medium: acetone. DH(K1)=-55.2 kJ mol-1, TDS=-4.7

Na+ ISE oth/un 25°C 0.05M M K1=7.97 1992BUb (98657)1005
K1=7.95 (by potentiometry), K1=7.31 (by calorimetry)

Na+ ISE non-aq 25°C 100% U K1=9.51 1992CSc (98658)1006
Ag/Ag+ electrode. Medium: MeCN, 0.05 M Bu4NClO4

Na+ sp non-aq 20°C 100% U K1=5.6 1992PSa (98659)1007
Medium: DMF, 0.01 M Me4NI

Na+ ISE non-aq 25°C 100% C K1=5.7 1989MGa (98660)1008
Medium: DMF, 0.10 M Et4NClO4

Na+ ISE non-aq 25°C 100% U H K1=10.68 1986BUb (98661)1009
In CH3CN. DH=-61.9 kJ mol-1

Na+ cal alc/w 25°C 100% U H K1=7.97 1986BUd (98662)1010
In MeOH. DH=-39.8 kJ mol-1

Na+ nmr non-aq 25°C 100% U K1=10.56 1986CHc (98663)1011
In CDCl3 saturated with D2O

Na+ cal non-aq 25°C 100% U H 1986DGa (98664)1012
DH1 = -85.7 kJ mol-1. Medium: nitromethane

Na+ ISE non-aq 25°C 100% C K1=5.12 1985CKa (98665)1013
Medium: DMSO

Na+ cal non-aq 25°C 100% U H 1985DGa (98666)1014
Medium: propylene carbonate. DH1 = -64.1 kJ mol-1

Na+ cal non-aq 25°C 100% U H 1985DGa (98667)1015
Medium: acetonitrile. DH1 = -60.9 kJ mol-1

Na+ ISE non-aq 25°C 100% M K1=13.56 1985DGb (98668)1016
Medium: nitromethane

Na+ cal non-aq 25°C 100% U H 1984DGa (98669)1017
Medium: N,N-dimethylformamide. DH1=-39.9 kJ mol-1; DS1=-18.4 J K-1 mol-1.

Na+ cal non-aq 25°C 100% U H 1984DGa (98670)1018
Medium: DMSO. DH1=-44.6 kJ mol-1; DS1=-47.3 J K-1 mol-1

Na+ gl alc/w 25°C 95% C K1=7.4 1981ANa (98671)1019

Medium: 95% MeOH, 0.1 M Me4NCl

Na+ ISE non-aq 25°C 100% U I K1=6.17 1981CRa (98672)1020
Medium: DMF. In EtOH: 8.57, in DMSO: 5.32; in N-methylpropionamide: 5.82

Na+ ix non-aq 25°C 100% U K1=5.28 1981SAa (98673)1021
Medium: DMSO, 0.1 M R4NX. In propylene carbonate: K1=10.83

Na+ ISE non-aq 25°C 100% U K1=10.5 1980CRa (98674)1022
Medium: Propylene carbonate

Na+ con non-aq 25°C 100% U K1=>7 1980KMb (98675)1023
Medium: MeCN

Na+ EMF non-aq 25°C 100% C I K1=7.8 1979BLb (98676)1024
Method: Ag electrode. Medium: MeOH, 0.05 M Me4NClO4.
Also K1=3.9 (H2O), 5.4 (DMSO), 10.9 (CH3CN), 5.6 (tetramethylurea).

Na+ ISE alc/w 25°C 100% U K1=7.98 1978CSb (98677)1025
Medium: MeOH

Na+ EMF oth/un 25°C 0.05M C I K1=3.9 1978YTa (98678)1026
Method: competition with Tl+, using Tl amalgam electrode.
Electrolyte not stated. In MeOH, 0.05 M: K1=7.9. In DMSO, 0.10 M: K1=5.4

Na+ cal alc/w 25°C 100% C 1977ADa (98679)1027
Medium: methanol. DH(K1)=-46.0 kJ mol-1. In H2O, DH(K1)=-31.8 kJ mol-1.

Na+ cal R4N.X 25°C 0.06M C IH 1976KLc (98680)1028
Medium: 0.057 M Me4NBr. Method: flow microcalorimetry. DH(K1)=-31.0 kJ mol-1, DS(K1)=-29 J K-1 mol-1. In 95% (v/v) MeOH/H2O, DH(K1)=-44.4, DS=-11

Na+ gl R4N.X 25°C 0.10M C H K1=4.11 1975ANa (98681)1029
Medium: Me4NCl. DH(K1)=-31.0 kJ mol-1, DS=-15

Na+ gl R4N.X 25°C 0.05M C I K1=3.9 1975LSc (98682)1030
In 95% MeOH: K1=7.21; 100%: > 8

****

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

---

Na+ cal alc/w 25°C 100% U H K1=3.01 1990KMb (98783)1031
Medium: MeOH. DH=-37.6 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

---
Na+ gl R4N.X 25°C 0.10M M K1=4.22 1990KMb (98800)1032
Medium: 0.10 M Me4NNO3
****
C18H36O9 L 27-Crown-9 (7043)
1,4,7,10,13,16,19,22,25-Nonaoxacycloheptacosane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sol non-aq 25°C 100% C K1=3.67 1999KCa (98808)1033
Medium: acetonitrile.

Na+ cal alc/w 25°C 100% U H K1=2.03 1993ILa (98809)1034
Medium: MeOH. DH=-27.1 kJ mol-1.
****
C18H37NO4 L (1721)
1-Octyl-1-aza-4,7,10,13-tetraoxacyclopentadecane; C8H17.N(CH2.CH2.O)4.CH2CH2)

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE alc/w 25°C 100% U K1=3.08 1983MKa (98812)1035
****
C18H38N2O6 L CAS 72911-99-0 (1760)
1-Methyl-10-methyldioxyethyl-1,10-Diaza-4,7,13,16-tetraoxa-cyclooctadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ gl alc/w 25°C 95% C K1=3.35 1975LSc (98820)1036
Medium: 95% MeOH
****
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
---
Na+ sol non-aq 20°C 100% C K1=5.46 1983SLa (98823)1037
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
---
Na+ sol non-aq 20°C 100% C K1=5.39 1983SLa (98842)1038
Medium: CHCl3
****
C18H38N2O7 L (6930)
N,N'-Bis(1-hydroxy-2-ethoxyethyl)-1,4-diaza-7,10,13-trioxacyclopentadecane;

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

---
Na+ cal alc/w 25°C 90% U H K1=3.50 1994IZa (98855)1039
Medium: 90% v/v MeOH/H2O. DH(K1)=-26.7 kJ mol-1, DS(K1)=-22.8 J K-1 mol-1
Data also for several other 'lariat' analogues
****
C18H38O9 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
---
Na+ dis non-aq 25°C 100% C K1=9.08 1998KSc (98876)1040
Medium: 1,2-dichloroethane.
****
C19H22O5 L Dibz-16-crown-5 CAS 14696-06-1 (655)
2,3:9,10-Dibenzo-1,4,8,11,14-pentaoxacyclohexadecan-2,9-diene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp non-aq 25°C 100% C K1=3.8 2000KBb (99335)1041
Medium: MeOH. Method: electrospray ionization mass spectrometry.
****
C19H23O6P L (5731)
1,2:8,9-Dibenzo-5-methylphosphinyl-3,7,10,13,16-pentaoxacyclohexadeca-1,8-diene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ con non-aq 25°C 100% U K1=3.29 1989TKb (99347)1042
Medium: tetrahydrofuran/CHCl3 4:1 (volume)
****
C19H27NO7 L (7048)
5'-(N-Acrylamide)-benzo-18-crown-6; CH2:CH.CO.NH.C16H23O6

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp non-aq 25°C 100% U K1=6.08 1979KMb (99395)1043
Medium: CHCl3
****
C19H27N3O6 L (2156)
1,10-Diaza-4,7,13,16,21-tetraoxacyclooctadecane-N,N-2,6-pyridinecarboxaldehyde;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp alc/w 25°C 100% U 1977TMa (99398)1044
Keff=4.58
Medium: MeOH
****
C19H30O5 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

---
Na+ dis non-aq 22°C 100% C 1984CBa (99432)1045
K(Na+A+L(org)=NaAL(org))=0.85
Extraction of metal picrate from H2O into CDCl3. HA is picric acid.
****
C19H30O5 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
---
Na+ dis non-aq 22°C 100% C 1984CBa (99434)1046
K(Na+A+L(org)=NaAL(org))=0.78
Extraction of metal picrate from H2O into CDCl3. HA is picric acid.
****
C19H30O6 L (643)
2,3-Benzo-8,11,15-trimethyl-1,4,7,10,13,16-hexaoxacyclooctadeca-2-ene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ nmr alc/w 29°C 100% U K1=3.57 1987LLa (99437)1047
Medium: MeOH

Na+ con alc/w 25°C 100% U K1=3.53 1983LSa (99438)1048
Medium: MeOH
****
C19H31N3O4 L (2158)
1,10-Diaza-4,7,13,16,21-tetraoxacyclooctadecane-N,N-2,6-methylpyridine;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp alc/w 25°C 100% U 1977TMa (99447)1049
Keff=4.89
Medium: MeOH
****
C19H32N2O4 L (8540)
1-Benzyl-4,7,13,16-tetraoxa-1,10-diazacyclooctadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE alc/w 25°C 100% U H K1=1.54 1998SSf (99453)1050
Medium: 100% MeOH, 0,05 M Et4NI. By calorimetry DH(K1)=-15.8 kJ mol-1
****
C19H38O6 L CAS 83585-72-2 (1675)
2-Octoxymethylene-1,4,7,10,13-pentaoxacyclopentadecane,
2-Octoxymethylene-15-crown-5

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE alc/w 25°C 100% U I K1=3.18 B2=5.50 1984IEa (99476)1051
Medium: MeOH. In 90% MeOH: 2.73

****
C19H39NO5 L (1693)
N-n-Heptanyl-1,4,7,10,13-pentaoxa-16-azacyclooctadecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	ISE	alc/w	25°C	10%	U		K1=2.98	1986HAa	(99479)1052

Medium: 10% MeOH/H2O
****
C19H39N3O5 L CAS 60598-00-7 (1537)
4-Methyl-1,4,10-triaza-7,13,16,21,24-pentaoxa-bicyclo[8,8,8]hexacosane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	gl	R4N.X	25°C	0.10M	U		K1=3.2	1978LMa	(99494)1053

****
C20H22N2O10 L CAS 29721-41-3 (5295)
cis-4,4'-Dinitrodibenzo-18-crown-6

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	con	non-aq	30°C	100%	U		K1=1.99	1973SJb	(99919)1054

Medium: HCON(CH3)2
****
C20H22O4 L CAS 82645-28-1 (8945)
o,o'-(Triethyleneglycoldiyl)-(Z)-stilbene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	con	non-aq	25°C	100%	C		K1=3.83	2000ICa	(99929)1055

Medium: nitromethane.
****
C20H22O6 L (6834)
1,8-Bis(2-Formyphenoxy)-3,6-dioxaoctane; (CH2.O.CH2.CH2.O.C6H4.CHO)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	con	non-aq	25°C	100%	U		K1=2.9	1993EVa	(99933)1056

Medium: THF+CHCl3 (4:1 vol)
****
C20H22O9 H2L (5624)
1,7-bis(2-Carboxymethoxyphenyl)-1,4,7-trioxaheptane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	ISE	alc/w	25°C	100%	U		K1=2.21	1981PTb	(99939)1057

Medium: MeOH
****
C20H24N2O5 L CAS 165815-06-5 (8936)
N-(2-Pyridylmethylene)-4-aminobenzo-15-crown-5;

```
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Na+        sp  non-aq 25°C 100%  C  I M                  2002YPc (99953)1058
                                          K(ZnA2L+Na)=3.73
Medium: MeCN, 0.10 M n-Bu4NPF6. By 1H nmr in CDCl3, K(ZnA2L+Na)=3.53.
A is p-thiocresol.
********************************************************************************
C20H24O5                L                          (5620)
5,9-Dimethyl-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
--------------------------------------------------------------------------------
Na+        ISE alc/w  25°C 100%  C        K1=1.1         1981PTa (100046)1059
Medium: MeOH. Data for racemic ligand.  For meso ligand K1=1.5
********************************************************************************
C20H24O5                L                          (5619)
6,8-Dimethyl-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
--------------------------------------------------------------------------------
Na+        ISE alc/w  25°C 100%  C        K1=1.9         1981PTa (100048)1060
Medium: MeOH. Data for racemic ligand.  For meso ligand K1=2.1
********************************************************************************
C20H24O6                L    DiBz-18-Crown-6  CAS 14187-32-7  (604)
2,3:11,12-Dibenzo-1,4,7,10,13,16-hexaoxacyclooctadeca-2,11-diene
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Na+        EMF alc/w  25°C 100%  C        K1=4.15        2004ZTa (100173)1061
Medium: 100% methanol, 0.05 M Bu4NClO4. Method: Ag electrode,
competition with Ag+ ion.
--------------------------------------------------------------------------------
Na+        oth NaCl   25°C 0.05M C        K1=1.22        2002KTa (100174)1062
Method: capillary electrophoresis. Medium: 0.03-0.06 M NaCl.
--------------------------------------------------------------------------------
Na+        dis non-aq 24°C 100%  C                       2002MRd (100175)1063
                                        K(Na+A+L)=5.46
Medium: CDCl3. HA is picric acid.
--------------------------------------------------------------------------------
Na+        con non-aq 25°C 100%  C        K1=6.7         2000ICa (100176)1064
Medium: nitromethane.
--------------------------------------------------------------------------------
Na+        sp  non-aq 25°C 100%  C        K1=4.4         2000KBb (100177)1065
Medium: MeOH.  Method: electrospray ionization mass spectrometry.
--------------------------------------------------------------------------------
Na+        oth alc/w  25°C   3%  U    M                  2000MTa (100178)1066
                                        K(NaL+phenolate)=1.34
                                        K(NaL+o-nitrophenolate)=1.54
                                        K(NaL+m-nitrophenolate)=1.49
```

K(NaL+p-nitrophenolate)=1.56
Method: CZE. Medium: 3% v/v EtOH/H2O. K(NaL+2,4-dinitrophenolate)=2.03, K(NaL+picrate)=2.18, K(NaL+SCN)=1.54, K(NaL+ClO4)=1.31.

Na+ dis oth/un 25°C 0.06M C 2000YYa (100179)1067
K(NaL+A)=-0.14
K(Na+L(org)+A=NaLA(org))=2.99
Method: extraction of metal picrate (0.06 M, pH 12) into dichloromethane/ ligand solution. HA: picric acid. Data for many additional solvents.

Na+ sp mixed 25°C C TIH K1=2.16 1999EDa (100180)1068
In 60 % mass H2O/acetonitrile; For80% H20 K1=1.77, DH1=-23.5 kJ/mol
For 100% acetonitrile K1=4.89, the same at 35 C: 4.68; 40 C: 4.52

Na+ oth alc/w 35°C 3.0% C K1=1.18 1999MTd (100181)1069
Method: capillary zone electrophoresis. Medium: 3% v/v EtOH/H20, 0.005 M phosphate buffer, pH 7.0

Na+ dis non-aq 25°C 100% U K1=8.47 1998KSb (100182)1070
Medium: 1,2-dichloroethane

Na+ oth oth/un 25°C 0.04M C K1=1.24 1998TIa (100183)1071
K(NaL+ClO4)=<0.0
K(NaL+picrate)=2.23
Method: capillary electrophoresis.
Medium: 0.005 M phosphate buffer, pH 7.1, 0.04 M MCl.

Na+ sp non-aq 25°C 100% U T H K1=4.89 1997EKa (100184)1072
Medium: CH3CN. Also data for H2O/CH3CN mixtures

Na+ sp mixed 10°C 60% C T H K1=2.42 1997EYa (100185)1073
Medium: 60% w/w CH3CN/H2O; For 45 C and 60% CH3CN K1=2.22;
For 80% CH3CN and 10 C K1=2.87; For 45 C and 80% CH3CN K1=2.80

Na+ nmr non-aq 27°C 100% U I K1=4.17 1996KAa (100186)1074
Method: 23Na nmr. Medium: acetonitrile. Also data for 20 and 40 wt% DMSO in AN. For 20% DMSO, K1=3.06; for 40% K1=2.15.

Na+ dis oth/un 25°C 0 U K1=4.35 1994OUa (100187)1075

Na+ dis non-aq 23°C 100% C K1=6.9 1992HGb (100188)1076
K(Na+A+L(org)=NaAL(org))=4.54
Extraction of metal chloride (A) from aqueous solution into nitrobenzene/ 0.01M Bu4NB(Ph)4. Peak potential voltammetry and distribution of 22Na.

Na+ sp non-aq 25°C 100% U K1=2.84 1991NTa (100189)1077
Medium: DMF

Na+ vlt non-aq 23°C 100% C I K1=4.92 1990LUa (100190)1078
Medium: MeCN, 0.05 M Bu4NClO4. Data also in DMF (K1=3.30), DMSO (3.10),

benzonitrile (5.22), propylene carbonate (5.12) and other solvents
---
Na+ vlt non-aq 25°C 100% U K1=11.2 1990SPa (100191)1079
Medium: 1,2-dichloroethane

Na+ cal non-aq 25°C 100% C H K1=4.89 1988BUb (100192)1080
Medium: acetonitrile. DH(K1)=-15.0 kJ mol-1, DS(K1)=43.0 J K-1 mol-1.

Na+ con non-aq 25°C 100% U K1=5.60 1986STb (100193)1081
Medium: THF:CHCl3 4:1 v/v. M as 2,4-dinitrophenolate

Na+ con non-aq 25°C 100% U K1=4.51 1985YKa (100194)1082
Medium: EtOH+CHCl3 1:1; M is used in nitrophenolate form

Na+ ISE non-aq 25°C 100% C K1=5.03 1984FLa (100195)1083
In propylenecarbonate; electrolyte Et4NClO4

Na+ ISE non-aq 25°C 100% U T H K1=5.00 1982NYa (100196)1084
Medium: MeCN

Na+ vlt non-aq 25°C 100% U I K1=5.00 1978HKc (100197)1085
Medium: CH3CN, 0.05M Bu4NClO4

Na+ nmr non-aq 29°C 100% U K1=3.75 1977SZa (100198)1086
Medium: DMF

Na+ sp alc/w 30°C 96% U K1=0.23 1975DBb (100199)1087

Na+ dis non-aq 25°C 100% C T HM 1975SIc (100200)1088
K(Na+A+L(org)=NaAL(org))=2.2
Method: Extraction from H2O into benzene. HA is picric acid. DH(NaAL(org))
=-37 kJ mol-1, DS(NaAL(org))=-84 J K-1 mol-1.

Na+ sol none 25°C 0.0 U I K1=1.16 1975SNa (100201)1089

Na+ con non-aq 40°C 100% U T K1=3.56 1973SJb (100202)1090
Medium:dimethoxyethane. 10 C: K1=3.86; 20 C: K1=3.73;
30 C: K1=3.66. Na+ present as tetraphenylboron ion-pair.

