

SC-Database

Software version = 5.81 Data version = 4.62
 Experiment list contains 1456 experiments for
 (no ligands specified)
 Metal : K+
 (no references specified)
 (no experimental details specified)

e- HL Electron (442)
 Electron;

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

K+ EMF KCl 25°C 0.0 C I 1997BMa (612) 1
 $K(K+e=K(Hg))=-37.15(-2.19766V)$

Method: K(Hg) amalgam electrode. Data for 0-0.6 mass fraction MeOH/H2O,
 0.05-2.0 m KCl. $K=-36.43 (E=-2.1554 V, x=0.2)$; $K=-35.75 (E=-2.1149, x=0.4)$

 K+ EMF mixed 25°C 10% U I 1974DKb (613) 2
 $K(K+e=K(s))=-49.27(-2.915V)$

Medium: 10% w/w DMSO/H2O; $K=-49.04(-2.901V, 20\%)$, $-48.43(-2.865V, 40\%)$,
 $-47.74(-2.824V, 60\%)$

 K+ oth none 25°C 0.0 U I 1972C0a (614) 3
 $K(K+e=K(s))=-49.87 (-2950mV)$

Method: Estimated. MeOH: $-54.02(-3.196V)$. EtOH: $-52.63(-3.131V)$. BuOH: -50.36
 $(-2.979V)$. PentOH: $-50.36(-2.979V)$. Me2CO: $-49.26(-2.914V)$

 K+ oth none 25°C 0.0 U I 1972C0a (615) 4
 $K(K+e=K(s))=-49.87 (-2950mV)$

Method: Estimated. MeCN: $-56.58(-3.347V)$. HCOOH: $-59.52(-3.521V)$.
 Also NH3 and N2H4

 K+ EMF mixed 25°C 30% U I 1972KRb (616) 5
 $K(K+e=K(s))=-49.29(-2.916V)$

In: 30% w/w ethylene glycol/H2O; $K=-49.17(-2.909V, w=50)$, $-49.04(-2.901V, w=70)$
 $-49.46(-2.926V, w=90)$, $-50.68(-2.998V, 100\%)$

 K+ EMF non-aq 25°C 100% U I 1972KRc (617) 6
 $K(K+e=K(s))=-49.73(-2.942V)$

Medium: 30% w/w propylene glycol/MeOH; 0% PG: $K=-49.60(-2.934V)$. 50%: -49.92
 $(-2.953V)$. 70%: $-50.19(-2.969V)$. 90%: $-50.37(-2.980V)$. 100%: $-50.64(-2.996V)$

 K+ con non-aq -34°C 100% U 1969DLa (618) 7
 $K(K + e(soln))=2.24$
 $K(2K=K2)=3.18$

Medium: NH3(liquid)

 K+ EMF alc/w 25°C 100% U I 1968DIb (619) 8

K(K+e=K(s))=-48.43, -2865 mV

At I=0 corr: K=-49.41, -2923.0 mV. Also values for 6 EtOH/H2O mixtures

K+	EMF none	25°C	0.0	U					1967BHc (620)	9
									K(K+e=K/Hg)=-33.33, -1971 mV	

K+	EMF non-aq	25°C	100%	U					1966LcA (621)	10
									K'=-51.073, -3020.2 mV	
Medium: CH3NHCHO. K': K + Cl + Ag(s)=K(s) + AgCl(s)										

K+	EMF alc/w	25°C	100%	U					1958BSb (622)	11
									K(K+e=K(s))=-49.38(-2921 mV)	
Medium: MeOH										

K+	EMF non-aq	25°C	100%	U T					1954PSa (623)	12
									K(K+e=K(s))=-48.55(-2.872V)	
Medium: formamide; K=-49.65(-2.868V, 18 C)(M units)										

K+	EMF none	25°C	0.0	U					1923LRa (624)	13
									K(K+e=K(s))=-49.42(-2922.4 mV)	

BF4-	HL								(2497)	
Tetrafluoroborate;										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
K+	con	non-aq	25°C	100%	U			K1=1.7	1975YKa (1194)	14
Medium: MeCN										

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
K+	sp	oth/un	25°C	1.00M	U	I		K1=0.45	1990RAa (1312)	15
Medium: KCl. Data at I=0 M and at pressures to 2041 atmos.										

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
K+	con	non-aq	25°C	100%	U	T		K1=2.37	1993TAa (2070)	16
Medium: 2-methoxyethanol, -10 to 80 C										

K+	con non-aq	25°C	100%	U	I				1978CAa (2071)	17
Medium: Acetonitrile. Data also for (hexyl)4N+ and (amyl)4N+										

K+	con non-aq	25°C	100%	U					1974HPb (2072)	18
Medium: hexamethylphosphotriamide. K1 by Pitts eqn. K1=1.70 (Fuoss-Hsia eqn)										

 K+ con non-aq 25°C 100% U K1=4.35 1973TKb (2073) 19
 Medium: liquid SO2, 0 corr

K+ con non-aq 25°C 100% U K1=1.8 1971ENa (2074) 20
 Medium: trifluoroethanol. K1=1.68 to 1.91

K+ con mixed 25°C 8% U I K1=0.70 1970BKb (2075) 21
 Medium: 8% t-butanol/H2O. K1=0.90(10%), 0.62(15%), 1.08(20%), 2.60(50%)

K+ con non-aq 25°C 100% U K1=-0.25 1970CDa (2076) 22
 Medium: DMSO

K+ sol non-aq 25°C 100% U I Kso=-2.4 1967AKa (2077) 23
 Medium: DMF. In (Me3N)3PO: Kso=-4.0

K+ con non-aq 25°C 100% U K1=3.38 1965BFb (2078) 24
 Medium: diaminoethane

K+ con non-aq 0°C 100% U T H K1=3.84 1956LLa (2079) 25
 Medium: liquid SO2. K1=3.70(-8.93C), DH(K1)=22.0 kJ mol-1, DS=155 J K-1 m-1

K+ con non-aq 30°C 100% U K1=6.96 ? 1954JGa (2080) 26
 Medium: CH3CO2H

K+ con non-aq -34°C 100% U K1=2.72 1949HKa (2081) 27
 Medium: liquid NH3

BrO3- HL Bromate (6017)
 Bromate;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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K+	cal	none	25°C	0.0	C	IH		1992BVa (2414)	28
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DH(Kso)=41.5 kJ mol-1, measured for I=0.002-0.02 M self medium.
 Also data for 0.047-0.228 mol fraction MeOH/H2O.

K+	con	none	25°C	0.0	U		K1=-0.33	1971JBa (2415)	29
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K+	con	none	25°C	0.0	U		K1=-0.35	1969BJa (2416)	30
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K+	con	none	25°C	0.0	U		K1=-0.32	1969GUc (2417)	31
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K+	oth	oth/un	25?°C	0.0	M		K1=0.1	1966MBb (2418)	32
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K+	con	alc/w	25°C	50%	U		K1=1.22	1958DTa (2419)	33
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Medium: 50% EtOH/H2O

K+	con	none	25°C	0.0	U		K1=-0.60	1948MOa (2420)	34
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 K+ con none 18°C 0.0 U K1=-0.35 1927DAb (2421) 35

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
K+	con	oth/un	25°C	0.0	U			K(K+Ru(CN)6)=2.48	1970FKb (2735)	36

C6N6Co---		H3L						Cyanocobaltate (5470)		
Hexacyanocobaltate; [Co(CN)6]---										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
K+	con	oth/un	25°C		U			K1=1.0	1974FIb (3494)	37
K+	con	none	18°C	0.0	U T			K1=1.26	1950JMc (3495)	38
K1=1.22(25 C)										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
K+	con	none	25°C	0.0	U			K1=1.47	1947JAa (3496)	39

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
K+	gl	KCl	25°C	0.10M	C	TIH		K1=1.80	1986CDc (3571)	40
B(K2Fe(CN)6)=2.14										
B(KHFe(CN)6)=4.63										
Data for 10-35 C and 0.05-1.0 M KCl. DH(K1)=7.5 kJ mol ⁻¹ , DS(K1)=71										
J K ⁻¹ mol ⁻¹ ; DH(K2Fe(CN)6)=35.6, DS=184; DH(KHFe(CN)6)=32.2, DS=222										

K+	ISE	oth/un	25°C	0.0	C			K1=2.39 B2= 5.46	1984DRa (3572)	41
K(2K+Fe(CN)6)=3.20										
K(3K+Fe(CN)6)=3.72										
Method: potassium ISE. Extrapolated from data for 0.01-1.0 M KCl.										
At I=1.0, K1=1.68, K(2K+Fe(CN)6)=1.96, K(3K+Fe(CN)6)=2.13.										

K+	con	oth/un	25°C		U			K1=2.0	1974FIb (3573)	42
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K+	sol	KNO3	25°C	2.00M	U			K1=2.6	1971HFa (3574)	43
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K+	EMF	oth/un	25°C		U			K1=2.28	1969NSa (3575)	44
Assuming K(K+Fe(CN)6)=1.30										

K+	ISE	oth/un	25°C	.004M	U	I		K1=1.78	1967EGa (3576)	45
Method:K+ sensitive glass electrode. Medium: K4L. K1=2.13(0.0004 M),										
2.35(0 corr)										

 K+ gl oth/un 40°C .001M U T H K1=2.01 1967EGa (3577) 46
 Medium: K4L. K1=1.95(10 C), 2.00(25 C). DH(K1)=2.5 kJ mol⁻¹. By calorimetry:
 DH=4.1, DS=54

K+ ISE R4N.X 39°C 0.10M U TIH K1=1.6 1966CLb (3578) 47
 Method:K+ glass electrode. Medium: Me4NCl. K1=1.5(25 C). At I=0 corr:
 K1=2.2(25 C), 2.4(39 C); DH=17 kJ mol⁻¹, DS=96 J K⁻¹ mol⁻¹

K+ sp none 25°C 0.0 U K1=2.37 1957CPa (3579) 48

K+ con none 25°C 0.0 U K1=2.3 1949JAa (3580) 49

K+ con none 25°C 0.0 U K1=2.3 1937DAa (3581) 50

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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K+	gl	oth/un	25°C	1.30M	U			K1=1.9	1974HIa (3654)	51
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K+	ISE	oth/un	25°C	.005M	U			K1=1.03	1967EGa (3655)	52
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Medium: K3L. K1=1.29(I=0.001),1.46(0 corr). When I=0.00125: K1=1.21(10 C),
 1.25(25 C), 1.28(45 C). By calorimetry: DH(K1)=2.1 kJ mol⁻¹, DS=34 J K⁻¹ m⁻¹

K+	sol	oth/un	25°C	3.0M	U			K1=0.30	1967Rmd (3656)	53
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Medium: LiNO3

K+	sol	oth/un	25°C	3.0M	U	I		K1=0.30	1967Rmd (3657)	54
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Medium: LiNO3. K1=0.18(I=2), -0.24(I=0.5), 0.90(I=0)
 In LiCl: K1=-0.42(I=3), -0.49(I=2), -0.27(I=1), -0.22(I=0.5), 0.90(I=0)

K+	sol	oth/un	25°C	3.0M	U			K1=0.30	1967Rmd (3658)	55
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Medium: LiNO3

K+	ISE	R4N.X	25°C	0.10M	U	T		K1=0.85	1966CLb (3659)	56
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Medium: Me4NCl. 39 C: K1=0.9

K+	ISE	oth/un	25°C	0.0	U	T	H	K1=1.4	1966CLb (3660)	57
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Medium: 0 corr. 39 C: K1=1.5. DH=-12 kJ mol⁻¹, DS=-62 J K⁻¹ mol⁻¹

K+	sol	oth/un	25°C	3.0M	U		H	K1=-0.42	1966MRb (3661)	58
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Medium: LiCl. By calorimetry: DH(K1)=-22.6 kJ mol⁻¹, DS=-84 J K⁻¹ mol⁻¹

K+	con	none	18°C	0.0	U	T		K1=1.30	1950JMc (3662)	59
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K1=1.22(25 C)

K+	con	none	25°C	0.0	U			K1=1.40	1949MOa (3663)	60
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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
K+	con	oth/un	25°C	0.00	U			K1=1.36	1976LLa (3703)	61

Cl-		HL		Chloride				CAS 7647-01-0	(50)	
Chloride;										
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
K+	con	mixed	25°C	20%	C	I		K1=1.73	2001BSa (5116)	62
Medium: 20 % w/w ethylene carbonate/water. Data for 20-80 % w/w ethylene carbonate/water.										
K+	ISE	none	25°C	0	C	I		K1=-0.51	1995RGa (5117)	63
I=0.16 (Me4N.X) K1=-0.69; I=0.5 (Me4N.X) K1=-0.68.										
K+	oth	alc/w	25°C	100%	U			K1=1.08	1982GBa (5118)	64
Medium: MeOH										
K+	sol	alc/w	25°C	50%	U	I		Kso(KCl)=-0.706	1982MPe (5119)	65
Method: K ion selective electrode. Data for 10-90% w/w MeOH/H2O.										
K+	nmr	KCl	25°C	0.10M	U	M		K(K(18-crown-6)+L)=0.7	1982SYa (5120)	66
K+	con	mixed	25°C	50%	U			K1=2.2	1974KKc (5121)	67
Medium: 50% w/w EtOH/acetone. K1=2.02 to 2.32(depending upon eqn used)										
K+	con	non-aq	25°C	100%	U			K1=4.73	1973TKb (5122)	68
Medium: liquid sulfur dioxide										
K+	con	mixed	20°C	89%	U			K1=2.79	1973YKa (5123)	69
Medium: 89% w/w butanol/H2O										
K+	con	non-aq	25°C	100%	U			K1=2.0	1971ENa (5124)	70
Medium: trifluoroethanol. K1=1.85 to 2.08										
K+	con	none	25°C	0.0	U			K1 < -1.59	1971HPa (5125)	71
K+	con	non-aq	25°C	100%	U			K1=0.07	1971PGa (5126)	72
Medium: N-methylformamide										
K+	con	none	25°C	0.0	U			K1=-0.76	1971PJa (5127)	73
K+	con	mixed	25°C	9.9%	U	I		K1=0.30	1970BKb (5128)	74

Medium: 9.9% w/w t-butanol/H₂O. K₁=0.81(15.1%), 0.91(20.1%)

K+ con non-aq 25°C 100% U K₁=0.38 1970CDa (5129) 75
Medium: DMSO

K+ con diox/w 25°C 50% U I K₁=0.91 1970PSa (5130) 76
Medium: 50% w/w dioxan/H₂O at 1 bar. K₁=0.87(500 bar), 0.84(1000 bar),
In 70% dioxan: K₁=2.32(1 bar), 2.21(500 bar), 2.14(1000 bar). Also 80% diox.

K+ con non-aq 25°C 100% U I K₁=1.17 1970SAf (5131) 77
Medium: 9.57% w/w butanol/MeOH. K₁=1.21(19.7%), 1.40(39.8%), 1.51(51.4%)

K+ con mixed 440°C 90% U I K₁=-3.28 1969HFa (5132) 78
Medium: 90% argon/H₂O. K₁=-2.52(10%). Also other ratios

K+ con mixed 25°C 50% U I K₁=1.0 1968BTc (5133) 79
Medium: 50% THF. K₁=1.59(70%), 2.52(80%), 2.97(85%), 3.87(90%)

K+ con none 25°C 0.0 U K₁=-0.10 1968CFa (5134) 80

K+ sol alc/w 25°C 100% U K_{so}=-2.5 1967AKa (5135) 81
K_{so}=-5.4 in DMF

K+ oth oth/un 25°C 0.0 U K_{so}(KCl, sylvite)=0.898 1967LEa (5136) 82

K+ con alc/w 25°C 60% U I K₁=0.48 1965HKa (5137) 83
Medium: 60.3% EtOH. K₁=1.06(79.3%), 1.37(87.9%)

K+ con non-aq 25°C 100% U I K₁=1.43 1962SHd (5138) 84
Medium: HCOOH. K₁=3.78 in CH₃COOH

K+ con none 281°C 0.0 U T K₁=0.31 1961WLa (5139) 85
I=0 corr. K₁=0.92(306 C)

K+ con alc/w 25°C 100% U K₁=2.10 1957GKa (5140) 86
Medium: EtOH

K+ gl diox/w 25°C 70% U K₁=2.63 1957PGa (5141) 87

K+ EMF non-aq 25°C 100% U K₁=6.88 1956BKa (5142) 88
Medium: CH₃COOH

K+ con non-aq 0°C 100% U T H K₁=4.13 1956LLa (5143) 89
Medium: liquid SO₂. K₁=3.97 (-8.93 C). DH(K₁)=24.8 kJ mol⁻¹, DS=170

K+ con alc/w 25°C 100% U K₁=1.0 1951EKa (5144) 90
Medium: MeOH

K+ con non-aq -34°C 100% U K1=3.06 1949HKa (5145) 91
Medium: liquid NH3

K+ sol oth/un 25°C 0.0 U Kso(KCl)=0.932 1934AKa (5146) 92

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

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

K+ cal none 25°C 0.0 C IH 1992BVa (6037) 93
DH(Kso)=41.5 kJ mol⁻¹, measured for I=0.002-0.02 M self medium.
Also data for 0.047-0.228 mol fraction MeOH/H2O.

K+ con none 25°C 0.0 C I K1=-0.22 1986SDa (6038) 94
Value derived from data for 0.001-0.05 self medium.

K+ con non-aq 25°C 100% U K1=0.69 1975AJa (6039) 95
Medium: DMSO

K+ nmr non-aq 25°C 100% U K1=1.44 1975SAd (6040) 96
Medium: hexamethylphosphoramide

K+ con none 25°C 0.0 U K1=-0.15 1972DDa (6041) 97

K+ con mixed 25°C 1.0% U I K1=-0.16 1972DDb (6042) 98
Medium: 1.0% w/w sulfolane/H2O. K1=-0.09(31.9%), 0.59(75.7%), 1.26(95.3%)

K+ con oth/un 18°C 0.0 U T K1=-0.18 1931BRb (6043) 99
K1=-0.04(25 C)

K+ con none 18°C 0.0 U K1=-0.17 1902KSa (6044) 100

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

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

K+ con non-aq 25°C 100% M K1=1.45 1999DSd (6252) 101
Medium: acetonitrile.

K+ con mixed 25°C 20% C K1=0.87 1994SSb (6253) 102
Medium: 20% w/w propylene carbonate/ethylene carbonate.

K+ con non-aq 25°C 100% C K1=0.031 1990SAb (6254) 103
Medium: propylene carbonate. K1 derived from literature data.

K+ con none 25°C 0.0 C T H K1=0.196 1988YOa (6255) 104
Data for 0-50 C. DH(K1)=-1.8 kJ mol⁻¹, DS(K1)=-2.4 J K⁻¹ mol⁻¹.

K+ con none 25°C 0.0 C I K1=-0.46 1986SDa (6256) 105
 Value derived from data for 0.001-0.05 self medium.

K+ con non-aq 25°C 100% U I K1=1.3 1982Gcb (6257) 106
 Medium: DMF. In DMF and 1,1,3,3-Tetramethylurea: K1=1.1; in DMF and DMSO:
 1.0; in DMF and Hexamethylphosphotriamide: 0.9

K+ con non-aq 25°C 100% U I K1=1.3 1982Gcb (6258) 107
 Medium: DMF. In DMF and beta-picoline: K1=1.3. Other data given

K+ gl non-aq 25°C 100% U H K1=5.69 1981TMb (6259) 108
 Medium: Glacial acetic acid. Alternative method: Spectrophotometry.
 DH(K1)=-27 kJ mol⁻¹

K+ sol oth/un 25°C 1.0M U K1=0.18 1980FSb (6260) 109
 In 1.0 M LiClO₄;
 in 2.0 M K1=-0.04; ; in 3.0 M K1=0.4 in 4.0 M K1=0.6

K+ con non-aq 25°C 100% U K1=1.43 1978CAa (6261) 110
 Medium: Acetonitrile

K+ con non-aq 25°C 100% U K1=10.7 1975AJa (6262) 111
 Medium: hexamethylphosphoramidate

K+ con non-aq 25°C 100% U K1=1.4 1975YKa (6263) 112
 Medium: MeCN

K+ con oth/un 25°C ? U I K1=1.63 1974ADb (6264) 113
 Medium: benzene/CH₃CN. K1=0.146 in ethylene carbonate. Data for other media

K+ con non-aq 25°C 100% U I K1=1.45 1974ADb (6265) 114
 Medium: MeCN. K1=0.20 in 19.2% MeCN in ethylene carbonate; 0.35 (29.3%);
 0.74(53.1%); 1.00(69.2%). In H₂O, I-0 corr: K1=-0.01

K+ con non-aq 25°C 100% U K1=0.95 1974HPb (6266) 115
 Medium: hexamethylphosphotriamide. K1 by Pitts eqn, by Fuoss-Hsia: K1=1.25

K+ con non-aq 25°C 100% U I K1=1.54 1973DDa (6267) 116
 in 14.6% w/w methanol-sulfolane; K1=1.05(14.6%), 1.14(39.6%), 1.29(60.1%),
 1.47(88.0%), 1.50(95.9%). Also MeCN-sulfolane and MeCN-benzene

K+ con non-aq 25°C 100% U K1=-0.2 1973JYa (6268) 117
 Medium: propene carbonate; 0 corr

K+ con alc/w 25°C 100% U K1=1.53 1972DAa (6269) 118
 Medium: MeOH

K+ con non-aq 25°C 100% U K1=2.49 1971BHa (6270) 119
 Medium: acetone

K+	con none	25°C	0.0	U	K1=0.00	1971DAa	(6271)	120
K+	con non-aq	25°C	100%	U T	K1=2.78	1971HEa	(6272)	121
Medium: acetone. -50 C: K1=2.64								
K+	con non-aq	25°C	100%	U	Kso=-8.35	1971JKa	(6273)	122
Medium: methylisobutyl ketone								
K+	con alc/w	25°C	100%	U	K1=1.92	1971NIa	(6274)	123
Medium: EtOH								
K+	con non-aq	25°C	100%	U	K1=0.31	1971PGa	(6275)	124
Medium: N-methylformamide								
K+	con mixed	25°C	70%	U I	K1=1.51	1970ALa	(6276)	125
Medium: 70% w/w t-butanol/H2O. K1=2.79(80%). Medium 0 Corr.								
K+	con non-aq	25°C	100%	U	K1=1.09	1969FOc	(6277)	126
Medium: MeCN. 0 corr.								
K+	sol none	25°C	0.0	U	Kso=-1.94	1969GUb	(6278)	127
K+	con none	25°C	0.0	U	K1=-0.08	1969GUc	(6279)	128
K+	con mixed	25°C	85%	U	K1=1.66	1968BTc	(6280)	129
Medium: 84.5% THF								
K+	con alc/w	25°C	100%	U	K1=1.04	1968CPb	(6281)	130
Medium: MeOH. In MeCN: K1=1.23, also for MeOH-MeCN mixtures								
K+	ISE none	25°C	0.0	U T	Kso=-2.02	1968HRb	(6282)	131
K+	sol alc/w	25°C	100%	U I	Kso=-4.5	1967AKa	(6283)	132
Medium: MeOH. In DMF: Kso=-0.1								
K+	con non-aq	25°C	100%	U	K1=1.13	1967KHe	(6284)	133
Medium: MeCN								
K+	con non-aq	25°C	100%	U T	K1=1.75	1966Mwb	(6285)	134
Medium: MeCN, also at 20 C, 30 C								
K+	con non-aq	25°C	100%	U	K1=1.99	1962Mwa	(6286)	135
Medium: MeCN								
K+	con none	25°C	0.0	U	K1=-0.48	1945JOa	(6287)	136

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

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

K+ oth none 25?°C 0.0 M K1=0.8 1966MBb (6494) 137

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

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

K+ sp oth/un 25°C 1.0M U I K1=0.10 1993MAa (6976) 138
K1 values over a range of pressures and ionic strengths

K+ ISE NaClO4 25°C 1.0M U TI K1=-1.7 1984CTd (6977) 139

HP03-- H2L Phosphite CAS 13598-36-2 (6305)
Phosphite;

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

K+ con oth/un 20°C 0.0 U K1=0.80
 K(K+HL)=0.74

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

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

K+ sol non-aq 20°C 100% U K1=-0.40 1971CBc (7594) 141
Medium:propene carbonate

K+ sol non-aq 25°C 100% U K1=0.0 1967CKa (7595) 142
Medium: MeCN

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

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

K+ con non-aq 25°C 100% C T K1=1.40 2001SSa (8187) 143
Medium: N,N-dimethylformamide. Data for -40 to 25 C.

K+ con mixed 25°C 20% C K1=1.82 1994SSb (8188) 144
Medium:20% w/w propylene carbonate/ethylene carbonate.

K+ con non-aq 25°C 100% U K1=0.70 1982GCa (8189) 145
Medium: DMF

K+	con non-aq	25°C	100%	U	K1=0.43	1976RMa	(8190)	146
Medium: 3-methylsulfonate								
K+	nmr non-aq	25°C	100%	U	K1=0.633	1975SAd	(8191)	147
Medium: hexamethylphosphoramide								
K+	con oth/un	25°C	?	U I	K1=-0.06	1974ADb	(8192)	148
In ethylenecarbonate: K1=0.11								
K+	con non-aq	25°C	100%	U	K1=0.79	1974HPb	(8193)	149
Medium: hexamethylphosphotriamide. Calculated using Pitts eqn. By Fuoss-Hsia K1=1.22								
K+	con alc/w	25°C	100%	U T H	K1=1.51	1974SKa	(8194)	150
Medium: MeOH. DH(K1)=2.1 kJ mol ⁻¹ . K1=1.49 (15 C), 1.51 (35 C), 1.53 (45 C). Data in alcohols up to nonyl alcohol. In BuOH:DH=25.5;K1=2.87(15 C)3.32(45C)								
K+	con non-aq	25°C	100%	U T H	K1=3.97	1974SKa	(8195)	151
Medium: hexanol. DH(K1)=23.0 kJ mol ⁻¹ . K1=3.80(15 C), 4.09(35 C), 4.20(45 C) In nonyl alcohol: DH(K1)=39.3; K1=4.25(15 C),4.69(25 C),4.76(35 C),4.98(45C)								
K+	oth none	25°C	0.0	M	K1=-1.54	1973SOb	(8196)	152
Estimated from literature data. K(Rb+I)=-1.52, K(Cs+I)=-0.70								
K+	con non-aq	25°C	100%	U	K1=3.98	1973TKb	(8197)	153
Medium: liquid SO ₂								
K+	con non-aq	25°C	100%	U	K1=2.15	1972IWa	(8198)	154
Medium: acetone								
K+	con alc/w	25°C	93.7M	U	K1=1.28	1971BPa	(8199)	155
Medium: 93.7% w/w EtOH/H ₂ O								
K+	con non-aq	25°C	100%	U	K1=1.75	1971ENa	(8200)	156
Medium: trifluoroethanol								
K+	con non-aq	25°C	100%	U	K1=2.45	1971HNb	(8201)	157
Medium: propanol								
K+	con alc/w	25°C	100%	U I	K1=0.96	1971SSb	(8202)	158
Medium:MeOH. K1=1.83 (EtOH), 2.52 (PrOH), 3.02 (BuOH), 3.58 (PentOH) 3.97 (HexOH), 4.38 (HeptOH), 4.66 (OctOH), 5.14 (NonOH).								
K+	con alc/w	25°C	100%	U I	K1=0.36	1970Bwc	(8203)	159
Medium: MeOH; K1=1.59 in EtOH								
K+	con non-aq	25°C	100%	U	K1=-1.10	1970CDa	(8204)	160
Medium: DMSO								

K+ con oth/un 55°C 0.0 U T K1=-0.14 1968ATb (8205) 161
K1=-0.20(5 C), -0.19(15,25 C), -0.15(35 C), -0.14(45 C)

K+ sol non-aq 25°C 100% U Kso=-0.5 1967AKa (8206) 162

Medium: DMF

K+ con non-aq 140°C 100% U K1=2.07 1967BNb (8207) 163
K(K+KI)=4.4

Medium: liquid I2

K+ con non-aq 25°C 100% U I K1=1.00 1967JTa (8208) 164
Medium: HOC2H4NH2. K1=2.62(EtCOMe), 1.83(PhCOMe), 3.56(pyridine), 1.09(MeCN),
2.02(PhCN), 1.98(acetone), 2.41(PrOH)

K+ dis none 25°C 0.0 U Kd(K+I=K(TBP)+I(TBP))=-1.64 1967RMe (8209) 165

With (i-amylO)2MePO: Kd=-1.57

K+ con non-aq 25°C 100% U K1=2.25 1966SAa (8210) 166
Medium: acetone

K+ con non-aq 25°C 100% U K1=2.98 1965BFb (8211) 167
Medium: diaminoethane

K+ con non-aq 25°C 100% U I K1=3.32 1964FMb (8212) 168
Medium: diaminoethane. K1=3.82(diaminopropane)

K+ con non-aq 35°C 100% U T K1=-1.29 1964JMb (8213) 169
Medium: MeCN. K1=-2.02(C), -1.05(25 C)

K+ con alc/w 25°C 100% U T K1=1.68 1961BKb (8214) 170
Medium: EtOH. K1=1.55(15 C), 1.82(40 C)

K+ con non-aq 25°C 100% U K1=2.29 1957HUa (8215) 171
Medium: PhCOMe. Alternative value K1=2.35

K+ con non-aq 25°C 100% U K1=2.67 1956HUa (8216) 172
Medium: EtCOMe

K+ con non-aq 0°C 100% U T H K1=3.52 1956LLa (8217) 173
Medium: liquid SO2. K1=3.37(-8.93 C). DH(K1)=23 kJ mol⁻¹, DS=154 J K⁻¹ mol⁻¹

K+ con non-aq -34°C 100% U K1=2.39 1949HKa (8218) 174
Medium: liquid NH3

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

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

K+ sol oth/un 25°C 3.0M U H K1=-0.28 1984DSa (8522) 175
in 3.0 M LiClO4; Also in 2.0 M LiClO4 K1=-0.40; in 4.0 M LiClO4 K1=0.04
in 1.0 M LiClO4 K1=0.

K+ EMF none 25°C 0.0 U 1973KCb (8523) 176
Kso(KL(s))=-1.64
By conductivity: Kso=-1.6

K+ EMF non-aq 25°C 100% U TI 1973KCb (8524) 177
Kso=-7.2
Medium: MeOH. By conductivity: Kso=-7.3. In DMSO: Kso=-7.7; by cond.: -7.4

K+ con none 25°C 0.0 U K1=-0.3 1971JBa (8525) 178

K+ con none 25°C 0.0 U K1=-0.24 1969BJa (8526) 179

K+ con mixed 25°C 14% U I K1=0.16 1969SHe (8527) 180
Medium: 14.3% w/w glycerol/H2O. K1=-0.08(0%), 0.35(25.7%), 0.75(32.0%),
0.88(44.5%), 1.02(58.7%), 1.33(70.2%)

K+ con diox/w 25°C 30% U I K1=0.37 1959BOa (8528) 181
Medium: dioxan/H2O, I=0 corr. K1=-0.39(0%), -0.11(9.5%), 0.16(17.9%),
0.59(37.2%), 0.89(43.8%), 1.18(49.6%), 1.57(57.1%)

K+ con none 25°C 0.0 U K1=-0.25 1956SPc (8529) 182

K+ con none 25°C 0.0 U K1=-0.23 1948MOa (8530) 183

K+ con none 18°C 0.0 U K1=-0.30 1927DAb (8531) 184

I04- HL Periodate CAS 13444-71-8 (6063)
Periodate;

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

K+ con none 25°C 0.0 U 1948MOa (8606) 185
K(K+HL)=0.24

IrCl6--- H3L (1615)
Hexachloroiridate;

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

K+ gl KCl 25°C 0.10M U T K1=1.56 1978SKc (8623) 186
Data also available when T=35, 42 and 50.
Alternative method: Kinetic studies.

MnO4- HL Permanganate CAS 13456-41-3 (5678)
Manganate(VII), Permanganate;

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

K+ ISE none 25°C 0.0 C 2003KUa (8633) 187

K(KA+L)=1.97
K(K+A(org))+L=KAL(org))=5.26

Distribution from water into 1,2-dichloroethane. K 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

K+ sp oth/un 25°C ? U M 1997STa (8737) 188

K(2K+H2L=K2L+2H)=-2.3

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

NO2- HL Nitrite CAS 7782-77-6 (635)
Nitrite;

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

K+ cal none 25°C 0.0 C IH 1992BVa (9384) 189

DH(Kso)=13.1 kJ mol⁻¹, measured for I=0.002-0.02 M self medium.
Also data for 0.047-0.228 mol fraction MeOH/H2O.

K+ con oth/un 25°C 0.0 U K1=-0.11 1964PSh (9385) 190

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

Nitrate;

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

K+ con mixed 25°C 20% C I K1=1.87 2001BSa (9717) 191

Medium: 20 % w/w ethylene carbonate/water. Data for 20-80 % w/w ethylene carbonate/water.

K+ con none 25°C 0.0 C T H K1=0.083 1988Y0a (9718) 192
Data for 0-50 C. DH(K1)=-0.5 kJ mol⁻¹, DS(K1)=0.0 J K⁻¹ mol⁻¹.

K+ con none 25°C 0.0 C I K1=-0.22 1986SDa (9719) 193
Value derived from data for 0.001-0.05 self medium.