Na+ ISE alc/w 25°C 100% A K1=4.36 1971FRa (100203)1091
Medium: MeOH

Na+ con non-aq 25°C 100% U K1=2.78 1971SJb (100204)1092
Medium: HCON(CH3)2.
****
C20H24O6 L CAS 72011-24-6 (8872)
2,3:5,6-Dibenzo-1,4,7,10,13,16-hexaoxacyclooctadeca-2,5-diene;

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

```
Na+        dis non-aq 23°C 100%  C        K1=7.0         1992HGb (100263)1093
                                          K(Na+A+L(org)=NaAL(org))=4.71
Extraction of metal chloride (A) from aqueous solution into nitrobenzene/
0.01M Bu4NB(Ph)4. Peak potential voltammetry and distribution of 22Na.
**************************************************************************
C20H24O6                L                     CAS 14262-61-4  (8871)
2,3:8,9-Dibenzo-1,4,7,10,13,16-hexaoxacyclooctadeca-2,8-diene;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Na+        ISE mixed  25°C  50%  C        K1=2.27   B2= 5.28  2004YYb (100270)1094
Method: Na ion specific electrode. Medium: 50% THF/H2O.
--------------------------------------------------------------------------
Na+        sp  non-aq 25°C 100%  C        K1=3.860       2002YEa (100271)1095
Method: fluorescence spectroscopy. Medium: acetonitrile.
--------------------------------------------------------------------------
Na+        dis non-aq 23°C 100%  C        K1=6.3         1992HGb (100272)1096
                                          K(Na+A+L(org)=NaAL(org))=4.91
Extraction of metal chloride (A) from aqueous solution into nitrobenzene/
0.01M Bu4NB(Ph)4. Peak potential voltammetry and distribution of 22Na.
**************************************************************************
C20H24O8             H2L                      (5630)
1-(2-Hydroxyphenyl)-10-(2-carboxymethoxyphenyl)-1,4,7,10-tetraoxadecane;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Na+        ISE alc/w  25°C 100%  U        K1=1.91        1981PTb (100276)1097
Medium: MeOH
**************************************************************************
C20H26N2O6              L                     CAS 31352-45-1  (5298)
cis-4,4'-Diaminodibenzo-18-crown-6
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Na+        con non-aq 40°C 100%  U T      K1=2.54        1973SJb (100321)1098
Medium: HCON(CH3)2.  K1(10 C)=3.03, K1(20 C)=2.86, K1(30 C)=2.76
**************************************************************************
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
--------------------------------------------------------------------------
Na+        dis non-aq 25°C 100%  U   H                    1979KLa (100349)1099
                                          K(Na(picrate)+L)=6.09
Medium: CHCl3
**************************************************************************
C20H26O7                L                      (5626)
1,7-bis(2-Hydroxyethoxyphenyl)-1,4,7-trioxaheptane;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
```

Na+ ISE alc/w 25°C 100% U K1=1.39 1981PTb (100352)1100
Medium: MeOH
****
C20H27N2O5Cl HL CAS 199472-61-2 (8623)
5-Chloro-7-(1,4,7,10-tetraoxa-13-azacyclopentadec-13-ylmethyl)-8-quinolinol;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ cal non-aq 25°C 100% C H 1997ZBb (100357)1101
K(Na+HL)=3.00
Medium: MeOH. DH(K)=-17.8 kJ mol-1, DS(K)=-2.3 J K-1 mol-1.
****
C20H28O7 L CAS 123295-30-7 (5571)
14,14-Dimethyl-15,16-(1,4-Benzodioxinic)-1,4,7,10,13-pentaoxacycloheptadeca-15-ene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ gl alc/w 25°C 100% U K1=0.95 1989MGb (100400)1102
Medium: MeOH
****
C20H31N2O4F L CAS 173417-87-3 (6461)
26-Fluoro-4,7,13,16-tetraoxa-1,10-diazatricyclo[8.8.7.1,20,24]hexacosa-20,22,24(26)
-triene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ EMF non-aq 25°C 100% C H K1=7.02 1999BHa (100441)1103
Medium: MeOH, 0.05 M Et4NClO4. By calorimetry DH(K1)=-36.2 kJ mol-1.
Method: by competition with Ag+, using Ag/Ag+ electrode.
****
C20H32N2O4 L CAS 61696-66-0 (6497)
4,7,13,16-Tetraoxa-1,10-diazatricyclo[8.8.7.1,20,24]hexacosa-20,22,24(26)-triene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ EMF non-aq 25°C 100% C H K1=4.90 1999BHa (100458)1104
Medium: MeOH, 0.05 M Et4NClO4. By calorimetry DH(K1)=-26.7 kJ mol-1.
Method: by competition with Ag+, using Ag/Ag+ electrode.
****
C20H32O7 L AN(MOEOEO)2E (2248)
24-Methoxy-22-methyl-3,6,9,12,15,18-hexaoxabicyclo[18.3.1]-tetracosa-1(24),20,22-tr
iene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ dis non-aq 25°C 100% U H 1979KLa (100494)1105
K(Na(picrate)+L)=4.66
Medium: CHCl3
****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	sp	non-aq	22°C	100%	U		K1=5.42	1987CCc	(100498)1106

In deuterochloroform

****

C20H33NO6 L CAS 105495-12-3 (1692)
N-(2-(2-Phenyloxy)ethoxy)ethyl-1,4,7,10-tetraoxa-13-azacyclopentadecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	ISE	alc/w	25°C	10%	U		K1=3.43	1986HAa	(100502)1107

Medium: 10% MeOH/H2O

****

C20H34O8 L (2504)
2,5,8,11,14,17,20,23-Octaoxa-12,13-benzotetracosa-12-ene; C6H4(O.(CH2.CH2.O)3.CH3)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	ISE	alc/w	25°C	100%	U		K1=1.61	1975CJa	(100526)1108

Medium: MeOH

****

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
Na+	EMF	alc/w	25°C	100%	C		K1=4.33	2004ZTa	(100678)1109

Medium: 100% methanol, 0.05 M Bu4NClO4. Method: Ag electrode, competition with Ag+ ion.

Na+	dis	non-aq	25°C	100%	U		K1=10.91	2000KSa	(100679)1110

Medium: 1,2-dichloroethane

Na+	nmr	non-aq	27°C	100%	U	I	K1=4.85	1996KAa	(100680)1111

Method: 23Na nmr. Medium: acetonitrile. Also data for 20, 40, 60, 80 wt% DMSO in AN. For DMSO: K1=1.35. For 20% DMSO, K1=3.86.

Na+	dis	non-aq	25°C	100%	U			1995BSa	(100681)1112
							K(Na(pic)+L=Na(pic),L)=5.99		

Medium:CHCl3. Data for host-guest associations; pic: picrate. L is a cis-syn -cis and cis-anti-cis mixture. Also data for syn-L (K=7.12) and anti-L(5.94)

Na+	cal	non-aq	25°C	100%	C	H	K1=5.33	1988BUb	(100682)1113

Medium: acetonitrile. DH(K1)=-20.0 kJ mol-1, DS(K1)=34.6 J K-1 mol-1.

Na+	con	none	25°C	0.0	C T	H	K1=4.93	1988TMc	(100683)1114

Data for 15-35 C. DH(K1)=-51.7 kJ mol-1, DS(K1)=-78.9 J K-1 mol-1.

Anion is tetraphenyl borate.

Na+ ISE non-aq 25°C 100% C K1=5.70 1984FLa (100684)1115
In propylenecarbonate; electrolyte Et4NClO4

Na+ dis non-aq 25°C 100% U H 1979KLa (100685)1116
K(Na(picrate)+L)=3.37
Medium: CHCl3

Na+ cal oth/un 25°C 0.10M U H 1976ITb (100686)1117
K1=1.21 (cis-syn-cis isomer)
K1=0.69 (cis-anti-cis isomer)
DH(Syn)=0.67 and DH(Anti)=-6.57 kJ mol-1.

Na+ ISE oth/un 25°C dil A K1=1.4 1971FRa (100687)1118
Isomer B. In MeOH, K1=3.68. For isomer A: K1=1.7; in MeOH: K1=4.08
****
C20H38N2O6 L CAS 178822-46-3 (8615)
6-Methylene-4,8,14,17,22,25-hexaoxa-1,11-diazabicyclo[9.8.8]heptacosane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ cal alc/w 25°C 80% C H K1=5.60 1995KZa (100740)1119
Medium: 80% v/v CH3OH/H2O. DH(K1)=-46.3 kJ mol-1, DS(K1)=-48.0 J K-1 mol-1
****
C20H38N4O10 H3L CAS 214461-75-3 (1659)
10-(2-Hydroxypropyl)-1,4,7,10-tetraazacyclododecane-1,4,7-tris(2-hydroxymethylethan
oic acid);

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ gl R4N.X 25°C 0.10M C K1=2.50 2000BCa (100749)1120
Medium: 0.10 M NMe4Cl.
****
C20H38O8 L (617)
3-Hexyl-1,4,7,10,13,16,19-heptaoxacycloheneicosan-2-one, 3-Hexyl-2-one-21-crown-7;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE alc/w 25°C 100% U K1=2.40 1982MKa (100756)1121
Medium: MeOH
****
C20H38O9 L CAS 94618-61-8 (8712)
1,11-Dimethyl-3,6,9,13,16,19,21,24,27-nonaoxabicyclo[9.9.7]heptacosane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE non-aq 25°C 100% M K1=4.33 1984NMb (100759)1122
Medium: MeOH.
****

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
---
Na+ gl non-aq 25°C 100% C I K1=4.86 1992LSc (100777)1123
Medium: MeCN, 0.05 M Et4NClO4. In MeOH K1=3.4; in DMF K1=2.3; in pyridine K1=3.94; in H2O K1<2
****
C20H40N2O6 L Cryptand 2,2,2H (6606)
1,10-Diaza-4,7,14,17,23,26-Hexaoxabicyclo[10.8.8]octacosane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ gl alc/w 25°C 95% M K1=4.36 1990LNa (100786)1124
Medium: 95% MeOH, 0.05 M Bu4NBr. For the 12,19-dihydroxy- analogue: K1=5.75
****
C20H40N2O6 L Cryptand 3,2,1H (6589)
1,7-Diaza-4,11,14,17,23,26-hexaoxabicyclo[13.8.5]octacosane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ gl alc/w 25°C 95% M K1=4.46 1990LNa (100795)1125
Medium: 95% MeOH, 0.05 M Bu4NBr. For the 9,19-dihydroxy- analogue: K1=5.12
****
C20H40N2O7 L CAS 132162-59-5 (8958)
4,7,10,13,19,22,25-Heptaoxa-1,16-diazabicyclo[14.11.2]nonacosane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ cal alc/w 25°C 90% C H K1=3.56 1992DJa (100799)1126
Medium: 90% v/v MeOH/H2O. DH(K1)=-35.4 kJ mol-1, DS(K1)=-51 J K-1 mol-1.
****
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
---
Na+ ISE alc/w 25°C 95% C K1=4.57 1977LSc (100816)1127
Medium: 95% (w/w) MeOH/H2O, 0.1 M Et4NBr.

Na+ gl R4N.X 25°C 0.05M C I K1=1.65 1975LSc (100817)1128
In 95% MeOH: K1=4.57; 100%: 4.8
****
C20H40O6 L CAS 103748-82-9 (1672)
2-Octoxymethylene-1,4,7,10,13,16-hexaoxacyclooctadecane,
2-Octoxymethylene-18-crown-6

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

Na+ ISE alc/w 25°C 100% U I K1=3.91 1984IEa (100849)1129
Medium: MeOH: In 90% MeOH: K1=3.17
****
C20H40O10 L 30-Crown-10 (7044)
1,4,7,10,13,16,19,22,25,28-Decaoxacyclotriacontane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sol non-aq 25°C 100% C K1=3.6 1999KCa (100853)1130
Medium: acetonitrile.

Na+ cal alc/w 25°C 100% U H K1=2.14 1993ILa (100854)1131
Medium: MeOH. DH=-25.6 kJ mol-1.
****
C20H41NO5 L (1714)
N-Octyl-monoaza-18-crown-6

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE alc/w 25°C 100% U K1=3.59 1983MKa (100857)1132
****
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
---
Na+ ISE R4N.X 25°C 0.10M U I K1=2.5 1978LMa (100890)1133
In CH3OH, K1>5.0
****
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
---
Na+ dis non-aq 25°C 100% C K1=2.08 1999KKb (100903)1134
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
---
Na+ EMF non-aq 25°C 100% C I K1=5.98 1997DMd (100929)1135
Method: Ag electrode; competitive titration. Medium: acetonitrile, 0.05 M
Et4NClO4. Also data for PC (K1=5.3), DMF (3.76), 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
-------------------------------------------------------------------------
Na+        gl  non-aq 25°C 100%  U  I     K1=9.13        1996SDa (100944)1136
Medium: MeCN, 0.05 M Et4NClO4. In MeOH: K1=6.2, DMF: 5.68, DMSO: 4.95,
propylene carbonate: 8.2
-------------------------------------------------------------------------
Na+        gl  R4N.X  25°C 0.10M C        K1=2.20        1993SFb (100945)1137
Medium: 0.1 M Et4NClO4.
*************************************************************************
C21H23NO9                L                        (6799)
2,3-(4'-(4"-Nitrophenoxycarbonyl))benzo-1,4,7,10,13-pentaoxacyclopentadeca-2-ene;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Na+        kin alc/w  25°C  54%  U        K1=0.65        1991HHb (101224)1138
Medium: 54% w/w EtOH/H2O
*************************************************************************
C21H24O3Si3              L                      CAS 546-45-2  (1286)
Trimethyl-triphenyl-cyclotrisiloxane; ((CH3)(C6H5)SiO)3
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Na+        con alc/w  25°C 100%  U        K1=0.10        1980OPa (101259)1139
Medium: MeOH, 0.1 M Me4NBr
*************************************************************************
C21H24O6                 L                        (672)
4'-Benzoyl-(3-benzo-15-crown-5);
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Na+        cal alc/w  26°C  80%  C   H    K1=-0.024      1986CCa (101260)1140
Medium: 80% EtOH/H2O
*************************************************************************
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
-------------------------------------------------------------------------
Na+        sp  non-aq 25°C 100%  C        K1=3.7         2000KBb (101268)1141
Medium: MeOH.  Method: electrospray ionization mass spectrometry.
-------------------------------------------------------------------------
Na+        gl  alc/w  25°C  80%  M  IH    K1=3.27        1986ALb (101269)1142
                                        K(NaL+H)=4.93
                                        K(Na+HL)=2.35
Medium: 80% w/w MeOH/H2O. DH(K1)=-24.7 kJ mol-1, DS(K1)=-20.4 J K-1 mol-1.
In 99% w/w MeOH/H2O, K1=3.9, K(Na+HL)=2.72, K(NaL+H)=7.06.
*************************************************************************
C21H26O6                 L                      CAS 88847-18-1  (6847)
Dibenzo-4-methyl-18-crown-6;
-------------------------------------------------------------------------
```

```
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Na+        sp  non-aq 25°C 100%  U        K1=2.56        1991NTa (101287)1143
Medium: DMF. Data also for 4-ethyl, 4-hexyl and 4,13-dihexyl analogues
*************************************************************************
C21H27N7O14P2         H2L    beta-NAD         CAS 53-84-9  (5577)
beta-Nicotinamide adenine dinucleotide;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Na+        nmr R4N.X  22°C 0.10M U        K1=-0.27       1985PHb (101297)1144
*************************************************************************
C21H27O8P              L                      CAS 71817-08-8  (6905)
1,2:10,11-Dibenzo-16-methylphosphonyl)-3,6,9,12,15,17,20-heptaoxacycloeicosane;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Na+        nmr non-aq 20°C 100%  U        K1=2.4         1982BGe (101301)1145
Medium: Acetone-D6 ; Method - NMR H1.
*************************************************************************
C21H29NO6              L                      CAS 83260-79-1  (9010)
2-Methyl-2-(8-quinolyloxy)methyl-15-crown-5;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Na+        sp  non-aq 25°C 100%  C        K1=5.30        2002NMa (101339)1146
Medium: THF, using metal picrate salt.
*************************************************************************
C21H30O2P2             L                        (7851)
P'P'-Diphenyl-P,P-dibutylmethylenediphosphinedioxide;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Na+        con non-aq 25°C       C        K1=4.5         1999ESa (101386)1147
In tetrahydrofuran; alkali metal is used as 2,4-dinitrophenolate
*************************************************************************
C21H31O7P3             L                      CAS 82154-48-1  (2916)
Methyldi((2-dimethylphosphinylmethoxy)phenoxymethyl)phosphineoxide;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Na+        con non-aq 25°C 100%  U        K1=3.85        1982YSa (101421)1148
Medium: tetrahydrofuran+CHCl3 4:1(vol); M is 2,4-dinitrophenolate
L=CH3.PO(CH2.O.C6H4.O.CH2.PO(CH3)2)2
*************************************************************************
C21H33NO7              L                      CAS 60835-76-9  (1766)
2,3-(4'(N-Butyl)carboxyamidobenzo)-1,4,7,10,13,16-hexaoxacyclooctadeca-2-ene,
R-18-crown-6
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
```

Na+ con non-aq 25°C 100% U K1=4.51 1976UHa (101423)1149
Medium: acetone
****
C21H40O10 L Spiro-O6-O4 (2362)
Spiro-19-crown-6-13-crown-4;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ nmr non-aq 33°C 100% U T K1=1.78 1982BDb (101450)1150
K(NaL+Na)=1.41
Medium: pyridine. At 13.4 C: K1=2.15, K(NaL+Na=Na2L)=1.30;
at 24 C: 1.90, 1.26
****
C21H40O10 L Spiro-O5-O5 (2364)
Spiro-bis-16-crown-5;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ nmr non-aq 20°C 100% U T H K1=2.88 1982BDb (101451)1151
K(NaL+Na)=1.26
Medium: pyridine. At 5 C: K1=2.90, K(NaL+Na)=1.4; at 34 C: 2.74, 1.5;
at 65 C: 2.6, 1.6; at 80 C: 2.5, 1.4. DH(K1)=-9.6 kJ mol-1
****
C21H42N4O6S L CAS 503465-05-2 (9248)
4,12,18,21,26,29-Hexaoxa-1,7,9,15-tetraazabicyclo[13.8.8]hentriacontane-8-thione;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ gl alc/w 25°C 95% C K1=4.39 2004KVa (101465)1152
Medium: 95% MeOH/H2O, 0.01 M Et4NClO4.
****
C21H42N6O3 L (6791)
1,5,9-Tris(N,N-dimethylethanamido)-1,5,9-triazacyclododecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ gl R4N.X 25°C 0.10M M K1=4.02 1990KMb (101476)1153
Medium: 0.10 M Me4NNO3
****
C21H42O7 L CAS 91318-76-2 (1674)
2-Octyloxyethyleneoxymethylene-1,4,7,10,13-pentaoxacyclopentadecane, R-15-crown-5

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE alc/w 25°C 100% U I K1=3.18 1984IEa (101478)1154
Medium: MeOH. In 90% MeOH: K1=2.73
****
C22H20N2O4 L CAS 207461-96-9 (8955)
(5Z)-12,13,20,21-Tetrahydrotribenzo[b,f,l][1,8,11,14,4,5]tetraoxadiazacyclohexadeci

ne;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp non-aq RT 100% C I K1=2.85 2000GDa (101697)1155
Medium: acetonitrile. In MeOH, K1=2.1.
****
C22H24O8 L CAS 81279-93-8 (5566)
11,12-(1,4-Benzodioxinic)-2,3-benzo-18-crown-6

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ gl alc/w 25°C 100% U K1=1.53 1989MGb (101917)1156
Data also for various 14,14-disubstituted analogues
****
C22H25O3P L CAS 97745-35-2 (2069)
Adamantyl(diphenoxy)phosphonyl

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sol non-aq 25°C 100% U K1=3.55 1987TCa (101925)1157
Medium: CH2Cl2, 2% MeCN. Metal as picrate
****
C22H26N4O12 L CAS 74044-87-4 (2796)
4'-Picrylaminobenzo-18-crown-6

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp oth/un 25°C 0.10M U K1=1.30 1980NTa (101992)1158
K(Na+HL)=1.00
At pH 11.5 in Li4(EDTA)
****
C22H26O5 L (673)
(3-Phenylacrylyl)-3-benzo-15-crown-5;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ cal alc/w 26°C 80% C H K1=0.098 1986CCa (101994)1159
Medium: 80% EtOH/H2O
****
C22H26O5 L CAS 160978-39-2 (8944)
o,o'-(Tetraethyleneglycoldiyl)-(Z)-stilbene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ con non-aq 25°C 100% C K1=4.92 2000ICa (101999)1160
Medium: nitromethane.
****
C22H26O8 L (5632)
1,4-bis(2-Carboxymethoxyphenyl)-1,4-dioxabutane diethyl ester;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE alc/w 25°C 100% U K1=1.48 1981PTb (102002)1161
Medium: MeOH
****
C22H26O8 HL CAS 80186-74-9 (9071)
sym-Dibenzo-16-crown-5-oxypropanoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ gl alc/w 25°C 80% M H K1=2.83 1986ALb (102004)1162
K(Na+HL)=2.38
Medium: 80% w/w MeOH/H2O. DH(K1)=-31 kJ mol-1, DS(K1)=-49 J K-1 mol-1.
****
C22H26O10 H2L (5628)
1,10-bis(2-Carboxymethoxy-phenyl)-1,4,7,10-tetraoxadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE alc/w 25°C 100% U K1=2.30 1981PTb (102009)1163
Medium: MeOH
****
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
---
Na+ sp non-aq 25°C 100% C I M 2002YPc (102018)1164
K(ZnA2L+Na)=3.26
Medium: MeCN, 0.10 M n-Bu4NPF6. By 1H nmr in CDCl3, K(ZnA2L+Na)=3.19.
A is p-thiocresol.
****
C22H28O6 L CAS 52755-95-0 (5622)
5,9-Dimethyl-2,3:11,12-dibenzo-18-crown-6

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE alc/w 25°C 100% C K1=3.77 1981PTa (102030)1165
Medium: MeOH. Data for racemic ligand. For meso ligand K1=3.56
****
C22H28O6 L CAS 34368-73-5 (5621)
6,8-Dimethyl-2,3:11,12-dibenzo-18-crown-6

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE alc/w 25°C 100% C K1=3.03 1981PTa (102032)1166
Medium: MeOH. Data for racemic ligand. For meso ligand K1=2.79
****
C22H28O7 L Dibenzo-21-Cr-7 CAS 14098-41-0 (2876)

2,3:11,12-Dibenzo-1,4,7,10,13,16,19-heptaoxacycloheneicosane-2,11-diene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE mixed 25°C 50% C K1=2.58 B2= 7.14 2004YYb (102052)1167
Method: Na ion specific electrode. Medium: 50% THF/H2O.

Na+ dis none RT dil C M K1=0.36 2003AGa (102053)1168
K(Na+A+L(org)=NaAL(org))=1.9
Method: extraction of picrate ion pair into dichloromethane. HA is picric acid.

Na+ con non-aq 25°C 100% U K1=4.6 1993EVa (102054)1169
Medium: THF+CHCl3 (4:1 vol)

Na+ ISE alc/w 25°C 100% A K1=2.40 1971FRa (102055)1170
Medium: MeOH
****
C22H28O7 L CAS 133560-78-8 (8962)
2,3:17,18-Dibenzo-1,4,7,10,13,16,19-heptaoxacycloheneicosa-2,17-diene, Dibenzo[21]crown-7;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE mixed 25°C 50% C K1=1.83 B2= 4.67 2004YYb (102066)1171
Method: Na ion specific electrode. Medium: 50% THF/H2O.

Na+ sp non-aq 25°C 100% C K1=>1.74 2002YEa (102067)1172
Method: fluorescence spectroscopy. Medium: acetonitrile.

Na+ sp non-aq 25°C 100% C K1=2.56 2002YEb (102068)1173
Method: steady state fluorescence spectroscopy. Medium: acetonitrile.
****
C22H28O9S HL CAS 104716-44-1 (9072)
sym-Dibenzo-16-crown-5-oxypropanesulfonic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ gl alc/w 25°C 80% M K1=2.73 1986ALb (102072)1174
Medium: 80% w/w MeOH/H2O.
****
C22H29N3O5 L CAS 75897-28-8 (661)
4-Dimethylaminophenylazo-benzo-15-crown-5;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE alc/w 25°C 100% C K1=3.06 1985ZFa (102084)1175
****
C22H29O9P HL CAS 104716-45-2 (9073)
sym-Dibenzo-16-crown-5-oxymethylphosphonic acid monoethyl ester;