K+ sol oth/un 25°C 1.0M U K1=0.04 1980FSb (9720) 194
In 1.0 M LiClO4; in 2.0 M K1=-0.1; in 3.0 M K1=-0.05; in 4.0 M K1=0.04
in 1.0 M LiNO3 K1=-0.7

K+ con non-aq 25°C 100% U K1=2.03 1974HPb (9721) 195
Medium: Hexamethylphosphotriamide. K=2.05 using Fuoss-Hsia equation

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K+          con non-aq 25°C 100% U          K1=1.77          1973Bmd (9722) 196
Medium: Hexamethylphosphotriamide
-----
K+          con diox/w 25°C 45% U I       K1=2.79          1972SAc (9723) 197
Medium: Dioxan/MeOH mixtures. In 0% dioxan: K1=1.26. 29.3%: 2.00.
52.6%: 3.27. 62.3%: 4.09
-----
K+          con oth/un 25°C 0.0 U          K1=-0.22         1971HPa (9724) 198
-----
K+          con oth/un 25°C 0.0 U          K1=-0.135        1971JBa (9725) 199
-----
K+          con oth/un 25°C 0.0 U          K1=-0.16         1971PJa (9726) 200
-----
K+          con oth/un 25°C 0.0 U          K1=-0.12         1969BJa (9727) 201
-----
K+          con oth/un 25°C 0.0 U          K1=-0.26         1969GUc (9728) 202
-----
K+          con diox/w 25°C 0.0 U I       K1=0.20          1969MFb (9729) 203
Also data for dioxan/H2O mixtures
-----
K+          con diox/w 25°C 65% U I       K1=1.60          1969SBe (9730) 204
In 59.8% dioxan, K1=1.18; 71.8%: 2.25; 76.3%: 2.70
-----
K+          con alc/w 25°C 100% U I       K1=1.18          1969SBe (9731) 205
In MeOH/dioxan mixtures, 43.9% MeOH: K1=3.62; 53.2%: 2.91; 61.4%: 2.44;
69.6%: 2.17
-----
K+          ISE R4N.X 25°C 0.10M U T H     K1=-0.4          1966CLb (9732) 206
Medium: Me4NCl. K1=-0.5(39 C). I=0 corr: K1=-0.15(25 C), -0.25(39 C).
DH=-13 kJ mol-1, DS=-52 J K-1 mol-1
-----
K+          con none 25°C 0.0 U          K1=0.1           1966MBb (9733) 207
-----
K+          con alc/w 25°C 83% U          K1=1.59          1963PSa (9734) 208
Medium: 83% EtOH, I=0 corr.
-----
K+          con oth/un 25°C 0.0 U          K1=-0.24         1955RSa (9735) 209
-----
K+          oth oth/un 25°C 0.0 U          K1=0.06 to -0.08 1937ROa (9736) 210
Method: Partial prssure of H2O. K1=0.06 to -0.08
-----
K+          oth oth/un 18°C 0.0 U          K1=-0.14         1927DAb (9737) 211
-----
K+          oth oth/un 18°C 0.0 U          K1=-0.11         1927ONa (9738) 212
*****
OH-
Hydroxide;          HL      Hydroxide          (57)
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values          Reference ExptNo

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 K+ nmr R4N.X 25°C 3.4M C K1=-0.8 2002PLa (11659) 213
 Method NMR K-39
 Medium: 3.4 M Me4NCl/Me4NOH

 PF6- HL (2404)
 Hexafluorophosphate;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
K+	con	non-aq	25°C	100%	U		K1=1.3	1975YKa (12765)	214

 Medium: MeCN

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
K+	gl	none	25°C	0.0	C	TI	K1=1.37 B(KHL)=13.21 B(KH2L)=19.79 B(K2L)=2.20 B(K2HL)=13.44	1991DDa (13226)	215

Data also for 10-50 C and 0.04-1.0 M NaCl, KCl or Et4NI

K+	gl	KCl	37°C	0.15M	C		K(K+HL)=0.48	1985DSa (13227)	216
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K+	gl	KNO3	25°C	0.50M	C		K1=0.54 K(K+HL)=0.36 K(K+H2L)=0.18	1983DGa (13228)	217
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K+	gl	KNO3	37°C	0.15M	C		K1=0.6 K(K+HL)=0.48 K(K+H2L)=-0.2	1983DGa (13229)	218
----	----	------	------	-------	---	--	---	-----------------	-----

K+	gl	R4N.X	25°C	0.20M	U	T HM	K(K+HL)=0.49	1956SAc (13230)	219
----	----	-------	------	-------	---	------	--------------	-----------------	-----

Medium: Pr4NCl. K=0.08(0 C). DH(K)=25 kJ mol⁻¹, DS=100 J K⁻¹ mol⁻¹

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
K+	gl	R4N.X	25°C	0.50M	U		K1=0.36	1967CMc (13414)	220

Ligand: O3POPHO2---, Medium: Me4NCl

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

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

K+ gl NaCl 25°C 0.25M U I K1=1.6 1994SFb (13603) 221
B(KHL)=9.7
B(KH2L)=15.3
B(K2L)=2.0
B(K2HL)=9.5
Medium: Me4NCl. At I=0 corr. K1=2.4, B(KHL)=11.1, B(KH2L)=17.2,
B(K2L)=3.4, B(K2HL)=11.3

K+ gl KNO3 25°C 0.10M C TIH K1=1.51 1985DRb (13604) 222
B(KHL)=9.81
B(KH2L)=15.5
B(K2L)=2.14
B(K2HL)=9.47
Data at 10-45 C and I=0.02-1.0 M. DH(K1)=-18 kJ mol⁻¹; DS=-33. DH(KHL)=-9;
DS=154. DH(K2L)=27; DS=129. DH(K2HL)=36; DS=298 (by T coeff).

K+ gl KCl 25°C 0.50M U K1=1.51 1982DNa (13605) 223
K(K+HL)=0.46

K+ gl R4N.X 25°C 0.50M C K1=1.50 1979DHa (13606) 224
K(K+HL)=0.46
K(KL+H)=7.4
K(K+H2L=KHL+H)=5.5
Medium: 0.50 M Me4NCl.

K+ cal R4N.X 5°C 1.00M U H 1973VAa (13607) 225
Medium: Me4NNO3, DH(K1)=2.9 kJ mol⁻¹. 35 C, I=0, DH(K1)=7.2

K+ gl none 25°C 0.0 U T K1=2.3 1959W0a (13608) 226
K1=2.3(40 C)

K+ gl R4N.X 25°C 1.00M U K1=0.80 1957LWa (13609) 227
Medium: Me4NCl

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

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

K+ gl R4N.X 25°C 1.00M U K1=1.01 1960CEa (13691) 228
Medium: Me4NCl

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

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

K+ gl R4N.X 25°C 1.0M U K1=1.17 1982CCb (13720) 229
K1=1.17

alpha2 isomer

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

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

K+ gl NaCl 25°C 0.25M U I K1=1.7 1994SFb (13868) 230
B(KHL)=9.9
B(KH2L)=14.7
B(KH3L)=15.7
B(K2L)=2.7

Medium: Me4NCl. B(K2HL)=9.7. At I=0 corr. K1=2.6, B(NaHL)=11.6, B(NaH2L)=
17.0, B(NaH3L)=18.1, B(Na2L)=4.4, B(Na2HL)=12.0

K+ gl KNO3 25°C 0.10M C TIH K1=1.55 1985DRb (13869) 231
B(KHL)=9.76
B(K2L)=2.81

Data at 10-45 C and I=0.02-1.0 M. DH(K1)=-9 kJ mol⁻¹; DS(K1)=-3. DH(KHL)=
-8; DS(KHL)=156. DH(K2L)=-10; DS(K2L)=17. (by T coeff)

K+ gl oth/un 25°C 0.10M U K1=2.53 1975SMa (13870) 232
B(KH(P3010))=11.64

K+ gl none 25°C 0.0 U T K1=2.8 1959W0a (13871) 233
K1=2.8(40 C)

K+ gl R4N.X 25°C 1.00M U K1=1.39 1957WLa (13872) 234
Medium: Me4NCl

P4012----- H4L CAS 13598-74-8 (234)
Cyclotetrametaphosphate;

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

K+ gl R4N.X 25°C 0.10M U K1=1.84 1976K0b (14008) 235

P4013----- H6L Tetrphosphate (1102)
Tetrphosphate;

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

K+ gl R4N.X 25°C 1.0M U K1=1.71 1967WMa (14046) 236
K(K+HL)=1.11

Medium: Me4NCl

K+ EMF oth/un 25°C dil U K1=0.5 1950WCa (14047) 237

Ligand: mostly P5016 7-. Data for many metals given but ligand uncertain

P6012----- H6L CAS 25268-83-1 (6590)
Dodecaoxohexaphosphate(III); anion of (PO.OH)₆

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

K+ gl R4N.X 25°C 1.0M U K1=1.01 1960CEa (14060) 238

P6018----- H6L (233)
Cyclohexametaphosphate;

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

K+ gl R4N.X 25°C 0.10M U K1=2.30 B2=4.30 1976KOb (14071) 239

P8024----- H8L (232)
Cyclooctametaphosphate;

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

K+ gl R4N.X 25°C 0.10M U K1=2.70 B2=4.90 1976KOb (14083) 240
B3=6.78

ReO4- HL Perrhenate (2581)
Rhenate(VII), Perrhenate;

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

K+ sol none 25°C 0.0 C Kso(KReO4)=-2.59
1988HHb (14101) 241

Method: perrhenate ion selective electrode.

K+ con oth/un 18°C 0.0 U K1=1.2 1963SKa (14102) 242

K+ oth none 25°C 0.0 U K1=0.72 1948MOa (14103) 243

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

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

K+ cal none 25°C 0.0 C IH 1992BVa (15112) 244
DH(Kso)=24.2 kJ mol⁻¹, measured for I=0.002-0.02 M self medium.
Also data for 0.047-0.228 mol fraction MeOH/H₂O.

K+ con non-aq 25°C 100% C K1=0.734 1990SAb (15113) 245
Medium: propylene carbonate.

K+ con non-aq 25°C 100% U K1=1.60 1978CAa (15114) 246
Medium: Acetonitrile

 K+ con non-aq 25°C 100% U 1976DCa (15115) 247
 K(KA+NCS)=2.00
 In nitrobenzene. In 70% C6H5NO2/30% toluene, K=3.40, in 50%/50%, K=4.00
 A=Dinitro-18-crown-6.

K+ con non-aq 25°C 100% U K1=1.86 1976RMa (15116) 248
 Medium: 3-methylsulfonate

K+ con non-aq 25°C 100% U I K1=0.85 1976RMb (15117) 249
 Medium: 1,3-Dimethylethyleneurea. In 1,3-Dimethylpropyleneurea K1=-0.078

K+ con non-aq 25°C 100% U K1=1.36 1973GKb (15118) 250
 Medium: MeCN, I=0 corr

K+ con non-aq 25°C 100% U K1=0.5 1973JYa (15119) 251
 Medium: propene carbonate, I=0 corr

K+ con non-aq 25°C 100% U K1=4.33 1973TKb (15120) 252
 Medium: Liquid SO2, I=0 corr

K+ con non-aq 25°C 100% U K1=0.15 1971PGa (15121) 253
 Medium: MeHNCHO

K+ con non-aq 25°C 100% U K1=1.41 1970YKb (15122) 254
 Medium: MeCN, I=0 corr

K+ con non-aq 25°C 100% U K1=1.3 1967SCa (15123) 255
 Medium: NC(CH2)4CN

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
K+	gl	R4N.X	25°C	1.0M	C		K1=0.22	1997CHa (15465)	256

Medium: 1.0 M Me4NCl.

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
K+	con	none	25°C	0.0	C	H	K1=0.91	1989Y0a (16267)	257

Data for 0-50 C. DH(K1)=2.4 kJ mol⁻¹, DS(K1)=25.7 J K⁻¹ mol⁻¹.

K+	EMF	KCl	25°C	1.0M	C		K1=0.27	1988M0c (16268)	258
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Method: Pt/H2 electrode. Data for 25-200 C.

K+	sol	oth/un	25°C	3.0M	U		K1=-0.51	1984DSa (16269)	259
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in 3.0 M LiClO₄;

K+ gl NaCl 37°C 0.10M C I K1=0.54 1982DRb (16270) 260
Data for I=0.03-0.50 M NaCl. At I=0.0 M, K1=0.87

K+ oth oth/un 25°C 0.50M U TI K1=0.85 1980GAb (16271) 261
Method: Ultrasonic absorption. Medium: Na₂SO₄

K+ con none 25°C 0.0 U K(K+KSO₄)=0.093 1978FFa (16272) 262

K+ con none 25°C 0.0 C K1=1.02 1977FFa (16273) 263
P=1 atm. Also data for P=250-2000 atm.

K+ sol oth/un 25°C 0.70M C K1=0.265 1975EWa (16274) 264
Mixed medium of NaCl, KCl, MgCl₂, NaClO₄, Mg(ClO₄)₂, Na₂SO₄.
Method: solubility of gypsum.

K+ oth none 25°C 0.0 U T K1=0.84 1969HEa (16275) 265
Estimated from literature data. K1=1.00 (50 C), 1.06 (60 C), 1.30 (100 C),
1.60 (150 C); 1.94 (200 C)

K+ cal none 25°C 0.0 U H K1=0.75 1969IEa (16276) 266
DH(K1)=4.22 kJ mol⁻¹, DS(K1)=0 (?)

K+ ISE R4N.X 39°C 0.10M U TI K1=0.5 1966CLb (16277) 267
Medium: Me₄NCl. K1=0.4(25 C). At I=0 corr: K1=0.85(25 C), 0.95(39 C).
DH(K1)=12 kJ mol⁻¹, DS=59 J K⁻¹ mol⁻¹

K+ ISE R4N.X 25°C 0.10M U T K1=0.52 1966CLb (16278) 268
Ligand: peroxodisulfate, S₂O₈²⁻, not SO₄²⁻. Medium: Me₄NCl. K1=0.56(39 C).
At I=0 corr: K1=0.92(25 C), 0.97(39 C); DH(K1)=8 kJ mol⁻¹, DS=42 J K⁻¹ mol⁻¹

K+ con oth/un 700°C 0.0 U T K(K+HL)=4.3 1966QMa (16279) 269
Medium:0 corr. p=0.40 g cm⁻³. K=1.16(p=0.70,400 C), 3.25(p=0.40,400 C),
1.95(p=0.7,700 C), also for many other p and T

K+ con oth/un 100°C 0.0 U T K1=1.3 1963QFa (16280) 270
K1=1.96(200 C), 1.35(300 C,density 1.0), 1.5(300 C,density 0.8)

K+ con diox/w 35°C 10% U I K1=0.9 1959DDa (16281) 271
I=0 corr. K1=1.0(20% dioxan), 1.3(30%)

K+ con oth/un 25°C 0.0 U K1=0.96 1950JMa (16282) 272

K+ con oth/un 18°C 0.0 U K1=0.82 1930RDa (16283) 273

S2O3²⁻ H2L Thiosulfate CAS 73686-28-7 (177)

Thiosulfate;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
K+	cal	R4N.X	25°C	0.50M	U		K1=0.26	1997MKa (16862)	274
DH(K1)=8.0 kJ mol ⁻¹									
K+	cal	oth/un	25°C	0.50M	U	H	K1=0.28	1974ARa (16863)	275
DH=8.20 kJ mol ⁻¹ .									
K+	con	alc/w	25°C	44%	U		K1=1.93	1956BMa (16864)	276
Medium: 44% EtOH									
K+	sp	alc/w	25°C	50%	U		K1=2.34	1956TMa (16865)	277
Medium: 50% EtOH									
K+	sp	none	25°C	0.0	U	T	K1=0.85	1955GMa (16866)	278
K1=0.85(15 C)									
K+	sol	none	25°C	0.0	U		K1=0.92	1951DMb (16867)	279

S207--				L	Pyrosulfate		CAS 16057-15-1	(8430)	
Pyrosulfate;									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
K+	con	none	25°C	0.0	C	T H	K1=1.66	1996DPc (16918)	280
Data for 30-40 C. DH(K1)=10.2 kJ mol ⁻¹ , DS(K1)=66 J K ⁻¹ mol ⁻¹ .									

SeO4--				H2L	Selenate		CAS 7783-08-6	(459)	
Selenate;									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
K+	oth	oth/un	25°C	var	C			19990Ca (17104)	281
							Kso(K2SeO4)=0.902		
Method: osmotic coefficients. Medium: 1.1-4.7 m K2SeO4									

SiO3--				H2L	Silicate		CAS 7699-41-4	(747)	
Silicate; SiO2(OH)2--									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
K+	oth	none	150°C	0.0	U	T		1969HEa (17213)	282
							*Ks(KAlSi2O6+4H)=4.70		
Method: est. data. *Ks=-1.14(microcline), -2.31(adularia), -1.25(highsanidine)									
3.80(KAl3Si3O10(OH)2); -2.37(mantmorillanite). also other data, 60-300 C									

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
K+	gl	R4N.X	25°C	1.0M	U		K1=1.17	1982CCb (17236)	283

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
K+	con	oth/un	18°C	0.0	U		K1=0.91	1963SKa (17248)	284
K+	oth	oth/un	25°C	0.0	U			1953CSa (17249)	285
							Kso=-0.89		

Method: Estimated value

 V04--- H3L CAS 15457-75-7 (1586)
 Vanadate; V02(OH)3-- or polymers

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
K+	gl	NaClO4	25°C	1.00M	U			1975KIC (17379)	286
							K(K+H7PV12036)=2.42		

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
K+	gl	R4N.X	20°C	1.0M	U	I	K1=0.04	1963SGd (17380)	287
Medium: Me4NCl. In 0.1 M Me4NCl: K(K+H15L10)=1.4, K(K+H14L10)=2.4, K(K+KH14L10)=1.0									

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
K+	con	non-aq	30°C	100%	U		K1=6.94	1954JGa (17620)	288
Medium: ethanoic acid									

CH4O3S			HL				CAS 75-75-2	(595)	
Methanesulfonic acid; CH3.SO3H									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
K+	con	mixed	25°C	20%	C	I	K1=1.77	2001BSa (17938)	289
Medium: 20 % w/w ethylene carbonate/water. Data for 20-80 % w/w ethylene carbonate/water.									
K+	con	mixed	25°C	20%	C		K1=2.06	1994SSb (17939)	290
Medium: 20% w/w propylene carbonate/ethylene carbonate.									

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
K+	gl	R4N.X	25°C	0.10M	U			K1=0.34	1972WFa (18148)	291
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
K+	gl	R4N.X	25°C	0.50M	U			K1=1.02 K(K+HL)=0.2	1967CIa (18283)	292
Medium: Me4NCl										

		C2H2O4		H2L	Oxalic acid			CAS 144-62-7	(24)	
Ethanedioic acid; (COOH)2										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
K+	gl	NaCl	25°C	0.04M	C	TIH		K1=0.43 B(KHL)=3.60	1992DDb (18932)	293
DH(K1)=14 kJ mol ⁻¹ , DS(K1)=56 J K ⁻¹ mol ⁻¹ ; DH(KHL)=8, DS(KHL)=96. Data for 0.04-1.0 M NaCl and 10-45 C. At I=0.0 M, K1=0.71.										

K+	gl	KCl	37°C	0.15M	C			K1=0.41	1985DSa (18933)	294

K+	gl	KNO3	37°C	0.15M	C	IH		K1=0.41	1983DRb (18934)	295
Method: determination of protonation constant in KNO3 and [Et4N]NO3 media Data for I=0.0-1.0 M KNO3. At I=0.0, K1=0.81; DH(K1)=4.2 kJ mol ⁻¹ , DS=29										

K+	gl	KNO3	37°C	0.10M	C			K1=0.43	1981DRa (18935)	296
Calculated from protonation data for I=0.03-0.3 M KNO3										

K+	sol	KNO3	37°C	dil	C			K1=1.00	1979TNa (18936)	297
Method: solubility in 0.03-0.30 M KCl or NaCl. At I=0.0 M: Kso(CaL.3H2O)=-8.10; Kso(CaL.H2O)=-8.69.										

		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
K+	gl	R4N.X	25°C	0.25M	C	TIH		K1=-0.43	1985DRa (20011)	298
I=0.02-1 M Et4NI. 10-45 C. DH = 5 kJ mol ⁻¹										

K+	gl	R4N.X	25°C	0.16M	U	TI		K1=-0.43	1985RSa (20012)	299
At 10 C: K1=-0.32 (I=0.04); 35 C: -0.35 (I=0.25); 45 C: -0.18 (I=0.16)										

K+	gl	non-aq	25°C	100%	U	H		K1=6.18	1981TMb (20013)	300
Medium: Glacial acetic acid. Alternative method: Spectrophotometry.										

DH(K1)=-19.0 kJ mol⁻¹

K+ gl non-aq 25°C 100% U K1=6.11 1964KLa (20014) 301
Medium: ethanoic acid

K+ sp non-aq 25°C 100% U K1=6.93 1961PSa (20015) 302
Medium: ethanoic acid

K+ EMF non-aq 25°C 100% U K1=6.15 1956BKa (20016) 303
Method: chloranil electrode. Medium: ethanoic acid

K+ con non-aq 30°C 100% U K1=6.44 1954JGa (20017) 304
Medium: ethanoic acid

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

K+ gl R4N.X 37°C 0.25M C TI B(KHL)=8.78 1985DRa (21591) 305

Medium: 0.02-1 M NEt4I

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

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

K+ ISE non-aq 25°C 100% M K1=0.46 B2=0.36 1988NHa (22103) 306
Medium: MeCN, 0.01 M Et4NClO4

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

K+ gl R4N.X 25°C 0.50M U K1=1.2 1967CIa (23269) 307
K(K+HL)=0.28

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

K+ gl KCl 25°C 0.15M M I K1=1.73 1987MKb (23377) 308
K(K+HL)=1.60
K(K+H2L)=1.57

for 0.3 M KCl K1=1.10; K(K+HL)=1.02; K(K+H2L)=0.98

for 0.5 M KCl K1=0.73; K(K+HL)=0.66; K(K+H2L)=0.64

K+ gl R4N.X 25°C 0.10M U 1972WFa (23378) 309
K(K+HL)=0.62
B(2K+L)=2.04

Medium: (CH3)4NC1

K+ gl R4N.X 25°C 0.50M U K1=1.79 1967CIa (23379) 310
K(K+HL)=0.36

Medium: Me4NC1

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

K+ gl KNO3 20°C 1.89M M I K1=0.60 1999JDa (24472) 311
B(KHL)=5.98
B(K2L)=0.54

Also data for I=1.64 and 1.52 M.

K+ gl R4N.X 25°C 0.25M C TIH K1=0.68 1985DRa (24473) 312
B(KHL)=5.31

I=0.02-1 M Et4NI.T=10-45. DH(K1)=4;DH(KHL)=11 kJ mol⁻¹. DS1=33; DS(KHL)=148

K+ gl KNO3 37°C 0.15M C IH K1=0.44 B2= 0.67 1983DRb (24474) 313
Method: determination of protonation constant in KNO3 and [Et4N]NO3 media
Data for I=0.0-1.0 M KNO3. At I=0.0, K1=0.85; DH(K1)=4.2 kJ mol⁻¹, DS=30

K+ gl KNO3 37°C 0.15M C K1=0.44 1982DRa (24475) 314
K(K+HL)=0.2

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

K+ ISE non-aq 25°C 100% M K1=0.18 B2=0.04 1988NHa (25658) 315
Medium: MeCN, 0.01 M Et4NC1O4

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

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

K+ gl R4N.X 25°C 0.25M U K1=1.08 1957WBa (27302) 316
Medium: 0.1-0.4 M (C3H7)4NI

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
K+	gl	R4N.X	25°C	0.25M	U		K1=1.18	1957WBa (27331)	317
Medium: 0.1-0.4 M (C3H7)4NI									

		C3H10O6P2		H4L			(3556)		
Propane-2,2-diphosphonic acid; CH3.C(P03H2)2.CH3									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
K+	gl	R4N.X	25°C	0.50M	U		K1=1.60 K(K+HL)=0.35	1967CIa (28400)	318
Medium: Me4NCl									

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
K+	sp	non-aq	?	100%	U		K(KSCN+L)=-0.68 K(2KSCN+L=(KSCN)2L)=0.84	1971TGa (28621)	319
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
K+	gl	R4N.X	25°C	0.25M	C	TI	K1=0.84 B(KHL)=6.0	1985DRa (29090)	320
I=0.02-1 M Et4NI. Also 37 C									

K+	gl	KNO3	37°C	0.15M	C	IH	K1=0.48	1983DRb (29091)	321
Method: determination of protonation constant in KNO3 and [Et4N]NO3 media									
Data for I=0.0-1.0 M KNO3. At I=0.0, K1=0.83; DH(K1)=4.2 kJ mol ⁻¹ , DS=30									

		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
K+	gl	R4N.X	25°C	0.25M	C	TIH	K1=0.48 B(KHL)=5.28	1985DRa (29981)	322
I=0.02-1M Et4NI.T=15-45 C. DH(K1)=4; DH(KHL)=3 kJ mol ⁻¹ . DS1=30; DS(KHL)=121									

K+	gl	KNO3	37°C	0.15M	C	IH	K1=0.11 B2= 0.11	1983DRb (29982)	323
Method: determination of protonation constant in KNO3 and [Et4N]NO3 media									
Data for I=0.0-1.0 M KNO3. At I=0.0, K1=0.53; DH(K1)=4.2 kJ mol ⁻¹ , DS=24									

C4H604S H2L Thiodiacetic CAS 123-93-3 (140)
2,2'-Thiodiglycolic acid, Thiodiethanoic acid; HOOC.CH2.S.CH2.COOH

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

K+ gl R4N.X 25°C 0.25M C I K1=0.32 1987DDd (30220) 324
B(KHL)=4.07

Medium: 0.012-0.975 Et4NI. At I=0.0 M, K1=0.78, B(KHL)=4.6

C4H605 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

K+ gl R4N.X 25°C 0.25M C TIH K1=0.38 1985DRa (30653) 325
B(KHL)=4.5

0.02-1 M NEt4I. 10-37 C. DH1=1; DH(KHL)=3 kJ mol-1. DS1=17; DS(KHL)=107

K+ gl KNO3 37°C 0.15M C K1=0.11 B2= 0.01 1983DRb (30654) 326
Method: determination of protonation constant in KNO3 and [Et4N]NO3 media
Data for I=0.0-1.0 M KNO3. At I=0.0, K1=0.45; DH(K1)=4.2 kJ mol-1, DS=23

K+ ISE oth/un 25°C 0.10M U K1=0.18 1964RZa (30655) 327

K+ gl R4N.X ? 0.28M U K1=0.23 1963EDa (30656) 328
Medium: Me4NBr

C4H605 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

K+ gl oth/un 25°C 0.0 C I K1=0.62 1999DGa (30886) 329
B(KHL)=4.04

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

K+ gl R4N.X 25°C 0.25M C TIH K1=0.25 1985DRa (30887) 330
B(KHL)=3.5

0.02-1 M NEt4I. 12.5-48 C. DH(K1)=9 kJ mol-1, DS=42; DH(KHL)=5, DS=94

C4H606 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

K+ gl R4N.X 25°C 0.1M U IH K1=0.48 2005ZZa (30976) 331
Medium: Et4NCl; L or D isomer is not specified. For 0.3 mol/L K1=0.20

C4H606 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

K+ ISE R4N.X 25°C 0.20M U K1=0.0 1972DMc (31286) 332
K(K+HL)=-0.2

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

K+ nmr R4N.X 37°C 0.25M C K(K+HL)=-0.3 2002CFb (34638) 333
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

K+ con non-aq 25°C 100% U K1=2.30 1974ESa (34658) 334
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

K+ con non-aq 25°C 100% C K1=3.6 1992MSe (34701) 335
Medium: 100% MeOH. Anion: picrate. Also data for nitrophenolate anions.

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

K+ sp non-aq 25°C 100% U K1=1.399 1984AMa (38000) 336
In Dimethyl Sulfoxide (DMSO);
Data also for other di- and triketones and esters and their alkali enolates

K+ gl diox/w 30°C 75% U K1=5.60 B2=9.87 1975MMa (38001) 337

K+ gl alc/w 25°C 100% U I K1=0.9 1965LIa (38002) 338
Medium: MeOH, 0.1 M KI. In EtOH, 0.1 M KSCN: K1=2.1

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

 K+ dis non-aq 25°C 100% C K1=2.97 1999KKb (42111) 339
 Medium: MIBK. Method: distribution of metal picrates into MIBK
 containing HO(CH2.CH2.O)n.C12H25, n=4, 6 or 8.

K+ con non-aq 25°C 100% C T K1=2.58 1999VMa (42112) 340
 Medium: 2-methoxyethanol. Data for 15-35 C.

K+ oth oth/un 25°C 0.04M C K1=0.15 1998TIa (42113) 341
 Method: capillary electrophoresis.
 Medium: 0.005 M phosphate buffer, pH 7.1, 0.04 M MCl.

K+ dis oth/un 25°C dil C K(KA+L)=4.76 1998TKa (42114) 342
 Self medium, I<0.03 M. Method: Extraction of KAL into dichloromethane.
 A is 18-crown-6.

K+ sol none 25°C 0.0 C I Kso(KL)=-3.39 1979LPf (42115) 343
 Method: spectrophotometry. Also data for 10-100% w/w MeOH/H2O.

K+ con none 30°C 0.0 U I M K1=1.42 1979PSa (42116) 344
 K(KL+2Trien-glycol)=1.39
 K(KL+2Tetraen-glycol)=1.44

K+ sp non-aq 20°C 100% U K1=4.6 1978JId (42117) 345
 Medium: CH2Cl2

K+ dis none 25°C 0.00 U I K1=1.64 1972Iwc (42118) 346
 In nitrobenzene: K1=2.92

K+ con none 25°C 0.00 M K1=1.64 1971YIa (42119) 347

K+ dis oth/un 25°C var U K1=2.4 1970SSb (42120) 348
 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
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K+ con non-aq 25°C 100% U K1=1.94 1973FGa (42230) 349
 Medium: tetrahydrofuran

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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K+ sp non-aq 20°C 100% U K1=4.6 1978JId (42243) 350

Medium: CH2Cl2

C6H4N2O5 HL CAS 329-71-5 (1941)
2,6-Dinitrophenol; HO.C6H3(NO2)2

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

K+ sp non-aq 20°C 100% U K1=4.7 1978JId (42247) 351

Medium: CH2Cl2

C6H4O3Cl2S HL CAS 88-42-6 (594)
2,5-Dichlorobenzenesulfonic acid; HO3S.C6H3(Cl)2

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

K+ con mixed 25°C 20% C K1=2.14 1994SSb (42294) 352

Medium: 20% w/w propylene carbonate/ethylene carbonate.

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

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

K+ gl oth/un 25°C 0.0 C I K1=1.39 1994DFc (45566) 353

B(KHL)=7.27
B(KH2L)=11.50
B(K2L)=1.75
B(K2HL)=6.66

Values at I=0 calculated from data for 0.04-1.0 M KCl.

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

K+ gl R4N.X 25°C 0.1M U IH K1=0.84 2005ZZa (46144) 354

K(2K+L)=1.09
K(2Na+L)=0.92

Mediumt: Et4NCl. For 0.3 mol/L K1=0.72;

K+ gl oth/un 25°C 0.0 C I K1=1.42 1999DGa (46145) 355

B(KHL)=7.13
B(KH2L)=11.3
B(K2HL)=7.0
B(K2L)=1.93

Medium: artificial seawater. Extrapolated from data for 5-45% salinity.
B(NaKL)=2.47, B(NaKHL)=7.3.

K+ ISE none 25°C 0 C I K1=1.42 1995RGa (46146) 356
B(K2L)=1.95
I=0.1 (Me4N.X) K1=0.92, B(K2L)=1.11; I=0.16 (Me4N.X) K1=0.87, B(K2L)=1.04.

 K+ gl KNO3 37°C 0.15M U H K1=0.56 1980DRa (46147) 357
 B(KHL)=5.5
 At 25C and zero ionic strength, DH1=5.44 kJ mol⁻¹

K+ ISE oth/un 25°C 0.10M U K1=0.59 1964RZa (46148) 358

K+ sp R4N.X 25°C 0.10M C K1=0.43 1961WAa (46149) 359
 Medium: 0.16 M Me4NCl.

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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K+ gl KNO3 25°C 0.10M C TIH T K1=0.79 1985DRb (46868) 360
 B(KHL)=9.86
 Data at 10-45 C and I=0.02-1.0 M in KNO3. DH(K1)=17 kJ mol⁻¹; DS=(K1)=70.
 DH(KHL)=-3; DS(KHL)=176 (by T coeff.)

K+ sp R4N.X 25°C 0.10M C K1=0.47 1985HAd (46869) 361

 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
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K+ gl R4N.X 37°C 0.25M C B(KHL)=8.44 1985DRa (47571) 362
 Medium: NEt4I

 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
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K+ con non-aq 25°C 100% C K1=3.6 1992MSe (51049) 363
 Medium: 100% MeOH. Anion: picrate. Also data for nitrophenolate anions.

K+ cal non-aq 25°C 100% U IH K1=0.34 1991TNa (51050) 364
 Medium: MeOH. DH(K1)=-24.5 kJ mol⁻¹; TDS=-25.0. In MeCN: K1=0.71

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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K+ con non-aq 25°C 100% U M K1=2.46 1976FGb (51296) 365
 K(KA+L)=1.30
 A=Tetra-n-butylammonium-2,4-dinitrophenolate. Medium: Tetrahydrofuran

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

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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
K+         gl  R4N.X  25°C 0.10M U      K1=2.58      1991BSa (51536) 366
                                  B(KHL)=11.46
                                  B(KH2L)=18.06
                                  B(K2L)=3.84

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*****
C6H16O3P2          L              (2075)
Di(dimethylphosphinylmethyl) ether; Me2P(O)CH2.O.CH2.P(O)Me2

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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
K+         con non-aq 25°C 100% U      K1=2.26      1989K Sa (51771) 367
Medium: tetrahydrofuran/CHCl3 4:1 (vol)

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K+         con non-aq 25°C 100% U      K1=2.26      1982Y Sa (51772) 368
Medium: tetrahydrofuran+CHCl3 4:1(vol); M is 2,4-dinitrophenolate

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

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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
K+         ISE non-aq 25°C 100% M      K1=0.84      B2=1.00      1988NHa (51980) 369
Medium: MeCN, 0.01 M Et4NC104

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*****
C6H18O3Si3        L              CAS 541-05-9 (1283)
Hexamethyl cyclotrisiloxane; ((CH3)2SiO)3

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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
K+         con alc/w 25°C 100% U      K1=< -0.3      19800Pa (52215) 370
Medium: MeOH, 0.1 M Me4NBr

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*****
C7H6O3           H2L      Salicylic acid  CAS 69-72-7 (14)
2-Hydroxybenzoic acid, Salicylic acid; HO.C6H4.COOH

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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
K+         gl  R4N.X  25°C 0.25M C TIH    K1=-0.5      1985DRa (54240) 371
I=0.02-1 M Et4NI. 10-45 C. DH = 8 kJ mol-1

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*****
C7H6O4           H3L              CAS 303-38-8 (1398)
2,3-Dihydroxybenzoic acid; C6H3(OH)2.COOH

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

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K+ gl NaClO4 25°C 0 C I K1=1.19 1992CRa (54467) 372
K(K+KL)=-0.01
K(K+HL)=0.54

Extrapolated to I=0 from I=0.04 to I=0.81

C7H8O3S HL CAS 6192-52-5 (561)
4-Toluenesulfonic acid; CH3.C6H4.SO3H

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

K+ con mixed 25°C 20% C I K1=1.95 2001BSa (56119) 373
Medium: 20 % w/w ethylene carbonate/water. Data for 20-80 % w/w ethylene carbonate/water.

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

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

K+ sp non-aq ? 100% U 1971TGa (58396) 374
K(KSCN+L=(KSCN)L)=-0.11
K(2KSCN+L=(KSCN)2L)=0.99

Medium: CH3CN

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

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

K+ sp non-aq 20°C 100% U K1=2.72 1992PSa (58513) 375
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

K+ dis non-aq 25°C 100% C M 2002IIa (58634) 376
K(KL+phen)=3.41
K(KL+2(phen))=5.74

Medium: chlorobenzene. For extraction from 0.10 M KCl:

K(K+HL(o)=KL(o)+H)=-12.21; K(K+HL(o)+phen(o)=KL(phen)(o)+H)=-8.75.

K+ gl alc/w 25°C 100% U I K1=1.6 1965LIa (58635) 377

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

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
K+	gl	R4N.X	25°C	0.25M	C	TIH	K1=0.83 B(KHL)=5.16	1985DRa (58976)	378
0.02-1 M NEt4I. 10-37 C. DH(K1)=1 kJ mol-1, DS=25; DH(KHL)=8, DS=134									
K+	gl	KNO3	37°C	0.15M	C	IH	K1=0.41 B2= 0.19	1983DRb (58977)	379
Method: determination of protonation constant in KNO3 and [Et4N]NO3 media Data for I=0.0-1.0 M KNO3. At I=0.0, K1=0.76; DH(K1)=3.8 kJ mol-1, DS=26 *****									
C8H8		L					CAS 629-20-9	(2539)	
1,3,5,7-Cyclooctatetraene; cyclo(-CH:CH.CH:CH.CH:CH.CH:CH-)									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
K+	nmr	non-aq	23°C	100%	U		K1=2.66	1976SCa (59248)	380

C8H8O3		HL				Phenoxyacetic	CAS 122-59-8	(1153)	
Phenoxyethanoic acid; C6H5.O.CH2.CO0H									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
K+	gl	none	25°C	0.0	C	TIH	K1=-0.01	1985CDb (60037)	381
Calculated from protonation data for I=0.04-0.9 M KCl. Data for 10-45 C. DH(K1)=1.0 kJ mol-1, DS(K1)=4 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
K+	cal	R4N.X	20°C	0.1M	C			1976ANb (60633)	382
DH1= -1.67 kJ/mol in Me4NCl									
K+	gl	KNO3	39°C	0.10M	U	TIH	K1=0.70	1963IFb (60634)	383
K1=1.23(20 C),1.00(27 C),0.81(34 C), DH(K1)=-49.3 kJ mol-1, DS=-146 J K-1m-1 At I=0 corr:K1=1.94(20 C) *****									
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
K+	oth	diox/w	25°C	75%	U		K1=3.34 B2=7.17	1979MMa (61303)	384

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

K+ gl alc/w 25°C 100% U I K1=0.8 1965LIa (61685) 385
Medium: MeOH, 0.1 M KI. In EtOH, 0.1 M KSCN: K1=1.8

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

K+ ISE alc/w 25°C 100% C I T K1=1.60 B2= 2.10 2003ADa (62670) 386
IUPAC Tentative. Medium: 0-0.1 M. In PC K1=2.08

K+ oth oth/un 25°C U K1=-0.06 2000MTa (62671) 387
Method: capillary zone electrophoresis.
Medium: 0.005 M H3BO3/Me4NOH, pH 9.2.

K+ cal non-aq 25°C 100% C H K1=0.68 B2= 1.18 19960Ka (62672) 388
Medium: DMF, 0.10 M Et4NCl. DH(K1)=-19.5 kJ mol⁻¹, DS(K1)=-52 J K⁻¹ mol⁻¹;
DH(K2)=6, DS(K2)=29.

K+ con alc/w 25°C 100% U I K1=1.408 1995DSb (62673) 389
Medium : MeOH. In MeCN K1=2.231

K+ con non-aq 25°C 100% U K1=3.1 1993EVa (62674) 390
Medium: THF+CHCl3 (4:1 vol)

K+ ISE non-aq 25°C 100% M IH K1=2.02 B2=4.67 1988BUa (62675) 391
Medium: propylene carbonate (also CH3CN), 0.05 M (CH3CH2)4NClO4.
DH(K1)=-14.6, DH(K2)=-8.7 kJ mol⁻¹; DS(K1)=-10.4, DS(K2)=21.5 J K⁻¹ mol⁻¹

K+ con non-aq 25°C 100% C K1=1.73 B2= 2.59 1987ZBb (62676) 392
Medium: MeOH.

K+ nmr alc/w 30°C 100% U K1=1.7 B2=2.4 1983AAa (62677) 393

K+ ISE alc/w 25°C 100% U K1=1.74 1983GGa (62678) 394
Medium: MeOH

K+ gl alc/w 25°C 100% U H T K1=1.59 B2=2.18 1982MRa (62679) 395
Medium: MeOH. DH(K1)=23.0 kJ mol⁻¹

K+ ISE alc/w 25°C 100% U T K1=1.58 B2=1.73 1982MYc (62680) 396
Medium: MeOH

K+ vlt non-aq 25°C 100% U K1=2.15 1980MDa (62681) 397
Medium: propylene carbonate

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
K+	con	non-aq	25°C	100%	U	I		K1=2.4	1993EVa (62986)	398

Medium: THF+CHCl3 4:1(vol). In 100% THF: K1=2.2

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
K+	con	non-aq	25°C	100%	C			K1=3.7	1992MSe (63003)	399

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

C8H20N4	L	Cyclen	CAS 294-90-6	(10)						
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1,4,7,10-Tetraazacyclododecane; cyclo(-(NH.CH2.CH2.)4-)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
K+	EMF	non-aq	25°C	100%	U	I		K1=2.90	1996WPa (63293)	400

Medium: acetonitrile, 0.05 M NEt4ClO4. In propylene carbonate K1=4.8; in dimethylformamide K1<2

C8H20O4P2	L		CAS 86536-56-3	(2076)						
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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
K+	con	non-aq	25°C	100%	U			K1=3.15	1989KSa (63310)	401

Medium: tetrahydrofuran/CHCl3 4:1 (vol)

C9H6O4	HL	Ninhydrin	CAS 485-47-2	(2536)						
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1,2,3-Indantrione monohydrate, Trioxohydrindene monohydrate;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
K+	nmr	non-aq	25°C	100%	U	I		K1=1.85	1976AFa (63951)	402

Medium: Hexamethylphosphoramide. Data also for a variety of mixed media

C9H11N3O7	H3L		(3877)							
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N-(1-Methyl-2,4,6-trioxo-perhydropyrimidinyl)iminodiethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
K+	gl	R4N.X	20°C	0.10M	U			K1=1.11	1963IFb (66525)	403

Medium: Me4NNO3

C9H11O2F5	HL		CAS 2145-68-8	(1251)						
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1,1,1,2,2-Pentafluoro-6,6-dimethyl-3,5-heptanedione;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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 K+ oth diox/w 25°C 75% U K1=3.67 B2=7.30 1979MMa (66535) 404

 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

K+ gl diox/w 30°C 75% U K1=3.86 B2=7.45 1975MMa (67745) 405

 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

K+ con alc/w 25°C 100% U K1=<-0.3 1980Pa (67967) 406
 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

K+ con non-aq 22°C 100% U K1=0.88 1981SKd (68122) 407
 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

K+ sp non-aq ? 100% U 1971TGa (68419) 408
 K(KSCN+L)=-0.42
 K(2KSCN+L=(KSCN)2L)=0.9
 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

K+ gl none 25°C 0.0 C 1990CDc (68517) 409
 B(KH3L)=14.33
 B(K2L)=3.4
 B(K2HL)=8.8
 B(K2H2L)=12.8
 Additional technique: spectrophotometry. Kso(KH3L)=-17.18.

K+ gl R4N.X 25°C 0.25M C I 1990DDb (68518) 410
 B(KHL)=6.15

B(KH2L)=9.95
B(KH3L)=12.20
B(K2HL)=5.9

Medium: 0.25 M Et4NI. Data for 0.08-0.99 M. B(K2L)=1.2

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

K+ gl alc/w 25°C 100% U I K1=1.2 1965LIa (70738) 411
Medium: MeOH, 0.1 M KI. In EtOH, 0.1 M KSCN: K1=2.4

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

K+ oth diox/w 25°C 75% U K1=3.61 B2=7.30 1979MMa (71110) 412

C10H13NO3 H3L (3912)
1,3-Dimethyluramil-N,N-diethanoic acid;

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

K+ gl R4N.X 20°C 0.10M U K1=0.94 1963IFb (71805) 413
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

K+ gl R4N.X 25°C 0.10M C TI R K1=0.70 1991SMa (72455) 414
IUPAC evaluation. 37 C, 0.15 NaCl: K1=0.36

K+ ISE oth/un 25°C 0.0 C K1=1.91 1976KRb (72456) 415
Method: K 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

K+ gl R4N.X 25°C 0.10M C TI R K1=1.00 1991SMa (72985) 416
IUPAC evaluation

K+ ISE oth/un 25°C 0.20M U K1=0.67 1954MEa (72986) 417

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
K+	gl	R4N.X	25°C	0.15M	M			K1=1.60 K(KL+H)=10.32 K(KHL+H)=6.05	1993CRa (73889)	418

Medium: 0.15 M Me4NCl.

K+	gl	mixed	25°C	0.10M	U			K1=1.41	1991SBa (73890)	419
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Medium: 0.34 mol parts CH3CN/H2O, 0.1 M R4NX

K+	gl	KNO3	25°C	0.10M	C	TIH		K1=0.80	1985DRb (73891)	420
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Data at 10-45 C and I=0.02-1.0 M in KNO3. DH(K1)=5 kJ mol⁻¹; DS=30.

K+	gl	R4N.X	25°C	0.10M	U	I	T	K1=0.55	1968WSa (73892)	421
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Medium: (CH3)4NCl. I=1.0: K1=0.69

K+	gl	oth/un	25°C	0.32M	U			K1=0.96 K(K+HL)=-0.31	1965BCa (73893)	422
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Medium: CsCl

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
K+	gl	R4N.X	25°C	0.10M	C	IH	R	K1=1.17	1991SMa (74741)	423

IUPAC evaluation. DH(K1)=1.3 kJ mol⁻¹ (tentative)

K+	gl	oth/un	25°C	0.25M	U	H		K1=1.20 B(KHL)=6.58	1986RSa (74742)	424
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K+	gl	R4N.X	25°C	0.10M	U	H		K1=1.42	1981CMd (74743)	425
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Method: effect of Na on ligand protonation.
By calorimetry, DH(K1)=1.3 kJ mol⁻¹, DS(K1)=33 J K⁻¹ mol⁻¹.

K+	ISE	oth/un	25°C	0.01M	U			K1=1.95	1971MEb (74744)	426
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K+	ISE	oth/un	25°C	0.0	U			K1=2.35	1970MRb (74745)	427
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Method: K-glass electrode. Using a valinomycin electrode, K1=2.34

K+	ISE	oth/un	25°C	0.0	U			K1=2.34	1970RMb (74746)	428
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K+	gl	oth/un	25°C	0.32M	U			K1=0.9 B2=0.70 K(K+HL)=-0.3	1965BCa (74747)	429
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Medium: CsCl

K+	ISE	oth/un	25°C	0.20M	U			K1=0.99	1954MEa (74748)	430
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C10H17N5O16P4 H5L AQP CAS 1062-98-2 (3341)
Adenosine-5'-tetrphosphoric acid;

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

K+ gl R4N.X 25°C 0.10M C T K1=1.54 1991SMa (75158) 431
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

K+ ISE alc/w 25°C 100% U K1=2.12 1982MKa (75609) 432
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

K+ ISE alc/w 25°C 100% C IH T K1=3.5 B2= 6.00 2003ADa (76006) 433
IUPAC Tentative. Medium: 0-0.1 M various. DH(K1)=-32.4 kJ mol⁻¹.
In H2O: K1=0.75, DH(K1)=-17.2. In PC: K1=3.6

K+ sp non-aq 25°C 100% C K1=3.80 2002NMa (76007) 434
Medium: THF, using metal picrate salt.

K+ oth oth/un 25°C U K1=0.53 2000MTa (76008) 435
Method: capillary zone electrophoresis.
Medium: 0.005 M H3BO3/Me4NOH, pH 9.2.

K+ con non-aq 25°C 100% C H K1=3.90 B2= 5.55 1999WBa (76009) 436
Medium: N,N-dimethylformamide. By calorimetry: DH(K1)=-24.0 kJ mol⁻¹,
DH(K2)=-27.7 kJ mol⁻¹.

K+ vlt non-aq 25°C 100% C I K1=4.4 1999WKb (76010) 437
Medium: acetonitrile, 0.10 M Et4NClO4. Also data for TMS, propylene
carbonate, acetone, formamide, DMF, DMA, DMSO, MeOH, EtOH.

K+ ISE alc/w 25°C 100% U H K1=3.40 B2= 5.83 1998SSf (76011) 438
Medium: 100% MeOH, 0,05 M Et4NI

K+ con alc/w 25°C 100% U I K1=2.385 1995DSb (76012) 439
Medium : MeOH. In MeCN K1=3.670

K+ cal non-aq 25°C 100% M H K1=4.26 1994BCd (76013) 440
Medium: acetone. DH(K1)=-26.9 kJ mol⁻¹, TDS=-2.7

K+ ISE non-aq 25°C 100% M IH K1=3.78 B2=6.62 1988BUa (76014) 441

Medium: propylene carbonate (also CH₃CN), 0.05 M (CH₃CH₂)₄NC10₄.
DH(K₁)=-30.5, DH(K₂)=-29.5 kJ mol⁻¹; DS(K₁)=-30.2, DS(K₂)=-44.9 J K⁻¹ mol⁻¹

K+ cal non-aq 25°C 100% C H K1=4.33 1988BUb (76015) 442
Medium: acetonitrile. DH(K₁)=-32.0 kJ mol⁻¹, DS(K₁)=-25 J K⁻¹ mol⁻¹.

K+ con non-aq 25°C 100% C T K1=4.0 1988TKa (76016) 443
Medium: MeCN

K+ ISE alc/w 25°C 90% U K1=3.00 B2=5.24 1987KHa (76017) 444
Medium: 90% w/w MeOH/H₂O

K+ con non-aq 25°C 100% C I K1=3.38 B2= 6.00 1987ZBb (76018) 445
Medium: MeOH. In 70% w/w MeOH/H₂O, K₁=2.79, K₂=2.04.

K+ ISE alc/w 25°C 100% U K1=3.35 B2=5.97 1984IEa (76019) 446
Medium: MeOH

K+ ISE non-aq 25°C 100% M K1=3.34 1984NMb (76020) 447
Medium: MeOH.

K+ ISE alc/w 25°C 100% U K1=3.43 1983GGa (76021) 448
Medium: MeOH

K+ gl alc/w 25°C 100% M H T K1=3.61 1982MRa (76022) 449
Medium: MeOH. DH(K₁)=-32.1 kJ mol⁻¹

K+ ISE alc/w 25°C 100% U T K1=3.34 B2=5.55 1982MYc (76023) 450
Medium: MeOH

K+ ISE alc/w 25°C 100% C K1=3.1 B2=6.0 1981PTa (76024) 451
Medium: MeOH

K+ con non-aq 25°C 100% U K1=2.98 1980HNa (76025) 452
Medium: MeCN

K+ cal alc/w 25°C 100% U H T K1=3.77 B2=6.48 1980LIa (76026) 453
Medium: MeOH. DH(K₁)=-32.2 and DH(K₂)=-33.9 kJ mol⁻¹.

K+ dis non-aq 25°C 100% U K1=3.4 1980TYa (76027) 454
Medium: propylene carbonate

K+ EMF oth/un 25°C var C T K1=0.76 1979HRa (76028) 455
Method: ISE based on cation exchange membrane. Medium: aqueous,
containing 0.06-0.25 m ligand.

K+ oth oth/un 25°C ? U K1=0.74 1977RLa (76029) 456
Method: ultrasound absorption

K+ cal oth/un 25°C 0.10M U H T K1=0.74 1976ITb (76030) 457

DH=-17.0 kJ mol⁻¹.

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

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

K+ cal non-aq 25°C 100% M H K1=2.61 1994BCd (76319) 458
Medium: acetone. DH(K1)=-0.9 kJ mol⁻¹, TDS=13.9

K+ sp non-aq 20°C 100% U K1=2.5 1992PSa (76320) 459
Medium: DMF, 0.01 M Me4NI

K+ ISE non-aq 25°C 100% M H K1=2.25 1988BUa (76321) 460
Medium: propylene carbonate, 0.05 M (CH3CH2)4NC1O4. DH(K1)=-7.7 kJ mol⁻¹;
DS(K1)=17.1 J K⁻¹ mol⁻¹

K+ cal non-aq 25°C 100% U H K1=2.11 1986BUb (76322) 461
In CH3CN. DH=-10.8 kJ mol⁻¹

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

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

K+ dis non-aq 25°C 100% C K1=5.57 1998KSc (76450) 462
Medium: 1,2-dichloroethane.

K+ con non-aq 25°C 100% U I K1=3.1 1993Eva (76451) 463
Medium: THF+CHCl3 4:1(vol). In 100% THF: K1=3.0

K+ con non-aq 25°C 100% C K1=3.7 1992MSe (76452) 464
Medium: 100% MeOH. Anion: picrate. Also data for nitrophenolate anions.

K+ cal non-aq 25°C 100% U IH K1=1.68 1991TNa (76453) 465
Medium: MeOH. DH(K1)=-26.9 kJ mol⁻¹; TDS=-17.6. In MeCN: K1=2.06

K+ ISE alc/w 25°C 100% U K1=1.72 1975CJa (76454) 466
Medium: MeOH

C10H22O6 L Penta-Et-Glycol CAS 4792-15-8 (5466)
1,14-Dihydroxy-3,6,9,12,-Tetraoxatetradecane; HO.(CH2.CH2.O)4.CH2.CH2.OH

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

K+ cal alc/w 25°C 90% U IH K1=1.91 1982HLA (76481) 467
Medium: 90% w/w MeOH/H2O. DH=-19.1 kJ mol⁻¹, DS=-8.20 J K⁻¹ mol⁻¹

C11H6O10 H5L (6712)
Benzenepentacarboxylic acid;

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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
K+         gl  KCl    25°C 0.30M U          K1=2.98      1991RSa (76885) 468
                               B(K2L)=4.56
                               B(K+HL)=2.21
                               B(K+H2L)=1.36
                               K(K+H3L)=0.61
K(K+H4L)=0.26, K(2K+HL)=2.1

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*****
C11H18N2O8      H4L      PDTA      CAS 4408-81-5 (1655)
1,2-Diaminopropane-N,N,N',N'-tetraethanoic acid;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
K+         oth R4N.X 25°C 0.50M U          K1=0.91      1971CSb (79299) 469
                               K(K+H2L)=0.79

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Method: polarimetry. Medium: Me4NOH

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K+         nmr oth/un 35°C  ?  U T          K1=0.75      1968SSa (79300) 470
K1(100 C)=0.18
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K+         nmr oth/un 100°C 0.50M U          K1=0.1       1968SSc (79301) 471
Medium: K4L

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*****
C11H18O7      HL      (6800)
1,4,7,10,13-Pentaoxacyclohexadecan-14,16-dione;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
K+         kin alc/w  ?  76% U          K1=0.78      1991HHb (79671) 472
Medium: 76% w/w EtOH/H2O

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*****
C11H20O2      HL      Dipivaloylmeth. CAS 1118-71-4 (363)
2,2,6,6-Tetramethyl-3,5-heptanedione; (CH3)3C.CO.CH2.CO.C(CH3)3
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
K+         gl  diox/w 30°C 75% U          K1=3.89      1975MMa (79749) 473

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*****
C11H22O5      L      16-Crown-5      CAS 55477-28-8 (1592)
1,4,7,10,13-Pentaoxacyclohexadecane; cyclo(-(O.CH2.CH2)5.CH2.CH2-)
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
K+         dis none 25°C 0.0 U          Keff=3.60    1991IOa (79854) 474

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By solvent extraction of the metal picrate into dichloromethane.

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K+         ISE none 25°C 0.0 C          K1=0.40      1991TKa (79855) 475

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

 K+ dis none 25°C 0.0 C M 1989TKc (79856) 476
 K(KL+A=KAL(org))=1.63

Method: extraction of metal picrate/L from H2O into benzene.
 K(K+HA(org)+L(org)=KAL(org)+H)=0.041. HA is picric acid.

 K+ con non-aq 25°C 100% C I K1=3.6 1988TKa (79857) 477
 Medium: MeCN. In propylene carbonate K1=3.2; in MeOH 2.9

 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

 K+ ISE a/c/w 25°C 100% U K1=2.53 1983IKa (79878) 478

 C12H5N5O9S HL CAS 27050-59-3 (4943)
 1,3,7,9-Tetranitrophenothiazine-5-oxide;

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

 K+ dis oth/un 25°C var U K1=1.11 1972IWb (80064) 479

 K+ con non-aq 25°C 100% U K1=1.67 1972IWb (80065) 480

Medium: nitrobenzene.

 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

 K+ dis non-aq 25°C 100% C K1=4 1998KSc (80073) 481

Medium: 1,2-dichloroethane.

 K+ sp non-aq 20°C 100% U K1=4.9 1978JId (80074) 482

Medium: CH2Cl2

 K+ dis oth/un 25°C var U K1=2.05 1972IWb (80075) 483

 K+ con non-aq 25°C 100% U K1=1.51 1972IWb (80076) 484

Medium: nitrobenzene

 K+ dis oth/un 25°C var U K1=1.9 1970SSb (80077) 485

Method: paper chromatography

 C12H6O3 L CAS 81-84-8 (4892)
 1,8-Naphthalenedicarboxylic anhydride;

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

K+ sp non-aq ? 100% U 1971TGa (80101) 486
K(KSCN+L)=-0.25
K(2KSCN+L)=0.95

Medium: CH3CN

C12H6O12 H6L Mellitic acid (7400)
Benzenehexacarboxylic acid; (C(COOH))6

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

K+ ISE R4N.X 25°C 0 C I K1=3.42 1996RSb (80112) 487
B(NaHL)=10.31
B(NaH2L)=16.41
B(NaH3L)=20.93
B(NaH4L)=23.66

B(K2L)=4.65, B(K2HL)=12.36, B(K2H2L)=17.60, B(K2H3L)=20.93

B(K3L)=7.35, B(K3HL)=13.10, B(K4L)=7.33. I=0-3 M Et4NI etc.

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

K+ cal non-aq 25°C 100% U H K1=1.76 1989SSd (81673) 488
Medium: CH3CN

K+ cal non-aq 25°C 100% U H K1=1.76 B2=2.84 1988SSc (81674) 489
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

K+ oth R4N.X 25°C 0.50M U K1=1.56 1973CSa (82310) 490
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

K+ con non-aq 25°C 100% U K1=2.54 1982YSa (82641) 491
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
K+	cal	alc/w	25°C	100%	U	H	K1=2.79	1980BMa (82652)	492

Medium: MeOH. DH=-24.6 kJ mol⁻¹.

K+	cal	alc/w	25°C	100%	U	H	K1=2.79	1980LIb (82653)	493
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Medium: MeOH. DH=-24.6 kJ mol⁻¹.

K+	cal	alc/w	25°C	100%	U	H	K1=2.79	1977ILa (82654)	494
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Medium: MeOH. DH(K1)=-24.6 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
K+	ISE	alc/w	25°C	100%	U		K1=2.70	1982MKa (82660)	495

Medium: MeOH

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
K+	oth	diox/w	25°C	75%	U		K1=3.58 B2=7.22	1979MMa (82858)	496

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
K+	ISE	alc/w	25°C	100%	U		K1=4.18	1982MKa (82862)	497

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
K+	cal	alc/w	25°C	100%	U	H		1990KMb (82945)	498

Medium: MeOH. DH=-13.1 kJ mol⁻¹

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
K+	ISE	alc/w	25°C	100%	U		K1=1.17	1975CJa (83052)	499

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

K+ EMF alc/w 25°C 100% A K1=1.15 1971FRa (83138) 500

Medium: MeOH

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

K+ cal alc/w 25°C 100% U H K1=3.61 1980LIa (83155) 501

Medium: MeOH. DH=-37.7 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

K+ cal R4N.X 25°C 0.10M C TIH K1=2.04 2004WTa (83372) 502

Medium: 0.1 M Et4NCl. Also data for 0.043-0.759 mol fraction acetonitrile/
H2O, and for 20 and 30 C. DH(K1)=-26.2 kJ mol⁻¹, DS(K1)=-48.8 J K⁻¹ mol⁻¹.

K+ EMF alc/w 25°C 100% C K1=5.06 2004ZTa (83373) 503

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

K+ ISE alc/w 25°C 100% C IH R K1=6.11 2003ADa (83374) 504

IUPAC Recommended. Medium: 0-0.1 M various. DH(K1)=-55.3 kJ mol⁻¹
In H2O: K1=2.05, DH(K1)=-25.0. In PC K1=6.2, DH(K1)=-46

K+ dis oth/un 25°C dil C 2002KCa (83375) 505

KL extracted from Li acetate buffer into benzene in the presence of
bromocresol green, HA. K(K+L(org))+A=KLA(org))=6.68.

K+ ISE mixed 25°C 0.8M U TI K1=3.63 2002ZRa (83376) 506

in H2O K1=1.64

Medium: 0.8 mass parts n-Propanol in H2O; for 0.2 m.p. PrOH/H2O K1=2.15;
for 0.6 m. p. PrOH/H2O K1=2.75; K-selective electrode; also data for 45 C

K+ gl mixed 25°C 1.0M U I K1=5.65 2001ZKb (83377) 507

in 100% H2O K1=2.04

Medium: 1.0 mass parts CH3CN;

for 0.6 m.p. CH3CN/H2O K1=3.41; for 0.2 m.p. K1=2.41

K+ sp non-aq 25°C 100% C K1=4.8 2000KBb (83378) 508

Medium: MeCN. Method: electrospray ionization mass spectrometry.

K+ dis non-aq 25°C 100% U K1=11.21 2000Ksa (83379) 509
 Medium: 1,2-dichloroethane

K+ oth oth/un 25°C U K1=1.90 2000MTa (83380) 510
 K(KL+picrate)=0.41
 Method: capillary zone electrophoresis.
 Medium: 0.005 M H3BO3/Me4NOH, pH 9.2.

K+ con non-aq 25°C 100% C TIH K1=6.31 1999Rmb (83381) 511
 Medium: 100% MeOH. Data for 15-55 C. Also data for DMF/MeOH mixtures.
 DH(K1)=-56.0 kJ mol⁻¹, DS(K1)=-67.9 J K⁻¹ mol⁻¹. In 100% DMF, K1=4.28.

K+ cal non-aq 25°C 100% C H K1=4.47 1999Wba (83382) 512
 Medium: N,N-dimethylformamide. DH(K1)=-38.1 kJ mol⁻¹.

K+ gl mixed 25°C 20% U TI K1=2.33 1998Kba (83383) 513
 Medium: 20% w/w acetone/H2O. In 40% K1=2.95; in 60% K1=3.50;
 In 80%, K1=4.36. Also data for 10, 15, 35 and 40 C

K+ ISE alc/w 25°C C TI K1=3.86 1998Kbb (83384) 514
 Medium 60% mass MeOH in H2O; also for 0% K1=2.10; for 100% K1=6.43
 Method: gl. electrode, reversible to K+; for 55 C, 60% K1=3.26;

K+ ISE alc/w 25°C 100% U I K1=6.22 1998SSf (83385) 515
 Medium: 100% MeOH, 0,05 M Et4NI.

K+ dis non-aq 25°C 100% C I 1998TKa (83386) 516
 K(K+A+L(org))=KAL(org))=6.78
 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.

K+ cal non-aq 25°C 100% C K1=6.11 1997DZa (83387) 517
 Medium: benzonitrile. DH(K1)=-54.70 kJ mol⁻¹, DS(K1)=-66.5 J K⁻¹ mol⁻¹.

K+ oth non-aq 15°C 100% U T H K1=4.70 1997EKa (83388) 518
 Medium: CH3CN. Also data for H2O/CH3CN mixtures. For 40% CH3CN w/w K1=3.14;
 for 100% H2O: K1=2.17

K+ con non-aq 25°C 100% C T H K1=5.72 1997TAa (83389) 519
 Medium: acetonitrile. DH(K1)=-43.6 kJ mol⁻¹, DS(K1)=-36.6 J K⁻¹ mol⁻¹.
 Data for 10-25 C.

K+ cal R4N.X 25°C 0.10M C H T K1=2.27 1996BCh (83390) 520
 Medium: 0.10 M Et4NC104. DH(K1)=-15.4 kJ mol⁻¹.

K+ EMF alc/w 25°C U TIH K1=3.80 1996DBa (83391) 521
 K1=2.04 (100%H2O)
 80% mass 2-propanol /H2O; also for T=10 C K1=3.86; for T=45 C K1=3.73

K+ ISE R4N.X 25°C 0.03M U H K1=1.98 1996SSb (83392) 522

Method: K-selective electrode; in 0.025 M Me4NCl
DH1=-24.7 kJ/mol

K+ ISE non-aq 25°C 0.03M U H K1=4.92 1996SSb (83393) 523
Method: K-selective electrode; Medium: 0.025 M Me4NCl in isopropanol
DH1=-68.1 kJ/mol

K+ ISE non-aq 25°C 0.03M U H K1=5.52 1996SSb (83394) 524
Method: K-selective electrode; Medium: 0.025 M Me4NCl in MeCN
DH1=-15.9 kJ/mol

K+ ISE non-aq 25°C 0.03M U H K1=4.19 1996SSb (83395) 525
Medium: 0.025 M Me4NCl in N,N-dimethylformamide
Method: K-selective electrode; DH1=-36.8 kJ/mol

K+ ISE non-aq 25°C 0.03M U H K1=3.24 1996SSb (83396) 526
Medium: 0.025 M Me4NCl in hexamethylphosphoric triamide
Method: K-selective electrode; DH1=-37.4 kJ/mol

K+ ISE non-aq 25°C 0.03M U H K1=3.35 1996SSb (83397) 527
Medium: 0.025 M Me4NCl in DMSO
Method: K-selective electrode; DH1=-27.6 kJ/mol

K+ ISE mixed 25°C 0.03M U IH K1=2.47 1996SSb (83398) 528
Medium: 0.025 M Me4NCl in H2O/dioxane 2:8 v/v; for 8:2 K1=4.21
Method: K-selective electrode; DH1=-24.7 kJ/mol

K+ vlt non-aq 25°C 100% C K1=9.3 1995KTb (83399) 529
Method: ion transfer polarography. Medium: nitrobenzene, 0.05 M
tetrabutylammonium tetraphenylborate.