```
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Na+        gl  alc/w  25°C  80%  M        K1=3.2         1986ALb (102098)1176
                                         K(Na+HL)=2.45
Medium: 80% w/w MeOH/H2O.
******************************************************************************
C22H30O4P2              L                     CAS 470454-09-2  (8993)
4,10-Dibenzyl-1,7-dioxa-4,10-diphosphacyclododecan-4,10-dioxide;
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Na+        dis non-aq 24°C 100%  C                        2002MRd (102132)1177
                                         K(Na+A+L)=4.51
Medium: CDCl3. HA is picric acid.
******************************************************************************
C22H30O6                L                       (2506)
2,5,8,13,16,19-Hexaoxa-9,10:11,12-dibenzoeicosa-9,11-diene;
(-C6H4.O.(CH2.CH2.O)2.CH3)2
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Na+        ISE alc/w  25°C 100%  U                        1975CJa (102135)1178
                                         K1 < 0.01
Medium: MeOH
******************************************************************************
C22H31N2O6Cl           HL                     CAS 184647-21-0  (8621)
5-Chloro-2-(1,4,7,10,13-pentaoxa-16-azacyclooctadec-16-ylmethyl)-8-quinolinol;
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Na+        cal non-aq 25°C 100%  C   H                    1997ZBb (102140)1179
                                         K(Na+HL)=3.98
Medium: MeOH. DH(K)=-27.4 kJ mol-1, DS(K)=-15.7 J K-1 mol-1.
******************************************************************************
C22H31N2O6Cl           HL                     CAS 184647-19-6  (8620)
5-Chloro-7-(1,4,7,10,13-pentaoxa-16-azacylooctadec-16-ylmethyl)-8-quinolinol;
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Na+        cal non-aq 25°C 100%  C   H                    1997ZBb (102144)1180
                                         K(Na+HL)=3.60
Medium: MeOH. DH(K)=-27.5 kJ mol-1, DS(K)=-17.3 J K-1 mol-1.
******************************************************************************
C22H32O7P2              L                       (2078)
1,5-Bis(2-(dimethylphosphinylmethoxy)phenoxy)-3-oxapentane;
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Na+        con non-aq 25°C 100%  U        K1=3.86         1989KSa (102208)1181
```

Medium: tetrahydrofuran/CHCl3 4:1 (vol)
****
C22H32O8 L CAS 123295-31-8 (5572)
17,17-Dimethyl-18,19-(1,4-Benzodioxinic)-1,4,7,10,13,16-hexaoxacyclocosa-18-ene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	gl	alc/w	25°C	100%	U		K1=1.54	1989MGb	(102210)1182

Medium: MeOH
****
C22H36N2O6 L Bz-Cryptand 222 CAS 31250-18-7 (2269)
5,6-Benzo-4,7,13,16,21,24-hexaoxa-1,10-diazabicylo[8:8:8]hexacosa-5-ene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	gl	R4N.X	25°C	0.05M	U	H	K1=3.9	1998DBa	(102278)1183

Medium: 0.05 M Et4NClO4. By calorimetry: DH(K1)=-26.2 kJ mol-1,
---
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	gl	oth/un	25°C	0.02M	U	H	K1=7.50	1980CKa	(102279)1184

DH=-39.7 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-nonanoxacycloheptacosa-2-ene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	sp	non-aq	22°C	100%	U		K1=5.09	1987CCc	(102301)1185

In deuterochloroform
****
C22H37NO7 L CAS 105495-13-4 (1691)
N-(2-(2-Phenyloxy)ethoxy)ethyl-1,4,7,10,13-pentaoxa-16-azacyclooctadecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	ISE	alc/w	25°C	10%	U		K1=3.48	1986HAa	(102306)1186

Medium: 10% MeOH/H2O
****
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
Na+	nmr	non-aq	24°C	100%	U	M	K(Na(picrate)+L)=5.8	1981BEb	(102373)1187

Medium: CDCl3
****
C22H40O7 L (6596)
2,3,11,12,-Dicyclohexano-1,4,7,10,13,16,19-heptaoxacycloheneicosane;
dicyclohexyl-21-crown-7;

```
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Na+        sol non-aq 25°C 100%  C  I     K1=5.05        1999KCa (102380)1188
Medium: acetonitrile. In propylene carbonate, K1=5.19
*************************************************************************
C22H44N2O7              L    Cryptand 3,2,2H    (6607)
1,10-Diaza-4,7,14,17,20,26,29-Heptaoxabicyclo[13.8.8]hentriacontane;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Na+        gl  alc/w  25°C  95%  M        K1=4.65        1990LNa (102416)1189
Medium: 95% MeOH, 0.05 M Bu4NBr. For the 12,22-dihydroxy- analogue: K1=5.15
*************************************************************************
C22H44N2O8              L    Cryptand 4,2,2     (7304)
1,10-Diaza-4,7,13,16,21,24,27,30-octaoxabicyclo[8,8,14]dotricontane;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Na+        cal alc/w  25°C  50%  U   H    K1=4.26        1997ZIa (102422)1190
Medium: 95% v/v MeOH/H2O, 0.1 M. DH(K1)=-29.4 kJ mol-1, DS=-17.1 J K-1 mol-1
*************************************************************************
C22H44N2O8              L    Cryptand 3,3,2   CAS 132162-57-3  (1762)
Cryptand 3,3,2
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Na+        gl  alc/w  25°C 100%  C  I     K1=3.2         1975LSc (102430)1191
Medium: MeOH
*************************************************************************
C22H44N6O5S2            L                      CAS 503465-08-5  (9241)
9,20,23,28,31-Pentaoxa-1,4,6,12,14,17-hexaazabicyclo[15.8.8]tritriacontane-5,13-dit
hione;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Na+        gl  alc/w  25°C  95%  C        K1=2.55        2004KVa (102440)1192
Medium: 95% MeOH/H2O, 0.01 M Et4NClO4.
*************************************************************************
C22H44O11               L    33-Crown-11        (7045)
1,4,7,10,13,16,19,22,25,28,31-Undecaoxacyclotritriacontane;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Na+        cal alc/w  25°C 100%  U   H    K1=1.96        1993ILa (102444)1193
Medium: MeOH. DH=-33.9 kJ mol-1.
*************************************************************************
C22H45NO4               L                      CAS 75006-56-3  (1717)
N-Dodecyl-monoaza-15-crown-5
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
```

Na+ ISE alc/w 25°C 100% U I K1=3.06 1983MKa (102446)1194
****
C22H45NO6 L CAS 75006-58-5 (1720)
N-(Octyl-di(oxyethylene))-monoaza-15-crown-5

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE alc/w 25°C 100% U K1=3.83 1983MKa (102448)1195
****
C22H46N2O4 L CAS 69703-24-8 (2449)
N,N'-Bis(2-dimethylpropane)-cyclo-1,10-diaza-4,7,13,16-tetraoxaoctadecane)

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ gl alc/w 25°C 93% U K1=2.2 1978WVa (102452)1196
Medium: 93% MeOH/H2O
****
C22H46N2O8 L CAS 85726-96-1 (647)
4,10-Dimethyloxyethoxyethoxyethylidene-1,7-dioxo-4,10-diazacyclododecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sol non-aq 20°C 100% C K1=5.45 1983SLa (102456)1197
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
---
Na+ sol non-aq 20°C 100% C K1=5.15 1983SLa (102459)1198
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
---
Na+ ISE alc/w 25°C 95% U K1=4.2 1978LMa (102489)1199
****
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
---
Na+ sp diox/w 25°C 50% C I K1=1.15 2001INa (102646)1200
Medium: 50% v/v dioxane/H2O, 3% v/v triethylamine, pH 12. In 50%
v/v dioxane/H2O with Et4NOH, K1=2.51.

****
C23H23NO5 L CAS 218619-58-0 (7808)
Dibenzo-pyridino-18-crown-6;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ EMF alc/w 25°C 100% C K1=3.96 2004ZTa (102661)1201
Medium: 100% methanol, 0.05 M Bu4NClO4. Method: Ag electrode,
competition with Ag+ ion.
****
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
---
Na+ sp non-aq RT 100% C K1=2.60 2001AVa (102752)1202
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-azacyclopentadecan
e;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp alc/w RT 50% C I K1=1.25 2002GNe (102769)1203
Medium: 50% v/v MeOH/H2O, pH 7.4 (0.1M Tris buffer), 0.1 M Me4NCl.
In 0.5% MeOH/H2O, K1=0.8.
****
C23H32N2O5 L (7369)
9-(2'-Pyridylmethyl)-3,6,12,15-tetraoxa-19-methyl-21-hydroxy-9-azabicyclo[15.3.1]he
neicosatriene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ cal alc/w 25°C 100% U H K1=2.75 1997ZBa (102786)1204
Medium: MeOH
****
C23H33N2O6Cl L CAS 184647-23-2 (8622)
5-Chloro-8-methoxy-2-(1,4,7,10,13-pentaoxa-16-azacyclooctadec-16-ylmethyl)-quinolin
e;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ cal non-aq 25°C 100% C H K1=4.06 1997ZBb (102796)1205
Medium: MeOH. DH(K)=-20.2 kJ mol-1, DS(K)=9.97 J K-1 mol-1.
****
C23H42N2O9 HL CAS 111216-12-7 (5568)
2-Carboxy-3-monopiperidine-18-crown-6 derivative;

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

---
Na+ nmr alc/w 25°C 90% U K1=4.4 1987DDa (102841)1206
K(Na+HL)=4.3
Medium: 90% MeOH/H2O
****
C23H46O8 L CAS 91318-80-8 (1673)
2-Octyl-di(oxyethylene)-oxymethylene-1,4,7,10,13-pentaoxacyclopentadecane, R-15-crown-5

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE alc/w 25°C 100% U I K1=3.23 1984IEa (102843)1207
Medium: MeOH. In 90% MeOH: K1=2.75
****
C23H46O8 L CAS 91318-78-4 (1671)
2-Octyl-oxyethylene-oxymethylene-1,4,7,10,13,16-hexaoxacyclooctadecane, R-18-crown-6

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE alc/w 25°C 100% U I K1=3.97 1984IEa (102845)1208
Medium: MeOH. In 90% MeOH: 3.27
****
C24H20B- HL CAS 4358-26-3 (2489)
Tetraphenylborate;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ con non-aq 25°C 100% U I K1=1.0 1982GCa (102901)1209
Medium: DMF. Data available in a variety of media

Na+ con non-aq 25°C 100% U K1=0.48 1978CAa (102902)1210
Medium: Acetonitrile

Na+ con non-aq 25°C 100% U K1=0.16 1976RMb (102903)1211
Medium: 1,3-Dimethylethyleneurea (1,3-dimethyl-2-imidazolidinone)

Na+ con non-aq 25°C 100% U K1=0.6 1975YKa (102904)1212
Medium: MeCN

Na+ con non-aq 25°C 100% U I K1=2.61 1974TAb (102905)1213
Medium: MIBK(methyl-i-butyl ketone). K1=2.41(MIBK sat. with H2O), 0.94(H2O)
****
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
---
Na+ con non-aq 25°C 100% U K1=5.8 1989BEa (102939)1214
Medium: tetrahydrofuran/CHCl3 4:1 (volume)

****
C24H24O6 L CAS 99700-19-3 (8873)
2,3:5,6:8,9-Tribenzo-1,4,7,10,13,16-hexaoxacyclooctadeca-2,5,8-triene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ dis non-aq 23°C 100% C K1=6.2 1992HGb (102954)1215
Extraction of metal chloride (A) from aqueous solution into nitrobenzene/
0.01M Bu4NB(Ph)4. Peak potential voltammetry and distribution of 22Na.
****
C24H24O6 L TriBz18-Crown-6 (6069)
2,3:8,9:11,12-Tribenzo-1,4,7,10,13,16-hexaoxacyclooctadeca-2,8,11-triene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ dis non-aq 23°C 100% C K1=6.1 1992HGb (102960)1216
Extraction of metal chloride (A) from aqueous solution into nitrobenzene/
0.01M Bu4NB(Ph)4. Peak potential voltammetry and distribution of 22Na.
****
C24H25O7P L (2067)
Phenylphosphonyldibenzo-17-crown-6

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sol non-aq 25°C 100% U K1=3.49 1987TCa (102966)1217
Medium: CH2Cl2, 2% MeCN
****
C24H26N2O6 HL (664)
2-Hydroxynaphthylazo-benzo-15-crown-5;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE alc/w 25°C 100% C K1=3.38 1985ZFa (102970)1218
****
C24H30O7 HL (6603)
2-[(7,8,16,17-Tetrahydro-6H,15H-dibenzo[1,4,8,11]tetraoxacyclotetradeca-7-yl)oxy)-h
exanoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ dis oth/un 25°C ? U K1=1.61 1991BUa (103033)1219
With the butanoic acid analogue: K1=1.58
****
C24H30O8 L CAS 67655-22-5 (8710)
7,8,16,17-Tetrahydro-7,16-(epoxyethanoxyethanoxyethanoxy)-6H,15H-dibenzotetraoxacyc
lotetradecin;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE none 25°C 0.0 C K1=5.4 1978PAa (103035)1220

Method: Na-sensitive electrode.

****

C24H30O9 L (5625)

1,7-bis(2-Carboxymethoxyphenyl)-1,4,7-trioxaheptane diethylester;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	ISE	alc/w	25°C	100%	U		K1=1.89	1981PTb	(103038)1221

Medium: MeOH

****

C24H32N2O7 L (2350)

1,11-Bis(2-(methylamido)phenoxy)-3,6,9-trioxaundecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	nmr	non-aq	13°C	100%	U	T	K1=1.4	1981GLb	(103065)1222

Medium: acetonitrile. K1=1.5 between 24 and 51 C

****

C24H32N2O7 L (2347)

1,11-Bis(ortho(methylamido)phenoxy)-3,6,9-trioxaundecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	nmr	non-aq	5°C	100%	U	T H	K1=2.7	1981GLb	(103066)1223

Medium: pyridine. DH=-66 kJ mol-1. K1=2.4 (17 C); 1.9 (32 C); 1.1 (53 C)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	nmr	non-aq	0°C	100%	U	T H	K1=2.8	1981GLb	(103067)1224

Medium: pyridine. DH=-45 kJ mol-1. K1=2.3 (10 C); 1.7 (33 C); 1.6 (43 C)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	nmr	non-aq	24°C	100%	U	T	K1=1.5	1981GLb	(103068)1225

Medium: acetonitrile. K1=1.5 between 0 and 51 C

****

C24H32O6 L ANAN(MOEO)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
Na+	dis	non-aq	25°C	100%	U	H	K(Na(picrate)+L)=6.39	1979KLa	(103073)1226

Medium: CHCl3

****

C24H32O6 L AN(MOEOM)2AN (2244)

23,24-Dimethoxy-10,21-dimethyl-3,6,14,17-tetraoxatricyclo-tetracosa-1(23),8(24),9,11,19,21hexaene

---

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	dis	non-aq	25°C	100%	U	H	K(Na(picrate)+L)=3.30	1979KLa	(103079)1227

Medium: CHCl3
****
C24H32O6 L DP(OEOEO)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
---
Na+ dis non-aq 25°C 100% U H 1979KLa (103085)1228
K(Na(picrate)+L)=5.22
Medium: CHCl3
****
C24H32O8 L (5617)
2,3:11,12-Dibenzo-1,4,7,10,13,16,19,22-octaoxacyclotetracosa-2,11-diene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ oth alc/w 25°C 100% U K1=2.15 1980WAa (103088)1229
Medium: MeOH
****
C24H32O8 L DiBz-24-Crown-8 CAS 14174-09-5 (580)
2,3:14,15-Dibenzo-1,4,7,10,13,16,19,22-octaoxacyclotetracosa-2,14-diene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE mixed 25°C 50% C K1=2.11 B2= 4.68 2004YYb (103148)1230
Method: Na ion specific electrode. Medium: 50% THF/H2O.

Na+ dis none RT dil C M K1=0.91 2003AGa (103149)1231
K(Na+A+L(org)=NaAL(org))=4.38
Method: extraction of picrate ion pair into dichloromethane. HA is picric acid.

Na+ oth NaCl 25°C 0.1M C K1=-0.3 2002KTa (103150)1232
Method: capillary electrophoresis. Medium: 0.08-0.11 M NaCl.

Na+ sp non-aq 25°C 100% C K1=3.37 2002YEb (103151)1233
Method: steady state fluorescence spectroscopy. Medium: acetonitrile.

Na+ nmr non-aq 27°C 100% C I K1=>8 1998KZa (103152)1234
K(NaL+Na)>6
Method: 23Na nmr. Medium: nitromethane. Also data for 20-100% acetonitrile/nitromethane. In 100% acetonitrile, K1=3.60, K(NaL+Na)=1.22

Na+ sp non-aq 25°C 100% U TIH K1=3.52 1995KSa (103153)1235
Medium: 10% w/w DMF/MeCN. DH(K1)=-10.7 kJ mol-1, DS=33 J K-1 mol-1.
Data also for 20 30, 40 w/w% DMF

Na+ con non-aq 25°C 100% U K1=5.3 1993EVa (103154)1236
Medium: THF+CHCl3 (4:1 vol)

Na+ vlt non-aq 25°C 100% U K1=13.3 1990SPa (103155)1237
Medium: 1,2-dichloroethane

Na+ vlt alc/w 25°C 100% U K1=2.35 1985ZBa (103156)1238
Medium: MeOH

Na+ ISE alc/w 25°C 100% U K1=2.35 1983GGa (103157)1239
Medium: MeOH

Na+ dis non-aq 35°C 100% U TI K1=4.1 1980TYb (103158)1240
Medium: propylene carbonate

Na+ cal alc/w 25°C 70% U H K1=1.54 1976ITa (103159)1241
Medium: 70% w/w MeOH/H2O. DH(K1)=-32.0 kJ mol-1
****
C24H32O8 L CAS 75832-82-5 (5618)
2,3:8,9-Dibenzo-1,4,7,10,13,16,19,22-octaoxacyclotetracosa-2,8-diene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp non-aq 25°C 100% C K1=3.356 2002YEa (103185)1242
Method: fluorescence spectroscopy. Medium: acetonitrile.

Na+ oth alc/w 25°C 100% U K1=2.55 1980WAa (103186)1243
Medium: MeOH
****
C24H33N3O7 L (662)
4-Dihydroxyethylaminophenylazo-benzo-15-crown-5;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE alc/w 25°C 100% C K1=3.06 1985ZFa (103200)1244
****
C24H34N2O5 L CAS 182926-58-5 (8848)
7,13-Bis(2-methoxyphenyl)-1,4,10-trioxa-7,13-diazacyclopentadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp alc/w RT 50% C K1=3.1 2002GLb (103211)1245
Medium: 50% MeOH/H2O, pH 7.4 (0.1 M Tris buffer), 0.1 M Me4NCl.
****
C24H34O5P2 L CAS 470454-11-6 (8994)
7,13-Dibenzyl-1,4,10-trioxa-7,13-diphosphacyclopentan-7,13-dioxide;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ dis non-aq 24°C 100% C 2002MRd (103233)1246
K(Na+A+L)=4.28
Medium: CDCl3. HA is picric acid.
****

C24H34O10 HL CAS 143585-81-3 (7847)
1-Methyl-1,4,7,10,13,16-hexaoxacycloeicosino[18,19-b][1,4]benzodioxin-1-propanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	gl	non-aq	25°C	100%	U		K1=3.06 K(Na+HL)=2.30 K(NaL+H)=8.86	1992BCe	(103239)1247

Medium: methanol. Method: glass/Na+ and glass/H+ electrodes.
Data for many structurally related macrocycles and linear analogues.

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	sp	mixed	25°C	10%	C		K1=4.06	2001LWa	(103244)1248

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-diyldimethylferrocene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	nmr	non-aq	25°C	100%	U		K1=6.28	1992MGa	(103257)1249

Method:NMR. Medium: MeCN, 0.1 M Bu4NPF6. Data also for other ferrocene[2.2] cryptands. In MeOH K=3.72

****

C24H36O6 L (1703)
Decalino-benzo-18-crown-6

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	ISE	alc/w	25°C	?	U		K1=4.49	1983KTa	(103291)1250

****

C24H36O9 L (5573)
20,20-Dimethyl-21,22-(1,4-Benzodioxinic)-1,4,7,10,13,16,19-heptaoxacyclotricos-21-ene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	gl	alc/w	25°C	100%	U		K1=1.64	1989MGb	(103293)1251

Medium: MeOH

****

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
-------------------------------------------------------------------------
Na+        con non-aq 25°C 100%  U        K1=3.6         1989EVa (103297)1252
Medium: tetrahydrofuran/CHCl3 4:1 (volume)
*************************************************************************
C24H40O4               HL    Deoxycholic ac.  CAS 83-44-3  (6085)
3,12-Dihydroxy-5-beta-cholic acid;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Na+        gl  R4N.X  25°C 0.50M C  I     K1=0.02        1986BFb (103349)1253
                                         *B(2,2)=1.51
                                         *B(2,3)=5.30
                                         *B(4,4)=7.80
                                         B(NaHL2)=8.15
-------------------------------------------------------------------------
Na+        EMF R4N.X  25°C 0.50M C        K1=0.01        1985BPc (103350)1254
                                         *B(2,2)=1.03
                                         *B(3,3)=2.20
                                         *B(2,3)=1.80
                                         B(NaHL)=7.77
*************************************************************************
C24H42N2O6             L                      CAS 129242-36-0  (8616)
6,16,25-Tris(methylene)-4,8,14,18,23,27-hexaoxa-1,11-diazabicyclo[9.9.9]nonacosane;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Na+        cal alc/w  25°C  80%  C   H    K1=6.50        1995KZa (103355)1255
Medium: 80% v/v CH3OH/H2O. DH(K1)=-71.7 kJ mol-1, DS(K1)=-116 J K-1 mol-1
*************************************************************************
C24H42O6               L                      CAS 88692-14-2  (1705)
Decalino-cyclohexano-18-crown-6
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Na+        ISE alc/w  25°C    ?  U        K1=4.34        1983KTa (103392)1256
*************************************************************************
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
-------------------------------------------------------------------------
Na+        sp  non-aq 22°C 100%  U        K1=5.02        1987CCc (103398)1257
In deuterochloroform
-------------------------------------------------------------------------
Na+        ISE alc/w  25°C 100%  U        K1=1.74        1975CJa (103399)1258
Medium: MeOH
*************************************************************************
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
--------------------------------------------------------------------------------
Na+        nmr non-aq 24°C 100%  U    M                  1981BEb (103412)1259
                                        K(Na(picrate)+L)=4.9
Medium: CDCL3
********************************************************************************
C24H44O8                L    Dicy-24-crown-8  CAS 17455-23-1  (2401)
2,3,14,15-Dicyclohexyl-1,4,7,10,13,16,19,22-octaoxacyclotetracosane;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Na+        ISE mixed  25°C  50%  C        K1=2.05   B2= 5.60  2004YYb (103432)1260
Method: Na ion specific electrode. Medium: 50% THF/H2O.
--------------------------------------------------------------------------------
Na+        sol non-aq 25°C 100%  C  I     K1=5.45        1999KCa (103433)1261
Medium: acetonitrile. In propylene carbonate, K1=5.48
********************************************************************************
C24H48N2O9              L    BOA15C5          CAS 31255-19-3  (6119)
3-Oxa-1,5-bis-(1-aza-4,7,10,13-tetraoxacyclopentadecyl)pentane;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Na+        ISE alc/w  25°C  90%  U        K1=3.63        1988HKa (103459)1262
Medium: 90% w/w MeOH/H2O
********************************************************************************
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
--------------------------------------------------------------------------------
Na+        gl  alc/w  25°C 100%  C  I     K1=2.7         1975LSc (103466)1263
Medium: MeOH
********************************************************************************
C24H48N4O6              L                     CAS 56698-26-1  (1536)
4,10,16,22,27,32-Hexaoxa-1,7,13,19-tetraazatricyclo-tetratriacontane;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Na+        gl  R4N.X  25°C 0.10M U        K1=1.6         1981GLa (103487)1264
--------------------------------------------------------------------------------
Na+        ISE non-aq 25°C 100%  C        K1=4.5         1977LSc (103488)1265
Medium: 0.10 M Et4NBr in MeOH.
********************************************************************************
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-d
ithione;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
```