K+ cal alc/w 25°C 80% C H K1=4.70 1995KZa (83400) 530
Medium: 80% v/v CH3OH/H2O. DH(K1)=-45.3 kJ mol⁻¹, DS(K1)=-62.1 J K⁻¹ mol⁻¹

K+ cal non-aq 25°C 100% U IH T K1=5.73 1995OKb (83401) 531
Medium: Acetonitrile, 0.1 M Et4NClO4. DH(K1)=-17 kJ mol⁻¹
In propylene carbonate K1=6.24, DH(K1)=-47

K+ cal KCl 25°C 0.00 C T H K1=2.06 1995WIa (83402) 532
Method: isothermal flow calorimetry. Measurements at 1.52 MPa. Data for
50-125 C. Medium: 0.005 m KCl. DH(K1)=-26.0 kJ mol⁻¹, DS(K1)=-48 J K⁻¹ m⁻¹

K+ cal non-aq 25°C 100% M H K1=5.89 1994BCd (83403) 533
Medium: acetone. DH(K1)=-50.4 kJ mol⁻¹, TDS=-15.4

K+ cal non-aq 25°C 100% U H T K1=4.21 199400a (83404) 534
Medium: DMF, 0.1 M Et4NClO4. DH(K1)=-38.8 kJ mol⁻¹, DS=-50 J K⁻¹ mol⁻¹

K+ dis non-aq 25°C 100% U 1993INa (83405) 535
B(KPL)=6.20

K is the equilibrium constant for extraction of the metal picrate (P) into CH₂Cl₂. For extraction from D₂O, B=6.38

K+	EMF oth/un	25°C	0.05M	M	K1=6.15	1992BUb (83406)	536
K1=6.29 (by calorimetric competitive titration)							
K+	cal R4N.X	25°C	0.10M	C H	K1=2.04	19920Ia (83407)	537
DH(K1)=-26.3 kJ mol ⁻¹ , DS=-49 J K ⁻¹ mol ⁻¹							
K+	cal none	45°C	0.0	U H	K1=1.77	1992V0a (83408)	538
DH(K1)=-22.3 kJ mol ⁻¹ , DS=-36.1 J K ⁻¹ mol ⁻¹							
K+	ix none	25°C	0.0	U I	K1=1.8	1991BMb (83409)	539
Ligand bound to silica gel. In MeOH:K=3.8, in EtOH:K=4.0, in acetone, K=4.0							
K+	nmr oth/un	30°C	dil	C	K1=2.470	B2= 5.64	1991ERa (83410) 540
					B(K2L2)=9.435		
					B(K2L3)=12.474		
					B(K3L3)=16.889		
Medium: D ₂ O. Method: 13C nmr.							
K+	ISE alc/w	25°C	70%	C	K1=3.71	B2= 5.71	1991GTa (83411) 541
Medium: 70% v/v MeOH/H ₂ O, 0.10 M Bu ₄ NI. Method of corresponding solutions.							
K+	ix alc/w	RT	50%	C	K1=3.38	1990MBb (83412)	542
Medium: 50% v/v MeOH/H ₂ O.							
K+	con non-aq	25°C	100%	C M	K1=6.013	1990SAb (83413)	543
					K(KSCN+L)=4.33		
					K(KL+SCN)=-0.947		
Medium: propylene carbonate.							
K+	oth non-aq	25°C	100%	C	K1=4.65	1989BBh (83414)	544
Method: FABMS. Medium: glycerol.							
K+	ISE non-aq	25°C	100%	M H	K1=6.08	1988BUa (83415)	545
Medium: propylene carbonate, 0.05 M (CH ₃ CH ₂) ₄ NC104. DH(K1)=-45.4 kJ mol ⁻¹ ; DS(K1)=-36.6 J K ⁻¹ mol ⁻¹							
K+	cal non-aq	25°C	100%	C H	K1=5.72	1988BUb (83416)	546
Medium: acetonitrile. DH(K1)=-9.9 kJ mol ⁻¹ , DS(K1)=75.8 J K ⁻¹ mol ⁻¹ .							
K+	ISE alc/w	25°C	90%	U	K1=5.50	1987KHa (83417)	547
Medium: 90% w/w MeOH/H ₂ O							
K+	ix KCl	25°C	0.05M	C	K1=2.03	1987MGb (83418)	548
Medium: KCl/HCl.							
K+	con none	25°C	0.0	C T H	K1=2.034	1985TAa (83419)	549
Data for 10-45 C. DH(K1)=-25.01 kJ mol ⁻¹ , DS(K1)=-44.34 J K ⁻¹ mol ⁻¹ .							

K+ ISE non-aq 25°C 100% M K1=6.02 1984NMb (83420) 550
Medium: MeOH.

K+ oth oth/un RT 0.01M C K1=2.02 1984STb (83421) 551
Method: isotachophoresis. Medium: 0.01 M Bu4NCl or 0.01 M Tris.

K+ ISE alc/w 25°C 100% U K1=6.08 1983GGa (83422) 552
Medium: MeOH

K+ con alc/w 25°C 100% U K1=6.20 1983LSa (83423) 553

K+ sol non-aq 20°C 100% C K1=5.70 1983SLa (83424) 554
Medium: CHCl3

K+ cal alc/w 25°C 90% U IH K1=5.35 1982HLA (83425) 555
Medium: 90% MeOH. DH=-49.28 kJ mol⁻¹, DS=-18.7 J K⁻¹ mol⁻¹

K+ ISE alc/w 25°C 100% U K1=6.02 1982MKa (83426) 556
Medium: MeOH

K+ gl alc/w 25°C 100% M H T K1=6.18 1982MRa (83427) 557
Medium: MeOH. DH(K1)=-53.1 kJ mol⁻¹

K+ ISE alc/w 25°C 100% C K1=5.93 1981PTa (83428) 558
Medium: MeOH

K+ sp diox/w 25°C 100% U M K(K(Picrate)+L)=6.0 1981SSd (83429) 559

K+ cal alc/w 25°C 100% U H K1=6.06 1980BMA (83430) 560
Medium: MeOH. DH=-56.1 kJ mol⁻¹.

K+ cal alc/w 25°C 100% U H T K1=6.06 1980LIA (83431) 561
Medium: MeOH. DH=-56.1 kJ mol⁻¹.

K+ ISE alc/w 25°C 90% C K1=5.23 1980LVb (83432) 562
Method: K ion selective glass electrode. Medium: 90% v/v MeOH/H₂O, 0.10 M Me₄NBr. Also data for MeNH₃⁺, EtNH₃⁺ and C₆H₅.(CH₂)₂NH₃⁺ cations.

K+ dis non-aq 25°C 100% U K1=6.2 1980TYa (83433) 563
Medium: propylene carbonate

K+ oth alc/w 25°C 100% U K1=6.15 1980WJa (83434) 564
Method: fluorimetry in CH₃OH

K+ EMF oth/un 25°C var C T K1=2.05 1979HRa (83435) 565
Method: ISE based on cation exchange membrane. Medium: aqueous, containing 0.06-0.25 m ligand.

K+ oth KCl 25°C var U H K1=2.04 1979JLa (83436) 566
From heat capacity measurements, 0.02 - 0.4 M KCl. DH(K1)=-26 kJ mol-1

K+ cal alc/w 25°C 100% U H K1=6.05 1977ILa (83437) 567
Medium: MeOH. DH(K1)=-56.1 kJ mol-1

K+ cal alc/w 25°C 70% U H K1=4.33 1976ITa (83438) 568
Medium: 70% w/w MeOH/H2O. DH(K1)=-40.5 kJ mol-1.

K+ cal oth/un 25°C 100% U H T K1=2.03 1976ITb (83439) 569
DH=-26.0 kJ mol-1

K+ kin none 25°C 0.0 U K1=3.4 1976Lfa (83440) 570

K+ ISE alc/w 25°C 100% A K1=6.10 1971FRa (83441) 571
Medium: MeOH. In H2O: K1=2.06

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

K+ cal alc/w 25°C 100% U IH K1=3.78 1998SSf (83705) 572
Medium: 100% MeOH, 0,05 M Et4NI. DH(K1)=-22.0 kJ mol-1

K+ ISE alc/w 25°C 100% A K1=3.90 1971FRa (83706) 573
Medium: MeOH

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

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

K+ con non-aq 25°C C K1=2.5 1999ESa (83719) 574
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

K+ cal alc/w 25°C 100% U H K1=2.31 1994IZa (83731) 575
Medium: MeOH. DH(K1)=-28.9 kJ mol-1, DS(K1)=-52.7 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

K+ ISE alc/w 25°C 100% U I K1=1.76 1998SSf (83846) 576

Medium: 100% MeOH, 0,05 M Et4NI. Many other crown ethers studied

K+ cal non-aq 25°C 100% M H K1=3.85 1994BCd (83847) 577
Medium: acetone. DH(K1)=-16.1 kJ mol⁻¹, TDS=5.8

K+ sp non-aq 20°C 100% U K1=2.82 1992PSa (83848) 578
Medium: DMF, 0.01 M Me4NI

K+ ISE non-aq 25°C 100% C K1=<2 1989MGa (83849) 579
Medium: DMF, 0.10 M Et4NC104

K+ ISE non-aq 25°C 100% M H K1=4.43 1988BUa (83850) 580
Medium: propylene carbonate, 0.05 M (CH3CH2)4NC104. DH(K1)=-21.9 kJ mol⁻¹;
DS(K1)=11.0 J K⁻¹ mol⁻¹

K+ cal non-aq 25°C 100% U H K1=4.13 1986BUb (83851) 581
In CH3CN. DH=-15.3 kJ mol⁻¹

K+ cal alc/w 25°C 100% U H K1=1.83 1986BUd (83852) 582
In MeOH. DH=-4.7 kJ mol⁻¹

K+ sol non-aq 20°C 100% C K1=5.11 1983SLa (83853) 583
Medium: CHCl3

K+ con non-aq 25°C 100% U K1=4.32 1980K Mb (83854) 584
Medium: MeCN

K+ ISE alc/w 25°C 100% A K1=2.04 1971FRa (83855) 585
Medium: MeOH

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

K+ con non-aq 25°C 100% U K1=4.1 1993EVa (84001) 586
Medium: THF+CHCl3 (4:1 vol). Also data for other solvents

K+ cal oth/un 25°C 0.05M M K1=2.07 1992BUb (84002) 587
K1=2.40 (by conductivity)

K+ cal mixed 25°C 90% U IH K1=1.95 1982HLa (84003) 588
Medium: 90% MeOH. DH=-29.3 kJ mol⁻¹, DS=-18.2 J K⁻¹ mol⁻¹

K+ ISE alc/w 25°C 100% U K1=2.20 1975CJa (84004) 589
Medium: MeOH

K+ ISE alc/w 25°C 100% A K1=2.20 1971FRa (84005) 590
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

K+ EMF non-aq 25°C 100% C K1=3.23 1997WWa (84087) 591
Medium: MeOH, 0.05M Et4NC1O4.

Method: Ag/Ag+ electrode; by competition with Ag+.

C12H30N6 L CAS 296-35-5 (143)
1,4,7,10,13,16-Hexaazacyclooctadecane; cyclo(-(NH.CH2.CH2)6-)

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

K+ gl NaClO4 25°C 0.20M U K1=0.8 1980KKb (84336) 592

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

K+ gl R4N.X 25°C 0.10M M 1990DSa (84412) 593

B(KHL)=15.98

B(KH2L)=27.49

B(KH3L)=36.36

B(KH4L)=43.79

Medium: Me4NNO3

C13H20N2O8 H4L CAS 123064-92-6 (7929)

trans-1,3-Cyclopentanediaminotetraethanoic acid;

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

K+ gl KCl 25°C 1.0M U K1=0.90 1989CMb (86122) 594

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

K+ ISE alc/w 25°C 100% U K1=1.45 1975CJa (86148) 595

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

K+ kin alc/w ? 76% U I K1=1.91 1991HHb (86377) 596

Medium: 76% w/w EtOH/H2O. Also data for 65, 54 and 39% w/w ethanol/H2O:

K1=1.69, 1.49 and 1.11 respectively.

K+ cal alc/w 25°C 100% U H K1=2.55 1980LIb (86378) 597
Medium: MeOH. DH=-33.1 kJ mol⁻¹.

K+ cal alc/w 25°C 100% U H K1=2.55 1977ILa (86379) 598
Medium: MeOH. DH(K1)=-33.1 kJ mol⁻¹

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

K+ ISE alc/w 25°C 100% U K1=4.05 1982MKa (86426) 599
Medium: MeOH

C13H26O5 L (8408)
1,4,7,10,13-Pentaoxacyclooctadecane;

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

K+ cal non-aq 25°C 0.05M U K1=2.79 1996RSc (86463) 600
Medium: 0.05 M Et4NI in MeOH; by K-selective electrode K1=2.64
DH(K1)=-25.3 kJ mol⁻¹. In 0.05 M Et4NI in H2O K1=1.31

K+ cal non-aq 25°C 0.05M U K1=2.82 1996RSc (86464) 601
Medium: 0.05 M Et4NI in MeCN. DH(K1)=-9.0 kJ mol⁻¹

C13H26O5 L (6410)
15,15-Dimethyl-1,4,7,10,13-pentaoxacyclohexadecane;

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

K+ con none 25°C 0.0 C K1=0.1 2001KMb (86473) 602

K+ con non-aq 25°C 100% C I K1=3.13 1992TFa (86474) 603
Medium: acetonitrile. In propylene carbonate, K1=2.89.

K+ con alc/w 25°C 100% U K1=2.54 1991IOa (86475) 604
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

K+ con non-aq 25°C 100% C I K1=4.62 2000TMb (86496) 605
Medium: CH3CN. In other media, K1=4.49 (propylene carbonate), 4.21 (MeOH),
2.60 (DMF), 2.01 (DMSO).

K+ con oth/un 25°C dil C K1=1.27 1999TMa (86497) 606
Self medium (KCl).

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

K+ ISE alc/w 25°C 100% U K1=4.03 1983IKa (86507) 607

C13H27NO5 L (8611)
16-Methyl-1,4,7,10,13-Pentaoxa-16-azacyclooctadecane;

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

K+ ISE alc/w 25°C 100% U H K1=5.46 1998SSf (86509) 608

Medium: 100% MeOH, 0,05 M Et4NI

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

K+ sp non-aq ? 100% U 1971TGa (86631) 609

K(KSCN+L)=-0.19

K(2KSCN+L)=0.91

Medium: CH3CN

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

K+ dis non-aq 24°C 100% C 2002MRd (88271) 610

K(K+A+L)=5.90

Medium: CDCl3. HA is picric acid.

K+ dis none 25°C dil C I M 2002THb (88272) 611

K(KL+A)=0.71

K(K+A+L(org))=KAL(org))=3.73

HA is picric acid. Data for several aryl and alkyl solvents.

Method: extraction of metal picrate into dichloromethane/L.

K+ con non-aq 25°C 100% C K1=4.46 B2= 8.66 2000ICa (88273) 612

Medium: nitromethane.

K+ con non-aq 25°C 100% C H K1=2.87 B2= 4.11 1999WBa (88274) 613

Medium: N,N-dimethylformamide. By calorimetry: DH(K1)=-19.8 kJ mol⁻¹,
DH(K2)=-27.3 kJ mol⁻¹.

K+ vlt non-aq 25°C 100% C I K1=4.2 1999WKb (88275) 614
Medium: acetonitrile, 0.10 M Et4NClO4. Also data for TMS, propylene carbonate, acetone, formamide, DMF, DMA, DMSO, MeOH, EtOH.

K+ dis oth/un 25°C 0 U K1=2.87 19940Ua (88276) 615

K+ ISE alc/w ? 100% U K1=2.73 B2=6.13 1992CLb (88277) 616
Medium: MeOH

K+ ISE alc/w 25°C 100% C K1=2.88 B2= 6.03 1992PTa (88278) 617
Method: Na ion selective electrode. Medium: methanol, 1-5 mM KBr.
Data for 4,5-dibromo-, 4,5-dimethoxy- and 4,5-dibutoxybenzo-15-crown-5.

K+ ISE mixed 25°C 50% C K1=2.0 B2= 4.60 1991LMc (88279) 618
Method: K ion selective glass electrode. Medium: 50% w/w MeOH/DMF.

K+ cal non-aq 25°C 100% U H K1=3.58 1989SSd (88280) 619
Medium: CH3CN

K+ cal non-aq 25°C 100% C H K1=4.17 1988BUb (88281) 620
Medium: acetonitrile. DH(K1)=-23.4 kJ mol⁻¹, DS(K1)=1.0 J K⁻¹ mol⁻¹.

K+ con non-aq 25°C 100% C I K1=2.49 1988TKb (88282) 621
Medium: MeCN. In propylene carbonate K1=2.78; in MeOH 2.71

K+ con non-aq 25°C 100% C T H K1=3.24 1988TMb (88283) 622
Medium: acetonitrile. Data for 15-35 C. Anion: tetraphenylborate.
DH(K1)=-24.5 kJ mol⁻¹, DS(K1)=-20.0 J K⁻¹ mol⁻¹.

K+ sp non-aq 22°C 100% U K1=5.90 1987CCc (88284) 623
In deuteriochloroform

K+ ISE alc/w 25°C 90% U K1=2.63 1987KHa (88285) 624
Medium: 90% w/w MeOH/H2O

K+ con non-aq 25°C 100% C I K1=2.96 B2= 6.16 1987ZBb (88286) 625
Medium: MeOH. In 70% w/w MeOH/H2O, K1=1.97, K2=2.40.

K+ sp mixed 25°C 20% U I K1=0.81 1986GSa (88287) 626
In 0.015 M Et4N.Cl, 20% CH3CN/H2O. In 40%, K1=1.34; 60%, K1=2.00;
80%, K1=2.88; 100% CH3CN, K1=4.27.

K+ cal alc/w 25°C ? C K1=1.50 B2=6.24 1986LWa (88288) 627

K+ ISE alc/w 25°C 100% C K1=3.05 B2=6.43 1985ZFa (88289) 628

K+ con non-aq 25°C 100% U H K1=2.78 1982TAa (88290) 629
Medium: propylene carbonate

K+ ISE alc/w 25°C 100% C K1=2.8 B2=5.95 1981PTa (88291) 630

Medium: MeOH

C14H20O5 HL CAS 65112-35-8 (6061)
3,6,9,12-Tetraoxabicyclo[12.3.1]octadeca-1(18),14,16-trien-18-ol;

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

K+ cal alc/w 25°C 100% U H K1=1.26 1987ZBa (88388) 631
Medium: MeOH. DH=-12.5 kJ mol⁻¹; DS=-17.8.

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

K+ gl KCl 25°C 1.00M U K1=0.18 1984MFa (88695) 632

K+ oth R4N.X 25°C 0.50M U K1=1.83 1971CSa (88696) 633
K(K+HL)=0.78

Method: polarimetry. Medium: Me4NOH

K+ gl oth/un 25°C 0.10M U K1=1.52 1970CSa (88697) 634

Medium: CsNO3

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

K+ cal alc/w 25°C 100% U H K1=1.94 1980LIb (90043) 635

Medium: MeOH. DH=-23.0 kJ mol⁻¹.

C14H24O8S L CAS 63689-67-8 (2274)
1,4,7,10,13,16-Hexaoxa-19-thia-cyclohenicos-17,21-dione;

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

K+ cal alc/w 25°C 100% U H K1=2.09 1980LIb (90047) 636

Medium: MeOH. DH=-16.1 kJ mol⁻¹.

C14H24O9 L CAS 63689-61-2 (2273)
1,4,7,10,13,16,19-Heptaoxacyclohenicos-17,21-dione;

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

K+ cal alc/w 25°C 100% U H K1=2.32 1980LIb (90057) 637

Medium: MeOH. DH=-27.0 kJ mol⁻¹.

C14H24O10 HL 18-6A2 CAS 76871-57-3 (5407)
1,2-Bis-carboxy-18-crown-6;

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

K+ gl alc/w 25°C 90% U K1=6.17 1984FWa (90061) 638
B(KHL)=12.0

Medium: 90% v/v MeOH/H2O, 0.05 M R4NX

C14H25N3O7 H3L (5397)
1-Oxa-4,7,10-triazacyclododecane-4,7,10-triethanoic acid;

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

K+ gl R4N.X 25°C 0.10M U K1=2.78 1988ADa (90087) 639

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

K+ gl R4N.X 25°C 0.10M C K1=1.69 1987DDb (90193) 640

C14H26N2O8 H2L (6658)
1,4,10,13-Tetraoxa-7,16-diaza-2,3-dicarboxycyclooctadecane;

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

K+ gl R4N.X 25°C 0.10M U K1=2.00 1990AFa (90222) 641

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

K+ ISE non-aq 25°C 100% M IH K1=3.70 B2=6.90 1988BUa (90270) 642

Medium: propylene carbonate (also CH3CN), 0.05 M (CH3CH2)4NC1O4.

DH(K1)=-26.2, DH(K2)=-20.1 kJ mol⁻¹; DS(K1)=-17.4, DS(K2)=-6.37 J K⁻¹ mol⁻¹

K+ ISE alc/w 25°C 100% A K1=3.58 B2=5.46 1971FRa (90271) 643

Medium: MeOH. In H2O: K1=0.6

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

K+ ISE alc/w 25°C 100% U K1=3.99 1982MKa (90274) 644

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
K+	cal	non-aq	25°C	100%	C	H			1999WBa (90373)	645
Medium: N,N-dimethylformamide. DH(K1)=-3.4 kJ mol ⁻¹ .										
K+	gl	R4N.X	25°C	0.05M	C	H		K1=2.7	1996BCh (90374)	646
Medium: 0.05 M Et4NClO4. By calorimetry: K1=2.5, DH(K1)=-0.9 kJ mol ⁻¹ .										
K+	cal	non-aq	25°C	100%	M	H		K1=2.47	1994BCd (90375)	647
Medium: acetone. DH(K1)=-15.8 kJ mol ⁻¹ , TDS=-1.8										
K+	sp	non-aq	20°C	100%	U			K1=2.3	1992PSa (90376)	648
Medium: DMF, 0.01 M Me4NI										
K+	ISE	non-aq	25°C	100%	M	IH		K1=3.49 B2=5.92	1988BUa (90377)	649
Medium: propylene carbonate (also CH3CN), 0.05 M (CH3CH2)4NClO4. DH(K1)=-30.0, DH(K2)=-5.0 kJ mol ⁻¹ ; DS(K1)=-33.9, DS(K2)=29.5 J K ⁻¹ mol ⁻¹										
K+	cal	non-aq	25°C	100%	U	H		K1=3.50	1986BUb (90378)	650
In CH3CN. DH=-29.3 kJ mol ⁻¹										
K+	cal	alc/w	25°C	100%	U	H		K1=2.36	1986BUd (90379)	651
In MeOH. DH=-23.2 kJ mol ⁻¹										
K+	ISE	non-aq	25°C	100%	C	I		K1=3.22	1985CKa (90380)	652
Medium: propylenecarbonate. In DMF K1=1.51										
K+	ISE	non-aq	25°C	100%	U			K1=2.84	1981CRa (90381)	653
Medium: MeCN. In DMF: K1<2.5; in DMSO: <2.0; in EtOH: <2.6; in NMP: 2.44										
K+	ISE	non-aq	25°C	100%	U			K1=3.3	1980CRa (90382)	654
Medium: Propylene carbonate										
K+	EMF	non-aq	25°C	100%	C			K1=<2.0	1979BLb (90383)	655
Method: Ag electrode; competition with Ag+. Medium: MeOH, 0.05 M Me4NClO4.										
K+	gl	R4N.X	25°C	0.05M	C	I		K1=<2.0	1975LSc (90384)	656
In 95% MeOH: K1=2.26; 100%: 2.3										

 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
K+	ISE	R4N.X	25°C	0.05M	U	I		K1=<2	1991LSb (90461)	657
Medium: 0.05 M Et4NClO4. In MeCN: K1=7.2; DMF: K1=3.2										

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

K+ ISE alc/w 25°C 100% U K1=1.89 1975CJa (90492) 658

Medium: MeOH

C14H28O7 L 21-Crown-7 CAS 33089-36-0 (2264)

1,4,7,10,13,16,19-Heptaoxacycloheptacosane;

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

K+ sol non-aq 25°C 100% C K1=4.60 1999KCa (90523) 659

Medium: acetonitrile.

K+ ISE alc/w 25°C 100% U K1=4.35 1983GGa (90524) 660

Medium: MeOH

K+ cal alc/w 25°C 100% U H K1=4.22 1980LIa (90525) 661

Medium: MeOH. DH=-35.9 kJ mol⁻¹.

K+ ISE alc/w 25°C 100% A K1=4.41 1971FRa (90526) 662

Medium: MeOH

C14H30N2O2P L (2094)

P-(N,N-Diethylamidocarbonyl)methyl-P,P-dibutylphosphine oxide;

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

K+ con non-aq 25°C C K1=2.6 1999ESa (90552) 663

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

K+ con non-aq 25°C 100% U K1=2.35 1988YKa (90553) 664

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

K+ sol non-aq 20°C 100% C K1=3.97 1983SLa (90561) 665

Medium: CHCl₃

C14H30N2O4 L CAS 31255-13-7 (2448)

N,N'-Dimethyl-cyclo-1,10-diaza-4,7,13,16-tetraoxaocadecane;

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

K+ gl alc/w 25°C 95% C K1=4.55 2004KVa (90577) 666

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

K+ ISE a/c/w 25°C 100% U I K1=5.18 1998SSf (90578) 667
Medium: 100% MeOH, 0.05 M Et₄NI. Many other crown ethers studied

K+ ISE a/c/w 25°C 90% C K1=4.10 1980LVb (90579) 668
Method: K ion selective glass electrode. Medium: 90% v/v MeOH/H₂O, 0.10 M Me₄NBr. Also data for MeNH₃⁺, EtNH₃⁺ and C₆H₅.(CH₂)₂NH₃⁺ cations.

K+ gl a/c/w 25°C 93% U K1=3.30 1978WVa (90580) 669
Medium: 93% MeOH/H₂O

C₁₄H₃₀N₂O₅ L (6722)
7,13-Bis(2-hydroxyethyl)-1,4,10-trioxa-7,13-diazacyclopentadecane

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

K+ ISE non-aq 25°C 100% U K1=3.08 1993RPa (90629) 670
Medium: dimethylformamide, 0.05 M Et₄NClO₄. By competition with Ag⁺.

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

K+ cal a/c/w 25°C 90% U H K1=2.43 1994IZa (90638) 671
Medium: 90% v/v MeOH/H₂O. DH(K₁)=-33.0 kJ mol⁻¹,
DS(K₁)=-64.1 J K⁻¹ mol⁻¹

C₁₄H₃₀O₇ L CAS 1072-40-8 (2499)
2,5,8,11,14,17,20-Heptaioxaheneicosane; CH₃.O.(CH₂.CH₂.O)₆.CH₃

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

K+ dis non-aq 25°C 100% C K1=8.32 1998KSc (90694) 672
Medium: 1,2-dichloroethane.

K+ con non-aq 25°C 100% U K1=4.7 1993EVa (90695) 673
Medium: THF+CHCl₃ (4:1 vol). Also data for other solvents

K+ ISE a/c/w 25°C 100% U K1=2.55 1975CJa (90696) 674
Medium: MeOH

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

K+ gl a/c/w 25°C 100% U K1=1.6 1965LIa (91550) 675
Medium: MeOH, 0.1 M KI

 K+ gl diox/w 30°C 75% U K1=3.67 1954FUa (91551) 676

 C15H18N07Cl 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
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K+ cal alc/w 25°C 100% U H K1=4.73 1980BMa (91993) 677
 Medium: MeOH. DH=-33.3 kJ mol⁻¹.

C15H19N07 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
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K+ cal alc/w 25°C 100% U H K1=4.66 1981BBb (92117) 678
 Medium: MeOH. DH(K1)=-39.0 kJ mol⁻¹

K+ cal alc/w 25°C 100% U H K1=4.66 1980BMa (92118) 679
 Medium: MeOH. DH=-38.9 kJ mol⁻¹.

K+ cal alc/w 25°C 100% U H K1=4.66 1980LIb (92119) 680
 Medium: MeOH. DH=-38.9 kJ mol⁻¹

K+ sp alc/w 25°C 100% U H K1=4.66 1977ILc (92120) 681
 Medium: Methanol. DH(K1)= -38.9 kJ mol⁻¹

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
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K+ cal alc/w 25°C 100% U H K1=1.97 1987ZBa (92249) 682
 Medium: MeOH. DH=-19.9 kJ mol⁻¹; DS=-29.2. By potentiometry: K1=2.00.

C15H23N05 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
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K+ cal alc/w 25°C 100% U H K1=5.35 1980BMa (92268) 683
 Medium: MeOH. DH=-38.1 kJ mol⁻¹.

K+ cal alc/w 25°C 100% U H K1=5.35 1980LIa (92269) 684
 Medium: MeOH. DH=-38.1 kJ mol⁻¹.

K+ sp alc/w 25°C 100% U H K1=5.35 1977ILc (92270) 685
 Medium: Methanol. DH= -38.1 kJ mol⁻¹

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

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

 K+ con non-aq 25°C C K1=2.4 1999ESa (92328) 686
 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.C6H4.0(CH2CH2O)4CH3

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

 K+ sp alc/w 25°C 100% U K1=3.40 1981EMb (92343) 687
 Medium: MeOH

 K+ ISE alc/w 25°C 100% U K1=2.08 1975CJa (92344) 688
 Medium: MeOH

 C15H26O8 L CAS 96517-83-8 (2272)
 1,4,7,10,13,16-Hexaoxacycloheptacos-17,21-dione;

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

 K+ cal alc/w 25°C 100% U H K1=1.71 1980LIb (92457) 689
 Medium: MeOH. DH=-20.5 kJ mol⁻¹.

 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

 K+ EMF non-aq 25°C 100% U K1=2.28 2001WBa (92574) 690
 Medium: DMF, 0.05 M Et4NClO4. Also data for the 1,4,7-tris((S)-2-hydroxy-2-phenylethyl- derivative (K1=1.91). Competition with Ag+.

 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

 K+ ISE alc/w 25°C 90% C K1=3.78 1980LVb (92578) 691
 Method: K ion selective glass electrode. Medium: 90% v/v MeOH/H2O, 0.10 M Me4NBr. Also data for MeNH3+, EtNH3+ and C6H5.(CH2)2NH3+ cations.

 C15H36NO9P3 L CAS 37909-50-5 (2634)
 (N,N-Dimethylamine)methylenetrakis(phosphonic acid diethyl ester);
 (CH3)2N.C(CH2.PO(OC2H5)2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
K+	con	non-aq	22°C	100%	U		K1=1.66	1981SKd (92603)	692

Medium: CH3CN

C16H8N6O10		HL					CAS 2698-85-9 (5150)		
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N-(2,4,6-Trinitrobenzo)-2,4-dinitro-1-naphthylamine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
K+	dis	oth/un	25°C	var	U		K1=2.62	1972IWb (92633)	693

K+	con	non-aq	25°C	100%	U		K1=1.50 (dry nitrobenzene) K1=1.10 (wet nitrobenzene)	1972IWb (92634)	694
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Medium: nitrobenzene.

C16H16O6		H2L					(5634)		
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1-(2-Hydroxyphenyl)-4-(2-carboxymethoxyphenyl)-1,4-dioxabutane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
K+	ISE	alc/w	25°C	100%	U		K1=1.55	1981PTb (93715)	695

Medium: MeOH

C16H18O5		H2L					(5623)		
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1,7-bis(2-Hydroxy-phenyl)-1,4,7-trioxahseptane; O(CH2.CH2.O.C6H4.OH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
K+	ISE	alc/w	25°C	100%	U		K1=1.09	1981PTb (93875)	696

Medium: MeOH

C16H20N3O8F3		L					(1041)		
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2,4-Dinitro-6-trifluoromethylphenyl-aminomethyl-12-crown-4

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
K+	sp	mixed	25°C	16%	U		K1=2.93 K(K+HL)=1.33	1984BPa (94083)	697

C16H20O3P2		L					CAS 82154-46-9 (2914)		
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Dimethylphosphinomethyl-diphenylphosphinomethyl-ether; Me2PO.CH2.O.CH2.PO(C6H5)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
K+	con	non-aq	25°C	100%	U		K1=2.22	1982YSa (94098)	698

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

C16H22O6		L					(6667)		
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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

K+ ISE alc/w ? 100% U K1=2.83 B2=5.85 1992CLb (94240) 699
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

K+ kin alc/w 25°C 100% U K1=1.04 1992CDc (94243) 700
Medium: MeOH. Data also for other related ligands

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

K+ con non-aq 25°C 100% U K1=4.80 1976UHa (94267) 701
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

K+ dis non-aq 25°C 100% U H 1979KLa (94342) 702
K(K(picrate)+L)=5.03

Medium: CHCl3

K+ dis non-aq 24°C 100% C 1977MTc (94343) 703
K(KA+L)=5.04

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

K+ dis non-aq 25°C 100% U H 1979KLa (94353) 704
K(K(picrate)+L)=4.32

Medium: CHCl3

C16H24O5 L CAS 75507-20-9 (605)
Benzyloxymethyl-1,4,7,10-tetraoxacyclododecane, Benzyloxymethyl-12-crown-4;

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

K+ ISE alc/w 25°C 100% U K1=1.42 B2=2.71 1982MYc (94359) 705
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

K+ oth KCl 25°C 0.05M C K1=1.68 2002KTa (94400) 706
Method: capillary electrophoresis. Medium: 0.03-0.06 M KCl.
By conductivity in 0.001-0.004 M KCl, K1=1.664.

K+ dis NaClO4 25°C 0.1M C I K(KL+ClO4)=-0.49 2002TYa (94401) 707
Extraction of NaClO4 with L into dichloromethane.
K(K+L(org)+ClO4=KlClO4(org))=2.95. K(KL+ClO4=KlClO4(org))=3.73.

K+ con non-aq 25°C 100% C K1=>6 2000ICa (94402) 708
Medium: nitromethane.

K+ dis non-aq 25°C 100% U K1=10.16 2000Ksa (94403) 709
Medium: 1,2-dichloroethane

K+ oth alc/w 25°C 3% U M K(KL+phenolate)=0.33 2000MTa (94404) 710
K(KL+o-nitrophenolate)=0.54
K(KL+m-nitrophenolate)=0.68
K(KL+p-nitrophenolate)=0.89
Method: CZE. Medium: 3% v/v EtOH/H2O. K(KL+2,4-dinitrophenolate)=1.39,
K(KL+picrate)=1.49, K(KL+SCN)=0.82, K(KL+ClO4)=0.68

K+ oth alc/w 35°C 3.0% C K1=1.73 1999MTd (94405) 711
Method: capillary zone electrophoresis. Medium: 3% v/v EtOH/H2O, 0.005 M
phosphate buffer, pH 7.0

K+ cal non-aq 25°C 100% C H K1=3.63 1999Wba (94406) 712
Medium: N,N-dimethylformamide. DH(K1)=-32.6 kJ mol⁻¹.

K+ dis oth/un 25°C 0 U K1=4.76 19940Ua (94407) 713

K+ dis oth/un 25°C 0.01M U M K(K(picrate)+L)=3.12 1992TSb (94408) 714

K+ con none 20°C 0.0 C T H K1=1.80 1990TAa (94409) 715
Data for 15-32 C. At 15 C, K1=1.84; at 30 C, K1=1.685
At 25 C, DH(K1)=-18.1 kJ mol⁻¹, DS(K1)=-27.5 J K⁻¹ mol⁻¹.

K+ con none 25°C 0.0 U K1=1.744 1989TKa (94410) 716
K1=1.79 by potentiometry using an ion selective electrode

K+ sp non-aq 22°C 100% U K1=7.20 1987CCc (94411) 717
In deuteriochloroform

K+ ISE alc/w 25°C 90% U K1=4.75 1987KHa (94412) 718
Medium: 90% w/w MeOH/H2O

K+ cal non-aq 25°C 100% C H K1=5.29 1986ICa (94413) 719
Medium: MeOH. DH(K1)=-44.85 kJ mol⁻¹, DS(K1)=-49.0 J K⁻¹ mol⁻¹.

K+ cal alc/w 25°C 80% U H K1=3.82 1985LWa (94414) 720

K+ sp diox/w 25°C 0.0 U I K1=3.11 1983KOa (94415) 721
On PVA. In 24.4% w/w dioxan/H2O. Data given for 9.7-84.6 w/w mixtures.

K+ sp mixed 25°C 0.0 U I K1=2.88 1983KOa (94416) 722
On PVA. In 21.9% w/w tetrahydrofuran/H2O. Data given for 11.1-86.4 w/w mix

K+ ISE alc/w 25°C 100% U K1=4.9 1982GRc (94417) 723
Medium: MeOH

K+ sp alc/w 25°C 100% U K1=5.27 1981EMb (94418) 724
Medium: MeOH. By polarography at 22 C: K1=5.22

K+ ISE alc/w 25°C 100% C K1=5.2 1981PTa (94419) 725
Medium: MeOH

K+ sp diox/w 25°C 100% U M K(K(Picrate)+L)=5.24 1981SSd (94420) 726

K+ con non-aq 25°C 100% U K1=5.10 1976UHa (94421) 727
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

K+ cal alc/w 25°C 100% U H K1=3.18 1987ZBa (94472) 728
Medium: MeOH. DH=-33.5 kJ mol⁻¹; DS=-51.3. By ISE potentiometry: K1=3.15

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

K+ gl R4N.X 25°C 0.10M M K1=2.9 1991FGb (94493) 729
B(KHL)=7.4

Medium: 0.10 M Et4NNO3.

K+ ISE oth/un 25°C 0.10M C K1=5.48 1982BLc (94494) 730
Method: K ion selective electrode. Medium: 0.10 M Tris buffer, pH 7.0

K+ ISE R4N.X 25°C 0.10M U K1=5.48 1976BLb (94495) 731
Method: K ion selective electrode. Medium: 0.10 M (Me4N)H2PO4, pH 7.0

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

K+ nmr alc/w 20°C 100% C K1=9.26 1989GSc (94518) 732
Medium: 100% MeOH. Method: 1H pulsed gradient spin-echo nmr

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

K+ con non-aq 25°C C K1=2.5 1999ESa (94541) 733
In tetrahydrofuran; alkali metal is used as 2,4-dinitrophenolate

K+ con non-aq 25°C 100% U K1=2.48 1988YKa (94542) 734
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

K+ gl R4N.X 25°C 0.10M U K1=3.1 1990AFa (94588) 735

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

K+ gl R4N.X 25°C 0.10M U K1=3.3 1990AFa (94602) 736
B(KHL)=12.7

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

K+ con none 25°C 0.0 C K1=0.38 1998KTb (94630) 737

K+ ISE alc/w 25°C 100% U K1=2.15 1975CJa (94631) 738

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

K+ gl KCl 25°C 0.10M C K1=1.5 1991CMb (94907) 739

K+ gl R4N.X 25°C 0.10M C K1=1.64 1982DSa (94908) 740

C16H30N2O8 H2L CAS 72912-01-7 (1568)
1,4,10,13-Tetraoxa-7,16-diazacyclooctadecane-N,N'-diethanoic acid;

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

K+ gl R4N.X 25°C 0.10M U K1=3.91 1983CRb (95043) 741

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

K+ ISE alc/w 25°C 100% U K1=1.90 1982MKa (95096) 742
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

K+ ISE oth/un 25°C dil A I K1=1.90 1971FRa (95100) 743
In MeOH: K1=5.89

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

K+ ISE non-aq 25°C 100% M K1=2.66 1984NMb (95104) 744
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

K+ gl alc/w 25°C 95% M K1=2.60 1990LNa (95117) 745
Medium: 95% MeOH, 0.05 M Bu4NBr. For the 9,13-dihydroxy- analogue: K1 < 2

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
K+	con	non-aq	25°C	100%	M	M		K1=7.63 K(KL+ClO4)=0.96	1999DSd (95211)	746
Medium: acetonitrile.										
K+	ISE	non-aq	25°C	100%	C	H		K1=6.71	1999WBa (95212)	747
Medium: N,N-dimethylformamide. Method: competitive titration against Ag+, using Ag+ ISE. By calorimetry: DH(K1)=-53.5 kJ mol ⁻¹ .										
K+	gl	R4N.X	25°C	0.05M	C	H		K1=3.8	1996BCh (95213)	748
Medium: 0.05 M Et4NClO4. By calorimetry: K1=4.1, DH(K1)=-36.3 kJ mol ⁻¹ .										
K+	cal	non-aq	25°C	100%	M	H		K1=8.45	1994BCd (95214)	749
Medium: acetone. DH(K1)=-60.7 kJ mol ⁻¹ , TDS=-12.7										
K+	sp	non-aq	20°C	100%	U			K1=6.4	1992PSa (95215)	750
Medium: DMF, 0.01 M Me4NI										
K+	ISE	non-aq	25°C	100%	C			K1=6.1	1989MGa (95216)	751
Medium: DMF, 0.10 M Et4NClO4										
K+	ISE	non-aq	25°C	100%	M	H		K1=9.15	1988BUa (95217)	752
Medium: propylene carbonate, 0.05 M (CH3CH2)4NClO4. DH(K1)=-66.0 kJ mol ⁻¹ ; DS(K1)=-47 J K ⁻¹ mol ⁻¹										
K+	ISE	non-aq	25°C	100%	U	H		K1=9.10	1986BUb (95218)	753
In CH3CN. DH=-64.1 kJ mol ⁻¹										
K+	cal	alc/w	25°C	100%	U	H		K1=8.40	1986BUd (95219)	754
In MeOH. DH=-61.1 kJ mol ⁻¹										
K+	nmr	non-aq	25°C	100%	U			K1=11.22	1986CHc (95220)	755
In CDCl3 saturated with D2O										
K+	ISE	non-aq	25°C	100%	C	I		K1=6.00	1985CKa (95221)	756
Medium: DMSO. In propylenecarbonate K1=8.69; in DMF K1=6.59										
K+	ISE	non-aq	25°C	100%	U			K1=9.8	1980CRa (95222)	757
Medium: Propylene carbonate										
K+	kin	R4N.X	25°C	0.10M	U			K1=4.2	1980GBa (95223)	758
K+	ISE	alc/w	25°C	100%	U			K1=8.54	1978CSb (95224)	759
Medium: MeOH										
K+	cal	R4N.X	25°C	0.06M	C	H			1976KLc (95225)	760

Medium: 0.057 M Me4NBr. Method: flow microcalorimetry.
DH(K1)=-28.5 kJ mol⁻¹, DS(K1)=-20 J K⁻¹ mol⁻¹.

K+ gl R4N.X 25°C 0.05M C I K1=3.95 1975LSc (95226) 761
In 95% MeOH: K1=7.45; 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

K+ cal alc/w 25°C 100% U H K1=3.85 1990K Mb (95319) 762
Medium: MeOH. DH=-25.7 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

K+ gl NaClO4 25°C 0.50M U K1=<2 1981K Mb (95334) 763

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

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

K+ con non-aq 25°C 100% C I K1=3.06 1992TFa (95384) 764
Medium: acetonitrile. In propylene carbonate, K1=2.88.

K+ con alc/w 25°C 100% U K1=2.43 1991IOa (95385) 765
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

K+ sol non-aq 25°C 100% C K1=3.94 1999K Ca (95396) 766
Medium: acetonitrile.

K+ ISE alc/w 25°C 100% A K1=3.48 1971FRa (95397) 767
Medium: MeOH

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

K+ EMF alc/w 25°C 100% U I K1=4.69 1994LLa (95415) 768
Medium: MeOH, 0.05M Et4NClO4. Also data for acetonitrile: K=5.24, PC: K=5.0

DMF: K=3.31 and H2O: K<2. Method: 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

K+ cal alc/w 25°C 90% U H K1=4.00 1994IZa (95431) 769
Medium: 90% v/v MeOH/H2O. DH(K1)=-23.9 kJ mol⁻¹, DS(K1)=-3.7 J K⁻¹ mol⁻¹

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

K+ ISE non-aq 25°C 100% U K1=4.66 1993RPa (95449) 770
Medium: dimethylformamide, 0.05 M Et4NClO4. By competition with Ag+.

K+ gl NaClO4 25°C 0.50M U K1=<2 1981K Mb (95450) 771

C16H34O6 L CAS 57721-92-3 (2501)
2,5,8,15,18,21-Hexaoxadocosane; CH3.0.(CH2.CH2.0)2.(CH2)6.0.(CH2.CH2.0)2.CH3

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

K+ ISE alc/w 25°C 100% U K1=<0.1 1975CJa (95485) 772
Medium: MeOH

C16H34O8 L CAS 1191-91-9 (2500)
2,5,8,11,14,17,20,23-Octaoxatetracosane; CH3.0.(CH2.CH2.0)7.CH3

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

K+ con non-aq 25°C 100% U K1=4.9 1993EVa (95490) 773
Medium: THF+CHCl3 (4:1 vol). Also data for other solvents

K+ ISE alc/w 25°C 100% U K1=2.87 1975CJa (95491) 774

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

K+ gl non-aq 25°C 100% U K1=2.3 1986STb (95539) 775
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
K+	EMF	non-aq	25°C	100%	U	I	K1=3.40	1996WPa (95572)	776
Medium: acetonitrile, 0.05 M NEt4ClO4. In propylene carbonate K1=5.91									
K+	gl	alc/w	25°C	100%	C	I	K1=2.43	1993TCa (95573)	777
Medium: MeOH, 0.05 M Et4NClO4. In DMF, K1=1.59									

C17H20N4O6 HL Riboflavin CAS 83-88-5 (1438)									
7,8-Dimethyl-10(D-1'-ribityl)isoalloxazine, Vitamin B2, Vitamin H									
K+	sol	oth/un	22°C		U		K1=-0.097	1980LDA (96338)	778
Medium: variable KNO3 content 0.1-2.5 M									

C17H21O5P L (5732)									
Methyldi(2-methoxyphenoxy)methylphosphine oxide; Me.PO(CH2.O.C6H4.OMe)2									
K+	con	non-aq	25°C	100%	U		K1=1.88	1989TKb (96391)	779
Medium: tetrahydrofuran/CHCl3 4:1 (volume)									

C17H23NO6 L (7047)									
5'-(N-Acrylamide)-benzo-15-crown-5; CH2:CH.CO.NH.C14H19O5									
K+	sp	non-aq	25°C	100%	U		K1=9.67	1979KMb (96406)	780
Medium: CHCl3									

C17H24N4O11 L CAS 94616-60-1 (1039)									
2,4,6-Trinitrophenylaminomethyl-15-crown-5									
K+	sp	mixed	25°C	16%	U		K1=2.28 K(K+HL)=1.12	1984BPa (96463)	781

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									
K+	con	non-aq	25°C	100%	U		K1=4.89	1976UHa (96468)	782
Medium: acetone									