Na+ gl alc/w 25°C 95% C K1=2.22 2004KVa (103507)1266
Medium: 95% MeOH/H2O, 0.01 M Et4NClO4.
****
C24H48N7O5P3 L CAS 254441-66-2 (7955)
2,5,8,11,14-Pentaoxa-16,18,19-triaza-1,15,17-triphosphabicyclo[13.3.1]nonadeca-1,15
,17-triene,17,

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ EMF R4N.X RT 0.10M M K1=1.20 2001BSb (103513)1267
Method: Ag/Ag+ electrode. Medium: 0.10 M Et4NNO3.
****
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
---
Na+ gl R4N.X 25°C 0.10M M K1=5.84 1990KMb (103517)1268
Medium: 0.10 M Me4NNO3
****
C24H48O12 L 36-Crown-12 (7046)
1,4,7,10,13,16,19,22,25,28,31,34-Dodecaoxacyclohexatriacontane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ cal alc/w 25°C 100% U H K1=2.06 1993ILa (103521)1269
Medium: MeOH. DH=-31.1 kJ mol-1.
****
C24H49NO5 L CAS 86181-93-3 (1709)
N-Dodecyl-monoaza-18-crown-6

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE alc/w 25°C 100% U I K1=3.61 1983MKa (103523)1270
****
C24H49NO7 L CAS 75006-62-1 (1713)
N-(Octyl-di-(oxyethylene))-monoaza-18-crown-6

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE alc/w 25°C 100% U K1=4.21 1983MKa (103525)1271
****
C24H49NO7 L CAS 86170-86-7 (1719)
N-(Octyl-tri(oxyethylene))-monoaza-15-crown-5

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE alc/w 25°C 100% U K1=4.26 1983MKa (103527)1272
****
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
---
Na+ sol non-aq 20°C 100% C K1=5.52 1983SLa (103530)1273
Medium: CHCl3
****
C24H72O12Si12 L CAS 18919-94-3 (1287)
Tetracosamethyl-cyclododecasiloxane; ((CH3)2SiO)12

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ con alc/w 25°C 100% U K1=<-0.3 1980OPa (103592)1274
Medium: MeOH, 0.1 M Me4NBr
****
C25H19N3O2 L (2157)
2,6-(Di-(8-methoxyquinolyl)-pyridine; C9H6N.O.CH2.C5H3N.CH2.O.C9H7N

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp alc/w 25°C 100% U K1=3.92 B2=7.72 1977TMa (103596)1275
Medium: MeOH
****
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
---
Na+ con non-aq 25°C C K1=4.8 1999ESa (103636)1276
In tetrahydrofuran; alkali metal is used as 2,4-dinitrophenolate
---
Na+ con non-aq 25°C 100% U K1=4.4 1984YKa (103637)1277
Medium: tetrahydrofuran + CHCl3 4:1, Na as 2,4-dinitrophenolate
---
Na+ con non-aq 25°C 100% U 1969SSi (103638)1278
K(NaI+L)=1.90
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
---
Na+ sp diox/w 25°C 50% C K1=2.09 2001INa (103653)1279
Medium: 50% v/v dioxane/H2O, 3% v/v triethylamine, pH 12.
****
C25H28NO4S+ 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
---
Na+ sp non-aq 25°C 100% C K1=1.80 2002GVc (103661)1280
Medium: acetonitrile, 0.1 M Et4NClO4.
****
C25H30N3O5Cl HL CAS 172033-66-8 (8619)
5-Chloro-2-(3,6,12,15-tetraoxa-9,21-diazabicycloheneicosa-1,17,19-trien-9-ylmethyl-8-quinolinol;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ cal non-aq 25°C 100% C H 1997ZBb (103687)1281
K(Na+HL)=4.20
Medium: MeOH. DH(K)=-23.6 kJ mol-1, DS(K)=1.2 J K-1 mol-1.
****
C25H30N3O5Cl HL CAS 172033-54-4 (8618)
5-Chloro-7(3,6,12,15-tetraoxa-9,21-diazabicycloheneicosa-1,17,19-trien-9-ylmethyl)-8-quinolinol;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ cal non-aq 25°C 100% C H 1997ZBb (103691)1282
K(Na+HL)=3.85
Medium: MeOH. DH(K)=-17.5 kJ mol-1, DS(K)=15.0 J K-1 mol-1.
****
C25H32O8 HL (6604)
2-[(6,7,9,10,18,19-Hexahydro-17H-dibenzo[1,4,7,10,13]pentaoxacyclohexadeca-18-yl]oxyhexanoic acid
---
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ dis oth/un 25°C ? U K1=1.72 1991BUa (103749)1283
****
C25H37N2O7P L CAS 202407-79-2 (8035)
26,27-Dimethoxy-3,7,24-triMe-11,14,17,20-tetraoxa-2,4-diaza-phosphatricycloheptacosahexaeneoxide;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ dis non-aq 20°C 100% C 1998DDc (103760)1284
K(NaP+L)=3.48
Medium: CHCl3. P is picrate.
****
C25H40O12 L CAS 239470-22-5 (8948)
4'-Carboxybenzo-30-crown-10;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ con non-aq 25°C 100% C T H K1=4.01 1999RGa (103776)1285

Medium: acetonitrile. Data for 5-35 C. DH(K1)=-33.4 kJ mol-1, DS(K1)=
-35 J K-1 mol-1.

****

C25H48O12 L Spiro-O6-O6 CAS 69502-15-4 (2363)
Spiro-bis-19-crown-6;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	nmr	non-aq	31°C	100%	U	T	K1=2.96 K(NaL+Na)=2.15	1982BDb	(103826)1286

Medium: pyridine. At 45.3 C: K1=2.65, K(NaL+Na=Na2L)=2.02;
at 19 C: 3.25, 2.27

****

C25H50N2O8 L BCA15C5 CAS 71972-29-7 (6116)
1,5-Bis-(1-aza-4,7,10,13-tetraoxacyclopentadecyl)pentane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	ISE	alc/w	25°C	90%	U		K1=2.82	1988HKa	(103830)1287

Medium: 90% w/w MeOH/H2O

****

C25H50N4O5 L CAS 61136-92-3 (1535)
Pentaoxa-4,10,16,22,27-tetraaza-1,7,13,19-tricyclo-tetratriacontane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	gl	R4N.X	25°C	0.10M	U		K1=1.8	1981GLa	(103836)1288

****

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
Na+	gl	alc/w	25°C	95%	C		K1=4.22	2004KVa	(103846)1289

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

****

C25H50O9 L CAS 91318-82-0 (1670)
2-Octyl-di(oxyethylene)-oxymethylene-1,4,7,10,13,16-hexaoxacyclooctadecane,R-18-cro
wn-6

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	ISE	alc/w	25°C	100%	U	I	K1=3.97	1984IEa	(103850)1290

Medium: MeOH. In 90% MeOH: K1=3.26

****

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

---
Na+ sp non-aq 25°C 100% C I 2002YPb (103903)1291
K(CuLA2+Na)=2.72
Medium: MeCN, 0.10 M Bu4NPF6. By nmr, K=3.00. Also data for acetone/
0.01 M Bu4NPF6: K=2.51 (2.41 by nmr) and MeOH. A is triphenylphosphine.

Na+ sp non-aq 25°C 100% C I 2002YPb (103904)1292
K(ZnLA2+Na)=3.36
Medium: MeCN, 0.10 M Bu4NPF6. A is CH3.C6H4.SH

Na+ sp non-aq 25°C 100% U I M 1997YLa (103905)1293
K(Ru(II)(bpy)2L+Na)=3.08
Medium: CH3CN;0.1M NBu4PF6. In (CH3)2CO: K=2.31; in CH3OH: K=1.42. 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
---
Na+ con non-aq 25°C 100% U K1=3.1 1990EAb (103913)1294
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
---
Na+ con non-aq 25°C C K1=3.2 1999TEa (103921)1295
In: tetrahydrofurane/CHCl3 4:1 v/v

Na+ oth non-aq 25°C 100% U K1=3.2 1995TEa (103922)1296
Medium: tetrahydrofurane: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
---
Na+ sp alc/w 25°C 100% U K1=3.22 B2=5.71 1977TMa (103980)1297
Medium: MeOH
****
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
---
Na+ sp non-aq 25°C 100% C K1=5.12 2003GHa (104076)1298
K(NaL+Na)=2.62

Method: fluorescence spectroscopy. Medium: acetonitrile, 0.05 M Et4NClO4.
****
C26H34O9 L CAS 67655-23-6 (8711)
7,8,16,17-Tetrahydro-7,16-(epoxyethanoxyethanoxyethanoxyethanoxy)-dibenzotetraoxacyclotetradecin;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE none 25°C 0.0 C K1=3.5 1978PAa (104109)1299
Method: Na-sensitive electrode.
****
C26H34O10 L (5629)
1,10-bis(2-Carboxymethoxyphenyl)-1,4,7,10-tetraoxadecane diethyl ester;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE alc/w 25°C 100% U K1=2.38 1981PTb (104112)1300
Medium: MeOH
****
C26H35N3O5 HL CAS 254900-33-9 (8919)
7-(10-Hydroxybenzoquinoline-9-ylmethyl)-1,4,10,13-tetraoxa-7,16-diazacyclooctadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ cal alc/w 25°C 100% C H 1999SBg (104117)1301
K(Na+HL)=ca.3
Medium: MeOH. DH(K)=ca.5 kJ mol-1. K and DH(K) estimated by competitive titration with Zn++.
****
C26H36N2O6 L DiBzCryptand222 (746)
5,6,14,15-Dibenzo-4,7,13,16,21,24-hexaoxa-1,10-diazabicyclo[8.8.8]hexacosan-5,14-diene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ gl R4N.X 25°C 0.05M U H 1998DBa (104139)1302
Medium: 0.05 M Et4NClO4. By calorimetry: DH(K1)=-10.8 kJ mol-1,
---
Na+ cal non-aq 25°C 100% U IH 1988DSa (104140)1303
Medium: MeCN. DH(K1)=-61.4 kJ mol-1. Also data in propylene carbonate, dimethylformamide and dimethylsulphoxide
---
Na+ ISE non-aq 25°C 100% U M K1=5.15 1987DSa (104141)1304
Medium: N,N-dimethylformamide

Na+ ISE alc/w 25°C 100% C I K1=7.37 1985CKa (104142)1305
Medium: MeOH: In propylenecarbonate K1=9.20; in DMF K1=5.32; in DMSO K1=4.48
****
C26H36N2O6Cl2 H2L (7215)

7,16-Bis((5-chloro-2-hydroxybenzyl)-1,4,10,13-tetraoxa-7,16-diazacyclooctadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ cal non-aq 25°C 100% C H 1995ZBa (104157)1306
K(Na+H2L)=2.85
Medium: methanol. DH(K)=-16.0 kJ mol-1, DS(K)=1.0 J K-1 mol-1.
****
C26H36O9 L CAS 518019-36-8 (8969)
2,3:11,12-Dibenzo-1,4,7,10,13,16,19,22,25-nonaoxacycloseptacosa-2,11-diene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp non-aq 25°C 100% C K1=<2 2002YEb (104164)1307
Method: steady state fluorescence spectroscopy. Medium: acetonitrile.
****
C26H36O9 L DiBz-27-crown-9 CAS 61260-08-0 (1775)
Dibenzo-27-crown-9.
2,3:17,18-Dibenzo-1,4,7,10,13,16,19,22,25-nonaoxacycloseptacosa-2,15-diene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ cal non-aq 25°C 100% C H K1=2.41 1986ICa (104173)1308
Medium: MeOH. DH(K1)=-19.0 kJ mol-1, DS(K1)=-17.7 J K-1 mol-1.

Na+ cal alc/w 25°C 70% U H K1=1.50 1976ITa (104174)1309
Medium: 70% w/w MeOH/H2O. DH(K1)=-49.1 kJ mol-1
****
C26H38N2O4 L CAS 80757-23-9 (2450)
N,N'-Bis(benzyl)-1,10-diaza-4,7,13,16-tetraoxacyclooctadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE alc/w 25°C 100% U K1=2.68 1992MGa (104188)1310
Medium: MeOH, 0.1 M Bu4NPF6

Na+ gl alc/w 25°C 93% U K1=2.4 1978WVa (104189)1311
Medium: 93% MeOH/H2O
****
C26H38N2O6 L CAS 155581-87-6 (8849)
7,16-Bis(2-methoxyphenyl)-1,4,10,13-tetraoxa-7,16-diazacyclooctadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp alc/w RT 50% C K1=4.0 2002GLb (104195)1312
Medium: 50% MeOH/H2O, pH 7.4 (0.1 M Tris buffer), 0.1 M Me4NCl.
****
C26H38N4O6Cl2 H2L CAS 227796-03-4 (8914)
7,16-Bis(3-amino-5-chloro-2-hydroxybenzyl)-1,4,10,13-tetraoxa-7,16-diazacyclooctade
cane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ cal alc/w 25°C 100% C H 1999SBf (104198)1313
K(Na+H2L)=3.42
Medium: MeOH. DH(K)=-12.4 kJ mol-1, DS(K)=23.9 J K-1 mol-1.
****
C26H38O6P2 L CAS 470454-13-8 (8995)
7,16-Dibenzyl-1,4,10,13-tetraoxa-7,16-diphosphacyclooctadecane-7,16-dioxide;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ dis non-aq 24°C 100% C 2002MRd (104214)1314
K(Na+A+L)=4.58
Medium: CDCl3. HA is picric acid.
****
C26H38O8 L (2507)
2,5,8,11,16,19,22,25-Octaoxa-12,13:14,15-dibenzohexacosa-12,14-diene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE alc/w 25°C 100% U 1975CJa (104220)1315
K1 < 0.1
Medium: MeOH
****
C26H40N4O6 H2L CAS 227796-04-5 (8915)
7,16-Bis(5-amino-2-hydroxybenzyl)-1,4,10,13-tetraoxa-7,16-diazacyclooctadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ cal alc/w 25°C 100% C H 1999SBf (104227)1316
K(Na+H2L)=2.73
Medium: MeOH. DH(K)=-24.6 kJ mol-1, DS(K)=-30.2 J K-1 mol-1.
****
C26H40O10 L CAS 123313-39-3 (5574)
23,23-Dimethyl-24,25-(1,4-Benzodioxinic)-21,4,7,10,13,16,19,22-octaoxacyclohexacosa
-24-ene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ gl alc/w 25°C 100% U K1=1.34 1989MGb (104241)1317
Medium: MeOH
****
C26H40O11P2 L (5727)
1,7-Bis(2-(diethoxyphosphinylmethoxy)phenyl)-1,4,7-trioxaheptane;2(EtO)2PO.CH2OC6H4
C2H4OC2H4)2O

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ con non-aq 25°C 100% U K1=4.2 1989EVa (104245)1318

Medium: tetrahydrofuran/CHCl3 4:1 (volume)
****
C26H42O10 L (8166)
1',4'-Bis(methyloxymethyl-3-(1,4,7,10-tetraoxacyclododecane))benzene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ cal alc/w 25°C 80% C H 1991LTa (104269)1319
B(Na2L)=2.41
Medium: 80% MeOH/H2O. DH(K1)=-3.51 kJ mol-1.
Also data for the 1',2'- and 1',3'- derivatives.
****
C26H43NO6 HL Glycocholic ac. CAS 475-31-0 (5821)
N-Cholylglycine, N-3,7,12-Trihydroxy-24-oxocholan-24-yl-glycine;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ nmr oth/un 25°C ? U 1986KBb (104272)1320
K1eff=1.04
At pH 5.0
****
C26H45NO7S HL Taurocholic ac. CAS 145-42-6 (5822)
Cholyltaurine; 5-Cholan-24-oic acid N-(2-sulfoethyl)amide-3,7,12-triol;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ nmr oth/un 25°C ? U 1986KBb (104277)1321
K1eff=0.75
At pH 5.0
****
C26H45N3O6 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
---
Na+ dis none 25°C dil C K1=6.70 1987BBf (104281)1322
K(Na+A+L(org)=NaAL(org))=3.95
Method: extraction of metal picrate from H2O into CHCl3.
****
C26H48N2O6 L (6003)
5,6,14,15-Dicyclohexyl-4,7,13,16,21,24-hexaoxa-1,10-diazabicyclo[8.8.8]hexacosane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE alc/w 25°C 100% U H K1=6.02 1987BUb (104296)1323
In MeOH. DH=-27.2 kJ mol-1
****
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
-------------------------------------------------------------------------
Na+        nmr non-aq 24°C 100%  U    M                   1981BEb (104312)1324
                                        K(Na(picrate)+L)=5.8
Medium: CDCl3
*************************************************************************
C26H50N2O7              L                       (6931)
N,N'-Bis(1-tetrahydrofuranyl-2-ethoxyethyl)-1,4-diaza-7,10,13-trioxacyclopentadecan
e;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Na+        cal alc/w  25°C  90%  U   H    K1=3.82          1994IZa (104320)1325
L=N,N'-Bis(1-tetrahydrofuranyl-2-ethoxyethyl)-1,4-diaza-7,10,13-trioxacyclo-
pentadecane. Medium: 90% v/v MeOH/H2O. DH(K1)=-27.7 kJ mol-1.
*************************************************************************
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
-------------------------------------------------------------------------
Na+        con non-aq 25°C 100%  M    M   K1=>12           1999DSd (104323)1326
                                        K(NaL+ClO4)=1.21
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
-------------------------------------------------------------------------
Na+        gl  alc/w  25°C  95%  C        K1=3.87          2004KVa (104341)1327
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
-------------------------------------------------------------------------
Na+        gl  alc/w  25°C  95%  C        K1=2.43          2004KVa (104351)1328
Medium: 95% MeOH/H2O, 0.01 M Et4NClO4.
*************************************************************************
C26H53NO6               L                       CAS 75006-60-9  (1716)
N-(Dodecyl-di-(oxyethylene))-monoaza-15-crown-5
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Na+        ISE alc/w  25°C 100%  U  I     K1=3.76          1983MKa (104355)1329
*************************************************************************
```

C26H53NO8 L CAS 86170-85-6 (1718)
N-(Octyl-tetra(oxyethylene))-monoaza-15-crown-5

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE alc/w 25°C 100% U K1=4.36 1983MKa (104357)1330
****
C26H53NO8 L CAS 86170-87-8 (1712)
N-(Octyl-tri-(oxyethylene))-monoaza-18-crown-6

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE alc/w 25°C 100% U K1=4.27 1983MKa (104359)1331
****
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
---
Na+ sol non-aq 20°C 100% C K1=5.34 1983SLa (104362)1332
Medium: CHCl3
****
C27H26O2P2 L (6811)
1,2-Bis(2-Diphenylphosphinyl)-1-methylethane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ con non-aq 25°C 100% U K1=2.6 1990EAb (104398)1333
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
---
Na+ con non-aq 25°C 100% U K1=3.0 1990EAb (104403)1334
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
---
Na+ oth non-aq 25°C 100% U K1=3.9 1995TEa (104408)1335
Medium: tetrahydrofurane:CHCl3 4:1 (v/v).
Metal ion is used as 2,4-dinitrophenolate.
****

C27H32NO5S+ L CAS 423763-94-4 (8997)
3-Ethyl-2-[4-(2,3,5,6,8,9,11,12-octahydro-1,4,7,10,13-benzopentaoxacyclopentadecin-15-yl)butadien

---

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	sp	non-aq	25°C	100%	C		K1=3.89	2002GVc (104518)	1336

Medium: acetonitrile, 0.1 M Et4NClO4.

****

C27H47N3O6 L (8029)
Tripodal ionophore 3;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	sp	non-aq	25°C	100%	C			2001LFa (104626)	1337
							K(NaP+L=LiPL)=4.88		

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
Na+	con	non-aq	25°C	100%	U		K1=5.5	1989BEa (104677)	1338

Medium: tetrahydrofuran/CHCl3 4:1 (volume)

****

C28H24O6 L TetBz18-Crown-6 CAS 99700-20-6 (6070)
2,3:8,9:11,12:14,15-Tetrabenzo-1,4,7,10,13,16-hexaoxacyclooctadeca-2,8,11,14-tetraene

---

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	dis	non-aq	23°C	100%	C		K1=5.2	1992HGb (104683)	1339

Extraction of metal chloride (A) from aqueous solution into nitrobenzene/
0.01M Bu4NB(Ph)4. Peak potential voltammetry and distribution of 22Na.

****

C28H24O6 L CAS 72011-26-8 (8874)
2,3:8,9:11,12:17,18-Tetrabenzo-1,4,7,10,13,16-hexaoxacyclooctadeca-2,8,11,17-tetraene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	dis	non-aq	23°C	100%	C		K1=4.7	1992HGb (104688)	1340

Extraction of metal chloride (A) from aqueous solution into nitrobenzene/
0.01M Bu4NB(Ph)4. Peak potential voltammetry and distribution of 22Na.

****

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
-------------------------------------------------------------------------
Na+        con non-aq 25°C 100%  U        K1=6.0         1993EVa (104715)1341
Medium: THF+CHCl3 (4:1 vol)
-------------------------------------------------------------------------
Na+        con non-aq 25°C 100%  U        K1=3.9         1992BEa (104716)1342
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
-------------------------------------------------------------------------
Na+        con non-aq 25°C       C        K1=3.6         1999TEa (104723)1343
In: tetrahydrofurane/CHCl3 4:1 v/v
*************************************************************************
C28H30N2O2P2            L                      CAS 68745-29-9  (5707)
N,N'-Bis(diphenylphosphinylmethyl)-1,2-diaminoethane; ((C6H5)2PO.CH2.NH.CH2-)2
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Na+        con non-aq 25°C 100%  U        K1=3.7         1984YKa (104728)1344
Medium: tetrahydrofuran + CHCl3 4:1, Na 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
-------------------------------------------------------------------------
Na+        con non-aq 25°C 100%  U        K1=5.8         1989BEa (104751)1345
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
-------------------------------------------------------------------------
Na+        sol non-aq 25°C 100%  U        K1=4.65        1987TCa (104769)1346
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
-------------------------------------------------------------------------
Na+        sp  non-aq 18°C 100%  C        K1=1.4         1997LHa (104786)1347
Medium: acetonitrile.
*************************************************************************
C28H37N3O9              L                      CAS 99224-19-8  (663)
```