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

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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
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K+         sp  diox/w 25°C 100% U   M              1981SSd (96514) 783
              K(K(Picrate)+L)=5.73
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K+         ISE none 25°C 0.0 C      K1=2.04        1980WSb (96515) 784
Method: monovalent ion electrode. Also data for the 4'-polyvinylbenzene-
derivative: by spectrophotometry, K1=2.04
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K+         con non-aq 25°C 100% U      K1=5.58        1976UHa (96516) 785
Medium: acetone
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C17H26O6          L              CAS 99159-90-7 (688)
2,3-Benzo-1,4,7,10,13,16-hexaoxacyclononadeca-2-ene;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
K+         sp  non-aq 22°C 100% U      K1=6.35        1987CCc (96520) 786
In deuteriochloroform
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-----
K+         cal alc/w 25°C 80% U   H      K1=3.33        1985LWa (96521) 787
*****
C17H26O6          L              CAS 65112-34-7 (6059)
21-Methoxy-3,6,9,12,15-pentaoxabicyclo[15.3.1]heneicosa-1(21),17,19-triene;
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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
K+         cal alc/w 25°C 100% U   H      K1=3.52        1987ZBa (96527) 788
Medium: MeOH. DH=-24.7 kJ mol-1; DS=-15.4. By ISE potentiometry: K1=3.48
*****
C17H30O6          H2L             CAS 159029-04-6 (7605)
15-(Methoxymethoxy)-9,11-dioxo-pentadecanoic acid;
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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
K+         sp  alc/w  RT  80% C      K1=-0.09       1994HWc (96671) 789
Medium: 80%MeOH/H2O. Also data for many analogues.
*****
C17H34N2O4        L              CAS 142565-14-8 (6562)
4,7,13,16-Tetraoxa-1,10-diazabicyclo[8.8.5]tricosane;
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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
K+         EMF non-aq 25°C 100% C   I      K1=7.56        1993DLb (96743) 790
Medium: propylene carbonate, 0.05 M Et4NClO4. In acetonitrile, K1=6.26.
-----
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-----
K+         gl  R4N.X 25°C 0.05M C   I      K1=3.41        1992CGb (96744) 791
-----
```

Medium: Et4NC1O4. In MeOH: K1=5.8; in DMF K1=3.85

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

K+ gl alc/w 25°C 95% C K1=3.51 2004KVa (96758) 792
Medium: 95% MeOH/H2O, 0.01 M Et4NC1O4.

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

K+ ISE alc/w 25°C 100% U K1=1.36 1982MYc (96765) 793
Medium: MeOH

C17H35N04 L (1694)
N-n-Heptanyl-1,4,7,10-tetraoxa-13-azacyclopentadecane;

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

K+ ISE alc/w 25°C 10% U K1=2.29 1986HAa (96768) 794
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

K+ con non-aq 25°C C K1=3.0 1999ESa (96812) 795
In tetrahydrofuran; alkali metal is used as 2,4-dinitrophenolate

C18H18O8 H2L (5631)
1,4-bis(2-Carboxymethoxyphenyl)-1,4-dioxabutane;

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

K+ ISE alc/w 25°C 100% U K1=2.23 1981PTb (97304) 796
Medium: MeOH

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

K+ sp non-aq 25°C 100% C K1=>1.74 2002YEa (97475) 797
Method: fluorescence spectroscopy. Medium: acetonitrile.

K+ ISE alc/w 25°C 100% U B2=5.7 1982GRc (97476) 798
Medium: MeOH

K+ ISE alc/w 25°C 100% C K1=2.0 B2=5.21 1981PTa (97477) 799
Medium: MeOH

C18H2007 H2L (5627)
1-(2-Hydroxyphenyl)-7-(2-carboxymethoxyphenyl)-1,4,7-trioxahепtane;

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

K+ ISE alc/w 25°C 100% U K1=2.24 1981PTb (97482) 800
Medium: MeOH

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

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

K+ con non-aq 25°C C K1=2.9 1999ESa (97505) 801
In tetrahydrofuran; alkali metal is used as 2,4-dinitrophenolate

K+ con non-aq 25°C 100% U K1=2.73 1988YKa (97506) 802
Medium: tetrahydrofuran

C18H2205 L (5737)
1,7-Di(2-methoxyphenyl)-1,4,7-trioxahепtane; MeO.C6H4.O.C2H4.O.C2H4.O.C6H4.OMe

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

K+ con non-aq 25°C 100% U K1=2.19 1989TKb (97565) 803
Medium: tetrahydrofuran/CHCl3 4:1 (volume)

C18H2205 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

K+ ISE alc/w ? 100% U K1=2.71 B2=6.35 1992CLb (97568) 804
Medium: MeOH. Data also for 7'-t-butyl, 7'-(1,1-dibutylethyl) and
7'-(1-methyl-1-dodecylethyl) analogues

K+ dis non-aq 15°C 100% C 1985YIa (97569) 805
K(K+2L(org))+A=KL2A(org))=7.61
K(KL2(org))+A(org)=KL2A)=3.2

Media: H2O/dichloroethane. Analysis by spectrophotometry.

HA: picric acid.

C18H2206 L (5633)
1,4-bis(2-Hydroxyethoxyphenyl)-1,4-dioxabutane;

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

K+ ISE alc/w 25°C 100% U K1=1.74 1981PTb (97572) 806
Medium: MeOH

C18H23N08 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-]isoin-
ole18,20dione;

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

K+ sp non-aq 25°C 100% C K1=4.4 20010Ya (97575) 807
Medium: methanol. For the N-propyl derivative, K1=4.5.

C18H2607 L (5656)
2,3-Acetylbenzo-1,4,7,10,13,16-hexaoxacyclooctadeca-2-ene;

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

K+ ISE alc/w 25°C 100% U K1=4.93 1982GRc (97730) 808
Medium: MeOH

C18H2607 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

K+ ISE alc/w 25°C 100% U K1=4.23 1982MKa (97732) 809
Medium: MeOH

C18H27N203F L CAS 173417-90-8 (6571)
23-Fluoro-4,7,20-trioxa-1,10-diazatricyclo[8.7.5.1,12,16]tricoso-12,14,16(23)triene
;

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

K+ EMF non-aq 25°C 100% C H K1=2.52 1999BHa (97747) 810
Medium: MeOH, 0.05 M Et4NClO4. By calorimetry DH(K1)=-3.3 kJ mol⁻¹.

Method: by competition with Ag⁺, using Ag/Ag⁺ electrode.

C18H28N203 L CAS 154148-31-9 (6510)
4,7,20-Trioxa-1,10-diazatricyclo[8.7.5.1,12,16]tricoso-12,14,16(23)-triene;

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

K+ EMF non-aq 25°C 100% C H K1=2.50 1999BHa (97770) 811
Medium: MeOH, 0.05 M Et4NClO4. By calorimetry DH(K1)=-24.5 kJ mol⁻¹

Method: by competition with Ag⁺, using Ag/Ag⁺ electrode

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

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

K+ sp non-aq 22°C 100% U K1=5.28 1987CCc (97835) 812
In deuteriochloroform

C18H2806 L CAS 85556-93-0 (642)
2,3-Benzo-8,15-dimethyl-1,4,7,10,13,16-hexaoxacyclooctadeca-2-ene;

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

K+ con alc/w 25°C 100% U K1=4.39 1983LSa (97841) 813
Medium: MeOH

C18H2806 L AN(MOEOE)20 CAS 60232-73-7 (2247)
21-Methoxy-19-methyl-3,6,9,12,15-pentaoxabicyclo[15.3.1]heneicos-1(21),17,19-triene
;

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

K+ dis non-aq 25°C 100% U H 1979KLa (97846) 814
K(K(picrate)+L)=6.26

Medium: CHCl3

C18H2806 L CAS 100433-53-6 (607)
Benzyloxymethyl-1,4,7,10,13-pentaoxacyclopentadecane, Benzyloxymethyl-15-crown-5;

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

K+ ISE alc/w 25°C 100% U K1=5.2 1982GRc (97850) 815
Medium: MeOH

K+ ISE alc/w 25°C 100% U K1=3.16 B2=4.43 1982MYc (97851) 816
Medium: MeOH

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

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

K+ sp non-aq 22°C 100% U K1=6.81 1987CCc (97856) 817
In deuteriochloroform

C18H3006 L (2503)
3,6,9,12,15,18-Hexaoxa-10,11-benzo-eicosa-10-ene; C6H4(0.(CH2.CH2.0)2.C2H5)2

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

K+ ISE alc/w 25°C 100% U K1=1.78 1975CJa (98115) 818
Medium: MeOH

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

K+ ISE alc/w 25°C 100% A K1=1.30 1971FRa (98270) 819
Medium: MeOH

C18H33NO9 HL 4NH18-C6A CAS 83572-66-1 (5404)
2-Carboxy-3-N-butylformamide-1,4,7,10,13,16-hexaoxacyclooctadecane;

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

K+ gl alc/w 25°C 90% U K1=5.8 1984FWa (98287) 820
B(KHL)=10.7

Medium: 90% v/v MeOH/H2O, 0.05 M R4NX

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

K+ ISE alc/w 25°C 100% U K1=3.84 1982MKa (98392) 821
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

K+ ISE non-aq 25°C 100% M K1=5.94 1984NMB (98394) 822
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

K+ ISE alc/w 25°C 100% U K1=1.78 1975CJa (98397) 823
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

K+ gl alc/w 25°C 95% M K1=5.11 1990LNa (98406) 824

Medium: 95% MeOH, 0.05 M Bu4NBr. For the 12,16-dihydroxy- analogue: K1=3.40

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

K+ gl alc/w 25°C 95% M K1=4.14 1990LNa (98414) 825
Medium: 95% MeOH, 0.05 M Bu4NBr. For the 9,16-dihydroxy- analogue: K1=2.44

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

K+ cal none 25°C 0 U IH K1=4.00 1997ZiA (98420) 826
DH(K1)=-32.9 kJ mol⁻¹, DS=-33.9. In 95% v/v MeOH/H2O: K1=8.61, DH(K1)=55.7,
DS=-22.1

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

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

K+ con non-aq 25°C 100% M M K1=>12 1999DSd (98589) 827
K(KL+ClO4)=0.84

Medium: acetonitrile.

K+ vlt non-aq 25°C 100% C I K1=11.3 1999FKb (98590) 828

Medium: acetonitrile, 0.10 M Et4NClO4. Method: cyclic voltammetry.
Also in: DMF (K1=8.0), DMSO (7.0), MeOH (10.4), acetone (10.4) etc.

K+ ISE non-aq 25°C 100% C H K1=7.82 1999WBa (98591) 829

Medium: N,N-dimethylformamide. Method: competitive titration against
Ag⁺, using Ag⁺ ISE. By calorimetry: DH(K1)=-60.2 kJ mol⁻¹.

K+ gl R4N.X 25°C 0.05M C H K1=6.0 1996BCh (98592) 830

Medium: 0.05 M Et4NClO4. By calorimetry: DH(K1)=-52.3 kJ mol⁻¹.

K+ cal alc/w 25°C 80% C H K1=8.52 1995KZa (98593) 831

Medium: 80% v/v CH3OH/H2O. DH(K1)=-65.8 kJ mol⁻¹, DS(K1)=-57.7 J K⁻¹ mol⁻¹

K+ cal non-aq 25°C 100% M H K1=10.04 1994BCd (98594) 832

Medium: acetone. DH(K1)=-69.0 kJ mol⁻¹, TDS=-12.0

K+ ISE oth/un 25°C 0.05M M K1=10.49 1992BUb (98595) 833

K1=9.82 (by potentiometry)

K+ ISE non-aq 25°C 100% U K1=10.50 1992CSc (98596) 834

Ag/Ag⁺ electrode. Medium: MeCN, 0.05 M Bu4NClO4

K+ ISE non-aq 25°C 100% M H K1=11.00 1988BUa (98597) 835
Medium: propylene carbonate, 0.05 M (CH₃CH₂)₄NC104. DH(K1)=-72.8 kJ mol⁻¹;
DS(K1)=-34.5 J K⁻¹ mol⁻¹

K+ con none 25°C 0.0 U K1=5.4 1988DSb (98598) 836

K+ ISE non-aq 25°C 100% U H K1=9.56 1986BUb (98599) 837
In CH₃CN. DH=-74.0 kJ mol⁻¹

K+ cal alc/w 25°C 100% U H K1=9.82 1986BUd (98600) 838
In MeOH. DH=-75.0 kJ mol⁻¹

K+ nmr non-aq 25°C 100% U K1=13.20 1986CHc (98601) 839
In CDCl₃ saturated with D₂O

K+ cal non-aq 25°C 100% U H 1986DGa (98602) 840
DH1 = -80.3 kJ mol⁻¹. Medium: nitromethane

K+ ISE non-aq 25°C 100% C I K1=7.18 1985CKa (98603) 841
Medium: DMSO. In DMF K1=8.03

K+ cal non-aq 25°C 100% U H 1985DGa (98604) 842
Medium: propylene carbonate. DH1 = -71.9 kJ mol⁻¹

K+ cal non-aq 25°C 100% U H 1985DGa (98605) 843
Medium: acetonitrile. DH1 = -71.3 kJ mol⁻¹

K+ ISE non-aq 25°C 100% M K1=12.58 1985DGb (98606) 844
Medium: nitromethane

K+ cal non-aq 25°C 100% U H 1984DGa (98607) 845
Medium: N,N-dimethylformamide. DH1=-54.5 kJ mol⁻¹; DS1=-31.0 J K⁻¹ mol⁻¹.

K+ cal non-aq 25°C 100% U H 1984DGa (98608) 846
Medium: DMSO. DH1=-61.2 kJ mol⁻¹; DS1=-71.5 J K⁻¹ mol⁻¹

K+ gl oth/un 25°C 0.10M U I K1=5.6 1982CFb (98609) 847
In MeCN, mol fraction n: K1=6.5 (n=0.1); 7.1 (n=0.2); 8.1 (0.4); 8.9 (0.6);
9.7 (n=0.7); 10.3 (n=0.9)

K+ ISE non-aq 25°C 100% U I K1=11.31 1981CRa (98610) 848
Medium: MeCN. In DMSO: K1=7.11; in EtOH: 10.50; in DMF: 7.98;
in N-methylpropanoamide: 8.4

K+ sp diox/w 25°C 100% U M 1981SSd (98611) 849
K(K(Picrate)+L)=8.3

K+ ISE non-aq 25°C 100% U K1=11.1 1980CRa (98612) 850
Medium: Propylene carbonate

K+ kin R4N.X 25°C 0.10M U K1=5.4 1980GBa (98613) 851

K+ con non-aq 25°C 100% U K1=>7 1980KMb (98614) 852
Medium: MeCN

K+ ISE alc/w 25°C 100% U K1=10.4 1978CSb (98615) 853
Medium: MeOH

K+ EMF oth/un 25°C 0.05M C I K1=5.4 1978YTa (98616) 854
Method: competition with Tl+, using Tl amalgam electrode.
Electrolyte not stated. In MeOH, 0.05 M: K1=10.8. In DMSO, 0.10 M: K1=6.0

K+ cal alc/w 25°C 100% C 1977ADa (98617) 855
Medium: methanol. DH(K1)=-69.9 kJ mol⁻¹. In H₂O, DH(K1)=-48.5 kJ mol⁻¹.

K+ cal R4N.X 25°C 0.06M C IH 1976KLc (98618) 856
Medium: 0.057 M Me₄NBr. Method: flow microcalorimetry. DH(K1)=-47.7 kJ
mol⁻¹, DS(K1)=-59 J K⁻¹ mol⁻¹. In 95% (v/v) MeOH/H₂O, DH(K1)=-79.5, DS=-80

K+ gl R4N.X 25°C 0.10M C H K1=5.58 1975ANa (98619) 857
Medium: Me₄NCl. DH(K1)=-46.0 kJ mol⁻¹, DS=-48.1

K+ oth non-aq -30°C 100% U K1=4.9 1975HBb (98620) 858
Medium: THF

K+ gl R4N.X 25°C 0.05M C I K1=5.4 1975LSc (98621) 859
In 95% MeOH: K1=9.75

C18H36N4O4 L (6795)
4,10-Bis(N,N-dimethylpropanamido)-1,7-dioxo-4,10-diazacyclododecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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K+ cal alc/w 25°C 100% U H K1=3.03 1990KMb (98781) 860
Medium: MeOH. DH=-30.6 kJ mol⁻¹

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
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K+ sol non-aq 25°C 100% C K1=4.55 1999KCa (98806) 861
Medium: acetonitrile.

K+ cal alc/w 25°C 100% U H K1=3.47 1993ILa (98807) 862
Medium: MeOH. DH=-43.5 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

K+ ISE a/c/w 25°C 100% U K1=2.82 1983MKa (98811) 863

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

K+ gl a/c/w 25°C 95% C K1=4.80 1975LSc (98819) 864
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

K+ sol non-aq 20°C 100% C K1=5.22 1983SLa (98821) 865
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

K+ sol non-aq 20°C 100% C K1=5.48 1983SLa (98839) 866
Medium: CHCl3

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

K+ dis non-aq 25°C 100% C K1=9.27 1998KSc (98874) 867
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

K+ sp non-aq 25°C 100% C K1=3.8 2000KBb (99334) 868
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

K+ con non-aq 25°C 100% U K1=3.29 1989TKb (99345) 869
Medium: tetrahydrofuran/CHCl3 4:1 (volume)

C19H27N07 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

K+ sp non-aq 25°C 100% U K1=7.79 1979KMb (99394) 870
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

K+ sp alc/w 25°C 100% U Keff=5.25 1977TMa (99397) 871

Medium: MeOH

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

K+ con alc/w 25°C 100% U K1=3.91 1983LSa (99436) 872
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

K+ sp alc/w 25°C 100% U Keff=4.78 1977TMa (99446) 873

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

K+ ISE alc/w 25°C 100% U H K1=3.72 B2= 6.16 1998SSf (99452) 874
Medium: 100% MeOH, 0,05 M Et4NI. By calorimetry DH(K1)=-14.1 kJ mol-1
DH(B2)=-26.0.Many other crown ethers studied

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
K+	ISE	alc/w	25°C	100%	U	I	K1=3.05	1984IEa (99475)	875
Medium: MeOH. In 90% MeOH: K1=2.52									

C19H39N05		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
K+	ISE	alc/w	25°C	10%	U		K1=4.17 B2=7.38	1986HAa (99478)	876
Medium: 10% MeOH/H2O									

C19H39N305		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
K+	gl	R4N.X	25°C	0.10M	U		K1=4.2	1978LMa (99492)	877

C20H2204		L					CAS 82645-28-1 (8945)		
o,o'-(Triethyleneglycoldiyl)-(Z)-stilbene;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
K+	con	non-aq	25°C	100%	C		K1=ca.4.5	2000ICa (99927)	878
Medium: nitromethane.									

C20H2206		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
K+	con	non-aq	25°C	100%	U		K1=1.9	1993EVa (99931)	879
Medium: THF+CHCl3 (4:1 vol)									

C20H2209		H2L					(5624)		
1,7-bis(2-Carboxymethoxyphenyl)-1,4,7-trioxaheptane;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
K+	ISE	alc/w	25°C	100%	U		K1=3.07	1981PTb (99938)	880
Medium: MeOH									

C20H2405		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
K+	ISE	alc/w	25°C	100%	C		K1=0.9 B2=4.0	1981PTa (100045)	881

Medium: MeOH. Data for racemic ligand. For meso ligand K1=1.4, B2=4.67

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

K+ ISE alc/w 25°C 100% C K1=1.4 B2=4.57 1981PTa (100047) 882

Medium: MeOH. Data for racemic ligand

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

K+ EMF alc/w 25°C 100% C K1=4.86 2004ZTa (100125) 883

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

K+ oth KCl 25°C 0.05M C K1=1.74 2002KTa (100126) 884
Method: capillary electrophoresis. Medium: 0.03-0.06 M KCl.

K+ dis non-aq 24°C 100% C K(K+A+L)=7.04 2002MRd (100127) 885

Medium: CDCl3. HA is picric acid.

K+ con non-aq 25°C 100% C K1=5.39 2000ICa (100128) 886
Medium: nitromethane.

K+ sp non-aq 25°C 100% C K1=4.9 2000KBb (100129) 887
Medium: MeOH. Method: electrospray ionization mass spectrometry.

K+ oth alc/w 25°C 3% U M 2000MTa (100130) 888
K(KL+phenolate)=0.55
K(KL+o-nitrophenolate)=1.01
K(KL+m-nitrophenolate)=0.81
K(KL+p-nitrophenolate)=1.12

Method: CZE. Medium: 3% v/v EtOH/H2O. K(KL+2,4-dinitrophenolate)=1.73,
K(KL+picrate)=1.87, K(KL+SCN)=1.40, K(KL+ClO4)=0.60

K+ dis oth/un 25°C 0.06M C K(KL+A)=1.30 2000YYa (100131) 889
K(K+L(org)+A=KLA(org))=4.99

Method: extraction of metal picrate (0.06 M, pH 12) into dichloromethane/
ligand solution. HA: picric acid. Data for many additional solvents.

K+ sp mixed 25°C C TIH K1=2.66 1999EDa (100132) 890
In 60 % mass H2O/acetonitrile; For 80% H2O K1=2.37, DH1=-6.4 kJ/mol
For 100% acetonitrile K1=4.50 the same at 35 C: 4.42; 40 C: 4.38

K+ oth alc/w 35°C 3.0% C K1=1.66 1999MTd (100133) 891
Method: capillary zone electrophoresis. Medium: 3% v/v EtOH/H2O, 0.005 M
phosphate buffer, pH 7.0

K+ dis non-aq 25°C 100% U K1=9.36 1998KSb (100134) 892
Medium: 1,2-dichloroethane

K+ oth oth/un 25°C 0.04M C K1=1.67 1998TIa (100135) 893
K(KL+ClO4)=0.54
K(KL+picrate)=1.95

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

K+ sp non-aq 25°C 100% U T H K1=4.50 1997EKa (100136) 894
Medium: CH3CN. Also data for H2O/CH3CN mixtures

K+ sp mixed 10°C 60% C T H K1=2.97 1997EYa (100137) 895
Medium: 60% w/w CH3CN/H2O; For 45 C and 60% CH3CN K1=2.66;
For 80% CH3CN and 10 C K1=3.45; For 45 C and 80% CH3CN K1=3.23

K+ con non-aq 25°C 100% C T H K1=4.78 1997TAa (100138) 896
Medium: acetonitrile. DH(K1)=-20.1 kJ mol⁻¹, DS(K1)=23.8 J K⁻¹ mol⁻¹.
Data for 10-25 C.

K+ vlt non-aq 25°C 100% C K1=6.9 1995KTb (100139) 897
Method: ion transfer polarography. Medium: nitrobenzene, 0.05 M
tetrabutylammonium tetraphenylborate.

K+ dis oth/un 25°C 0 U K1=4.68 1994OUa (100140) 898

K+ dis non-aq 23°C 100% C K1=6.6 1992HGb (100141) 899
K(K+A+L(org))=KAL(org))=6.37

Extraction of metal chloride (A) from aqueous solution into nitrobenzene/
0.01M Bu4NB(Ph)4. Peak potential voltammetry and distribution of 42K.

K+ sp non-aq 25°C 100% U K1=3.17 1991NTa (100142) 900
Medium: DMF

K+ vlt non-aq 23°C 100% C I K1=4.75 1990LUa (100143) 901
Medium: MeCN, 0.05 M Bu4NClO4. Data also in DMF (K1=3.15), DMSO (2.60),
benzonitrile (5.15), propylene carbonate (5.06) and other solvents

K+ vlt non-aq 25°C 100% U K1=9.9 1990SPa (100144) 902
Medium: 1,2-dichloroethane

K+ cal non-aq 25°C 100% C H K1=4.78 1988BUb (100145) 903
Medium: acetonitrile. DH(K1)=-18.6 kJ mol⁻¹, DS(K1)=29 J K⁻¹ mol⁻¹.

K+ con non-aq 25°C 100% U K1=4.66 1986STb (100146) 904
Medium: THF:CHCl3 4:1 v/v. Metal as 2,4-dinitrophenolate

K+ con mixed 25°C ? U K1=7.16 1984MPa (100147) 905
Medium: 60%(vol) isopropanol+ 20% H2O + 20% CHCl3

K+ ISE alc/w 25°C 100% C K1=4.8 1981PTa (100148) 906
Medium: MeOH

K+ vlt non-aq 25°C 100% U I K1=4.70 1978HKc (100149) 907
Medium: CH3CN, 0.05M Bu4NClO4

K+ nmr non-aq 29°C 100% U K1=3.64 1977SZa (100150) 908
Medium: DMF

K+ sp alc/w 30°C 96% U K1=0.65 1975DBb (100151) 909

K+ dis non-aq 25°C 100% C T HM 1975SIc (100152) 910
K(K+A+L(org)=KAL(org))=4.65
Method: Extraction from H2O into benzene. HA is picric acid. DH(KAL(org))
=-68.2 kJ mol⁻¹, DS(KAL(org))=-140 J K⁻¹ mol⁻¹.

K+ sol none 25°C 0.0 U I K1=1.67 1975SNa (100153) 911

K+ ISE alc/w 25°C 100% A K1=5.00 1971FRa (100154) 912
Medium: MeOH

C20H2406 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
K+	dis	non-aq	23°C	100%	C			K1=6.4 K(K+A+L(org)=KAL(org))=6.19	1992HGb (100261)	913

Extraction of metal chloride (A) from aqueous solution into nitrobenzene/
0.01M Bu4NB(Ph)4. Peak potential voltammetry and distribution of 42K.

C20H2406 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
K+	sp	non-aq	25°C	100%	C			K1=2.968	2002YEa (100267)	914

Method: fluorescence spectroscopy. Medium: acetonitrile.

K+	dis	non-aq	23°C	100%	C			K1=5.4 K(K+A+L(org)=KAL(org))=6.25	1992HGb (100268)	915
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Extraction of metal chloride (A) from aqueous solution into nitrobenzene/
0.01M Bu4NB(Ph)4. Peak potential voltammetry and distribution of 42K.

C20H2408 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

K+ ISE a/c/w 25°C 100% U K1=2.47 1981PTb (100275) 916
Medium: MeOH

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

K+ dis non-aq 25°C 100% U H K(K(picrate)+L)=7.93 1979KLa (100346) 917
Medium: CHCl3

C20H26O7 L (5626)
1,7-bis(2-Hydroxyethoxyphenyl)-1,4,7-trioxahseptane;

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

K+ ISE a/c/w 25°C 100% U K1=2.23 1981PTb (100351) 918
Medium: MeOH

C20H27NO5 L (5296)
2,3:11,12-Dibenzo-1,4,7,10,13-pentaoxa-16-azaoctadeca-2,11-diene;

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

K+ ISE a/c/w 25°C 100% A K1=3.20 1971FRa (100353) 919
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

K+ cal non-aq 25°C 100% C H K(K+HL)=3.17 1997ZBb (100356) 920
Medium: MeOH. DH(K)=-19.4 kJ mol⁻¹, DS(K)=-4.40 J K⁻¹ mol⁻¹.

C20H28N2O4 L (5297)
2,3:11,12-Dibenzo-1,4,10,13-tetraoxa-7,16-diazaoctadeca-2,11-diene;

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

K+ ISE a/c/w 25°C 100% A K1=1.63 1971FRa (100388) 921
Medium: MeOH

C20H28O7 L CAS 123295-30-7 (5571)
14,14-Dimethyl-15,16-(1,4-Benzodioxinic)-1,4,7,10,13-pentaoxacycloheptadeca-15-ene;

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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
K+         gl  alc/w  25°C 100% U          K1=1.40      1989Mgb (100399) 922
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;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
K+         EMF non-aq 25°C 100% C H      K1=6.71      1999BHa (100440) 923
Medium: MeOH, 0.05 M Et4NClO4. By calorimetry DH(K1)=-39.6 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;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
K+         EMF non-aq 25°C 100% C H      K1=5.56      1999BHa (100457) 924
Medium: MeOH, 0.05 M Et4NClO4. By calorimetry DH(K1)=-41.5 kJ mol-1.
Method: by competition with Ag+, using Ag/Ag+ electrode.
*****
C20H32O6            L          CAS 14098-26-1 (5657)
2,3-tert.Butylbenzo-1,4,7,10,13,16-hexaoxacyclooctadeca-2-ene;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
K+         ISE alc/w  25°C 100% U          K1=5.12      1982GRc (100489) 925
Medium: MeOH
*****
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-tri-
ene;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
K+         dis non-aq 25°C 100% U H          K(K(picrate)+L)=5.26
1979KLa (100491) 926
Medium: CHCl3
*****
C20H32O8            L          Benzo24-crown-8 (6356)
2,3-Benzo-1,4,7,10,13,16,19,22-Octaoxatetracosa-2-ene;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
K+         sp non-aq  22°C 100% U          K1=5.96      1987CCc (100496) 927
In deuteriochloroform
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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

K+ ISE alc/w 25°C 10% U K1=3.64 B2=6.98 1986HAa (100501) 928
Medium: 10% MeOH/H2O

C20H34O8 L (2504)
2,5,8,11,14,17,20,23-Octaoxa-12,13-benzotetracos-12-ene; C6H4(0.(CH2.CH2.0)3.CH3)2

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

K+ ISE alc/w 25°C 100% U K1=2.83 1975CJa (100525) 929
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

K+ EMF alc/w 25°C 100% C K1=4.96 2004ZTa (100652) 930
Medium: 100% methanol, 0.05 M Bu4NClO4. Method: Ag electrode,
competition with Ag+ ion.

K+ dis non-aq 25°C 100% U K1=11.72 2000KSa (100653) 931
Medium: 1,2-dichloroethane

K+ dis non-aq 25°C 100% U K(K(pic)+L)=K(pic),L)=8.20 1995BSa (100654) 932
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=8.27) and anti-L(8.18)

K+ cal non-aq 25°C 100% C H K1=6.19 1988BUb (100655) 933
Medium: acetonitrile. DH(K1)=-29.6 kJ mol⁻¹, DS(K1)=19 J K⁻¹ mol⁻¹.

K+ con none 25°C 0.0 C T H K1=5.53 1988TMc (100656) 934
Data for 15-35 C. DH(K1)=-66.8 kJ mol⁻¹, DS(K1)=-122.8 J K⁻¹ mol⁻¹.
Anion is tetraphenyl borate.

K+ con mixed 25°C ? U K1=6.75 1984MPa (100657) 935
Medium: 20%(vol) isopropanol+ 80% H2O

K+ dis non-aq 25°C 100% U H K(K(picrate)+L)=8.3 1979KLa (100658) 936
Medium: CHCl3

K+ ISE oth/un 25°C dil A K1=1.78 1971FRa (100659) 937
Isomer B. In MeOH, K1=5.38. For isomer A: K1=2.18; in MeOH: K1=6.01

K+ cal oth/un 40°C 0.0 U T K1=1.50 1971INa (100660) 938
Isomer B. K1(10 C)=1.79, K1(25 C)=1.63. For isomer A: K1=2.15(10 C),
2.02(25 C), 1.91(40 C)

K+ cal oth/un 25°C 0.01M U K1=1.60 1969IRa (100661) 939
Isomer B. For isomer A: K1=2.01

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

K+ cal alc/w 25°C 80% C H K1=7.08 1995KZa (100739) 940
Medium: 80% v/v CH3OH/H2O. DH(K1)=-54.1 kJ mol⁻¹, DS(K1)=-46.0 J K⁻¹ mol⁻¹

C20H38O8 L (617)
3-Hexyl-1,4,7,10,13,16,19-heptaioxacycloheneicosan-2-one, 3-Hexyl-2-one-21-crown-7;

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

K+ ISE alc/w 25°C 100% U K1=3.39 1982MKa (100755) 941
Medium: MeOH

C20H38O9 L CAS 94618-61-8 (8712)
1,11-Dimethyl-3,6,9,13,16,19,21,24,27-nonaioxabicyclo[9.9.7]heptacosane;

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

K+ ISE non-aq 25°C 100% M K1=7.06 1984NMB (100758) 942
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

K+ gl non-aq 25°C 100% C I K1=5.09 1992LSc (100775) 943
Medium: MeCN, 0.05 M Et4NClO4. In DMF K1=2.6; 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

K+ gl alc/w 25°C 95% M K1=5.47 1990LNa (100785) 944
Medium: 95% MeOH, 0.05 M Bu4NBr. For the 12,19-dihydroxy- analogue: K1=5.13

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

K+ gl alc/w 25°C 95% M K1=3.23 1990LNa (100794) 945
Medium: 95% MeOH, 0.05 M Bu4NBr. For the 9,19-dihydroxy- analogue: K1=3.78

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

K+ cal alc/w 25°C 90% C H K1=4.35 1992DJa (100798) 946
Medium: 90% v/v MeOH/H2O. DH(K1)=-63.2 kJ mol-1, DS(K1)=-129 J K-1 mol-1.

C20H40N2O7 L CAS 147900-71-8 (8617)
4,7,10,16,19,22,27-Heptaoxa-1,13-diazabicyclo[11.11.5]nonacosane;

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

K+ cal alc/w 25°C 80% C H K1=3.99 1995KZa (100801) 947
Medium: 80% v/v CH3OH/H2O. DH(K1)=-32.8 kJ mol-1, DS(K1)=-33.6 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

K+ ISE alc/w 25°C 95% C K1=7.0 1977LSc (100812) 948
Medium: 95% (w/w) MeOH/H2O, 0.1 M Et4NBr.

K+ cal R4N.X 25°C 0.06M C H 1976KLc (100813) 949
Medium: 0.057 M Me4NBr. Method: flow microcalorimetry.
DH(K1)=-13 kJ mol-1, DS(K1)=0 J K-1 mol-1.

K+ gl R4N.X 25°C 0.05M C I K1=2.2 1975LSc (100814) 950
In 95% MeOH: K1=7.0; 100%: > 7

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

K+ ISE alc/w 25°C 100% U I K1=5.39 1984IEa (100848) 951
Medium: MeOH. In 90% MeOH: K1=4.7

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

K+ sol non-aq 25°C 100% C K1=4.62 1999KCa (100851) 952
Medium: acetonitrile.

K+ cal alc/w 25°C 100% U H K1=3.98 1993ILa (100852) 953
Medium: MeOH. DH=-48.7 kJ mol⁻¹.

C20H41NO5 L (1714)
N-Octyl-monoaza-18-crown-6

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

K+ ISE alc/w 25°C 100% U K1=4.87 1983MKa (100856) 954

C20H42N2O8 L (6935)
N,N'-Bis(1-hydroxy-2-ethoxyethyl)-1,4-diaza-7,10,13,16-tetraoxacyclooctadecane;

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

K+ cal alc/w 25°C 90% U IH K1=4.28 1994IZa (100871) 955
L=N,N'-Bis(1-Hydroxy-2-ethoxyethyl)-1,4-diaza-7,10,13,16-tetraoxacycloocta-
decane. Medium: 90% v/v MeOH/H₂O. DH(K1)=-37.1 kJ mol⁻¹. Also in 100% MeOH

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

K+ ISE R4N.X 25°C 0.10M U I K1=1.7 1978LMa (100888) 956
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

K+ dis non-aq 25°C 100% C K1=2.31 1999KKb (100901) 957
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

K+ EMF non-aq 25°C 100% C I K1=3.20 1997DMd (100927) 958
Method: Ag electrode; competitive titration. Medium: acetonitrile, 0.05 M
Et₄NClO₄. Also data for PC (K₁=5.2), MeOH (3.5), DMF (3.63), 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

K+ gl non-aq 25°C 100% U I K1=6.07 1996SDa (100940) 959
Medium: MeCN, 0.05 M Et4NClO4. In MeOH: K1=3.9, DMF: 3.62,
propylene carbonate: 6.7

K+ gl R4N.X 25°C 0.10M C K1=<2.0 1993SFb (100941) 960
Medium: 0.1 M Et4NClO4.

C21H22N3O9F3 L CAS 78857-86-0 (1040)
2",4"-Dinitro-6"-trifluoromethylphenyl-4'-aminobenzo-15-crown-5

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

K+ sp mixed 25°C 16% U K1=2.11 1984BPa (101199) 961
K(K+HL)=1.41
Medium: 16% MeCN/H2O

C21H23NO9 L (6799)
2,3-(4'-(4"-Nitrophenoxy-carbonyl))benzo-1,4,7,10,13-pentaoxacyclopentadeca-2-ene;

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

K+ kin alc/w 25°C 54% U K1=0.65 1991HHb (101223) 962
Medium: 54% w/w EtOH/H2O. K1=0.40(39%), 0.60(49%)

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

K+ con alc/w 25°C 100% U K1=<-0.3 19800Pa (101258) 963
Medium: MeOH, 0.1 M Me4NBr

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

K+ sp non-aq 25°C 100% C K1=4.9 2000KBb (101265) 964
Medium: MeOH. Method: electrospray ionization mass spectrometry.

K+ gl alc/w 25°C 80% M IH K1=3.11 1985AEb (101266) 965
Medium: 80% w/w MeOH/H2O, pH=11. By calorimetry: DH(K1)=-24.8 kJ mol⁻¹, DS=
-20.4 J K⁻¹ mol⁻¹. At pH=3, K(K+HL)=2.23, DH(K+HL)=-30.5, DS(K+HL)=-59.3.

C21H26O6 L CAS 88847-18-1 (6847)
Dibenzo-4-methyl-18-crown-6;

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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
K+         sp non-aq 25°C 100% U          K1=2.90      1991NTa (101286) 966
Medium: DMF. Data also for 4-ethyl, 4-hexyl and 4,13-dihexyl analogues
*****
C21H29NO6          L                      CAS 83260-79-1 (9010)
2-Methyl-2-(8-quinolyloxy)methyl-15-crown-5;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
K+         sp non-aq 25°C 100% C          K1=4.10      2002NMa (101338) 967
Medium: THF, using metal picrate salt.
*****
C21H30O2P2          L                      (7851)
P'P'-Diphenyl-P,P-dibutylmethylenediphosphinedioxide;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
K+         con non-aq 25°C          C          K1=3.2       1999ESa (101384) 968
In tetrahydrofuran; alkali metal is used as 2,4-dinitrophenolate
*****
C21H31O7P3          L                      CAS 82154-48-1 (2916)
Methyldi((2-dimethylphosphinylmethoxy)phenoxy)methyl)phosphineoxide;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
K+         con non-aq 25°C 100% U          K1=3.08      1982YSa (101419) 969
Medium: tetrahydrofuran+CHCl3 4:1(vol); M is 2,4-dinitrophenolate
L=CH3P(O)[CH2OC6H4OCH2P(O)(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
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
K+         con non-aq 25°C 100% U          K1=4.75      1976UHa (101422) 970
Medium: acetone
*****
C21H42N4O6S          L                      CAS 503465-05-2 (9248)
4,12,18,21,26,29-Hexaoxa-1,7,9,15-tetraazabicyclo[13.8.8]hentriacontane-8-thione;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
K+         gl alc/w 25°C 95% C          K1=4.89      2004KVa (101463) 971
Medium: 95% MeOH/H2O, 0.01 M Et4NClO4.
*****
C21H42O7          L                      CAS 91318-76-2 (1674)
2-Octyloxyethyleneoxymethylene-1,4,7,10,13-pentaoxacyclopentadecane, R-15-crown-5
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Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo

K+ ISE a/c/w 25°C 100% U I K1=3.22 B2=5.63 1984IEa (101477) 972
Medium: MeOH. In 90% MeOH: K1=2.56

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

K+ sp non-aq RT 100% C I K1=2.55 2000GDa (101695) 973
Medium: acetonitrile. In MeOH, K1=2.2.

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

K+ gl a/c/w 25°C 100% U K1=2.15 1989MGb (101916) 974
Data also for various 14,14-disubstituted analogues

C22H25N5O14 L CAS 74305-50-3 (2797)
4'-Picrylamino-(2''-nitrobenzo)-18-crown-6

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

K+ sp oth/un 25°C 0.10M U K1=1.70 1980NTa (101919) 975
At pH 12.35 in Li4(EDTA)

C22H25O3P L CAS 97745-35-2 (2069)
Adamantyl(diphenoxy)phosphonyl

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

K+ sol non-aq 25°C 100% U K1=3.85 1987TCa (101923) 976
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

K+ sp oth/un 25°C 0.10M U K1=1.92 1980NTa (101991) 977
K(K+HL)=1.62
At pH 11.5 in Li4(EDTA)

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

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

K+ con non-aq 25°C 100% C K1=4.25 2000ICa (101997) 978
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

K+ ISE alc/w 25°C 100% U K1=2.09 1981PTb (102001) 979
Medium: MeOH

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

K+ ISE alc/w 25°C 100% U K1=3.21 1981PTb (102008) 980
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

K+ sp non-aq 25°C 100% C M K(ZnA2L+K)=4.26 2002YPC (102016) 981
Medium: MeCN, 0.10 M n-Bu4NPF6. 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

K+ ISE alc/w 25°C 100% C K1=4.37 1981PTa (102029) 982
Medium: MeOH. Data for racemic ligand. For meso ligand K1=4.13

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

K+ ISE alc/w 25°C 100% C K1=4.04 1981PTa (102031) 983
Medium: MeOH. Data for racemic ligand. For meso ligand K1=3.42

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
K+	dis	none	RT	dil	C	M	K1=1.20 K(K+A+L(org))=KAL(org))=4.65	2003AGa (102044)	984

Method: extraction of picrate ion pair into dichloromethane. HA is picric acid.

K+	oth	alc/w	35°C	3.0%	C		K1=1.21	1999MTd (102045)	985
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Method: capillary zone electrophoresis. Medium: 3% v/v EtOH/H₂O, 0.005 M phosphate buffer, pH 7.0

K+	dis	oth/un	25°C	0	U		K1=4.09	19940Ua (102046)	986
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K+	con	non-aq	25°C	100%	U		K1=5.4	1993Eva (102047)	987
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Medium: THF+CHCl₃ (4:1 vol)

K+	cal	non-aq	25°C	100%	C	H	K1=4.19	1986ICa (102048)	988
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Medium: MeOH. DH(K1)=-34.6 kJ mol⁻¹, DS(K1)=-35.9 J K⁻¹ mol⁻¹.

K+	ISE	alc/w	25°C	100%	A		K1=4.30	1971FRa (102049)	989
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Medium: MeOH

 C22H28O7 L CAS 133560-78-8 (8962)
 2,3:17,18-Dibenzo-1,4,7,10,13,16,19-heptaoxacycloheptacosane-2,17-diene,
 Dibenzo[21]crown-7;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
K+	sp	non-aq	25°C	100%	C		K1=2.916	2002YEa (102064)	990

Method: fluorescence spectroscopy. Medium: acetonitrile.

K+	sp	non-aq	25°C	100%	C		K1=4.46	2002YEb (102065)	991
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Method: steady state fluorescence spectroscopy. Medium: acetonitrile.