4-Di(methyloxycarbonylethyl)aminophenylazo-benzo-15-crown-5;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE alc/w 25°C 100% C K1=3.07 1985ZFa (104794)1348
****
C28H40N2O6 L (2443)
Bicyclo-NcN'-1,10-diaza-4,7,13,16-tetraoxaoctadecane;(c=(CH2.C6H4.O.CH2)2)

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ gl alc/w 25°C 93% U K1=2.55 1978WVa (104818)1349
Medium: 93% MeOH/H2O
****
C28H40N2O9 L (2348)
1,20-Bis(ortho(methylamido)phenoxy)-3,6,9,12,15,18-hexaoxaeicosane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ nmr non-aq 0°C 100% U T H K1=2.9 1981GLb (104820)1350
Medium: pyridine. DH=-18 kJ mol-1. K1=2.8 (10 C); 2.5 (33 C), 2.4 (43 C)
****
C28H40O6 L CAS 29471-17-8 (1262)
2,3:11,12-Bis(4'-tert-butylbenzo)-1,4,7,10,13,16-hexaoxacyclooctadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ gl non-aq 25°C 100% U K1=5.41 1980MDb (104845)1351
Medium: Propylene carbonate.
Medium: propylene carbonate

Na+ con alc/w 25°C 100% U I M 1979BDa (104846)1352
K(NaCl+L)=4.32
Medium: MeOH. In DMSO: K(NaClO4+L)=3.30. In MeCN: K(NaBPh4+L)=5.08
****
C28H40O8 L AN(MOEOEOM)2AN (2243)
29,30-Dimethoxy-13,27-dimethyl-3,6,9,17,20,23-hexaoxatricyclo-triconta-1,11,13,15,25,27-hexaene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ dis non-aq 25°C 100% U H 1979KLa (104859)1353
K(Na(picrate)+L)=3.70
Medium: CHCl3
****
C28H40O10 L DiBz-30-crown10 CAS 104946-67-0 (1776)
2,3:17,18-Dibenzo-1,4,7,10,13,16,19,22,25,28-decaoxacyclotriaconta-2,17-diene;

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

Na+ con non-aq 25°C 100% U I K1=5.25 1991ASb (104895)1354
Medium: 1,2-dichlorethane. In nitromethane: K1=3.14; in MeCN: K=3.14;
in acetone: K=3.04

Na+ vlt non-aq 25°C 100% U K1=12.8 1990SPa (104896)1355
Medium: 1,2-dichloroethane

Na+ nmr non-aq 20°C 100% U K1=2.54 1976LCa (104897)1356
Medium: acetone

Na+ ISE alc/w 25°C 100% A K1=2.0 1971FRa (104898)1357
Medium: MeOH
****
C28H42N2O6 L (2451)
N,N'-Bis(4-methoxybenzyl)-1,10-diaza-4,7,13,16-tetraoxacyclooctadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ gl alc/w 25°C 93% U K1=2.2 1978WVa (104928)1358
Medium: 93% MeOH/H2O
****
C28H44N4O5 L (6932)
N,N'-Bis(1-pyridyl-2-ethoxyethyl)-1,4-diaza-7,10,13-trioxacyclopentadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ cal alc/w 25°C 90% U H K1=3.95 1994IZa (104936)1359
Medium: 90% v/v MeOH/H2O. DH(K1)=-30.0 kJ mol-1, DS(K1)=-25.2 J K-1 mol-1
****
C28H44N4O6 H2L CAS 227796-02-3 (8913)
7,16-Bis(3-amino-2-hydroxy-5-methylbenzyl)-1,4,10,13-tetraoxa-7,16-diazacyclooctade
cane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ cal alc/w 25°C 100% C H 1999SBf (104939)1360
K(Na+H2L)=3.00
Medium: MeOH. DH(K)=-7.9 kJ mol-1, DS(K)=30.9 J K-1 mol-1.
****
C28H44O6 L (1704)
Decalino-(tert-butyl-benzo)-18-crown-6

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE alc/w 25°C ? U K1=4.59 1983KTa (104941)1361
****
C28H44O11 L CAS 123295-33-0 (5575)
26,26-Dimethyl-27,28-(1,4-Benzodioxinic)-1,4,7,10,13,16,19,22,25-nonoxacyclononacos
a-27-ene;

```
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Na+        gl  alc/w  25°C 100%  U        K1=1.51        1989MGb (104943)1362
Medium: MeOH
*************************************************************************
C28H44O12P2             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
-------------------------------------------------------------------------
Na+        con non-aq 25°C 100%  U        K1=4.9         1989EVa (104947)1363
Medium: tetrahydrofuran/CHCl3 4:1 (volume)
*************************************************************************
C28H47NO11              L                        (1689)
N-(2-(2-(4'-Benzo-15-crown-5)-oxyethoxy)ethyl-1,4,7,10-tetraoxa-13-azacyclopentadec
ane;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Na+        ISE alc/w  25°C  10%  U        K1=3.10        1986HAa (104969)1364
Medium: 10% MeOH/H2O
*************************************************************************
C28H48O6                L                    CAS 88692-13-1  (1706)
Didecalino-18-crown-6
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Na+        ISE alc/w  25°C    ?  U        K1=4.81        1983KTa (104977)1365
*************************************************************************
C28H52O5                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
-------------------------------------------------------------------------
Na+        nmr non-aq 24°C 100%  U    M                   1981BEb (105012)1366
                                       K(Na(picrate)+L)=3.8
Medium: CDCl3
*************************************************************************
C28H52O6                L                        (5352)
Di(t-butylcyclohexyl)-18-crown-6
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Na+        oth oth/un 25°C  dil  U        K1=1.42        1970MSa (105018)1367
*************************************************************************
C28H52O10               L                    CAS 17455-26-4  (6071)
2,3:17,18-Dicyclohexyl-1,4,7,10,13,16,19,22,25,28-decaoxacyclotriacontane;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
```

Na+ sol non-aq 25°C 100% C I K1=4.33 1999KCa (105022)1368
Medium: acetonitrile. Also K1=4.41(propylene carbonate), K1=2.38 (MeOH), K1=3.82 (i-PrOH), K1=3.80 (n-BuOH).
****
C28H54N2O8 L (6936)
N,N'-Bis(1-furanyl-2-ethoxyethyl)-1,4-diaza-7,10,13,16-tetraoxacyclooctadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ cal alc/w 25°C 100% U H K1=4.5 1994IZa (105027)1369
thoxyethyl)-1,4-diaza-7,10,13,16-tetraoxacycloocta-
Medium: MeOH. DH(K1)=-28.6 kJ mol-1, DS(K1)=-10.1 J K-1 mol-1. DAta also for
****
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
---
Na+ con non-aq 25°C 100% M M K1=6.44 1999DSd (105031)1370
K(NaL+ClO4)=1.23
Medium: acetonitrile.
****
C28H56N2O11 L BOA18C6 (6118)
3-Oxa-1,5-Bis-(1-aza-4,7,10,13,16-pentaoxacyclooctadecyl)pentane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE alc/w 25°C 90% U K1=3.56 1988HKa (105034)1371
Medium: 90% w/w MeOH/H2O
****
C28H56N6O8S2 L CAS 503465-18-7 (9246)
4,12,15,23,29,32,37,40-Octaoxa-1,7,9,18,20,26-hexaazabicyclo[24.8.8]dotetracontane-8,19-dithione;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ gl alc/w 25°C 95% C K1=3.68 2004KVa (105042)1372
Medium: 95% MeOH/H2O, 0.01 M Et4NClO4.
****
C28H56N6O8S2 L CAS 503465-14-3 (9244)
9,12,15,18,29,32,37,40-Octaoxa-1,4,6,21,23,26-hexaazabicyclo[24.8.8]dotetratriconta
ne-5,22-dithio

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ gl alc/w 25°C 95% C K1=2.38 2004KVa (105052)1373
Medium: 95% MeOH/H2O, 0.01 M Et4NClO4.
****
C28H57NO7 L CAS 81239-49-8 (1708)

N-(Dodecyl-di(oxyethylene))-monoaza-18-crown-6

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	ISE	alc/w	25°C	100%	U	I	K1=4.23	1983MKa	(105056)1374

****

C28H57NO7 L CAS 81239-49-8 (1715)
N-(Dodecyl-tri-(oxyethylene))-monoaza-15-crown-5

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	ISE	alc/w	25°C	100%	U	I	K1=4.21	1983MKa	(105058)1375

****

C28H57NO9 L CAS 86181-95-5 (1711)
N-(Octyl-tetra-(oxyethylene))-monoaza-18-crown-6

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	ISE	alc/w	25°C	100%	U		K1=4.33	1983MKa	(105060)1376

****

C28H58N2O8 L CAS 85726-98-3 (651)
4,13-Dibutoxyethoxyethylidene-1,7,10,16-tetraoxo-4,13-diazacyclooctadecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	sol	non-aq	20°C	100%	C		K1=5.46	1983SLa	(105062)1377

Medium: CHCl3

****

C29H26N2O2 H2L CAS 97801-59-7 (8539)
2,2'-[1,3-Propanediylbis[nitrilo(phenylmethylidyne)]]bisphenol;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	cal	non-aq	25°C	100%	U	H	K1=2.97	1998SBb	(105073)1378

Medium: MeCN Calorimetric titration of LiNCS. DH(K1)=-16.1 kJ mol-1

****

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
Na+	oth	non-aq	25°C	100%	U		K1=3.3	1995TEa	(105081)1379

Medium: tetrahydrofurane: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

Na+ oth non-aq 25°C 100% U K1=2.6 1995TEa (105086)1380
Medium: tetrahydrofurane: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
---
Na+ con non-aq 25°C C K1=4.7 1999TEa (105091)1381
In: tetrahydrofurane/CHCl3 4:1 v/v
****
C29H35NO5 L CAS 201154-06-5 (7825)
N-(1-Pyrenylmethyl)-1,4,7,10,13-pentaoxa-16-azacyclooctadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp mixed 25°C 90% C 1997KKa (105103)1382
K(NaSCN+L)=3.00
Method: fluorescence emission. Medium: MeOH/CHCl3 (9:1 v/v).
****
C29H36NO6S+ 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
---
Na+ sp non-aq 25°C 100% C K1=4.68 2002GVc (105107)1383
Medium: acetonitrile, 0.1 M Et4NClO4.
****
C29H40N2O6Cl2 L CAS 181706-77-4 (8627)
3,18-Dichlorooctahydro-5H,16H-6,15-(ethanoxyethanoxyethano)-dibenzotetraoxaazacyclo
heneicosine;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ cal non-aq 25°C 100% C H K1=3.76 1998ZBc (105138)1384
Medium: MeOH. DH(K1)=-23.3 kJ mol-1, DS(K1)=-6.17 J K-1 mol-1.
****
C29H42N2O6 L (2444)
Bicyclo-NcN'-1,10-diaza-4,7,13,16-tetraoxaoctadecane;(c=(CH2.C6H4.O.CH2)2.CH2)

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ gl alc/w 25°C 93% U K1=2.1 1978WVa (105148)1385
Medium: 93% MeOH/H2O
****
C29H58N2O10 L BCA18C6 CAS 74776-87-7 (6117)
1,5-Bis-(1-aza-4,7,10,13,16-pentaoxacyclooctadecyl)pentane;

```
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Na+        ISE alc/w  25°C  90%  U        K1=3.10        1988HKa (105171)1386
Medium: 90% w/w MeOH/H2O
*************************************************************************
C30H30N20O10            L                     CAS 259886-49-2  (8959)
Cucurbit[5]uril;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Na+        sol none   25°C  dil  C        K1=1.85        2001BCf (105218)1387
Method: dissolution of ligand in a 0.002-0.02 M NaX solution; spectrophoto
metric measurement.
*************************************************************************
C30H32O4P2              L                       (6816)
1,8-Bis(diphenylphosphinyl)-3,6-dioxaoctane;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Na+        con non-aq 25°C 100%  U        K1=3.44        1993EBa (105231)1388
Medium: CH3CN. Data also for 3,5,8-trioxa, 3,5,8,11-tetraoxa and 3,5,8,11-pe
ntaoxa analogues
-------------------------------------------------------------------------
Na+        con non-aq 25°C 100%  U        K1=4.5         1992BEa (105232)1389
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
-------------------------------------------------------------------------
Na+        con non-aq 25°C       C        K1=4.2         1999TEa (105237)1390
In: tetrahydrofurane/CHCl3 4:1 v/v
*************************************************************************
C30H34N2O2P2            L                     CAS 68743-31-3  (2066)
Diaminoethane-N,N'-di-2-ethyldiphenylphosphine oxide; (CH2.NH.C2H4.P(O)(C6H5)2)2
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Na+        con non-aq 25°C 100%  U        K1=3.98        1986STb (105242)1391
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
-------------------------------------------------------------------------
Na+        sp  non-aq 25°C 100%  U        K1=2.47        1996AAb (105256)1392
Medium: MeCN
```

tacyclo[12.12.12.1(6,9).1(19,22).1(31,34]hentetetraconta-4,6,8.....dodecaene
****
C30H36O6 L ANANAN(MOE)2O (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
---
Na+ dis non-aq 25°C 100% U H 1979KLa (105263)1393
K(M(picrate)+L)=9.16
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
---
Na+ sp alc/w RT 50% C K1=2.3 2002GLb (105268)1394
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
---
Na+ nmr non-aq 25°C 100% U K1=8.49 1986CHc (105274)1395
In CDCl3
****
C30H38N2O8 L CAS 137571-97-2 (6821)
Anthraquinone[2.2]cryptand;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE non-aq 25°C 100% U K1=5.58 1992CSc (105279)1396
Ag/Ag+ electrode. Medium: MeCN, 0.05 M Bu4NClO4
****
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
---
Na+ con non-aq 25°C 100% U K1=4.16 1989KSa (105303)1397
Medium: tetrahydrofuran/CHCl3 4:1 (vol)
****
C30H44N2O6 L (2445)
Bicyclo-NcN'-1,10-diaza-4,7,13,16-tetraoxaoctadecane;(c=(CH2.C6H4.O.(C2H4)2)

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

---
Na+ gl alc/w 25°C 93% U K1=2.35 1978WVa (105311)1398
Medium: 93% MeOH/H2O
****
C30H44O10 L CAS 96011-79-9 (653)
4,4'(5')-Dimethylbenzo-30-crown-10;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sol non-aq 20°C 100% C K1=4.82 1983SLa (105319)1399
Medium: CHCl3
****
C30H48O12 L CAS 123313-40-6 (5576)
29,29-Dimethyl-30,31-(1,4-Benzodioxinic)-1,4,7,10,13,16,19,22,25,28-decaoxacyclodot
riaconta30ene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ gl alc/w 25°C 100% U K1=1.2 1989MGb (105341)1400
Medium: MeOH. Some other similar ligands also studied
****
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
---
Na+ con non-aq 25°C 100% U K1=4.8 1989EVa (105345)1401
Medium: tetrahydrofuran/CHCl3 4:1 (volume)
****
C30H61NO8 L CAS 86181-96-6 (1710)
N-(Dodecyl-tri(Oxyethylene))-monoaza-18-crown-6

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE alc/w 25°C 100% U I K1=4.27 1983MKa (105385)1402
****
C31H34O4P2 L (7157)
1,9-Bis(diphenylphosphinyl)-3,7-dioxononane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ oth non-aq 25°C 100% U K1=3.6 1995TEa (105527)1403
Medium: THF:CHCl3 4:1 v/v. Na as 2,4-dinitrophenolate. Also other si
milar ligands
****
C31H46N2O6 L (2446)
Bicyclo-NcN'-1,10-Diaza-4,7,13,16-tetraoxaoctadecane;(c=(CH2.C6H4.O.C2H4)2.CH2)

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

Na+ gl alc/w 25°C 93% U K1=2.0 1978WVa (105553)1404
Medium: 93% MeOH/H2O
****
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
---
Na+ con non-aq 25°C C K1=3.8 1999TEa (105578)1405
In: tetrahydrofurane/CHCl3 4:1 v/v

Na+ con non-aq 25°C 100% U K1=3.46 1989KSa (105579)1406
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
---
Na+ sp non-aq 25°C 100% U M 1981SPb (105584)1407
K(NaI+L)=2.66
Medium: CH3CN
****
C32H33N3O12F2 L CAS 149696-88-8 (7035)
2,3:14,15-Difluorobenzo-8,9-(4-dicarboxymethyliminobenza)-4,13-diaza-4,13-dicarboxy
methylcyclooc-

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp R4N.X 30°C 0.10M U 1993SKf (105618)1408
K1eff=3.84
Medium: Me4NCl. K1eff at pH 7.2
****
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
---
Na+ con non-aq 25°C 100% U K1=5.3 1992BEa (105647)1409
Medium: THF+CHCl3 (4:1 vol)
****
C32H36O6P2 L (7893)
1,12-Bis(diphenylphosphinyl)-2,5,8,11-tetraoxododecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ con non-aq 25°C C K1=4.5 1999TEa (105652)1410
In: tetrahydrofurane/CHCl3 4:1 v/v
****
C32H37NO5 L CAS 402920-62-1 (8843)

13-[4-(9-Anthracenylmethyl)-2-methoxyphenyl]-1,4,7,10-tetraoxa-13-azacyclopentadeca
ne;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp alc/w RT 50% C K1=2.5 2002GNe (105655)1411
Medium: 50% v/v MeOH/H2O, pH 7.4 (0.01 M Tris buffer), 0.1 M Me4NCl.
****
C32H38N2O7 L CAS 488759-47-3 (9009)
cis-2,12-Dimethyl-2,12-bis[(8-quinolyloxy)methyl]-15-crown-5;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp non-aq 25°C 100% C K1=6.27 2002NMa (105669)1412
Medium: THF, using metal picrate salt. For the trans- ligand, K1=5.63.
****
C32H38N2O7 L CAS 225792-57-4 (9008)
cis-2,6-Dimethyl-2,6-bis[(8-quinolyloxy)methyl]-15-crown-5;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp non-aq 25°C 100% C K1=6.41 2002NMa (105671)1413
Medium: THF, using metal picrate salt. For the trans- ligand, K1=5.60.
****
C32H38N2O7 L (9015)
cis-2,9-Dimethyl-2,6-bis[(8-quinolyloxy)methyl]-15-crown-5;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp non-aq 25°C 100% C K1=6.66 2002NMa (105673)1414
Medium: THF, using metal picrate salt. For the trans- ligand, K1=5.57.
****
C32H38N2O10 L (7073)
7,16-Bis(6-methoxy-2-oxo-2H-1-benzopyran-7-yl)-1,4,10,13-tetraoxa-7,16-diazacycloo
tadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp none RT 0 U K1=0.48 1994CGa (105675)1415
Method: fluorimetry
****
C32H38N4O6Cl2 HL CAS 172033-56-6 (8675)
2,2'-[1,4,10,13-Tetraoxa-7,16-diazacyclooctadecane-7,16-diylbis(methylene)]bis[5-Cl
-8-quinolinol]

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ cal non-aq 25°C 100% C H 1995ZBa (105680)1416
K(Na+HL)=3.74
Medium: methanol. DH(K)=-26.4 kJ mol-1, DS(K)=-17 J K-1 mol-1.

****
C32H38N4O6Cl2 H2L (7214)
7,16-Bis((5-chloro-8-hydroxy-7-quinolinyl)methyl)-1,4,10,13-tetraoxa-7,16-diazacycl
ooctadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ cal alc/w 25°C 100% U H 1996BBf (105691)1417
K(Na+H2L)=2.89
Medium: MeOH, 0.1 M Me4NCl. DH(K)=-14.1 kJ mol-1. Data also for similar
lariat ligands with substituted oxine side chains
****
C32H40N4O4 L CAS 340963-90-8 (8926)
8,8'-[1,4,10,13-Tetraoxa-7,16-diazacyclooctadecane-7,16-diylbis(methylene)bisquinol
ine;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ cal alc/w 25°C 100% C H K1=3.73 2001DXa (105715)1418
Medium: MeOH. DH(K1)=-22.5 kJ mol-1, DS(K1)=-4.0 J K-1 mol-1.
****
C32H40N4O6 H2L CAS 254900-38-4 (8920)
7,16-Bis(8-hydroxyquinoline-2-ylmethyl)-1,4,10,13-tetraoxa-7,16-diazacyclooctadecan
e;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ cal alc/w 25°C 100% C H 1999SBg (105720)1419
K(Na+H2L)=3.65
Medium: MeOH. DH(K)=-25.3 kJ mol-1, DS(K)=-15 J K-1 mol-1.
****
C32H40N6O6Cl2 H2L CAS 254900-39-5 (8921)
7,16-Bis(3-(5-chloro-2-hydroxyphenyl)pyrazol-1-ylmethyl)-1,4,10,13-tetraoxa-7,16-di
azacyclooctad;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ cal alc/w 25°C 100% C H 1999SBg (105730)1420
K(Na+H2L)=3.02
Medium: MeOH. DH(K)=-20 kJ mol-1, DS(K)=-9.4 J K-1 mol-1.
****
C32H41N5O8 HL CAS 552856-75-4 (8847)
7-[2-Methoxy-4-[(4-nitrophenyl)azo]phenyl]-16-(2-methoxyphenyl)-1,4,10,13-tetraoxa-
7,16-diazacyc;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp alc/w RT 50% C K1=2.5 2002GLb (105735)1421
Medium: 50% MeOH/H2O, pH 7.4 (0.1 M Tris buffer), 0.1 M Me4NCl.
****

C32H43N2O7S HL CAS 189057-31-6 (7756)
3-(4-Carboxybutyl)-2-[4-[N-(1,4,7,10,13-pentaoxa-16-azacyclooctadeca)]]styryl-benzo
thiazolium;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp non-aq 18°C 100% C K1=2.9 1997LHa (105759)1422
Medium: acetonitrile.
****
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;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ con non-aq 25°C 100% U K1=4.4 1989BEa (105778)1423
Medium: tetrahydrofuran/CHCl3 4:1 (volume)
****
C32H46N2O8Cl2 L CAS 181706-75-2 (8626)
3,18-Dichlorododecahydro-5H,16H-6,15-(ethanoxyethanoxyethano)dibenzohexaoxadiazacyc
lohexacosine;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ cal non-aq 25°C 100% C H K1=4.03 1998ZBc (105788)1424
Medium: MeOH. DH(K1)=-26.5 kJ mol-1, DS(K1)=-11.8 J K-1 mol-1.
****
C32H48N2O3 L CAS 170801-55-5 (8952)
1,5-Bis[2,2'-azo-4,4'-(1,1,3,3-tetramethylbutyl)phenoxy]-3-oxapentane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp alc/w RT 100% C K1=1.5 2000GDa (105796)1425
Medium: MeOH.
****
C32H48N2O4 L CAS 170801-51-1 (8953)
6,7,9,10-Tetrahydro-2,14-bis(1,1,3,3-tetramthylbutyl)dibenzotrioxadiazacyclotrideci
ne 16-oxide;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp alc/w RT 100% C K1=1.1 2000GDa (105799)1426
Medium: MeOH
****
C32H48N2O6 L (2447)
Bicyclo-NcN'-1,10-diaza-4,7,13,16-tetraoxaoctadecane;(c=(CH2.C6H4.O.C3H6)2)

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ gl alc/w 25°C 93% U K1=2.2 1978WVa (105803)1427

Medium: 93% MeOH/H2O
****
C32H52O14P2 L CAS 112120-15-7 (5730)
1,13-Bis(2-(diethoxyphosphinylmethoxy)phenyl)-1,4,7,10,13,16-hexaoxahexadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ con non-aq 25°C 100% U K1=4.7 1989EVa (105825)1428
Medium: tetrahydrofuran/CHCl3 4:1 (volume)
****
C32H55NO13 L CAS 105495-11-2 (1690)
N-(2-(2-(4'-Benzo-18-crown-6)-oxyethoxy)ethyl-1,4,7,10,13-pentaoxa-16-azacyclooctad
ecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE alc/w 25°C 10% U K1=2.93 B2=5.86 1986HAa (105833)1429
Medium: 10% MeOH/H2O
****
C32H64N4O10 L CAS 42133-16-4 (8579)
4,10,13,19,25,28,33,36,41,44-Decaoxa-1,7,16,22-tetraazatricyclo[20.8.8.87,16]hexate
tracontane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE alc/w 25°C 95% C K1=3.6 1977LSc (105851)1430
K(NaL+Na)=3.2
Medium: 95% (w/w) MeOH/H2O, 0.1 M Et4NBr.
****
C32H66N2O4 L 22DD Kryptofix CAS 79495-97-9 (6655)
1,10-Didecyl-1,10-diaza-4,7,13,16-tetraoxacyclooctadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ cal alc/w 25°C 100% U H 1986BUd (105864)1431
In MeOH. DH=-16.8 kJ mol-1
****
C33H41N3O6 L (8027)
Tripodal ionophore ;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp non-aq 25°C 100% C 2001LFa (105925)1432
K(NaP+L=LiPL)=4.45
Method: Analyses by spectrophotometry. Medium: chloroform. P is picrate.
****
C33H41N3O6Cl2 L CAS 181706-78-5 (8628)
3,18-Dichlorohexahydro(ethanoxyethanoxyethano)-23,27-nitrilodibenzotetraoxadiazacyc
lopentacosine;

```
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Na+        cal non-aq 25°C 100%  C   H    K1=3.43        1998ZBc (105928)1433
Medium: MeOH. DH(K1)=-17.7 kJ mol-1, DS(K1)=6.31 J K-1 mol-1.
*************************************************************************
C33H46N2O12            L                        (7049)
1,4-Diaza-1,4-di(5'-benzo-15-crown-5)-hepta-2,6-dione; CH2(CH2CONH.C14H19O5)2
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Na+        sp  non-aq 25°C 100%  U        K1=6.38        1979KMb (105982)1434
Medium: CHCl3
*************************************************************************
C33H57N3O9             L    Enniatin B       CAS 917-13-5  (4177)
Enniatin B
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Na+        gl  alc/w  20°C 100%  U        K1=2.38        1968WPa (105998)1435
Medium: MeOH, 1 M NaI
*************************************************************************
C34H34N4O11            L                     CAS 74145-44-1  (2351)
1,11-Bis(2-(2-nitrophenyl)amido)phenoxy)-3,6,9-trioxaundecane;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Na+        nmr non-aq 23°C 100%  U T      K1=1.4         1981GLb (106007)1436
Medium: acetonitrile. K1=1.1 (1 C); 1.3 (33 C)
*************************************************************************
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
-------------------------------------------------------------------------
Na+        sp  alc/w  25°C  70%  U        K1=8.90   B2=16.90  1995VZa (106009)1437
                                        K3=6.00
                                        K4=3.50
Medium: 70% MeOH
*************************************************************************
C34H38N2O14          H2L                       (7072)
7,16-Bis(3-carboxy-6-methoxy-2-oxo-2H-1-benzopyran-7-yl)-1,4,10,13-tetraoxa-diazacy
clooctadecane;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Na+        sp  none    RT     0  U        K1=0.70        1994CGa (106029)1438
Method: fluorimetry
*************************************************************************
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
Na+	oth	non-aq	22°C	100%	U		K1=1.7	1978YSa (106041)	1439

Medium: 1:1 v/v EtOH+CHCl3. Na 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
Na+	con	non-aq	25°C	100%	U		K1=6.0	1992BEa (106045)	1440

Medium: THF+CHCl3 (4:1 vol)

****

C34H40O7 L CAS 488759-49-5 (9011)
cis-2,9-Dimethyl-2,9-bis[(1-napthyloxy)methyl]-15-crown-5;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	sp	non-aq	25°C	100%	C		K1=4.12	2002NMa (106048)	1441

Medium: THF, using metal picrate salt.

****

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
Na+	con	non-aq	25°C		C		K1=5.2	1999TEa (106052)	1442

In: tetrahydrofurane/CHCl3 4:1 v/v

****

C34H42N2O6Cl2 L CAS 181706-79-6 (8629)
3,18-Dichlorooctahydro-5H,16H-6,15-(ethanoxyethanoxyethano)tribenzotetraoxadiazacyc
lodocosine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	cal	non-aq	25°C	100%	C	H	K1=3.67	1998ZBc (106059)	1443

Medium: MeOH. DH(K1)=-11.4 kJ mol-1, DS(K1)=32.1 J K-1 mol-1.

****

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
Na+	nmr	non-aq	25°C	100%	U		K1=15.11	1986CHc (106070)	1444

Medium: CDCl3

****

C34H46O10 L CAS 210485-26-0 (3146)

15,31-Diethylhexadecahydroanthra[2,3-b:6,7-b']bis[1,4,7,10,13]pentaoxacyclopentadec
in;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp mixed 20°C 80% C K1=4.40 1999OBa (106080)1445
K(NaL+Na)=1.94
Medium: 80% v/v CHCl3/MeOH.

Na+ vlt non-aq 20°C 100% C K1=1.9 1999OBa (106081)1446
Medium: DMF, 0.10 M Bu4N[BPh4]. Method: by competition with Tl(I).
Data for other 15,31-dialkyl derivatives.
****
C34H53O8Br H2L CAS 38784-08-6 (2336)
5-Bromolasalocid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ gl alc/w 25°C 100% M H 1988PJa (106100)1447
K(Na+HL)=2.68
Also used Na+ sensitive glass electrode. DH = 2.1 kJ mol-1; DS = 59
****
C34H54O8 H2L Lasalocid CAS 25999-20-6 (2335)
Lasalocid acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ nmr non-aq 20°C 100% C 1998MLa (106148)1448
K(Na+HL)=0.8
Medium: CD3OD. Method: 13C nmr. By 23Na nmr, K(Na+HL)=0.6.

Na+ dis oth/un 25°C 0.0 U K1=2.2 1992LPb (106149)1449

Na+ gl alc/w 25°C 100% M H 1988PJa (106150)1450
K(Na+HL)=2.8
K(Na+H2L)=0.7
Medium: MeOH. Also using Na+ sensitive glass elect. DH=1.2 kJ mol-1, DS=58

Na+ gl alc/w 25°C 100% U 1982BDc (106151)1451
K(Na+2HL)=2.61
Medium: MeOH
****
C34H68N4O8 L CAS 49811-34-9 (8578)
10,13,25,28,33,36,41,44-Octaoxa-1,7,16,22-tetraazatricyclo[20.8.8.87,16]hexatetraco
ntane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE alc/w 25°C 95% C K1=3.2 1977LSc (106182)1452
K(NaL+Na)=1.5

Medium: 95% (w/w) MeOH/H2O, 0.1 M Et4NBr.

****

C35H45N9 L CAS 312304-65-7 (7962)

29,32,35-TriMe-1,14,29,32,35,38,39,40,41-Nonaazahexacyclohentetraconta-3,5,7,8,10,12,16,18,20,21,

---

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	gl	R4N.X	25°C	0.10M	U		K1=7.0 K(NaL+H)=9.4 K(NaHL+H)=8.0 K(NaH2L+H)=5.2	2001BBa (106204)	1453

Medium: 0.10 M NMe4NO3.

****

C36H30O3Si3 L CAS 512-63-0 (1285)

Hexaphenyl-cyclotrisiloxane; ((C6H5)2SiO)3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	con	alc/w	25°C	100%	U		K1=0.10	1980OPa (106217)	1454

Medium: MeOH, 0.1 M Me4NBr

****

C36H32N2O6 L (5744)

5,6:11,12-Dibenzo-1,16-di(8-quinolyl)-1,4,7,10,13,16-hexaoxahexadecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	con	non-aq	25°C	100%	U		K1=5.8	1989BEa (106221)	1455

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
Na+	sol	none	25°C	dil	C		K1=3.49	2001BCf (106267)	1456

Method: dissolution of ligand in a 0.002-0.02 M NaX solution;
spectrophotometric measurement.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	cal	mixed	25°C	50%	C	IH	K1=3.23	1998BJb (106268)	1457

Medium: 50% (v/v) HCOOH/H2O. DH(K1)=-5.9 kJ mol-1.
Also data for 0-40% (v/v). In H2O, K1=3.47, DH(K1)=-2.3 kJ mol-1.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	sp	none	25°C	0	U		K1=3.16 B2=4.94	1994HKa (106269)	1458

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	sol	none	25°C	0.0	U		K1=7.38	1992BCa (106270)	1459

****

C36H36O4P2 L (2073)

3-t-Butyl-1,2-dihydroxybenzene bis(diphenylphosphinylmethyl) ether

---

```
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Na+        con non-aq 25°C 100%  U        K1=3.34        1989KSa (106282)1460
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
-------------------------------------------------------------------------
Na+        con non-aq 25°C 100%  U        K1=4.16        1989KSa (106286)1461
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
-------------------------------------------------------------------------
Na+        dis non-aq 25°C 100%  U   H                    1979KLa (106297)1462
                                        K(Na(picrate)+L)=3.08
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
-------------------------------------------------------------------------
Na+        dis non-aq 25°C 100%  U   H                    1979KLa (106303)1463
                                        K(Na(picrate)+L)=5.68
Medium: CHCl3
*************************************************************************
C36H40O6                L    ANAN(MOM)2ANAN   CAS 1129-06-1  (2241)
Tetra(1,3-(2-methoxy-5-methylbenzo))-9,18-dioxacyclooctadeca-2,5,10,14-tetraene;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Na+        dis non-aq 25°C 100%  U   H                    1979KLa (106308)1464
                                        K(Na(picrate)+L)=3.79
Medium: CHCl3
*************************************************************************
C36H44O7P2              L                       (5725)
1,17-Di(diphenylphosphinyl))-3,6,9,12,15-pentaoxaseptadecane;
Ph2PO.C2H4(O.C2H4)4OC2H4POPh2
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Na+        con non-aq 25°C 100%  U        K1=6.1         1992BEa (106339)1465
Medium: THF+CHCl3 (4:1 vol)
-------------------------------------------------------------------------
Na+        cal non-aq 25°C 100%  U        K1=3.82        1991SGa (106340)1466
```

Medium: CH3CN; Na as NaNCS
****
C36H44O8P2 L (7895)
1,18-Bis(diphenylphosphinyl)-hexaoxooctadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ con non-aq 25°C C K1=5.2 1999TEa (106346)1467
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
---
Na+ sp non-aq 25°C 100% C 2001LFa (106376)1468
K(NaP+L=LiPL)=4.24
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
---
Na+ nmr non-aq 25°C 100% U K1=15.41 1986CHc (106380)1469
In CDCl3
****
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
---
Na+ con non-aq 25°C 100% U K1=4.5 1989BEa (106398)1470
Medium: tetrahydrofuran/CHCl3 4:1 (volume)
****
C36H54O10 L CAS 86116-04-3 (5647)
1,8-Bis(4'-(2,3-benzo-1,4,7,10,13-pentaoxacyclopentadecane))-octane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE alc/w 25°C 90% U K1=2.90 1987KHa (106419)1471
90% w/w MeOH/H2O. Also data for the 1,4,7,10-tetraoxadecane-bridged
ligand: K1=2.78; K2=2.83.
****
C36H56O6 L CAS 54535-81-8 (1263)
2,3:11,12-Bis(3',5'-di-tert-butylbenzo)-1,4,7,10,13,16-hexaoxacyclooctadecane;

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

```
-------------------------------------------------------------------------------
Na+        con alc/w  25°C 100%  U  I M                  1979BDa (106437)1472
                                          K(NaCl+L)=2.20
Medium: MeOH. In DMSO: K(NaClO4+L)=3.16. In MeCN: K(NaBPh4+L)=4.21
*******************************************************************************
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
-------------------------------------------------------------------------------
Na+        gl  non-aq 20°C 100%  U        K1=2.11        1993EAa (106443)1473
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
-------------------------------------------------------------------------------
Na+        con non-aq 25°C 100%  C   H    K1=4.68        1997PBb (106518)1474
Medium: acetonitrile. Additional method: potentiometry with ISE.
By calorimetry, DH(K1)=-23.6 kJ mol-1, DS(K1)=17 J K-1 mol-1
-------------------------------------------------------------------------------
Na+        vlt non-aq 25°C 100%  C  I     K1=12.5        1997WRa (106519)1475
Method: cyclic voltammetry. Medium: acetonitrile, 0.05 M Et4NClO4. In DMSO
K1=5.6; in acetone, K1=11.7; in hexamethylphosphoric triamide, K1=2.1.
-------------------------------------------------------------------------------
Na+        vlt non-aq 23°C 100%  U  I     K1=12.5        1994FRa (106520)1476
Medium: MeCN. In PrCN: K1=11.8; acetone: 11.7; DMF: 8.7; Me-pyrrol.: 6.6;
NN-DMA: 6.5; DMSO: 5.6; Di-Et-formamide: 5.3; Di-Et-acetamide: 5.2; PC: 12.0
-------------------------------------------------------------------------------
Na+        ISE alc/w  25°C  90%  U  I     K1=6.1         1988ACb (106521)1477
Medium: 90% v/v MeOH/H2O. 80% MeOH/H2O, K1=5.4; 70%, K1=5.1; 60%, K1=4.7.
-------------------------------------------------------------------------------
Na+        gl  alc/w  25°C 100%  M T H                  1985CFc (106522)1478
                                          K(Na+HL)=3.77
Medium: EtOH
-------------------------------------------------------------------------------
Na+        ISE alc/w  25°C 100%  M        K1=6.37        1984CTa (106523)1479
Medium: MeOH
-------------------------------------------------------------------------------
Na+        ISE non-aq 25°C 100%  M        K1=8.95        1984CTa (106524)1480
Medium: N,N-dimethylformamide. In DMSO K1=5.70
-------------------------------------------------------------------------------
Na+        ISE alc/w  25°C 100%  U        K1=8.82        1984CTb (106525)1481
Medium: EtOH
-------------------------------------------------------------------------------
Na+        gl  alc/w  25°C 100%  U   H    K1=6.72        1978HPa (106526)1482
DH(K1)=-22.9 kJ mol-1, DS-51.8 J K-1 mol-1
-------------------------------------------------------------------------------
Na+        sp  non-aq 25°C 100%  C        K1=>6.0        1977CEb (106527)1483
```

Method: temperature jump relaxation. Medium: MeOH.

Na+ gl alc/w 25°C 100% U 1975GPa (106528)1484
K(Na+HL=NaL+H)=-0.5
Medium: MeOH. K varies (-0.10 to -0.76) with conc. of Monensin and NaClO4

Na+ oth alc/w 25°C 100% U H K1=6.0 1971LFa (106529)1485
Method: micro-calorimetry. Medium:MeOH. DH=-16.2 kJ mol-1, DS=61 J K-1 mol-1

Na+ ISE alc/w ? 100% U K1=5.85 1970LWb (106530)1486
Medium: MeOH. In methylcellosolve/H2O, 80:20, K1=4.93

****

C37H54N2O14 L (7050)
1,4-Diaza-1,4-di(5'-benzo-18-crown-6)-hepta-2,6-dione; CH2(CH2CONH.C16H23O6)2

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

---

Na+ sp non-aq 25°C 100% U K1=6.33 1979KMb (106633)1487
Medium: CHCl3

****

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

---

Na+ con non-aq 25°C 100% U K1=4.1 1993BEb (106644)1488
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

---

Na+ con non-aq 25°C 100% U K1=4.8 1991EBa (106650)1489
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

---

Na+ con non-aq 25°C 100% U K1=6.0 1993EVa (106661)1490
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-hexaoxaeicosane;

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

---
Na+ con non-aq 25°C 100% U K1=5.7 1992BEa (106682)1491
Medium: THF+CHCl3 (4:1 vol)
****
C38H48O9P2 L (7896)
1,21-Bis(diphenylphosphinyl)-2,5,8,11,14,17,20-heptaoxoheneeicozane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ con non-aq 25°C C K1=5.1 1999TEa (106687)1492
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
---
Na+ nmr non-aq 25°C 100% U K1=9.90 1986CHc (106692)1493
In CDCl3
****
C38H54O10 L CAS 210485-29-3 (3260)
Hexadecahydro-15,31-bis(2-methylpropyl)anthra[2,3:6,7]bis[1,4,7,10,13]pentaoxacyclo
pentadecin;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp mixed 20°C 80% C K1=4.62 1999OBa (106700)1494
K(NaL+Na)=3.67
Medium: 80% v/v CHCl3/MeOH.

Na+ vlt non-aq 20°C 100% C K1=0.9 1999OBa (106701)1495
Medium: DMF, 0.10 M Bu4N[BPh4]. Method: by competiton with Tl(I).
Data for other 15,31-dialkyl derivatives.
****
C39H50N2O16 L CAS 332843-42-2 (8210)
19,19'-(1,3-Propandiyl)bis(1,4,7,10,13,16-hexaoxacyclooctadecino[2,3]isoindole-18,2
0-dione;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp non-aq 25°C 100% C K1=3.2 2001OYa (106722)1496
Medium: methanol. For the 1,4-butanediyl- derivative, K1=3.4.
****
C40H36O4P2 L (6805)
1,6-Bis(2-Diphenylphosphinylphenyl)-2,5-dioxahexane; (CH2.O.CH2.C6H4(PO(6H5)2)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ con non-aq 25°C 100% U K1=4.5 1993BEb (106735)1497

Medium: THF+CHCl3 4:1(vol)
****
C40H36O5P2 L CAS 86341-96-0 (5724)
1,7-Di(2-diphenylphosphinyl)phenyl-1,4,7-trioxaheptane;Ph2PO.C6H4.O.C2H4.O.C2H4.O.C6H4.POPh2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ con non-aq 25°C 100% U K1=4.8 1991EBa (106747)1498
Medium: THF+CHCl3 4:1(vol). Data also for 1,4,7,10-tetraoxa,1,4,7,10,13-pentaoxa and 1,4,7,10,13,16-hexaoxa and 4-tributyl analogues
****
C40H44O4P2 L (2074)
3,5-Di(t-butyl)-1,2-dihydroxybenzene bis(diphenylphosphinylmethyl)ether
---
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ con non-aq 25°C 100% U K1=3.54 1989KSa (106766)1499
Medium: tetrahydrofuran/CHCl3 4:1 (vol)
****
C40H46O7 L CAS 177723-37-4 (8912)
25,27-Diethoxycalix[4]arenecrown-5, 1,3-alternate;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ dis non-aq 22°C 100% C M 1996CPa (106773)1500
K(NaA+L(org)=NaAL(org))=4.38
Medium: CHCl3 saturated with H2O. Method: extraction of NaA into CHCl3/L solution. HA is picric acid. For the cone conformation, K=<4.
****
C40H46O8 L CAS 161282-95-7 (8680)
25,27-Dimethoxycalix[4]arene-crown-6;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp non-aq 25°C 100% C K1=<=1 1995CUa (106778)1501
Medium: methanol, 0.01 M Et4NCl.
****
C40H48O8 L AN2DP(OEOEO)2E (2235)
3,4,5,6-Bis(3-methyl-5-(2-methoxy-5-methylbenzo))-2,7,10,13,16,19-hexaoxacyclodocosa-3,5-diene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ dis non-aq 25°C 100% U H 1979KLa (106797)1502
K(Na(picrate)+L)=7.69
Medium: CHCl3
****
C40H50N20O10 L CAS 143902-45-8 (8935)
Decamethylcucurbit[5]uril;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ cal mixed 25°C 50% C H K1=2.54 2000ZKb (106809)1503
Medium: 50% v/v formic acid/H2O. DH(K1)=-5.4 kJ mol-1, DS(K1)=31 J K-1 mol-1.
****
C40H52N4O4 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
---
Na+ ISE non-aq 25°C 100% C K1=4.25 1998WLc (106824)1504
Medium: DMF, 0.05 M Et4NClO4.
****
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
---
Na+ con non-aq 25°C 100% U K1=4.5 1989BEa (106829)1505
Medium: tetrahydrofuran/CHCl3 4:1 (volume)
****
C40H62O12 L CAS 86116-05-4 (5648)
1,8-Bis(4'-(2,3-benzo-1,4,7,10,13,16-hexaoxacyclooctadecane))-octane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE alc/w 25°C 90% U K1=3.84 B2=6.97 1987KHa (106836)1506
90% w/w MeOH/H2O. Also data for the 1,4,7,10-tetraoxadecane-bridged ligand: K1=3.49; K2=3.15.
****
C40H64O12 L Nonactin CAS 6833-84-7 (4179)
Nonactin

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp non-aq 25°C 100% C H K1=2.23 1977CEb (106851)1507
Method: temperature jump relaxation. Medium: MeOH. DH(K1)=-20.9 kJ mol-1.
By spectrophotometric titration, K1=2.36.

Na+ vlt non-aq 22°C 100% U K1=3.97 1974RKd (106852)1508
Medium: 0.025 NBu4ClO4 in CH3CN

Na+ cal alc/w 25°C 100% U H K1=2.71 1973ZFa (106853)1509
Method: micro-calorimetry. Medium: MeOH. DH=-11.1, DS=-14.6
In EtOH: K1=3.27, DH=-27.4 kJ mol-1, DS=-29.4 J K-1 mol-1

Na+ oth alc/w 30°C 100% U K1=2.32 1973ZFa (106854)1510

Method: vapour pressure osmometry. Medium: MeOH. In EtOH, K1=3.26

Na+ cal alc/w 25°C 100% U H 1971FCa (106855)1511
Method: micro-calorimetry. Medium: methanol. DH=-14.2 kJ mol-1

Na+ nmr non-aq 17°C 100% U K1=4.85 1970PCa (106856)1512
Medium: NaClO4,acetone. With 0.5 mol fraction water, K1=2.32

Na+ oth alc/w 30°C 100% U K1=2.20 1967PWb (106857)1513
Medium: MeOH, 0.1 M NaSCN. Method: osmotic vapour pressure
****
C40H68O11 HL CAS 28380-24-7 (5372)
Nigericin (Antibiotic K178);

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp non-aq 25°C 100% C K1=3.96 1977CEb (106865)1514
Method: temperature jump relaxation. Medium: MeOH. DH(K1)=9.6 kJ mol-1.

Na+ cal alc/w 25°C 100% U H K1=3.9 1971LFa (106866)1515
Method: micro-calorimetry. Medium:MeOH. DH=6.9 kJ mol-1, DS=98 J K-1 mol-1

Na+ ISE alc/w ? 100% U K1=4.38 1970LWb (106867)1516
Medium:MeOH. In methylcellosolve:H2O, 80:20, K1=3.82
****
C41H42O6 L CAS 151832-07-4 (6874)
9-(Dimethylethyl)-29,30,31,32,33-pentamethoxy-23-oxahexacyclotritriacontapentadecan
e;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ dis non-aq 25°C 100% U 1993HSa (106873)1517
K(Na(picrate)+L)=10.56
Medium: CDCl3. With 23-thia- analogue K=8.95
****
C41H66O12 L Monactin CAS 7182-54-9 (4180)
Monactin

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp non-aq 25°C 100% C H K1=2.70 1977CEb (106892)1518
Method: temperature jump relaxation. Medium: MeOH. DH(K1)=-25.1 kJ mol-1.
By spectrophotometric titration, K1=2.60.

Na+ vlt non-aq 22°C 100% U K1=4.28 1974RKd (106893)1519
Medium: 0.024 NBu4ClO4 in CH3CN

Na+ oth alc/w 30°C 100% U K1=2.52 1973ZFa (106894)1520
Method: vapour pressure osmometry. Medium:MeOH. In EtOH, K1=3.48