 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
K+	ISE	alc/w	25°C	100%	C		K1=3.10 B2=6.84	1985ZFa (102083)	992

 C22H30O4P2 L CAS 470454-09-2 (8993)
 4,10-Dibenzyl-1,7-dioxo-4,10-diphosphacyclododecan-4,10-dioxide;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
K+	dis	non-aq	24°C	100%	C		K(K+A+L)=5.16	2002MRd (102130)	993

Medium: CDCl₃. HA is picric acid.

C22H3006 L (2506)
2,5,8,13,16,19-Hexaoxa-9,10:11,12-dibenzoicosa-9,11-diene;
(-C6H4.O.(CH2.CH2.O)2.CH3)2

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

K+ ISE a/c/w 25°C 100% U K1=0.90 1975CJa (102134) 994
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

K+ cal non-aq 25°C 100% C H 1997ZBb (102139) 995
K(K+HL)=5.42

Medium: MeOH. DH(K)=-52.1 kJ mol⁻¹, DS(K)=-71.1 J K⁻¹ mol⁻¹.

C22H31N2O6Cl HL CAS 184647-19-6 (8620)
5-Chloro-7-(1,4,7,10,13-pentaoxa-16-azacyclooctadec-16-ylmethyl)-8-quinolinol;

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

K+ cal non-aq 25°C 100% C H 1997ZBb (102143) 996
K(K+HL)=4.47

Medium: MeOH. DH(K)=-40.0 kJ mol⁻¹, DS(K)=-48.7 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

K+ con non-aq 25°C 100% U K1=3.93 1989KSa (102206) 997
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-hexaoxacyclocoosa-18-ene;

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

K+ gl a/c/w 25°C 100% U K1=2.72 1989MGb (102209) 998
Medium: MeOH

C22H36N2O6 L Bz-Cryptand 222 CAS 31250-18-7 (2269)
5,6-Benzo-4,7,13,16,21,24-hexaoxa-1,10-diazabicyclo[8:8:8]hexacosane-5-ene;

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

K+ gl R4N.X 25°C 0.05M U H K1=5.1 1998DBa (102274) 999
Medium: 0.05 M Et4NClO4. By calorimetry: DH(K1)=-38.3 kJ mol⁻¹,

K+ gl oth/un 25°C 0.02M U H K1=4.21 1980CKa (102275)1000
DH=-65.3 kJ mol⁻¹. Alternative method, calorimetry

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

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

K+ sp non-aq 22°C 100% U K1=6.26 1987CCc (102299)1001
In deuteriochloroform

C22H37NO7 L CAS 105495-13-4 (1691)
N-(2-(2-Phenylloxy)ethoxy)ethyl-1,4,7,10,13-pentaoxa-16-azacyclooctadecane;

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

K+ ISE alc/w 25°C 10% U K1=4.78 B2=8.74 1986HAa (102305)1002
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

K+ nmr non-aq 24°C 100% U M 1981BEb (102370)1003
K(K(picrate)+L)=8.6

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

K+ sol non-aq 25°C 100% C I K1=4.98 1999KCa (102379)1004
Medium: acetonitrile. In propylene carbonate, K1=4.73

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

K+ gl alc/w 25°C 95% M K1=5.15 1990LNa (102415)1005
Medium: 95% MeOH, 0.05 M Bu₄NBr. For the 12,22-dihydroxy- analogue: K1=5.63

C22H44N2O8 L Cryptand 4,2,2 (7304)
1,10-Diaza-4,7,13,16,21,24,27,30-octaoxabicyclo[8,8,14]dotriacontane;

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

 K+ cal alc/w 25°C 95% U H K1=5.5 1997Z1a (102421)1006
 Medium: 95% v/v MeOH/H2O, 0.1 M. DH(K1)=-37.8 kJ mol⁻¹, DS=-21.5 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
K+	gl	alc/w	25°C	100%	C I			K1=6.0	1975LSc (102428)	1007
Medium: MeOH										

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
K+	gl	alc/w	25°C	95%	C			K1=3.84	2004KVa (102438)	1008
Medium: 95% MeOH/H2O, 0.01 M Et4NClO4.										

				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
K+	cal	alc/w	25°C	100%	U H			K1=3.16	1993ILa (102443)	1009
Medium: MeOH. DH=-48.9 kJ mol ⁻¹ .										

				L				CAS 75006-56-3 (1717)		
N-Dodecyl-monoaza-15-crown-5										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
K+	ISE	alc/w	25°C	100%	U I			K1=2.86	1983MKa (102445)	1010

				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
K+	ISE	alc/w	25°C	100%	U			K1=3.58	1983MKa (102447)	1011

				L				CAS 69703-24-8 (2449)		
N,N'-Bis(2-dimethylpropane)-cyclo-1,10-diaza-4,7,13,16-tetraoxaocadecane)										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
K+	gl	alc/w	25°C	93%	U			K1=2.4	1978WVa (102451)	1012
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

K+ sol non-aq 20°C 100% C K1=5.46 1983SLa (102454)1013
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

K+ sol non-aq 20°C 100% C K1=5.63 1983SLa (102457)1014
Medium: CHCl3

C22H46N4O8 L CAS 61136-93-4 (8201)
7,9-Dimethyl-4,10,16,22,27-pentaoxa-1,7,13,19-tetraazabicyclo[11.11.5]nonacosane;

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

K+ gl R4N.X 25°C 0.10M U K1=1.3 1982GKc (102460)1015
Medium: 0.10 M NMe4NO3.

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

K+ ISE R4N.X 25°C 0.10M U I K1=1.7 1978LMA (102487)1016

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

K+ sp diox/w 25°C 50% C I K1=0.73 2001INa (102644)1017
Medium: 50% v/v dioxane/H2O, 3% v/v triethylamine, pH 12. In 50%
v/v dioxane/H2O with Et4NOH, K1=1.91.

C23H23NO5 L CAS 218619-58-0 (7808)
Dibenzo-pyridino-18-crown-6;

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

K+ EMF alc/w 25°C 100% C K1=4.15 2004ZTa (102658)1018
Medium: 100% methanol, 0.05 M Bu4NClO4. Method: Ag electrode,
competition with Ag+ ion.

K+ con non-aq 25°C 100% C T H K1=4.06 1997TAa (102659)1019
Medium: acetonitrile. DH(K1)=-18.6 kJ mol⁻¹, DS(K1)=15.5 J K⁻¹ mol⁻¹.
Data for 10-25 C.

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
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K+ sp non-aq RT 100% C K1=2.40 2001AVa (102750)1020
Method: spectrophotometric titration. Medium: acetonitrile.

C23H32N2O5 L (7368)
9-(2'-Hydroxy-5'-methylbenzyl)-3,6,12,15-Tetraoxa-9,21-diazabicyclo[15.3.1]heneicosatriene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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K+ cal alc/w 25°C 100% U H K1=3.53 1997ZBa (102781)1021
Medium: MeOH. Data also for several similar 5'-substituted ligands

C23H32N2O5 L (7369)
9-(2'-Pyridylmethyl)-3,6,12,15-tetraoxa-19-methyl-21-hydroxy-9-azabicyclo[15.3.1]heneicosatriene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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K+ cal alc/w 25°C 100% U H K1=3.00 1997ZBa (102785)1022
Medium: MeOH

C23H33N2O6Cl L CAS 184647-23-2 (8622)
5-Chloro-8-methoxy-2-(1,4,7,10,13-pentaoxa-16-azacyclooctadec-16-ylmethyl)-quinoline;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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K+ cal non-aq 25°C 100% C H K1=5.64 1997ZBb (102795)1023
Medium: MeOH. DH(K)=-45.8 kJ mol⁻¹, DS(K)=-45.6 J K⁻¹ mol⁻¹.

C23H41N2O10 HL CAS 111216-09-2 (5567)
2-Carboxy-3-monopiperidinenitroxide-18-crown-6 derivative;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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K+ nmr alc/w 25°C 90% U K1=3.8 1987DDa (102835)1024
Medium: 90% MeOH/H₂O

C23H42N2O9 HL CAS 111216-12-7 (5568)
2-Carboxy-3-monopiperidine-18-crown-6 derivative;

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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
K+         nmr a/c/w  25°C  90%  U          K1=5.0          1987DDa (102840)1025
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
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
K+         ISE a/c/w  25°C 100% U I      K1=3.28  B2=5.48  1984IEa (102842)1026
Medium: MeOH. In 90% MeOH: K1=2.71
*****
C23H46O8          L          CAS 91318-78-4 (1671)
2-Octyl-oxyethylene-oxymethylene-1,4,7,10,13,16-hexaoxacyclooctadecane,
R-18-crown-6
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
K+         ISE a/c/w  25°C 100% U I      K1=5.64          1984IEa (102844)1027
Medium: MeOH. In 90% MeOH: K1=4.8
*****
C24H20B-          HL          CAS 4358-26-3 (2489)
Tetraphenylborate;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
K+         con non-aq 25°C 100% C T      K1=2.38          1999VMa (102895)1028
Medium: 2-methoxyethanol. Data for 15-35 C.
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K+         sol none   25°C  0.0  U I          1979LPf (102896)1029
Kso(KB(C6H5)4)=-7.33
Method: spectrophotometry. Also data for 10-100% w/w MeOH/H2O.
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K+         con non-aq 25°C 100% U          K1=0.40          1978CAa (102897)1030
Medium: Acetonitrile
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K+         con non-aq 25°C 100% U          K1=1.02          1976RMa (102898)1031
Medium: 3-methylsulfonate
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K+         con non-aq 25°C 100% U          K1=0.3           1975YKa (102899)1032
Medium: MeCN
*****
C24H24N2O4          L          (5741)
1,10-Di(8-quinolyl)-1,4,7,10-tetraoxadecane; C9H6N.O.C2H4.O.C2H4.O.C2H4.O.C9H6N
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
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K+ con non-aq 25°C 100% U K1=5.2 1989BEa (102937)1033
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

K+ dis non-aq 23°C 100% C K1=5.7 1992HGb (102952)1034
Extraction of metal chloride (A) from aqueous solution into nitrobenzene/
0.01M Bu4NB(Ph)4. Peak potential voltammetry and distribution of 42K.

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

K+ dis non-aq 23°C 100% C K1=5.4 1992HGb (102958)1035
K(K+A+L(org))=KAL(org))=5.24

Extraction of metal chloride (A) from aqueous solution into nitrobenzene/
0.01M Bu4NB(Ph)4. Peak potential voltammetry and distribution of 42K.

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

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

K+ sol non-aq 25°C 100% U K1=2.89 1987TCa (102964)1036
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

K+ ISE alc/w 25°C 100% C K1=3.25 B2=6.98 1985ZFa (102969)1037

C24H30O7 HL (6603)
2-[(7,8,16,17-Tetrahydro-6H,15H-dibenzo[1,4,8,11]tetraoxacyclotetradeca-7-yl)oxy]-hexanoic acid;

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

K+ dis oth/un 25°C ? U K1=1.97 1991BUa (103032)1038

C24H30O8 L CAS 67655-22-5 (8710)
7,8,16,17-Tetrahydro-7,16-(epoxyethoxyethoxyethoxy)-6H,15H-dibenzotetraoxacyclotetradecin;

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

K+ ISE none 25°C 0.0 C K1=5.7 1978PAa (103034)1039
Method: K-sensitive electrode.

C24H3009 L (5625)
1,7-bis(2-Carboxymethoxyphenyl)-1,4,7-trioxaheptane diethylester;

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

K+ ISE alc/w 25°C 100% U K1=2.79 1981PTb (103037)1040
Medium: MeOH

C24H3206 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

K+ dis non-aq 25°C 100% U H 1979KLa (103070)1041
K(K(picrate)+L)=7.20

Medium: CHCl3

C24H3206 L AN(MOEO)2AN (2244)
23,24-Dimethoxy-10,21-dimethyl-3,6,14,17-tetraoxatricyclo-tetracos-1(23),8(24),9,11,19,21hexaene

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

K+ dis non-aq 25°C 100% U H 1979KLa (103076)1042
K(K(picrate)+L)=3.59

Medium: CHCl3

C24H3206 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

K+ dis non-aq 25°C 100% U H 1979KLa (103082)1043
K(K(picrate)+L)=6.23

Medium: CHCl3

C24H3208 L (5617)
2,3:11,12-Dibenzo-1,4,7,10,13,16,19,22-octaoxacyclotetracos-2,11-diene;

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

K+ oth alc/w 25°C 100% U K1=3.45 1980WAa (103087)1044
Medium: MeOH

C24H3208 L DiBz-24-Crown-8 CAS 14174-09-5 (580)

2,3:14,15-Dibenzo-1,4,7,10,13,16,19,22-octaoxacyclotetracos-2,14-diene;

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

K+ dis none RT dil C M K1=0.95 2003AGa (103130)1045
K(K+A+L(org))=KAL(org))=4.52

Method: extraction of picrate ion pair into dichloromethane. HA is picric acid.

K+ oth KCl 25°C 0.05M C K1=0.63 2002Kta (103131)1046

Method: capillary electrophoresis. Medium: 0.03-0.06 M KCl.

K+ sp non-aq 25°C 100% C K1=2.62 2002Yeb (103132)1047

Method: steady state fluorescence spectroscopy. Medium: acetonitrile.

K+ con non-aq 25°C 100% C TIH K1=3.70 1999Rmb (103133)1048

Medium: 100% MeOH. Data for 15-55 C. Also data for DMF/MeOH mixtures.

DH(K1)=-27.4 kJ mol⁻¹, DS(K1)=-22.3 J K⁻¹ mol⁻¹. In 100% DMF, K1=1.83.

K+ dis oth/un 25°C 0 U K1=3.49 19940Ua (103134)1049

K+ con non-aq 25°C 100% U K1=5.3 1993Eva (103135)1050

Medium: THF+CHCl₃ (4:1 vol)

K+ vlt non-aq 25°C 100% U K1=10.4 1990SPa (103136)1051

Medium: 1,2-dichloroethane

K+ cal non-aq 25°C 100% C H K1=3.45 1986ICa (103137)1052

Medium: MeOH. DH(K1)=-31.1 kJ mol⁻¹, DS(K1)=-38.3 J K⁻¹ mol⁻¹.

K+ ISE alc/w 25°C 100% U K1=3.53 1983GGa (103138)1053

Medium: MeOH

K+ dis non-aq 35°C 100% U I K1=3.7 1980TYb (103139)1054

Medium: propylene carbonate

K+ cal alc/w 25°C 70% U H K1=2.42 1976ITa (103140)1055

Medium: 70% w/w MeOH/H₂O. DH(K1)=-35.7 kJ mol⁻¹

K+ ISE alc/w 25°C 100% A K1=3.49 1971FRa (103141)1056

Medium: MeOH

C24H32O8 L CAS 75832-82-5 (5618)

2,3:8,9-Dibenzo-1,4,7,10,13,16,19,22-octaoxacyclotetracos-2,8-diene;

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

K+ sp non-aq 25°C 100% C K1=3.730 2002YEa (103183)1057

Method: fluorescence spectroscopy. Medium: acetonitrile.

K+ oth alc/w 25°C 100% U K1=3.85 1980WAa (103184)1058

Medium: MeOH

C24H33N3O7 L (662)

4-Dihydroxyethylaminophenylazo-benzo-15-crown-5;

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

K+ ISE alc/w 25°C 100% C K1=3.28 B2=6.77 1985ZFa (103199)1059

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

K+ sp alc/w RT 50% C K1=<2.3 2002GLb (103209)1060

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

K+ dis non-aq 24°C 100% C 2002MRd (103231)1061

K(K+A+L)=5.24

Medium: CDCl3. HA is picric acid.

C24H34O7 L CAS 20740-88-9 (5612)

1,17-Diphenoxy-3,6,9,12,15-pentaoxaheptadecane;

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

K+ gl alc/w 25°C 100% M K1=1.57 1976FAa (103235)1062

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

K+ ISE non-aq 25°C 100% U K1=3.54 1992BCe (103238)1063

K(K+HL)=2.73

K(KL+H)=8.81

Medium: methanol. Method: glass/K+ 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
K+	sp	mixed	25°C	10%	C		K1=4.41	2001LWa (103242)	1064
Method: fluorimetry. Medium: 10%v/v acetonitrile/H2O.									

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
K+	nmr	non-aq	25°C	100%	U		K1=5.13	1992MGa (103255)	1065
Method:NMR. Medium: MeCN, 0.1 M Bu4NPF6. Data also for other ferrocene[2.2] cryptands. In MeOH K=3.77									

C24H36O6		L					(1703)		
Decalino-benzo-18-crown-6									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
K+	ISE	alc/w	25°C	?	U		K1=5.55	1983KTa (103290)	1066

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
K+	gl	alc/w	25°C	100%	U		K1=2.85	1989MGb (103292)	1067
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
K+	con	non-aq	25°C	100%	U		K1=3.7	1989EVa (103295)	1068
Medium: tetrahydrofuran/CHCl3 4:1 (volume)									

C24H36O18		H4L					(8196)		
2,3,11,12-Tetrakis[N-(carboxymethyl)carbamoyl]-1,4,7,10,13,16-hexaoxacyclooctadecane;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
K+	ISE	oth/un	25°C	0.10M	C		K1=2.81	1982BLc (103299)	1069
Method: K ion selective electrode. Medium: 0.10 M Tris buffer, pH 7.0									
Data for a large range of 2,3,11,12-substituted derivatives.									

C24H36O21		H6L					CAS 71735-94-9	(7414)	

1,4,7,10,13,16,19,22,25-Nonaoxacycloheptacosane-2,3,11,12,20,21-hexacarboxylic acid;

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

K+ gl R4N.X 25°C 0.10M M K1=2.9 1991FGb (103308)1070
B(KHL)=8.3

Medium: 0.10 M Et4NNO3.

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

K+ cal alc/w 25°C 80% C H K1=3.60 1995KZa (103354)1071
Medium: 80% v/v CH3OH/H2O. DH(K1)=-43.5 kJ mol⁻¹, DS(K1)=-77.2 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

K+ ISE alc/w 25°C ? U K1=5.95 1983KTa (103391)1072

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

K+ sp non-aq 22°C 100% U K1=6.58 1987CCc (103395)1073
In deuteriochloroform

K+ ISE alc/w 25°C 100% U K1=3.30 1975CJa (103396)1074
Medium: MeOH

C24H44N4O10 L CAS 57207-22-4 (8203)
N,N,N',N',N'',N''',N''''-Octamethyl-1,4,7,10,13,16-hexaoxacyclooctadecane-2,3,11,12-tetracarboxami

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

K+ ISE R4N.X 25°C 0.10M U K1=1.85 1976BLb (103403)1075
Method: K ion selective electrode. Medium: 0.10 M (Me4N)H2PO4, pH 7.0

Data for related N-substituted amides with K, NH4 and alkylammonium ions.

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

K+ nmr non-aq 24°C 100% U M 1981BEb (103409)1076
K(K(picrate)+L)=7.1

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

K+ sol non-aq 25°C 100% C K1=5.10 1999KCa (103430)1077
Medium: acetonitrile. In propylene carbonate, K1=4.79

C24H48N2O9 L BOA15C5 CAS 31255-19-3 (6119)
3-Oxa-1,5-bis-(1-aza-4,7,10,13-tetraoxacyclpentadecyl)pentane;

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

K+ ISE a/c/w 25°C 90% U K1=4.75 B2=7.82 1988HKa (103458)1078
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

K+ gl a/c/w 25°C 100% C I K1=5.4 1975LSc (103464)1079
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

K+ gl R4N.X 25°C 0.10M U K1=3.42 1982GKc (103483)1080
Medium: 0.10 M NMe4NO3.

K+ gl R4N.X 25°C 0.10M U K1=3.4 1981GLa (103484)1081

K+ kin non-aq 25°C 100% C K1=5.85 1977LSc (103485)1082
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]hexatricosane-5,16-dithione;

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

K+ gl a/c/w 25°C 95% C K1=3.87 2004KVa (103505)1083
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

K+ EMF R4N.X RT 0.10M M K1=1.02 2001BSb (103512)1084
Method: Ag/Ag+ electrode. Medium: 0.10 M Et4NN03.

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

K+ cal alc/w 25°C 100% U H K1=3.03 1993ILa (103520)1085
Medium: MeOH. DH=-50.3 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

K+ ISE alc/w 25°C 100% U I K1=4.98 1983MKa (103522)1086

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

K+ ISE alc/w 25°C 100% U K1=5.73 1983MKa (103524)1087

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

K+ ISE alc/w 25°C 100% U K1=4.57 1983MKa (103526)1088

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

K+ sol non-aq 20°C 100% C K1=5.57 1983SLa (103528)1089
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

K+ con alc/w 25°C 100% U K1=0.39 1980Pa (103591)1090
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

K+ sp alc/w 25°C 100% U K1=2.75 B2=4.75 1977TMa (103595)1091
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

K+ con non-aq 25°C C K1=3.7 1999ESa (103629)1092
In tetrahydrofuran; alkali metal is used as 2,4-dinitrophenolate

K+ con non-aq 25°C 100% U K1=3.5 1984YKa (103630)1093
Medium: tetrahydrofuran + CHCl3 4:1, K as 2,4-dinitrophenolate

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

K+ sp diox/w 25°C 50% C K1=1.17 2001INa (103651)1094
Medium: 50% v/v dioxane/H2O, 3% v/v triethylamine, pH 12.

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

K+ cal non-aq 25°C 100% C H K(K+HL)=5.16 1997ZBb (103686)1095
Medium: MeOH. DH(K)=-38.8 kJ mol⁻¹, DS(K)=-31.4 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

K+ cal non-aq 25°C 100% C H K(K+HL)=4.01 1997ZBb (103690)1096

Medium: MeOH. DH(K)=-28.3 kJ mol⁻¹, DS(K)=-18.2 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

K+ dis oth/un 25°C ? U K1=2.05 1991BUa (103748)1097

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

K+ dis non-aq 20°C 100% C 1998DDc (103757)1098

K(KP+L)=4.23

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

K+ con non-aq 25°C 100% C T H K1=5.31 1999RGa (103775)1099

Medium: acetonitrile. Data for 5-35 C. DH(K1)=-67.2 kJ mol⁻¹, DS(K1)=-125 J K⁻¹ mol⁻¹.

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

K+ ISE alc/w 25°C 90% U K1=2.69 1988HKa (103829)1100

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

K+ gl R4N.X 25°C 0.10M U K1=2.5 1981GLa (103835)1101

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

K+ gl alc/w 25°C 95% C K1=5.90 2004KVa (103844)1102
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

K+ ISE alc/w 25°C 100% U I K1=5.50 1984IEa (103849)1103
Medium: MeOH. In 90% MeOH: K1=4.8

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

K+ sp non-aq 25°C 100% U I M K(Ru(II)(bpy)2L+K)=2.28 1997YLa (103899)1104

Medium: CH3CN;0.1M NBu4PF6. In (CH3)2CO: K=2.13. 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

K+ con non-aq 25°C 100% U K1=2.1 1990EAb (103911)1105
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

K+ con non-aq 25°C C K1=2.7 1999TEa (103917)1106
In: tetrahydrofurane/CHCl3 4:1 v/v

K+ oth non-aq 25°C 100% U K1=2.7 1995TEa (103918)1107
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

K+ sp alc/w 25°C 100% U K1=3.51 B2=5.92 1977TMa (103978)1108
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

K+ sp non-aq 25°C 100% C K1=3.80 2003GHa (104074)1109
K(KL+K)=2.71

Method: fluorescence spectroscopy. Medium: acetonitrile, 0.05 M Et4NC104.

C26H34O9 L CAS 67655-23-6 (8711)

7,8,16,17-Tetrahydro-7,16-(epoxyethanoxyethanoxyethanoxyethanoxy)-dibenzotetraoxacy
clotetradecin;

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

K+ ISE none 25°C 0.0 C K1=4.3 1978PAa (104108)1110

Method: K-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

K+ ISE alc/w 25°C 100% U K1=3.42 1981PTb (104111)1111

Medium: MeOH

C26H35N3O5 HL CAS 254900-33-9 (8919)

7-(10-Hydroxybenzoquinoline-9-ylmethyl)-1,4,10,13-tetraoxa-7,16-diazacyclooctadecan
e;

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

K+ cal alc/w 25°C 100% C H K(K+HL)=3.52 1999SBg (104116)1112

Medium: MeOH. DH(K)=-31.2 kJ mol⁻¹, DS(K)=-37.3 J K⁻¹ mol⁻¹.

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-di
ene;

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

K+ gl R4N.X 25°C 0.05M U H 1998DBa (104133)1113

Medium: 0.05 M Et4NC104. By calorimetry: DH(K1)=-36.7 kJ mol⁻¹,

K+ cal non-aq 25°C 100% U IH 1988DSa (104134)1114
Medium: MeCN. DH(K1)=-71.3 kJ mol⁻¹. Also data in propylene carbonate,
dimethylformamide and dimethylsulphoxide

K+ ISE non-aq 25°C 100% U M K1=6.10 1987DSa (104135)1115

Medium: N,N-dimethylformamide

K+ ISE a/c/w 25°C 100% C I K1=8.60 1985CKa (104136)1116
Medium: MeOH. In propylenecarbonate K1=9.0; in DMF K1=6.73; in DMSO K1=6.12

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

K+ cal non-aq 25°C 100% C H K(K+H2L)=2.76 1995ZBa (104156)1117

Medium: methanol. DH(K)=-24.1 kJ mol⁻¹, DS(K)=-28 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-nonaoxacycloheptacos-2,11-diene;

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

K+ sp non-aq 25°C 100% C K1=2.43 2002YEB (104163)1118

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-nonaoxacycloheptacos-2,15-diene;

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

K+ cal a/c/w 25°C 70% U H K1=2.86 1976ITa (104172)1119

Medium: 70% w/w MeOH/H₂O. DH(K1)=-39.7 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

K+ ISE a/c/w 25°C 100% U K1=3.38 1992MGa (104186)1120

Medium: MeOH, 0.1 M Bu₄NPF₆

K+ gl a/c/w 25°C 93% U K1=3.0 1978WVa (104187)1121

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

K+ sp a/c/w RT 50% C K1=3.9 2002GLb (104194)1122

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

C26H3806P2 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

K+ dis non-aq 24°C 100% C K(K+A+L)=5.27 2002MRd (104212)1123

Medium: CDCl3. HA is picric acid.

C26H3808 L CAS 20740-89-0 (5613)
1,20-Diphenoxy-3,6,9,12,15,18-hexaoxaicosane;

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

K+ gl alc/w 25°C 100% M K1=1.99 1976FAa (104216)1124

C26H3808 L (2507)
2,5,8,11,16,19,22,25-Octaoxa-12,13:14,15-dibenzoheptacosane-12,14-diene;

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

K+ ISE alc/w 25°C 100% U K1=1.45 1975CJa (104219)1125

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

K+ cal alc/w 25°C 100% C H K(K+H2L)=2.81 1999SBf (104226)1126

Medium: MeOH. DH(K)=-34.8 kJ mol⁻¹, DS(K)=-63.1 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-octaoxacyclohexacosane-24-ene;

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

K+ gl alc/w 25°C 100% U K1=2.63 B2=4.73 1989Mgb (104240)1127

Medium: MeOH

C26H40O11P2 L (5727)
1,7-Bis(2-(diethoxyphosphinylmethoxy)phenyl)-1,4,7-trioxahexane;2(EtO)2PO.CH2OC6H4C2H4OC2H4)2O

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

K+ con non-aq 25°C 100% U K1=4.4 1989EVa (104243)1128

Medium: tetrahydrofuran/CHCl3 4:1 (volume)

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
K+	dis	none	25°C	dil	C			K1=7.79 K(K+A+L(org))=KAL(org)=5.19	1987BBf (104279)	1129

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
K+	ISE	alc/w	25°C	100%	U	H		K1=6.92	1987BUb (104295)	1130

In MeOH. DH=-36.1 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
K+	nmr	non-aq	24°C	100%	U	M		K(K(picrate)+L)=7.2	1981BEb (104309)	1131

Medium: CDCl3

C26H50N2O7 L (6931)
N,N'-Bis(1-tetrahydrofuran-2-ethoxyethyl)-1,4-diaza-7,10,13-trioxacyclopentadecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
K+	cal	alc/w	25°C	90%	U	H		K1=3.59	1994IZa (104319)	1132

L=N,N'-Bis(1-tetrahydrofuran-2-ethoxyethyl)-1,4-diaza-7,10,13-trioxacyclopentadecane. Medium: 90% v/v MeOH/H2O. DH(K1)=-43.2 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
K+	con	non-aq	25°C	100%	M	M		K1=6.91 K(KL+C104)=1.18	1999DSd (104321)	1133

Medium: acetonitrile.

C26H52N4O5 L CAS 78648-22-3 (1534)
4,10,16,22,33-Pentaoxa-1,7,13,19-tetraazatricyclo[11,11,6,5(7.19)pentatriacontane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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K+ gl R4N.X 25°C 0.10M U K1=2.52 1982GKc (104328)1134
Medium: 0.10 M NMe4NO3.

K+ gl R4N.X 25°C 0.10M U K1=<2 1981GLa (104329)1135

C26H52N6O7S2 L CAS 503465-16-5 (9245)
4,12,20,26,29,34,37-Hepta-oxa-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

K+ gl alc/w 25°C 95% C K1=5.33 2004KVa (104339)1136
Medium: 95% MeOH/H2O, 0.01 M Et4NClO4.

C26H52N6O7S2 L CAS 503465-12-1 (9243)
9,12,15,26,29,34,37-Hepta-oxa-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

K+ gl alc/w 25°C 95% C K1=3.76 2004KVa (104349)1137
Medium: 95% MeOH/H2O, 0.01 M Et4NClO4.

C26H53N06 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

K+ ISE alc/w 25°C 100% U I K1=3.55 1983MKa (104354)1138

C26H53N08 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

K+ ISE alc/w 25°C 100% U K1=4.74 1983MKa (104356)1139

C26H53N08 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

K+ ISE alc/w 25°C 100% U K1=5.74 1983MKa (104358)1140

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

K+ sol non-aq 20°C 100% C K1=5.65 1983SLa (104360)1141
Medium: CHCl3

C27H26O2P2 L (6811)

1,2-Bis(2-Diphenylphosphinyl)-1-methylethane;

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

K+ con non-aq 25°C 100% U K1=2 1990EAb (104396)1142

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

K+ con non-aq 25°C 100% U K1=1.9 1990EAb (104401)1143

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

K+ oth non-aq 25°C 100% U K1=2.9 1995TEa (104406)1144

Medium: tetrahydrofurane:CHCl3 4:1 (v/v).
Metal ion is used as 2,4-dinitrophenolate.

C27H32N05S+ L CAS 423763-94-4 (8997)

3-Ethyl-2-[4-(2,3,5,6,8,9,11,12-octahydro-1,4,7,10,13-benzopentaoxacyclopentadecin-
15-yl)butadien

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

K+ sp non-aq 25°C 100% C K1=3.11 2002GVc (104516)1145

Medium: acetonitrile, 0.1 M Et4NClO4.

C27H47N3O6 L (8029)

Tripodal ionophore 3;

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

K+ sp non-aq 25°C 100% C 2001Lfa (104624)1146

K(KP+L=LiPL)=4.37

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

K+ con non-aq 25°C 100% U K1=5.0 1989BEa (104675)1147
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-tetrae
ne

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

K+ dis non-aq 23°C 100% C K1=4.0 1992HGb (104681)1148
K(K+A+L(org))=KAL(org))=3.94

Extraction of metal chloride (A) from aqueous solution into nitrobenzene/
0.01M Bu4NB(Ph)4. Peak potential voltammetry and distribution of 42K.

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-tetrae
ne;

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

K+ dis non-aq 23°C 100% C K1=3.4 1992HGb (104686)1149
K(K+A+L(org))=KAL(org))=3.97

Extraction of metal chloride (A) from aqueous solution into nitrobenzene/
0.01M Bu4NB(Ph)4. Peak potential voltammetry and distribution of 42K.

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

K+ con non-aq 25°C 100% U K1=5.0 1993Eva (104710)1150
Medium: THF+CHCl3 (4:1 vol)

K+ con non-aq 25°C 100% U K1=2.7 1992BEa (104711)1151
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

K+ con non-aq 25°C C K1=3.2 1999TEa (104721)1152
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

K+ con non-aq 25°C 100% U K1=2.8 1984YKa (104726)1153
Medium: tetrahydrofuran + CHCl3 4:1, K 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

K+ con non-aq 25°C 100% U K1=5.9 1989BEa (104749)1154
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

K+ sol non-aq 25°C 100% U K1=3.69 1987TCa (104767)1155
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

K+ sp non-aq 18°C 100% C K1=1.3 1997LHa (104783)1156
Medium: acetonitrile.

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

K+ gl alc/w 25°C 93% U K1=2.65 1978WVa (104817)1157
Medium: 93% MeOH/H2O

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

K+ con non-aq 25°C 100% C I M 1983RCb (104841)1158

K(KL+Cl)=0.60
K(KL+ClO4)=078
K(KL+A)=1.29
K(KL+B(C6H5)4)=1.38

Medium: 100% methanol. HA=picric acid. Also data for 100% acetonitrile, propylene carbonate, dimethylformamide, isopropyl alcohol and butanol.

K+ con alc/w 25°C 100% U I M 1979BDa (104842)1159

K(KCl+L)=5.06

Medium: MeOH. In DMSO: K(KClO4+L)=3.42. In MeCN: K(KBPh4+L)=4.98

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

K+ dis non-aq 25°C 100% U H 1979KLa (104856)1160

K(K(picrate)+L)=3.94

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

K+ dis oth/un 25°C 0 U K1=4.33 19940Ua (104884)1161

K+ con non-aq 25°C 100% U I K1=5.96 1991ASb (104885)1162

Medium: 1,2-dichlorethane. In nitromethane: K1=5.37; in MeCN: K=4.63;

in acetone: K=4.39; in DMF: K=3.13

K+ vlt non-aq 25°C 100% U K1=12.4 1990SPa (104886)1163

Medium: 1,2-dichloroethane

K+ nmr non-aq 21°C 100% U 1987SRb (104887)1164

B(K2L)=1.72

Medium: CH3NO2.

K+ sp mixed 25°C 20% U I K1=2.42 1986GSa (104888)1165

In 0.015 M Et4N.Cl, 20% CH3CN/H2O. In 40%, K1=2.71; 60%, K1=3.23;

80%, K1=3.88; 100% CH3CN, K1=4.90.

K+ nmr non-aq 20°C 100% U K1=4.30 1976LCa (104889)1166

Medium: acetone

K+ ISE alc/w 25°C 100% A K1=4.60 1971FRa (104890)1167

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

K+ gl alc/w 25°C 93% U K1=2.8 1978WVa (104927)1168
Medium: 93% MeOH/H2O

C28H42O9 L CAS 97583-32-9 (5614)
1,13-Diphenoxy-3,6,9,12,15,18,21-heptaoxatricosane;

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

K+ gl alc/w 25°C 100% M K1=2.44 1976FAa (104930)1169

C28H43NO5 L CAS 36080-62-3 (5355)
2:3,11:12-Dibenzo-16-octyl-1,4,7,10,13-pentaoxa-16-azaoctadeca-2,11-diene;

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

K+ EMF alc/w 25°C 100% A K1=4.10 1971FRa (104932)1170

Medium: MeOH

C28H44N4O6 H2L CAS 227796-02-3 (8913)

7,16-Bis(3-amino-2-hydroxy-5-methylbenzyl)-1,4,10,13-tetraoxa-7,16-diazacyclooctadecane;

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

K+ cal alc/w 25°C 100% C H 1999SBf (104938)1171

K(K+H2L)=2.36

Medium: MeOH. DH(K)=-10.6 kJ mol⁻¹, DS(K)=9.6 J K⁻¹ mol⁻¹.

For the 3-trifluoroacetamidobenzyl derivative, DH(K)=-70, DS(K)=-133.

C28H44O6 L (1704)

Decalino-(tert-butyl-benzo)-18-crown-6

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

K+ ISE alc/w 25°C ? U K1=5.47 1983KTa (104940)1172

C28H44O11 L CAS 123295-33-0 (5575)

26,26-Dimethyl-27,28-(1,4-Benzodioxinic)-1,4,7,10,13,16,19,22,25-nonoxacyclononacosane-27-ene;

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

K+ gl alc/w 25°C 100% U K1=2.60 B2=4.90 1989MGb (104942)1173

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

K+ con non-aq 25°C 100% U K1=5.1 1989EVa (104945)1174
Medium: tetrahydrofuran/CHCl3 4:1 (volume)

C28H47N011 L (1689)
N-(2-(2-(4'-Benzo-15-crown-5)-oxyethoxy)ethyl)-1,4,7,10-tetraoxa-13-azacyclopentadecane;

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

K+ ISE a/c/w 25°C 10% U K1=3.16 1986HAa (104968)1175
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

K+ ISE a/c/w 25°C ? U K1=6.18 1983KTA (104976)1176

C28H52O5 L (2339)
16,16,18,18,23,23,25,25-Octamethyl-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

K+ nmr non-aq 24°C 100% U M K(K(picrate)+L)=5.2 1981BEb (105009)1177

Medium: CDCl3

C28H52O6 L (5352)
Di(t-butylcyclohexyl)-18-crown-6

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

K+ oth oth/un 25°C dil U K1=2.08 1970MSa (105015)1178

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

K+ sol non-aq 25°C 100% C I K1=4.86 1999KCa (105021)1179
Medium: acetonitrile. Also K1=4.66 (propylene carbonate), K1=4.50 (MeOH), K1=5.93 (i-PrOH), K1=5.47 (n-BuOH), K1=4.58 (acetone).

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

K+ cal alc/w 25°C 90% U IH K1=4.52 1994IZa (105026)1180
L=N,N'-Bis(1-furanyl-2-ethoxyethyl)-1,4-diaza-7,10,13,16-tetraoxacycloocta-
decane. Medium: 90% v/v MeOH/H2O. DH(K1)=-34.9 kJ mol⁻¹. Also in 100% MeOH

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

K+ con non-aq 25°C 100% M M K1=>12 1999DSd (105029)1181
K(KL+ClO4)=0.87

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

K+ ISE alc/w 25°C 90% U K1=4.75 B2=7.82 1988HKa (105033)1182
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

K+ gl alc/w 25°C 95% C K1=5.62 2004KVa (105040)1183
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]dotetradeconta
ne-5,22-dithio

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

K+ gl alc/w 25°C 95% C K1=3.61 2004KVa (105050)1184
Medium: 95% MeOH/H2O, 0.01 M Et4NClO4.

C28H57N07 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

K+ ISE alc/w 25°C 100% U I K1=5.62 1983MKa (105055)1185

C28H57N07 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

 K+ ISE a/c/w 25°C 100% U I K1=4.46 1983MKa (105057)1186

 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
K+	ISE	a/c/w	25°C	100%	U			K1=5.75	1983MKa (105059)	1187

									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
K+	sol	non-aq	20°C	100%	C			K1=6.03	1983SLa (105061)	1188
Medium: CHCl3										

									CAS 176849-77-7	(7160)
1,6-Bis(diphenylphosphinyl)-2-oxohexane;										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
K+	oth	non-aq	25°C	100%	U			K1=2.6	1995TEa (105079)	1189
Medium: tetrahydrofurane:CHCl3 4:1 (v/v).										
Metal ion is used as 2,4-dinitrophenolate.										

									CAS 176849-78-8	(7161)
1,6-Bis(diphenylphosphinyl)-3-oxohexane;										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
K+	oth	non-aq	25°C	100%	U			K1=2.3	1995TEa (105084)	1190
Medium: tetrahydrofurane:CHCl3 4:1 (v/v).										
Metal ion is used as 2,4-dinitrophenolate.										

									(7897)	
1,7-Bis(diphenylphosphinyl)-2,6-dioxoheptane;										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
K+	con	non-aq	25°C		C			K1=3.5	1999TEa (105089)	1191
In: tetrahydrofurane/CHCl3 4:1 v/v										

									CAS 201154-06-5	(7825)
N-(1-Pyrenylmethyl)-1,4,7,10,13-pentaoxa-16-azacyclooctadecane;										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
K+	sp	mixed	25°C	90%	C				1997KKa (105100)	1192