```
Na+        cal alc/w  25°C 100%  U   H                    1971FCa (106895)1521
Method: micro-calorimetry. Medium: MeOH.   DH=-22.4 kJ mol-1
--------------------------------------------------------------------------------
Na+        oth alc/w  30°C 100%  U        K1=3.15        1967PWb (106896)1522
Medium: MeOH, 0.1 M NaSCN. Method: osmotic vapour pressure
********************************************************************************
C42H40O4P2              L                        (7153)
1,2-Bis(2-(2-(diphenylphosphinyl)ethyl)phenoxy)ethane
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Na+        oth non-aq 25°C 100%  U        K1=3.5         1995TEa (106913)1523
Medium: THF:CHCl3 4:1 v/v. Na 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
--------------------------------------------------------------------------------
Na+        con non-aq 25°C 100%  U        K1=4.2         1993BEb (106918)1524
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
--------------------------------------------------------------------------------
Na+        con non-aq 25°C 100%  U        K1=5.0         1993BEb (106929)1525
Medium: THF+CHCl3   4:1(vol)
--------------------------------------------------------------------------------
Na+        con non-aq 25°C 100%  U        K1=3.98        1989KSa (106930)1526
Medium: tetrahydrofuran/CHCl3 4:1 (vol)
********************************************************************************
C42H40O7P2              L                     CAS 95651-36-8  (2079)
1,7-Di(2-(diphenylphosphinylmethoxy)phenyl)-1,4,7-trioxaheptane;
(Ph2PO.CH2.O.C6H4.O.C2H4)2O
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Na+        con non-aq 25°C 100%  U        K1=4.01        1989KSa (106939)1527
Medium: tetrahydrofuran/CHCl3 4:1 (vol)
--------------------------------------------------------------------------------
Na+        con non-aq 25°C 100%  U        K1=4.01        1989TKb (106940)1528
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
--------------------------------------------------------------------------------
```

Na+ sp non-aq 25°C 100% C K1=2.4 2000PBa (106953)1529
Medium: MeOH.

Na+ dis non-aq 22°C 100% C M 1996CPa (106954)1530
K(NaA+L(org)=NaAL(org))=4.30
Medium: CHCl3 saturated with H2O. Method: extraction of NaA into CHCl3/L solution. HA is picric acid. For the cone conformation, K=4.46.
****
C42H54O15 L CAS 104512-99-4 (7749)
Tris-(15-Crown-5)triphenylene ;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE mixed 25°C 50% C K1=2.9 1991LMc (106970)1531
K(NaL+Na)=2.7
K(Na2L+Na)=2.3
Method: Na ion selective glass electrode. Medium: 50% w/w MeOH/DMF.
****
C42H68N2O4 L CAS 188593-77-3 (8954)
2,17-Didodecyl-6,7,9,10,12,13-hexahydro-dibenzo[b,f][1,8,11,14,4,5]tetraoxadiazacyclohexadecine
---
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp non-aq RT 100% C I K1=4.0 2000GDa (106975)1532
Medium: acetonitrile. In MeOH, K1=2.60.
****
C42H68O12 L CAS 20261-85-2 (5373)
Dinactin;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp non-aq 25°C 100% C H K1=3.04 1977CEb (106984)1533
Method: temperature jump relaxation. Medium: MeOH. DH(K1)=-27.6 kJ mol-1.
By spectrophotometric titration, K1=3.04.

Na+ vlt non-aq 22°C 100% U K1=4.44 1974RKd (106985)1534
Medium: 0.025 NBu4ClO4 in CH3CN

Na+ oth alc/w 30°C 100% U K1=2.88 1973ZFa (106986)1535
Method: vapour pressure osmometry. Medium:MeOH. In EtOH, K1=3.63
****
C43H42O4P2 L (7156)
1,3-Bis((2-diphenylphosphinyl)phenoxy)propane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ oth non-aq 25°C 100% U K1=3.4 1995TEa (107001)1536
Medium: THF:CHCl3 4:1 v/v. Na as 2,4-dinitrophenolate. Also other similar ligands

****
C43H42O6P2 L (5734)
1,7-Di((2-diphenylphosphynylmethoxy)phenyl-1,7-dioxaheptane;
(Ph2PO.CH2O.C6H4.O.C2H4)2CH2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ con non-aq 25°C 100% U K1=2.60 1989TKb (107006)1537
Medium: tetrahydrofuran/CHCl3 4:1 (volume)
****
C43H70O12 L CAS 7561-71-9 (5374)
Trinactin;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp non-aq 25°C 100% C H K1=3.28 1977CEb (107032)1538
Method: temperature jump relaxation. Medium: MeOH. DH(K1)=-30.5 kJ mol-1.

Na+ oth alc/w 30°C 100% U K1=3.55 1973ZFa (107033)1539
Method: vapour pressure osmometry. Medium: EtOH
****
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
---
Na+ sp oth/un 25°C 0.10M C 1996RHb (107088)1540
K1eff=0
****
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
---
Na+ con non-aq 25°C 100% U K1=3.4 1993BEb (107092)1541
Medium: THF+CHCl3 4:1(vol)
****
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
---
Na+ con non-aq 25°C 100% U K1=5.2 1993BEb (107111)1542
Medium: THF+CHCl3 4:1(vol)
****
C44H44O5P2 L (5735)
1,7-Di((2-diphenylphosphinylmethoxy)phenyl)-4-oxaheptane; (Ph2PO.CH2O.C6H4.C3H6)2O

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

---
Na+ con non-aq 25°C 100% U K1=2.28 1989TKb (107115)1543
Medium: tetrahydrofuran/CHCl3 4:1 (volume)
****
C44H44O5P2 L (5733)
1,7-Di(2-(diphenylphosphynylethyl)phenyl)-1,4,7-trioxaheptane;
(Ph2PO.C2H2.C6H4.OC2H4)2O

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ oth non-aq 25°C 100% U K1=3.2 1995TEa (107121)1544
Medium: THF:CHCl3 4:1 v/v. Na as 2,4-dinitrophenolate

Na+ con non-aq 25°C 100% U K1=2.95 1989TKb (107122)1545
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
---
Na+ cal non-aq 25°C 100% U H K1=4.63 1998SBb (107129)1546
Medium: MeCN Calorimetric titration of LiNCS. DH(K1)=-33.0 kJ mol-1
****
C44H48O10 L CAS 155500-94-0 (7357)
5,17-Di-tert-butyl-26,28-bis(carboethoxymethoxy)calix[4]diquinone;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp non-aq 23°C 100% U K1=>6.0 1997BGa (107134)1547
Medium: 4/1 v/v CH2Cl2/CH3CN; 0.1 M Bu4NBF4
Data also for other related calix[4]diquinones
****
C44H50N2O6 L (9016)
4,13-Bis[2-(9-anthryloxy)ethyl]-4,13-diaza-18-crown-6;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp non-aq 20°C 100% C K1=4.11 2002MTb (107137)1548
Medium: methanol.
****
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
---
Na+ gl non-aq 25°C 100% C K1=4.6 2000ABb (107145)1549
B(Na2L)=8.71
Medium: MeOH, 0.05 M Et4NClO4.

****
C44H52N4O8 L CAS 246035-33-6 (2925)
25,27-Bis(N,N-diethylaminocarbonylmethoxy)-26,28-bis(aminocarbonylmethoxy)calix[4]arene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp non-aq 25°C 100% C K1=2.9 1999USa (107160)1550
Medium: MeOH, 0.10 M Et4NCl
****
C44H52O10 L CAS 163317-54-2 (9089)
1,3-Calix[4]-bis-crown-5;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp non-aq 25°C 100% C IH K1=3.5 1996AAe (107166)1551
Medium: acetonitrile. By calorimetry, DH(K1)= -4.56 kJ mol-1, DS(K1)=51 J K-1 mol-1. In 100% MeOH, K1=2.1.
****
C44H54O8 L CAS 162989-76-6 (8794)
1,3-Diisopropoxycalix[4]arene-crown-6, 1,3-alternate;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp non-aq 25°C 100% C K1=<2 2000PBa (107171)1552
Medium: MeOH.
****
C44H54O8 L CAS 161282-98-0 (8679)
25,27-Bis(1-proplyoxy)calix[4]arene-crown-6, 1,3-alternate;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp non-aq 25°C 100% C K1=<=1 1995CUa (107177)1553
Medium: methanol, 0.01 M Et4NCl.
****
C44H54O8 L CAS 161282-96-8 (8678)
25,27-Bis(2-proplyoxy)calix[4]arene-crown-6, 1,3-alternate;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp non-aq 25°C 100% C K1=<=1 1995CUa (107183)1554
Medium: methanol, 0.01 M Et4NCl.
****
C44H56O4 H4L (7294)
4-Tert-butyl-calix[4]arene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp non-aq 25°C 100% U I K1=1.3 1996ABa (107188)1555
Medium: MeCN. In acetone, 20 C (by NMR): K1=2.5

****
C44H72N4O8 L CAS 61894-23-3 (8580)
7,16:25,34-Bis(ethanoxyethanoxyethano)dibenzo[1,4,17,20,7,14,23,30]tetraoxatetraaza cyclodotriac..

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE alc/w 25°C 95% C K1=3.0 1977LSc (107194)1556
K(NaL+Na)=2.9
Medium: 90% (w/w) MeOH/H2O, 0.1 M Et4NBr. In H2O, K1=<1.5.
****
C45H39O3P3 L CAS 73218-92-5 (5679)
1,3,5-Tris(diphenylphosphinylmethyl)-benzene; C6H3(CH2.PO(C6H5)2)3

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ con non-aq 25°C 100% U K1=4.4 1984YKa (107214)1557
Medium: tetrahydrofuran + CHCl3 4:1, Na as 2,4-dinitrophenolate
****
C45H48NO6P3 L (7953)
Tris[2-(diphenylphosphorylmethoxy)ethyl]amine;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ cal non-aq 25°C 100% U H K1=3.73 1998SBb (107220)1558
B(Na2L)=7.59
B(Na3L)=7.41
Medium: MeCN Calorimetric titration of LiNCS. DH(K1)=-22.3 kJ mol-1
DH(Na2L)=-36.8, DH(Na3L)=-73.3
****
C45H48N3O3P3 L CAS 90179-28-5 (5682)
N,N',N"-tris(Diphenylphosphinylmethyl)-1,4,7-triazacyclononane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ con non-aq 25°C 100% U K1=4.5 1984YKa (107227)1559
Medium: tetrahydrofuran + CHCl3 4:1, Na as 2,4-dinitrophenolate
****
C46H40O6P2 L (6814)
1,2-Bis((2-(2-diphenylphosphinyl)phenoxy)ethoxy)benzene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ con non-aq 25°C 100% U K1=6.1 1991EBa (107242)1560
Solvent : Tetrahydrofurane + CHCl3 4:1(vol)
****
C46H46N2O4 L CAS 185118-12-1 (7824)
N,N'-Bis(1-pyrenylmethyl)-1,4,10,13-tetraoxa-7,16-diazacyclooctadecane;

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

---
Na+ sp mixed 25°C 90% C 1997KKa (107252)1561
K(NaSCN+L)=2.59
Method: fluorescence emission. Medium: MeOH/CHCl3 (9:1 v/v).
****
C46H46N2O16 H4L (7071)
7,16-Bis[2-(2,4-dicarboxyphenyl)-5-methoxy-1-benzofuran-6-yl]-tetraoxa-7,16-diazacyclooctadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp none RT 0 U K1=1.77 1994CGa (107257)1562
Method: fluorimetry
****
C46H46O7P2 L (6807)
1,15-Bis(2-Diphenylphosphinylphenyl)-2,5,8,11,14-pentaoxapentadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ con non-aq 25°C 100% U K1=5.5 1993BEb (107261)1563
Medium: THF+CHCl3 4:1(vol)
****
C46H48O6P2 L (7155)
1,8-Bis(2-(2-(diphenylphosphinyl)ethyl)phenoxy)-3,6-dioxyoctane
---
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ oth non-aq 25°C 100% U K1=3.7 1995TEa (107272)1564
Medium: THF:CHCl3 4:1 v/v. Na 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
---
Na+ con non-aq 25°C 100% U K1=5.12 1989KSa (107281)1565
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
---
Na+ con non-aq 25°C 100% U K1=4.34 1989KSa (107362)1566
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
-------------------------------------------------------------------------
Na+        con non-aq 25°C 100%  U        K1=5.4         1993BEb (107366)1567
Medium: THF+CHCl3   4:1(vol)
*************************************************************************
C48H54NO6P3             L                        (7975)
Tris(3-oxa-5-(diphenylphosphoryl)pentyl]amine;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Na+        cal non-aq 25°C 100%  U   H    K1=6.06   B2=11.23  1998SBb (107377)1568
Medium: MeCN  Calorimetric titration of LiNCS. DH(K1)=-34.8 kJ mol-1
DH(B2)=-34.3
*************************************************************************
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
-------------------------------------------------------------------------
Na+        con non-aq 25°C 100%  U        K1=4.51        1989KSa (107389)1569
Medium: tetrahydrofuran/CHCl3 4:1 (vol)
*************************************************************************
C48H60O8              H2L    R-Bu-Calixarene  CAS 147513-53-9  (6705)
4-tert-Butylcalix[4]arenedicarboxylic acid;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Na+        gl  alc/w  25°C 100%  C        K1=4.6         1993ABb (107404)1570
                                        B(Na2L)=8.3
                                        B(NaHL)=12.32
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
-------------------------------------------------------------------------
Na+        sp  non-aq 25°C 100%  C  I     K1=1.97        1996AAe (107412)1571
Medium: acetonitrile.  In 100% MeOH, K1=1.52.
*************************************************************************
C48H60O16             H4L                      (8251)
5,11,17,23-Tetrahydroxycalix[4]arene-bis(crown-6);
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Na+        sp  non-aq 25°C 100%  C        K1=3.5         2001PCa (107416)1572
Medium: methanol
*************************************************************************
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
---
Na+ sp non-aq 25°C 100% C K1=3.71 2004BCb (107422)1573
Medium: acetonitrile, 0.01 M Et4NClO4.

Na+ nmr mixed 47°C 50% C H K1=2.97 1995BDb (107423)1574
Method: 23Na and 1H nmr. Medium: 50% v/v CHCl3/CH3CN.
DH(K1)=-22 kJ mol-1, DS(K1)=-7 J K-1 mol-1.
****
C48H96N2O4 L CAS 72469-41-1 (5351)
N,N-Dioctadecyl-N',N'-dipropyl-3,6-dioxaoctanediamide;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE oth/un 21°C 100% C K1=5.5 1999CPa (107447)1575
Medium: PVC/DOS ion selective electrode membrane (DOS: bis(2-ethylhexyl)-
sebacate). Data for structurally related ionophores.
****
C52H64O12 H4L R-Bu-Calixarene CAS 113215-72-8 (6704)
5,11,17,23-Tetra-(t-butyl)-25,26,27,28-tetrakis[(hydroxycarbonyl)methoxy]calix[4]ar
ene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ gl alc/w 25°C 100% C K1=9.94 1993ABb (107492)1576
B(NaHL)=20.61
B(NaH2L)=30.67
B(NaH3L)=38.52
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
---
Na+ EMF non-aq 25°C 100% C H K1=7.2 1999USa (107500)1577
Medium: MeOH, 0.10 M Et4NCl. Method: by competition with Ag+
DH(K1)=-41 kJ mol-1
****
C52H68N4O8 L (4823)
25,27-Bis(N,N-diethylaminocarbonylmethoxy)-26,28-bis(N-butylaminocarbonylmethoxy)ca
lix[4]arene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp non-aq 25°C 100% C K1=2.1 1999USa (107509)1578
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
---
Na+ sp non-aq 25°C 100% C K1=4.67 2004BCb (107527)1579
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
---
Na+ dis non-aq 22°C 100% U K1=5.04 1996SCa (107543)1580
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
---
Na+ dis non-aq 22°C 100% C M 1996CPa (107556)1581
K(NaA+L(org)=NaAL(org))=6.09
Medium: CHCl3 saturated with H2O. Method: extraction of NaA into CHCl3/L solution. HA is picric acid.

Na+ cal alc/w 25°C 100% U K1=0.67 1977ILa (107557)1582
Medium: MeOH

Na+ sp alc/w 25°C 100% U K1=0.67 1972FEb (107558)1583
Medium: methanol/0.1M tetrabutyl-ammonium-perchlorate

Na+ gl alc/w 20°C 100% U K1=1.1 1968WPa (107559)1584
Medium: MeOH, 1 M NaI
****
C56H60O12 L CAS 157769-17-0 (9091)
1,3-Calix[4]-bis-benzo-crown-6;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp non-aq 25°C 100% C K1=1.5 1996AAe (107579)1585
Medium: acetonitrile.
****
C56H62O14 HL CAS 474540-94-8 (8852)
25,27-[4-Methyl-2-oxochromene-6,7-diylbis[2-(2-oxyethoxy)ethoxy]]-26,28-[ethylenebis[2-(2-oxyeth;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ oth non-aq RT 100% C I K1=2.3 2002LAa (107583)1586

Method: fluorimetry. Medium: EtOH. In CH3CN, K1=2.57.
****
C56H64O10 L CAS 405108-40-9 (8249)
1,2-Di-O-[2-(2-benzyloxyethoxy)ethyl]-3,4,5,6-tetra-O-benzyl-myo-inositol;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ dis non-aq 25°C 100% C 2001SSb (107589)1587
K(Na.pic+L(org)=NaL.pic)=1.36
Distribution of picrate salt into CHCl3/HL.
K: Na.pic(aq)+L(org)=NaL.pic(org). Data for series of myo-inositol ligands
****
C56H72O8 L CAS 123311-74-0 (6160)
Tetramethyl-t-butylcalix[4]arenetetraketone;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp alc/w 25°C 100% U I K1=5.1 1989ACb (107599)1588
Medium: MeOH. In CH3CN, K1=5.6
****
C56H72O12 L (8751)
Tetramethyl-4-t-Butylcalix[4]arenetetraethanoate;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ EMF non-aq 25°C 100% C IH K1=6.97 1995DGa (107603)1589
Medium: acetonitrile, 0.05 M Et4NClO4. In benzonitrile, K1=6.80
Competitive method: Ag/Ag+ electrode. DH(K1)=-63.0, DS=-77.8.
****
C56H78O8 L CAS 122356-76-7 (8681)
Tetra-tert-butyl-1,3-dimethoxycalix[4]arene-crown-6;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp non-aq 25°C 100% C K1=<=1 1995CUa (107608)1590
Medium: methanol, 0.01 M Et4NCl.
****
C56H80O8 L (9259)
5,11,17,23-Tetra(t-butyl)-25,26,27,28-tetramethoxyethoxycalix[4]arene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp non-aq 25°C 100% C H B2=9.64 2004BCb (107615)1591
Medium: acetonitrile, 0.01 M Et4NClO4. By calorimetry: DH(B2)=-46.4
kJ mol-1, DS(B2)=28.5 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
-------------------------------------------------------------------------
Na+        sp  alc/w  25°C 100%  C        K1=3.1         2001MAa (107624)1592
Medium: MeOH, 0.01 M Et4NCl.
*************************************************************************
C58H80O10               L                        (9264)
5,11,17,23-Tetra-t-butyl-25,27-di(2-methoxyethoxy)-26,28-di(ethylacetate)calix[4]ar
ene;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Na+        sp  non-aq 25°C 100%  C   H    K1=5.37   B2= 9.16  2004BCb (107633)1593
Medium: acetonitrile, 0.01 M Et4NClO4.  DH(K1)=-63.7 kJ mol-1,
DS(K1)=-111.0 J K-1 mol-1; DH(B2)=-65.4, DS(B2)=-44.6.
*************************************************************************
C60H54NO6P3             L                        (8067)
Tris[2-diphenylphosphoryl)phenoxyethyl]amine;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Na+        cal non-aq 25°C 100%  U   H    K1=4.32        1998SBb (107640)1594
                                          B(Li2L)=5.85
Medium: MeCN  Calorimetric titration of LiNCS. DH(K1)=-20.7 kJ mol-1
DH(Li2L)=-60.1
*************************************************************************
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
-------------------------------------------------------------------------
Na+        sp  non-aq 25°C 100%  C        K1=3.42        2004BCb (107644)1595
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
-------------------------------------------------------------------------
Na+        con non-aq 25°C 100%  C  IH    K1=7.40        2002ASc (107655)1596
Medium: acetonitrile. DH(K1)=-56.72 kJ mol-1, DS(K1)=-50.93 J K-1 mol-1.
In MeOH, K1=5.48, DH(K1)=-33.56, DS(K1)=-7.23.
-------------------------------------------------------------------------
Na+        nmr mixed  27°C  50%  C T H    K1=>5     B2= 1.26  1997IDa (107656)1597
Medium: 50% (v/v) CDCl3/CD3CN. Method: 1H and 23Na nmr. Data for K2 for
-33-37 C. DH(K2)=-16 kJ mol-1, DS(K2)=-28 J K-1 mol-1.
-------------------------------------------------------------------------
Na+        EMF non-aq 25°C 100%  C  IH    K1=7.68        1995DGa (107657)1598
Medium: acetonitrile, 0.05 M Et4NClO4. Competitive method: Ag/Ag+
electrode. DH(K1)=-69.2 kJ mol-1, DS=-85. Also data for tetrabutyl deriv.
-------------------------------------------------------------------------
```

Na+ sp alc/w 25°C 100% U I K1=5.0 1989ACb (107658)1599
Medium: MeOH. In CH3CN, K1=5.8
****
C60H82N2O10 L CAS 155377-20-1 (8806)
5,11,17,23-Tetra-butyl-25,27-bis(carboxymethoxy)-bis[(N,N-diethylaminocarbonyl)meth
oxy]calix[4]ar

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ gl non-aq 25°C 100% C K1=4.59 2000ABb (107668)1600
B(NaHL)=13.41
B(Na2L)=8.15
Medium: MeOH, 0.05 M Et4NClO4.
****
C60H84N4O8 L (8174)
25,26,27,28-Tetrakis-(N-ethylaminocarbonylmethoxy)calix[4]arene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp alc/w 25°C 100% U H K1=3.3 2000ABa (107673)1601
Medium: 100% MeOH, DH(K1)=-16.7 kJ mol-1 by colorimetry
K values for Na+, K+, Rb+, Cs+ less than 1
****
C60H84N4O8 L CAS 246035-32-5 (2735)
25,27-Bis(N,N-diethylaminocarbonylmethoxy)-26,28-bis(aminocarbonylmethoxy)-t-butylc
alix[4]arene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp non-aq 25°C 100% C K1=3.3 1999USa (107681)1602
Medium: MeOH, 0.10 M Et4NCl
****
C62H78N2O4S2 L (8158)
5,11,17,23-Tetrakis(1,1-dimethylethyl)-25,27-bis(2-methylthioethoxy)....calix(4)are
ne;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ cal non-aq 25°C 100% U H K1=5.22 2002NRa (107687)1603
Method: microcalorimetry. Medium: MeCN.. DH(K1)=-33.8 kJ mol-1
In benzonitrile K1=5.11, DH=-17.5
****
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
---
Na+ sp non-aq 25°C 100% C K1=3.5 1991ACc (107696)1604
Medium: acetonitrile, 0.01 M Et4NClO4.

****
C63H60NO6P3 L (8437)
Tris[2-(diphenylphosphorylmethyl)phenoxyethyl]amine;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ cal non-aq 25°C 100% U H K1=3.00 B2= 4.47 1998SBb (107721)1605
Medium: MeCN Calorimetric titration of LiNCS. DH(K1)=-19.6 kJ mol-1
DH(B2)=-17.6
****
C64H60O12 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
---
Na+ sp non-aq 25°C 100% C K1=<1 1999LDa (107736)1606
Medium: acetonitrile, 0.01 M Et4NClO4.
****
C64H62O6P4 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
---
Na+ con non-aq 25°C 100% U K1=4.4 1990EAb (107741)1607
Medium: THF+CHCl3 4:1(vol). Metal as 2,4-dinitrophenolate
****
C64H64O12 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
---
Na+ sp non-aq 25°C 100% C K1=1.4 1996AAe (107746)1608
Medium: acetonitrile.
****
C64H64O16 L CAS 474540-93-7 (8853)
25,27:26,28-Bis[4-methyl-2-oxochromene-6,7-diylbis[2-(2-oxyethoxy)ethoxy]]calix[4]a
rene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ oth non-aq RT 100% C I K1=2.48 2002LAa (107750)1609
Method: fluorimetry. Medium: EtOH. In CH3CN, K1=2.38.
****
C64H72N4O4P4 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
---
Na+ con non-aq 25°C 100% U K1=6.29 1986STb (107754)1610
Medium: THF:CHCl3 4:1 v/v. M as 2,4-dinitrophenolate

****
C64H80O6 L (9262)
5,11,17,23-Tetra-t-butyl-25,27-di(phenylmethoxy)-26,28-di(2-methoxyethoxy)-calix[4]arene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp non-aq 25°C 100% C H K1=3.80 2004BCb (107763)1611
Medium: acetonitrile, 0.01 M Et4NClO4. DH(K1)=-32.1 kJ mol-1, DS(K1)=-35.1 J K-1 mol-1.
****
C64H86O7 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
---
Na+ sp alc/w 25°C 100% U K1=1.5 1996AAc (107770)1612
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
---
Na+ sp non-aq 25°C 100% C K1=4.84 2004BCb (107778)1613
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
---
Na+ EMF non-aq 25°C 100% C IH K1=5.61 1999DCa (107786)1614
Medium: acetonitrile, 0.05 M Bu4NClO4. Method: by competition with Ag+.
By calorimetry: K1=5.36, DH(K1)=-25.61 kJ mol-1, DS(K1)=19.1 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
---
Na+ cal alc/w 25°C 100% U H 1995ABc (107792)1615
Medium: 100% Methanol. DH(K1)=-34.3 kJ mol-1, DS(K1)=23 J K-1 mol-1.
****
C68H96O8 L (6161)
Tetra-t-butyl-4-t-butylcalix[4]arenetetraketone;

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

Na+ sp alc/w 25°C 100% U K1=4.3 1989ACb (107796)1616
Medium: MeOH, 0.1 M Et4NCl
****
C68H96O12 L R-Bu-Calixarene CAS 170127-17-0 (2961)
25,26,27,28-Tetrakis(butoxycarbonylmethoxy)-5,11,17,23-tetra-t-butylcalix[4]arene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp alc/w 25°C 100% U K1=5.6 1992ABb (107799)1617
Medium: MeOH, 0.01 M Et4NClO4. Data also for many substituted p-tert-butyl-
calix[4]arenes
****
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
---
Na+ sp non-aq 25°C 100% C K1=>6 1999USa (107806)1618
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
---
Na+ nmr mixed 25°C 50% C K1=>4.0 2002MYa (107817)1619
Medium: 50% deutero-CHCl3/deutero-CH3CN. Method: 1H and 23Na nmr.

Na+ cal alc/w 25°C 100% U IH 1995ABc (107818)1620
Medium: 100% Methanol. DH(K1)=-50.6 kJ mol-1, DS(K1)=-20 J K-1 mol-1.
In acetonitrile, K1>8.5, DH(K1)=-79 kJ mol-1, DS(K1)=-103 J K-1 mol-1.

Na+ dis non-aq 20°C 100% C M 1988AGa (107819)1621
K(Na+A+L(org)=NaAL(org))=9.27
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
---
Na+ EMF alc/w 25°C 100% C H K1=7.23 2004MFa (107837)1622
Competitive potentiometry with Ag+. Medium: MeOH, 0.01 M Et4NCl.
By calorimetry, DH(K1)=-46 kJ mol-1, DS(K1)=-17 J K-1 mol-1.
****
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
-------------------------------------------------------------------------
Na+        con non-aq 25°C 100%  U        K1=3.86        1985YKa (107848)1623
Medium: EtOH+CHCl3 1:1;  M is used in nitrophenolate form
*************************************************************************
C72H72N6O15             L                        (2349)
1,3,5-Tris((2-(9-(8-quinolyloxy)-1,4,7-trioxanonyl)phenyl)amido)benzene;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Na+        nmr non-aq 30°C 100%  U T H    K1=3.3         1981GLb (107849)1624
Medium: pyridine. DH=-62 kJ mol-1. K1=3.1 (44 C); 2.4 (57 C); 1.6 (87 C)
*************************************************************************
C73H88O7                L    Calixspherand    CAS 154747-96-3  (7186)
2,26,31,41-Tetrakis(1,1-dimethylethyl)-45-ethoxy-35,38,44,46-tetramethoxy-9,14,19-t
rimethylcalix-
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Na+        kin mixed  25°C    0  U                        1994BHb (107853)1625
                                          K(NaX+L)=12.1
Medium: CDCl3, saturated with D2O. X=picrate. Data also for 2 analogues
calixspherands
*************************************************************************
C75H100O15              L                      CAS 152495-34-6  (7033)
Penta-tert-butylpentakis(ethoxycarbonylmethyloxy)calix[5]arene;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Na+        sp  alc/w  25°C 100%  U        K1=4.4         1993BMa (107861)1626
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
-------------------------------------------------------------------------
Na+        ISE non-aq 25°C 100%  C  IH    K1=8.89        2001DKa (107871)1627
Method: Na+ ion selective electrode. Medium: acetonitrile, 0.05 M Bu4NClO4
By calorimetry, DH(K1)=-76.0 kJ mol-1, DS(K1)=-85.1 J K-1 mol-1.
-------------------------------------------------------------------------
Na+        ISE non-aq 25°C 100%  U  IH    K1=7.45        2001NKa (107872)1628
Method: Na ion electrode. Medium: 75% MeCN, 25% DMF. DH(K1)=-62.4 kJ mol-1
In 25% MeCN K1=5.66, DH=-65.6. Calorimetric titns. also used
-------------------------------------------------------------------------
Na+        sp  non-aq 25°C 100%  U        K1=6.1         1989ACb (107873)1629
Medium: CH3CN
*************************************************************************
C77H82O9                L                      CAS 253317-20-3  (9288)
p-Tert-butyldihomooxacalix[4]arene tetraphenyketone;
```

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp alc/w 25°C 100% C I K1=3.7 1999MAb (107895)1630
Medium: MeOH, 0.01 M Et4NCl. In acetonitrile, K1=3.2.
****
C78H90O10P2 L CAS 160638-26-6 (9130)
5,11,17,23-Tetra-t-butyl-bis(diethylcarbamoylmethoxy)-bis(diphenylphosphinoylmethox
y)calix[4]aren

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp alc/w 20°C 100% C K1=4.90 2003YVa (107901)1631
Medium: 100% EtOH, 0.01 M Et4NBr. Ligand is cone isomer. For paco isomer,
K=4.96. Also data for bis(diethyl ester) analogues.
****
C80H112O24 L CAS 175349-59-4 (7498)
C-Heptylcalix[4]resorcinarene octa-alpha-(methyl ethanoate);

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ dis non-aq 25°C 100% U 1995FDa (107905)1632
K=3.50
Medium: CDCl3. Method: by H2O/CDCl3 extraction of picrate salt.
K: MA(org)+L(org)=MLA(org) where A=picrate.
****
C85H80O15 L CAS 269057-77-4 (3302)
5,11,17,23,29-Pentabenzylcalix[5]arene-31,32,33,34,35-pentaethanoate pentamethyl
ester;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp non-aq 25°C 100% C I K1=2.6 2000AAa (107912)1633
Medium: methanol, 0.01 M Et4NCl. Also data for acetonitrile, 0.01 M Et4NCl
and for the pentaethylester.
****
C85H120O15 L CAS 152495-35-7 (7034)
Penta-tert-butylpentakis(tert-butoxycarbonylmethoxy)calix[5]arene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ EMF alc/w 25°C 100% U K1=5.1 1993BMa (107918)1634
Medium: MeOH, 0.1 M Et4NClO4.
****
C88H78N2O12 L CAS 351183-45-4 (8252)
1,3-Calix[4]bis(10-cyano-9-anthrylmethyl-o-benzocrown-6);

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp mixed 25°C 50% C K1=3.1 2001JDa (107922)1635

K(NaL+Na)=1.6
Medium: 50% v/v CH2Cl2/MeOH, 0.01 M benzyl(trimethyl)ammonium hydroxide.
Method: fluorescence spectroscopy.
****
C88H96N8O12S4 L CAS 639027-46-6 (9277)
Tetra(benzoylthiocarbamido)cavitand;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE NaCl rt 0.01M C K1=4.9 2003MGa (107928)1636
Method: segmented sandwich membrane ISE.
****
C88H96N8O16 L CAS 639030-70-9 (9278)
Tetra(benzoylcarbamido)cavitand;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE NaCl rt 0.01M C K1=4.2 2003MGa (107936)1637
Method: segmented sandwich membrane ISE.
****
C90H120O18 L CAS 92003-62-8 (6159)
Hexaethyl-4-t-butylcalix[6]arenehexaethanoate;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ cal non-aq 25°C 100% C K1=5.31 1997DZa (107944)1638
Medium: benzonitrile. DH(K1)=-29.17 kJ mol-1, DS(K1)=3.8 J K-1 mol-1.

Na+ sp non-aq 25°C 100% U I K1=3.5 1989ACb (107945)1639
Medium: CH3CN
****
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;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ sp non-aq 25°C 100% C I K1=4.5 2000AAa (107952)1640
Medium: methanol, 0.01 M Et4NCl. Also data for acetonitrile, 0.01 M Et4NCl and the pentaethyl ester.
****
C96H144O24 L CAS 169888-22-6 (7534)
C-Undecylcalix[4]resorcinarene octa-alpha-(methyl ethanoate);

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ dis non-aq 25°C 100% U 1995FDa (107968)1641
K=3.22
Medium: CDCl3. Method: by H2O/CDCl3 extraction of picrate salt.
K: MA(org)+L(org)=MLA(org) where A=picrate.

****
C102H174N6O73 L CAS 571203-64-0 (9253)
4,13-Bis(2-(6-deoxy-b-cyclodextrin-6-yl)aminoethylamidomethyl)-4,13-diazatrioxacycl
opentadecane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ gl R4N.X 25°C 0.10M C K1=2.30 2003WWa (107973)1642
Medium: 0.10 M Et4NClO4.
****
C104H160O24 L CAS 175349-60-7 (7494)
C-Heptylcalix[4]resorcinarene octa-alpha-(tert-butyl ethanoate);

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ dis non-aq 25°C 100% U 1995FDa (107979)1643
K=3.74
Medium: CDCl3. Method: by H2O/CDCl3 extraction of picrate salt.
K: MA(org)+L(org)=MLA(org) where A=picrate.
****
C104H168N8O16 L CAS 175349-61-8 (7483)
C-Heptylcalix[4]resorcinarene octa-alpha-(N,N-diethyl acetamide);

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ dis non-aq 25°C 100% U 1995FDa (107983)1644
K=5.26
Medium: CDCl3. Method: by H2O/CDCl3 extraction of picrate salt.
K: MA(org)+L(org)=MLA(org) where A=picrate.
****
C112H120N4O16P4 L CAS 195455-62-0 (9276)
1,21,23,25-Tetrapentyl-7,11,15,28-tetra[(diphenylphosphinyl)acetamidomethylene]
cavitand;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ ISE NaCl rt 0.01M C K1=7.2 2003MGa (107992)1645
Method: segmented sandwich membrane ISE.
Phosphonic acid diethyl ester derivative: K1=12.0
****
C114H198N6O73 L CAS 571203-66-2 (9254)
4,13-Bis(8-(6-deoxy-beta-cyclodextrin-6-yl)aminooctylamidomethyl)-4,13-diazatrioxac
yclopentadecan

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Na+ gl R4N.X 25°C 0.10M C K1=3.26 2003WWa (108000)1646
K(Na+HL)=2.99
K(Na+H2L)=2.89
Medium: 0.10 M Et4NClO4.

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	dis	non-aq	25°C	100%	U			1995FDa (108011)	1647
							K=4.24		

Medium: CDCl3. Method: by H2O/CDCl3 extraction of picrate salt.
K: MA(org)+L(org)=MLA(org) where A=picrate.
****
C120H200N8O16 L CAS 169888-21-5 (7490)
C-Undecylcalix[4]resorcinarene octa-alpha-(N,N-diethyl acetamide);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	dis	non-aq	25°C	100%	U			1995FDa (108022)	1648
							K=5.25		

Medium: CDCl3. Method: by H2O/CDCl3 extraction of picrate salt.
K: MA(org)+L(org)=MLA(org) where A=picrate.
****
Polymer H2L X-14885A (4547)
Antibiotic X14885A, calcium ionophore

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	gl	alc/w	25°C	100%	U		K1=3.7	1989ABb (108077)	1649

Medium: MeOH
****
Polymer Myosin A (3529)
Myosin A;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	EMF	oth/un	5°C	?	U		K1=3.2 B2=5.80	1957LSa (108262)	1650
****
Polymer (4181)
Phosphatidic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	gl	oth/un	24°C	0.10M	U		K1=1.1	1966AKa (108272)	1651
****
Polymer (4204)
Pyruvate kinase;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	sp	R4N.X	25°C	0.10M	U			1966SSc (108409)	1652
							K'=0.68		

Medium: Me4NCl. See reference for definition

****

Polymer (1966)

poly(Benzo-1,4,7,10,13,16-hexaoxacyclooctadecane)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	sp	non-aq	25°C	100%	U		K1=6.53	1979KMb (108426)	1653

Medium: CHCl3

****

Polymer (1965)

poly(Benzo-1,4,7,10,13-pentaoxacyclopentadecane)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Na+	sp	non-aq	25°C	100%	U		K1=6.72	1979KMb (108430)	1654

Medium: CHCl3

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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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