K(KSCN+L)=4.75

Method: fluorescence emission. Medium: MeOH/CHCl3 (9:1 v/v).

C29H36N06S+ L CAS 423763-96-6 (8998)
2-[4-(2,3,5,6,8,9,11,12,14,15-Decahydro-1,4,7,10,13,16-benzohexaoxacyclooctadecin-1
8-yl)butadien

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

K+ sp non-aq 25°C 100% C K1=4.81 2002GVc (105105)1193
Medium: acetonitrile, 0.1 M Et4NClO4.

C29H40N206Cl2 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

K+ cal non-aq 25°C 100% C H K1=4.58 1998ZBc (105137)1194
Medium: MeOH. DH(K1)=-31.1 kJ mol⁻¹, DS(K1)=-16.6 J K⁻¹ mol⁻¹.

C29H42N206 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

K+ gl alc/w 25°C 93% U K1=2.8 1978WVa (105147)1195
Medium: 93% MeOH/H2O

C29H58N2010 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

K+ ISE alc/w 25°C 90% U K1=4.54 B2=7.62 1988HKa (105170)1196
Medium: 90% w/w MeOH/H2O

C30H30N20010 L CAS 259886-49-2 (8959)
Cucurbit[5]uril;

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

K+ sol none 25°C dil C K1=1.31 2001BCf (105216)1197
Method: dissolution of ligand in a 0.002-0.02 M KX solution; spectrophoto
metric measurement. For decamethylcucurbit[5]uril, K1=1.11.

C30H32O4P2 L (6816)
1,8-Bis(diphenylphosphinyl)-3,6-dioxaoctane;

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

K+ con non-aq 25°C 100% U K1=2.80 1993EBa (105227)1198
Medium: CH3CN. Data also for 3,5,8-trioxa, 3,5,8,11-tetraoxa and 3,5,8,11-pentaoxa analogues

K+ con non-aq 25°C 100% U K1=3.2 1992BEa (105228)1199
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

K+ con non-aq 25°C C K1=3.8 1999TEa (105235)1200
In: tetrahydrofuran/CHCl3 4:1 v/v

C30H34N2O2P2 L CAS 68743-31-3 (2066)
Diaminoethane-N,N'-di-2-ethylidiphenylphosphine oxide; (CH2.NH.C2H4.P(O)(C6H5)2)2

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

K+ con non-aq 25°C 100% U K1=2.56 1986STb (105240)1201
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

K+ sp non-aq 25°C 100% U K1=2.6 1996AAb (105254)1202
Medium: MeCN

tacyclo[12.12.12.1(6,9).1(19,22).1(31,34)]hentetetraconta-4,6,8....dodecaene

C30H36O6 L ANANAN(MOE)20 (2239)
2,3,4,5,6,7,8,9,10-Tri(1,3-(2-methoxy-5-methylbenzo))-12,15,18-trioxacyclooctadeca-
2,5,8-triene;

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

K+ dis non-aq 25°C 100% U H 1979KLa (105260)1203
K(K(picrate)+L)=9.06

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

K+ sp alc/w RT 50% C K1=1.6 2002GLb (105266)1204
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

K+ nmr non-aq 25°C 100% U K1=<8.68 1986CHc (105272)1205
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

K+ ISE non-aq 25°C 100% U K1=6.22 1992CSc (105277)1206
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

K+ con non-aq 25°C 100% U K1=3.72 1989Ksa (105301)1207
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

K+ gl alc/w 25°C 93% U K1=2.85 1978WVa (105310)1208
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

K+ sol non-aq 20°C 100% C K1=6.89 1983SLa (105318)1209
Medium: CHCl3

C30H46O10 L (5615)
1,26-Diphenoxy-3,6,9,12,15,18,21,24-octaohexacosane;

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

K+ gl alc/w 25°C 100% M K1=2.71 1976FAa (105324)1210

C30H48N4O6 L (6937)
N,N'-Bis(1-pyridyl-2-ethoxyethyl)-1,4-diaza-7,10,13,16-tetraoxacyclooctadecane;

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

K+ cal alc/w 25°C 90% U H K1=4.26 1994IZa (105326)1211
L=N,N'-Bis(1-pyridyl-2-ethoxyethyl)-1,4-diaza-7,10,13,16-tetraoxacyclooctadecane. Medium: 90% v/v MeOH/H2O. DH(K1)=-38.1 kJ mol⁻¹.

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-decaoxacyclodotriacontane;

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

K+ gl alc/w 25°C 100% U K1=2.54 B2=4.74 1989MGB (105340)1212
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

K+ con non-aq 25°C 100% U K1=5.4 1989Eva (105343)1213
Medium: tetrahydrofuran/CHCl₃ 4:1 (volume)

C30H57N08 HL 18NH15-C5A CAS 79145-86-1 (5405)
2-Carboxy-3-N-octadecanylformamide-1,4,7,10,13-pentaoxycyclopentadecane;

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

K+ gl alc/w 25°C 90% U K1=2.9 1984FWa (105382)1214
B(KHL)=8.3

Medium: 90% v/v MeOH/H2O, 0.05 M R4NX

C30H61N08 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

K+ ISE alc/w 25°C 100% U I K1=5.70 1983MKa (105384)1215

C31H34O4P2 L (7157)
1,9-Bis(diphenylphosphinyl)-3,7-dioxononane;

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

K+ oth non-aq 25°C 100% U K1=2.5 1995TEa (105525)1216
Medium: THF:CHCl₃ 4:1 v/v. K as 2,4-dinitrophenolate. Also other si

milar ligands

C31H46N2O6 L (2446)
 Bicyclo-NcN'-1,10-Diaza-4,7,13,16-tetraoxaocetadecane; (c=(CH2.C6H4.O.C2H4)2.CH2)

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

 K+ gl alc/w 25°C 93% U K1=2.65 1978WVa (105552)1217
 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

 K+ con non-aq 25°C C K1=3.1 1999TEa (105575)1218
 In: tetrahydrofurane/CHCl3 4:1 v/v

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

 K+ sp non-aq 25°C 100% U M K(KI+L)=1.77 1981SPb (105582)1219
 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

 K+ sp R4N.X 30°C 0.10M U K1eff=1.99 1993SKf (105617)1220
 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

 K+ con non-aq 25°C 100% U K1=3.9 1992BEa (105645)1221
 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

K+ con non-aq 25°C C K1=4.4 1999TEa (105650)1222
In: tetrahydrofuran/CHCl3 4:1 v/v

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

K+ sp non-aq 25°C 100% C K1=4.84 2002NMa (105668)1223
Medium: THF, using metal picrate salt. For the trans- ligand, K1=4.28.

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

K+ sp non-aq 25°C 100% C K1=4.88 2002NMa (105670)1224
Medium: THF, using metal picrate salt. For the trans- ligand, K1=4.26.

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

K+ sp non-aq 25°C 100% C K1=5.98 2002NMa (105672)1225
Medium: THF, using metal picrate salt. For the trans- ligand, K1=4.22.

C32H38N2O10 L (7073)
7,16-Bis(6-methoxy-2-oxo-2H-1-benzopyran-7-yl)-1,4,10,13-tetraoxa-7,16-diazacyclooctadecane;

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

K+ sp none RT 0 U K1=1.68 1994CGa (105674)1226
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-Chloro-8-quinolinol]

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

K+ cal non-aq 25°C 100% C H K(K+HL)=6.61
1995ZBa (105679)1227

Medium: methanol. DH(K)=-58.1 kJ mol⁻¹, DS(K)=-68.5 J K⁻¹ mol⁻¹.

C32H38N4O6Cl2 H2L (7214)
7,16-Bis((5-chloro-8-hydroxy-7-quinolinyloxy)methyl)-1,4,10,13-tetraoxa-7,16-diazacyclooctadecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
K+	cal	alc/w	25°C	100%	U	H			1996BBf (105690)	1228
K(K+H2L)=3.39										
Medium: MeOH; 0.1 M Me4NCl. DH(K)=-24.4 kJ mol ⁻¹ . Data also for similar ariat 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
K+	cal	alc/w	25°C	100%	C	H		K1=4.58	2001DXa (105714)	1229
Medium: MeOH. DH(K1)=-39.1 kJ mol ⁻¹ , DS(K1)=-43.6 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
K+	cal	alc/w	25°C	100%	C	H			1999SBg (105719)	1230
K(K+H2L)=5.88										
Medium: MeOH. DH(K)=-55.6 kJ mol ⁻¹ , DS(K)=-73.8 J K ⁻¹ mol ⁻¹ . K and DH(K) determined by competitive calorimetric titration.										

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
K+	cal	alc/w	25°C	100%	C	H			1999SBg (105729)	1231
K(K+H2L)=3.82										
Medium: MeOH. DH(K)=-47.8 kJ mol ⁻¹ , DS(K)=-87.3 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
K+	sp	alc/w	RT	50%	C			K1=2.1	2002GLb (105734)	1232
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
K+	sp	non-aq	18°C	100%	C			K1=2.0	1997LHa (105756)	1233
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
K+	con	non-aq	25°C	100%	U			K1=4.9	1989BEa (105776)	1234
Medium: tetrahydrofuran/CHCl3 4:1 (volume)										

C32H46N2O8Cl2			L					CAS 181706-75-2	(8626)	
3,18-Dichlorododecahydro-5H,16H-6,15-(ethanoxyethanoxyethano)dibenzohehexaoxadiazacyclohexacosine;										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
K+	cal	non-aq	25°C	100%	C	H		K1=4.66	1998ZBc (105787)	1235
Medium: MeOH. DH(K1)=-43.1 kJ mol ⁻¹ , DS(K1)=-55.4 J K ⁻¹ mol ⁻¹ .										

C32H46O10			L					CAS 77846-54-9	(5820)	
Biphenyl bis-19-crown-5, Octadecahydro-benzopentaoxacylononadecinobenzopentaoxacylononadecane;										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
K+	gl	non-aq	25°C	100%	U			K1=1.34 B2=1.22	1985RCa (105791)	1236
Medium: (CH3)2CO. L=Octadecahydro-4H,18H-[2,5,8,11,14]benzopentaoxacylononadecino[18,17,16-pqr][2,5,8,11,14]benzopentaoxacylononadecane										

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
K+	gl	alc/w	25°C	93%	U			K1=2.9	1978WVa (105802)	1237
Medium: 93% MeOH/H2O										

C32H48N2O10			L					CAS 84992-99-4	(665)	
Diaminoethane-N,N'-dimethenyl-di-(benzo-15-crown-5);										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
K+	cal	mixed	25°C	0.15M	C			K1=3.14	1986LWa (105805)	1238

C32H52O14P2			L					CAS 112120-15-7	(5730)	
1,13-Bis(2-(diethoxyphosphinylmethoxy)phenyl)-1,4,7,10,13,16-hexaoxahexadecane;										

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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
K+         con non-aq 25°C 100% U      K1=5.1      1989EVa (105823)1239
Medium: tetrahydrofuran/CHCl3 4:1 (volume)
*****
C32H55N013          L          CAS 105495-11-2 (1690)
N-(2-(2-(4'-Benzo-18-crown-6)-oxyethoxy)ethyl-1,4,7,10,13-pentaoxa-16-azacyclooctadecane;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
K+         ISE a/c/w 25°C 10% U      K1=4.66 B2=7.51 1986HAa (105832)1240
Medium: 10% MeOH/H2O
*****
C32H58N2012        H2L          CAS 88454-81-3 (5409)
2,11-Bis(carboxy)-3,12-bis(octanylformamide)-18-crown-6 (anti);
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
K+         gl a/c/w 25°C 90% U      K1=6.4      1984FWa (105837)1241
B(KHL)=11.8
Medium: 90% v/v MeOH/H2O, 0.05 M R4NX
*****
C32H58N2012        H2L          CAS 88454-82-4 (5408)
3,11-Bis-carboxy-2,12-bis(octanylformamide)-18-crown-6 (syn);
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
K+         gl a/c/w 25°C 90% U      K1=5.4      1984FWa (105843)1242
B(KHL)=11.0
Medium: 90% v/v MeOH/H2O, 0.05 M R4NX
*****
C32H64N4010        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;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
K+         ISE a/c/w 25°C 95% C      K1=4.8      1977LSc (105850)1243
K(KL+K)=3.9
Medium: 95% (w/w) MeOH/H2O, 0.1 M Et4NBr.
*****
C32H66N204          L      22DD Kryptofix CAS 79495-97-9 (6655)
1,10-Didecyl-1,10-diaza-4,7,13,16-tetraoxacyclooctadecane;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
K+         con non-aq 25°C 100% C T H      K1=5.53      1997TAa (105862)1244
Medium: acetonitrile. DH(K1)=-43.6 kJ mol-1, DS(K1)=-39.5 J K-1 mol-1.
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Data for 10-25 C.

K+ cal alc/w 25°C 100% U H 1986BUd (105863)1245
In MeOH. DH=-31.5 kJ mol⁻¹

C33H41N3O6 L (8027)

Tripodal ionophore ;

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

K+ sp non-aq 25°C 100% C 2001LFa (105923)1246

K(KP+L=LiPL)=3.42

Method: Analyses by spectrophotometry. Medium: chloroform. P is picrate.

C33H41N3O6Cl2 L CAS 181706-78-5 (8628)

3,18-Dichlorohexahydro(ethanoxyethanoxyethano)-23,27-nitrilodibenzotetraoxadiazacyclopentacosine;

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

K+ cal non-aq 25°C 100% C H K1=4.41 1998ZBc (105927)1247

Medium: MeOH. DH(K1)=-23.0 kJ mol⁻¹, DS(K1)=7.28 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

K+ sp non-aq 25°C 100% U K1=9.20 1979KMb (105981)1248

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

K+ gl alc/w 20°C 100% U K1=2.93 1968WPa (105997)1249

Medium: MeOH, 1 M KI

C34H38N2O14 H2L (7072)

7,16-Bis(3-carboxy-6-methoxy-2-oxo-2H-1-benzopyran-7-yl)-1,4,10,13-tetraoxa-diazacyclooctadecane;

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

K+ sp none RT 0 U K1=1.66 1994CGa (106028)1250

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
K+	oth	non-aq	22°C	100%	U			K1=1.0	1978YSa (106039)	1251
Medium: 1:1 v/v EtOH+CHCl3. K as acetate salt										

C34H40O6P2		L						CAS 137728-08-6	(6838)	
1,14-Bis(diphenylphosphinyl)-3,5,8,11-tetraoxatetradecane;										
K+	con	non-aq	25°C	100%	U			K1=5.0	1992BEa (106043)	1252
Medium: THF+CHCl3 (4:1 vol)										

C34H40O7		L						CAS 488759-49-5	(9011)	
cis-2,9-Dimethyl-2,9-bis[(1-naphthyloxy)methyl]-15-crown-5;										
K+	sp	non-aq	25°C	100%	C			K1=3.87	2002NMa (106047)	1253
Medium: THF, using metal picrate salt.										

C34H40O7P2		L						(7894)		
1,15-Bis(diphenylphosphinyl)-2,5,8,11,14-pentaoxopentadecane;										
K+	con	non-aq	25°C		C			K1=5.0	1999TEa (106050)	1254
In: tetrahydrofurane/CHCl3 4:1 v/v										

C34H42N2O6Cl2		L						CAS 181706-79-6	(8629)	
3,18-Dichlorooctahydro-5H,16H-6,15-(ethanoxyethanoxyethano)tribenzotetraoxadiazacyc lodocosine;										
K+	cal	non-aq	25°C	100%	C	H		K1=5.10	1998ZBc (106058)	1255
Medium: MeOH. DH(K1)=-17.0 kJ mol ⁻¹ , DS(K1)=40.6 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...										
K+	nmr	non-aq	25°C	100%	U			K1=11.00	1986CHc (106068)	1256
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

K+ sp mixed 20°C 80% C K1=5.65 19990Ba (106079)1257
K(KL+K)=2.27

Medium: 80% v/v CHCl3/MeOH.

C34H53O8Br H2L CAS 38784-08-6 (2336)
5-Bromolasalocid;

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

K+ gl alc/w 25°C 100% M H 1988PJa (106098)1258
K(K+HL)=3.49

Also used K+ sensitive glass electrode. DH = -8.8 kJ mol⁻¹; DS = 37

C34H54O8 H2L Lasalocid CAS 25999-20-6 (2335)
Lasalocid acid;

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

K+ nmr non-aq 20°C 100% C 1998MLa (106138)1259
K(K+HL)=1.8

Medium: CD3OD. Method: 13C nmr.

K+ dis oth/un 25°C 0.0 U K1=2.1 1992LPb (106139)1260

K+ gl alc/w 25°C 100% M H 1988PJa (106140)1261
K(K+HL)=3.56
K(K+H2L)=1.3

Medium: MeOH. Also using K+ sensitive glass elect. DH=-9.4 kJ mol⁻¹; DS=37

K+ gl alc/w 25°C 100% U 1982BDc (106141)1262
K(K+2HL)=3.45

Medium: MeOH

C34H58N4O14 H2L CAS 83458-45-1 (5569)
2,11-Dicarboxy-3,12-dipiperidinenitroxide-18-crown-6 derivative;

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

K+ nmr alc/w 25°C 90% U K1=5.4 1987DDa (106171)1263
K(K+HL)=4.4

Medium: 90% MeOH/H2O. Syn-isomer

K+ nmr alc/w 25°C 90% U K1=6.8 B2=11.90 1987DDa (106172)1264

Medium: 90% MeOH/H2O. Anti-isomer

C34H60N4O12 H2L CAS 111216-14-9 (5570)
syn-2,11-Dicarboxy-3,12-dipiperidine-18-crown-6 dervative;

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

K+ nmr alc/w 25°C 90% U K1=5.4 1987DDa (106174)1265
K(K+HL)=4.3
K(K+H2L)=4.2

Medium: 90% MeOH/H2O

C34H64O10 H2L D218-6A2 CAS 88454-79-9 (5406)
11,12-Bis(dodecanyl)-1,2-bis(carboxy)-1,4,7,10,13,16-hexaoxacyclooctadecane;

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

K+ gl alc/w 25°C 90% U K1=6.3 1984FWa (106178)1266
B(KHL)=12.1

Medium: 90% v/v MeOH/H2O, 0.05 M R4NX

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

K+ ISE alc/w 25°C 95% C K1=4.0 1977LSc (106181)1267
K(KL+K)=3.2

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-3,5,7,8,10,1
2,16,18,20,21,

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

K+ gl R4N.X 25°C 0.10M U K1=3.6 2001BBa (106202)1268
K(KL+H)=9.8
K(KHL+H)=9.3

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

K+ con alc/w 25°C 100% U K1=<-0.3 19800Pa (106216)1269

Medium: MeOH, 0.1 M Me4NBr

C36H32N2O6 L (5744)
5,6:11,12-Dibenzo-1,16-di(8-quinoly1)-1,4,7,10,13,16-hexaoxahexadecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
K+	con	non-aq	25°C	100%	U			K1=5.8	1989BEa (106219)	1270
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
K+	sol	none	25°C	dil	C			K1=2.85	2001BCf (106259)	1271
Method: dissolution of ligand in a 0.002-0.02 M KX solution; spectrophotometric measurement.										
K+	cal	mixed	25°C	50%	C	H		K1=2.79	1998BJb (106260)	1272
Medium: 50% (v/v) HCOOH/H2O. DH(K1)=-2.3 kJ mol ⁻¹ .										
K+	sp	none	25°C	0	U			K1=2.75 B2=4.05	1994HKa (106261)	1273
K+	sol	none	25°C	0.0	U			K1=7.91	1992BCa (106262)	1274

C36H36O4P2		L						(2073)		
3-t-Butyl-1,2-dihydroxybenzene bis(diphenylphosphinylmethyl) ether										
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
K+	con	non-aq	25°C	100%	U			K1=2.95	1989KSa (106280)	1275
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
K+	con	non-aq	25°C	100%	U			K1=4.02	1989KSa (106284)	1276
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
K+	dis	non-aq	25°C	100%	U	H			1979KLa (106294)	1277
K(K(picrate)+L)=3.28										
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
K+	dis	non-aq	25°C	100%	U	H			1979KLa (106300)	1278
K(K(picrate)+L)=4.82										

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
K+	dis	non-aq	25°C	100%	U	H			1979KLa (106306)	1279
K(K(picrate)+L)=3.38										

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
K+	con	non-aq	25°C	100%	U			K1=4.9	1992BEa (106334)	1280
Medium: THF+CHCl3 (4:1 vol)										

K+	cal	non-aq	25°C	100%	U			K1=2.75 B2=3.50	1991SGa (106335)	1281
Medium: CH3CN; K as KNCS										

 C36H44O8P2 L (7895)
 1,18-Bis(diphenylphosphinyl)-hexaoxooctadecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
K+	con	non-aq	25°C		C			K1=5.4	1999TEa (106344)	1282
In: tetrahydrofuran/CHCl3 4:1 v/v										

 C36H47N3O6 L (8028)
 Tripodal ionophore 2;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
K+	sp	non-aq	25°C	100%	C				2001Lfa (106374)	1283
K(KP+L=LiPL)=3.20										

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
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K+ nmr non-aq 25°C 100% U K1=>14.57 1986CHc (106378)1284
In CDCl3

C36H52N2O10 L CAS 84993-03-3 (666)

Hexadamine-N,N'-dimethenyl-di-(benzo-15-crown-5);

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

K+ cal mixed 25°C 0.15M C K1=3.56 1986LWa (106393)1285

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

K+ con non-aq 25°C 100% U K1=5.0 1989BEa (106396)1286

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

K+ ISE alc/w 25°C 90% U K1=4.17 B2=5.70 1987KHa (106418)1287

90% w/w MeOH/H2O. Also data for the 1,4,7,10-tetraoxadecane-bridged
ligand: K1=4.64; K2=2.01.

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

K+ con alc/w 25°C 100% U I M K(KCl+L)=3.20 1979BDa (106436)1288

Medium: MeOH. In DMSO: K(KClO4+L)=3.32. In MeCN: K(KBPh4+L)=4.04

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

K+ con non-aq 25°C 100% C H K1=2.97 1997PBb (106501)1289

Medium: acetonitrile. Additional method: potentiometry with ISE.

By calorimetry, DH(K1)=-22 kJ mol⁻¹, DS(K1)=-11 J K⁻¹ mol⁻¹.

K+ vlt non-aq 25°C 100% C I K1=9.7 1997WRa (106502)1290

Method: cyclic voltammetry. Medium: acetonitrile, 0.05 M Et4NClO4. In DMSO
K1=5.1; in acetone, K1=8.7; in hexamethylphosphoric triamide, K1=1.9.

K+ vlt non-aq 23°C 100% U I K1=9.7 1994FRa (106503)1291
 Medium: MeCN. In PrCN: K1=9.2; acetone: 8.7; DMF: 7.3; Me-pyrrol.: 6.0;
 NN-DMA: 5.6; DMSO: 5.1; Di-Et-formamide: 4.6; Di-Et-acetamide: 4.5; PC: 9.1

K+ ISE alc/w 25°C 100% M K1=4.97 1984CTa (106504)1292
 Medium: MeOH

K+ ISE non-aq 25°C 100% M K1=7.35 1984CTa (106505)1293
 Medium: N,N-dimethylformamide. In DMSO K1=5.05

K+ ISE alc/w 25°C 100% U K1=7.28 1984CTb (106506)1294
 Medium: EtOH

K+ gl alc/w 25°C 100% U K1=5.18 1978HPa (106507)1295

K+ oth alc/w 25°C 100% U H K1=4.48 1971FCa (106508)1296
 Method: micro-calorimetry. Medium: MeOH. DH=-16.2 kJ mol⁻¹, DS=31 J K⁻¹ m⁻¹

K+ oth alc/w 25°C 100% U H K1=4.60 1971LFA (106509)1297
 Method: micro-calorimetry. Medium: MeOH. DH=-15.6 kJ mol⁻¹, DS=35 J K⁻¹ mol⁻¹

K+ ISE alc/w ? 100% U K1=4.98 1970LWb (106510)1298
 Medium: MeOH. In methylcellosolve/H₂O, 80:20, K1=3.82

 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

K+ sp non-aq 25°C 100% U K1=8.03 1979KMb (106632)1299
 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

K+ con non-aq 25°C 100% U K1=3.2 1993BEb (106642)1300
 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

K+ con non-aq 25°C 100% U K1=3.7 1991EBa (106648)1301
 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

K+ con non-aq 25°C 100% U K1=4.6 1993EVa (106659)1302
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

K+ con non-aq 25°C 100% U K1=5.3 1992BEa (106680)1303
Medium: THF+CHCl3 (4:1 vol)

C38H48O9P2 L (7896)
1,21-Bis(diphenylphosphinyl)-2,5,8,11,14,17,20-heptaoxoheneeicosane;

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

K+ con non-aq 25°C C K1=5.1 1999TEa (106685)1304
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

K+ nmr non-aq 25°C 100% U K1=13.93 1986CHc (106690)1305
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

K+ sp mixed 20°C 80% C K1=4.87 19990Ba (106699)1306
K(KL+K)=2.27
Medium: 80% v/v CHCl3/MeOH.

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

K+ sp non-aq 25°C 100% C K1=3.9 20010Ya (106721)1307

Medium: methanol. For the 1,4-butanediyl- derivative, K1=4.1

C40H36O4P2 L (6805)
1,6-Bis(2-Diphenylphosphinylphenyl)-2,5-dioxahexane; (CH2.0.CH2.C6H4(PO(6H5)2)2

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

K+ con non-aq 25°C 100% U K1=3.2 1993BEb (106733)1308
Medium: THF+CHCl3 4:1(vol)

C40H36O5P2 L CAS 86341-96-0 (5724)
1,7-Di(2-diphenylphosphinyl)phenyl-1,4,7-trioxaheptane; Ph2PO.C6H4.0.C2H4.0.C2H4.0.C6H4.POPh2

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

K+ con non-aq 25°C 100% U K1=3.9 1991EBa (106745)1309
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

K+ con non-aq 25°C 100% U K1=2.66 1989KSa (106764)1310
Medium: tetrahydrofuran/CHCl3 4:1 (vol)

C40H46O7 L CAS 177723-37-4 (8912)
25,27-Diethoxycalix[4]arene-crown-5, 1,3-alternate;

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

K+ dis non-aq 22°C 100% C M 1996CPa (106771)1311
K(KA+L(org))=KAL(org))=9.77

Medium: CHCl3 saturated with H2O. Method: extraction of KA into CHCl3/L solution. HA is picric acid. For the cone conformation, K=5.71.

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

K+ sp non-aq 25°C 100% C K1=2.13 1995CUa (106776)1312
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
K+	dis	non-aq	25°C	100%	U	H			1979KLa (106794)	1313

K(K(picrate)+L)=8.51

Medium: CHCl3

 C40H50N2O010 L CAS 143902-45-8 (8935)
 Decamethylcucurbit[5]uril;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
K+	cal	mixed	25°C	50%	C	H		K1=3.48	2000ZKb (106806)	1314

Medium: 50% v/v formic acid/H2O. DH(K1)=-10 kJ mol⁻¹, DS(K1)=33 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
K+	ISE	non-aq	25°C	100%	C			K1=4.10	1998Wlc (106822)	1315

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
K+	con	non-aq	25°C	100%	U			K1=5.2	1989BEa (106827)	1316

Medium: tetrahydrofuran/CHCl3 4:1 (volume)

 C40H60N2O10 n L CAS 84993-07-7 (667)
 15,15'-Decamethylenedinitrilodimethylidyne-bis-(octahydro-1,4,7,10,13-benzopentaoxacyclopentadeci

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
K+	cal	mixed	25°C	0.15M	C			K1=3.12	1986LWa (106831)	1317

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
K+	kin	alc/w	23°C	100%	U			K1=4.08	1982HLc (106832)	1318

Medium: MeOH. Data also for nonamethylene(K=4.65) and tetramethylene(K=4.18) analogues

 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
K+	ISE	alc/w	25°C	90%	U			K1=4.98 B2=9.12	1987KHa (106835)	1319

90% w/w MeOH/H2O. Also data for the 1,4,7,10-tetraoxadecane-bridged ligand: K1=5.05; K2=3.93.

C40H64O12 L Nonactin CAS 6833-84-7 (4179)
Nonactin

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

K+ sp non-aq 25°C 100% C K1=4.15 1977CEb (106842)1320
Method: temperature jump relaxation. Medium: MeOH.

K+ vlt non-aq 22°C 100% U K1=4.43 1974RKd (106843)1321
Medium: 0.025 NBu4ClO4 in CH3CN

K+ cal alc/w 25°C 100% U H K1=4.49 1973ZFa (106844)1322
Method:micro-calorimetry. Medium:MeOH. DH=-43.6 kJ mol-1, DS=-60.3 J K-1 m-1
In EtOH: K1=5.26, DH=-52.2 kJ mol-1, DS=74.4 J K-1 mol-1

K+ oth alc/w 30°C 100% U K1=3.59 1973ZFa (106845)1323
Method: vapour pressure osmometry. Medium:MeOH. In EtOH, K1=4.61

K+ cal alc/w 25°C 100% U H K1=4.30 1971FCa (106846)1324
Method:micro-calorimetry. Medium:MeOH. DH=-45.9 kJ mol-1, DS=-71 J K-1 m-1

K+ nmr non-aq 17°C 100% U K1=4.85 1970PCa (106847)1325
Medium: KClO4,acetone. With 0.5 mol fraction water, K1=4.3

K+ ISE alc/w 20°C 100% U K1=3.59 1968WPa (106848)1326
Medium: MeOH, 0.1 M KSCN

K+ oth alc/w 30°C 100% U K1=3.80 1967PWb (106849)1327
Medium: MeOH, 0.1 M KSCN. 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

K+ cal alc/w 25°C 100% U H K1=5.6 1971LFa (106863)1328
Method: micro-calorimetry. Medium:MeOH. DH=-4.1 kJ mol-1, DS=93 J K-1 mol-1

K+ ISE alc/w ? 100% U K1=5.18 1970LWb (106864)1329
Medium:MeOH. In methylcellosolve:H2O, 80:40, K1=4.48

C40H80O20 L (5376)
Dibenzo-60-crown-20;

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

K+ ISE alc/w 25°C 100% A K1=3.90 1971FRa (106868)1330

Medium: MeOH

C41H42O6 L CAS 151832-07-4 (6874)
9-(Dimethylethyl)-29,30,31,32,33-pentamethoxy-23-oxahexacyclotritriacontapentadecane;

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

K+ dis non-aq 25°C 100% U K(K(picrate)+L)=7.72 1993HSa (106870)1331

Medium: CDCl3. With 23-thia- analogue K=7.15

C41H66O12 L Monactin CAS 7182-54-9 (4180)
Monactin

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

K+ sp non-aq 25°C 100% C K1=4.38 1977CEb (106887)1332
Method: temperature jump relaxation. Medium: MeOH.

K+ vlt non-aq 22°C 100% U K1=4.78 1974RKd (106888)1333
Medium: 0.025 NBu4ClO4 in CH3CN

K+ oth alc/w 30°C 100% U K1=4.04 1973ZFa (106889)1334
Method: vapour pressure osmometry. Medium: MeOH. In EtOH, K1=4.46

K+ oth alc/w 30°C 100% U K1=5.5 1967PWb (106890)1335
Medium: MeOH, 0.1 M KSCN. 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

K+ oth non-aq 25°C 100% U K1=2.4 1995TEa (106911)1336
Medium: THF:CHCl3 4:1 v/v. K 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

K+ con non-aq 25°C 100% U K1=3.1 1993BEb (106916)1337
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

K+ con non-aq 25°C 100% U K1=3.9 1993BEb (106925)1338
Medium: THF+CHCl3 4:1(vol)

K+ con non-aq 25°C 100% U K1=4.01 1989KSa (106926)1339
Medium: tetrahydrofuran/CHCl3 4:1 (vol)

C42H40O7P2 L CAS 95651-36-8 (2079)
1,7-Di(2-(diphenylphosphinylmethoxy)phenyl)-1,4,7-trioxahепtane;
(Ph2PO.CH2.O.C6H4.O.C2H4)2O

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

K+ con non-aq 25°C 100% U K1=4.19 1989KSa (106935)1340
Medium: tetrahydrofuran/CHCl3 4:1 (vol)

K+ con non-aq 25°C 100% U K1=4.19 1989TKb (106936)1341
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

K+ sp non-aq 25°C 100% C K1=>=10 2000PBa (106950)1342
Medium: MeOH.

K+ dis non-aq 22°C 100% C M 1996CPa (106951)1343
K(KA+L(org))=KAL(org))=9.83
Medium: CHCl3 saturated with H2O. Method: extraction of KA into CHCl3/L
solution. HA is picric acid. For the cone conformation, K=5.27.

C42H54O15 L CAS 104512-99-4 (7749)
Tris-(15-Crown-5)triphenylene ;

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

K+ ISE mixed 25°C 50% C K1=4.6 1991LMc (106969)1344
K(KL+K)=3.5
K(K2L+K)=1.7

Method: K 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]tetraoxadiazacyc
lohexadecine

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

K+ sp non-aq RT 100% C I K1=3.35 2000GDa (106973)1345
Medium: acetonitrile. In MeOH, K1=3.15.

C42H68O12 L CAS 20261-85-2 (5373)
Dinactin;

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

K+ sp non-aq 25°C 100% C K1=4.63 1977CEb (106980)1346
Method: temperature jump relaxation. Medium: MeOH.

K+ vlt non-aq 22°C 100% U K1=5.24 1974RKd (106981)1347
Medium: 0.025 NBu4ClO4,CH3CN

K+ oth alc/w 30°C 100% U K1=3.73 1973ZFa (106982)1348
Method: vapour pressure osmometry. Medium: MeOH

C43H42O4P2 L (7156)
1,3-Bis((2-diphenylphosphinyl)phenoxy)propane;

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

K+ oth non-aq 25°C 100% U K1=2.4 1995TEa (106999)1349
Medium: THF:CHCl3 4:1 v/v. K as 2,4-dinitrophenolate. Also other similar ligands

C43H42O6P2 L (5734)
1,7-Di((2-diphenylphosphinylmethoxy)phenyl)-1,7-dioxheptane;
(Ph2PO.CH2O.C6H4.O.C2H4)2CH2

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

K+ con non-aq 25°C 100% U K1=2.11 1989TKb (107004)1350
Medium: tetrahydrofuran/CHCl3 4:1 (volume)

C43H54N2O10 L (668)
4,4'-Diaminodiphenylmethane-N,N'-dimethenyl-di(3-benzo-15-crown-5);

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

K+ cal mixed 25°C 0.15M C K1=2.79 1986LWa (107010)1351

C43H70O12 L CAS 7561-71-9 (5374)
Trinactin;

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

K+ vlt non-aq 22°C 100% U K1=5.44 1974RKd (107031)1352
Medium: 0.025 NBu4ClO4 in CH3CN

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
K+	con	non-aq	25°C	100%	U		K1=2.4	1993BEb (107090)	1353
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
K+	con	non-aq	25°C	100%	U		K1=4.4	1993BEb (107109)	1354
Medium: THF+CHCl3 4:1(vol)									

C44H44O5P2		L					(5735)		
1,7-Di((2-diphenylphosphinylmethoxy)phenyl)-4-oxaheptane; (Ph2PO.CH2O.C6H4.C3H6)20									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
K+	con	non-aq	25°C	100%	U		K1=2?	1989TKb (107113)	1355
Medium: tetrahydrofuran/CHCl3 4:1 (volume)									

C44H44O5P2		L					(5733)		
1,7-Di(2-(diphenylphosphinylethyl)phenyl)-1,4,7-trioxaheptane; (Ph2PO.C2H2.C6H4.OC2H4)20									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
K+	oth	non-aq	25°C	100%	U		K1=2.3	1995TEa (107117)	1356
Medium: THF:CHCl3 4:1 v/v. K as 2,4-dinitrophenolate									

K+	con	non-aq	25°C	100%	U		K1=2.11	1989TKb (107118)	1357
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
K+	cal	non-aq	25°C	100%	U	H	K1=1.75 B2= 3.68	1998SBb (107127)	1358
Medium: MeCN Calorimetric titration of LiNCS. DH(K1)=-20.6 kJ mol ⁻¹ DH(B2)=-6.9									

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
K+	sp	non-aq	23°C	100%	U		K1=4.8	1997BGa (107132)	1359
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
K+	sp	non-aq	20°C	100%	C			K1=5.85	2002MTb (107136)	1360

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
K+	gl	non-aq	25°C	100%	C			K1=4.89 B(K2L)=7.74	2000ABb (107143)	1361

Medium: MeOH, 0.05 M Et4NClO4.

C44H52N4O8 L CAS 246035-33-6 (2925)
25,27-Bis(N,N-diethylaminocarbonylmethoxy)-26,28-bis(aminocarbonylmethoxy)calix[4]a
rene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
K+	sp	non-aq	25°C	100%	C			K1=4.1	1999USa (107158)	1362

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
K+	sp	non-aq	25°C	100%	C	IH		K1=4.47	1996AAe (107164)	1363

Medium: acetonitrile. By calorimetry, DH(K1)= -59 kJ mol⁻¹, DS(K1)=-114 J K⁻¹ mol⁻¹. In 100% MeOH, K1=4.76, DH(K1)=-57.0, DS(K1)=-100.

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
K+	sp	non-aq	25°C	100%	C			K1=4.6	2000PBa (107170)	1364

Medium: MeOH.

C44H54O8 L CAS 161282-98-0 (8679)
25,27-Bis(1-propyloxy)calix[4]arene-crown-6, 1,3-alternate;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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K+ EMF non-aq 25°C 100% C K1=4.3 1995CUa (107175)1365
Medium: methanol, 0.01 M Et4NClO4. Method: Ag-competitive potentiometry.

C44H54O8 L CAS 161282-96-8 (8678)

25,27-Bis(2-propyloxy)calix[4]arene-crown-6, 1,3-alternate;

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

K+ sp non-aq 25°C 100% C H K1=4.5 1995CUa (107181)1366

Medium: methanol, 0.01 M Et4NCl. Alternative method: Ag-competitive potentiometry. By calorimetry, DH(K1)=-18.1 kJ mol⁻¹, DS(K1)=25 J K⁻¹ mol⁻¹.

C44H56O4 H4L (7294)

4-Tert-butyl-calix[4]arene;

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

K+ sp non-aq 25°C 100% U K1=1.2 1996ABa (107186)1367

Medium: MeCN

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

K+ ISE alc/w 25°C 95% C K1=3.6 1977LSc (107193)1368

K(KL+K)=2.7

Medium: 90% (w/w) MeOH/H2O, 0.1 M Et4NBr. In H2O, K1=ca.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

K+ con non-aq 25°C 100% U K1=4.0 1984YKa (107212)1369

Medium: tetrahydrofuran + CHCl3 4:1, K as 2,4-dinitrophenolate

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

K+ con non-aq 25°C 100% U K1=3.2 1984YKa (107225)1370

Medium: tetrahydrofuran + CHCl3 4:1, K 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

K+ con non-aq 25°C 100% U K1=4.9 1991EBa (107240)1371
Solvent : Tetrahydrofuran + 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

K+ sp mixed 25°C 90% C K(KSCN+L)=3.38 1997KKa (107249)1372

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

K+ sp none RT 0 U K1=2.22 1994CGa (107256)1373
Method: fluorimetry. L=7,16-bis[2-(2,4-dicarboxyphenyl)-5-methoxy-1-benzofuran-6-yl]-1,4,10,13-tetraoxa-7,16-diazacyclooctadecane

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

K+ con non-aq 25°C 100% U K1=4.8 1993BEb (107259)1374
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

K+ oth non-aq 25°C 100% U K1=2.8 1995TEa (107270)1375
Medium: THF:CHCl3 4:1 v/v. K 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

K+ con non-aq 25°C 100% U K1=4.73 1989KSa (107279)1376
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

K+ con non-aq 25°C 100% U 1989KSa (107360)1377
Medium: tetrahydrofuran/CHCl3 4:1 (vol)

C48H5008P2 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

K+ con non-aq 25°C 100% U K1=5.3 1993BEb (107364)1378
Medium: THF+CHCl3 4:1(vol)

C48H54010P4 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

K+ con non-aq 25°C 100% U K1=4.12 1989KSa (107387)1379
Medium: tetrahydrofuran/CHCl3 4:1 (vol)

C48H6008 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

K+ gl alc/w 25°C 100% C K1=4.7 1993ABb (107402)1380
B(K2L)=8.3
B(KHL)=12.4
Medium: MeOH, 0.01 M Et4NClO4. Data also for di-tert-butyl ester

C48H60012 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

K+ sp non-aq 25°C 100% C IH K1=4.12 1996AAe (107410)1381
Medium: acetonitrile. By calorimetry, DH(K1)=-17 kJ mol⁻¹, DS(K1)=23
J K-1 mol⁻¹. In 100% MeOH, K1=4.1, DH(K1)=-31.7, DS(K1)=-28.

C48H60016 H4L (8251)
5,11,17,23-Tetrahydroxycalix[4]arene-bis(crown-6);

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

K+ sp non-aq 25°C 100% C K1=4.4 2001PCa (107415)1382
Medium: methanol

C48H96N204 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

K+ ISE oth/un 21°C 100% C K1=4.7 1999CPa (107446)1383
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

K+ gl alc/w 25°C 100% C K1=9.05 1993ABb (107489)1384
B(KHL)=19.77
B(KH2L)=29.35
B(KH3L)=37.35

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

K+ sp non-aq 25°C 100% C H K1=5.0 1999USa (107498)1385
Medium: MeOH, 0.10 M Et4NCl. DH(K1)=-33.3 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

K+ sp non-aq 25°C 100% C K1=2.2 1999USa (107507)1386
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

K+ sp non-aq 25°C 100% C K1=3.36 2004BCb (107525)1387
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

K+ dis non-aq 22°C 100% U K1=8.48 1996SCa (107541)1388

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

K+ dis non-aq 22°C 100% C M 1996CPa (107549)1389

K(KA+L(org))=KAL(org))=9.35

Medium: CHCl3 saturated with H2O. Method: extraction of KA into CHCl3/L solution. HA is picric acid.

K+ cal alc/w 25°C 100% U H K1=4.90 1977ILa (107550)1390

Medium: MeOH. DH(K1)=-19.0 kJ mol⁻¹

K+ sp alc/w 25°C 100% U K1=4.48 1972FEb (107551)1391

Medium: methanol/0.1M tetrabutyl-ammonium-perchlorate

K+ oth alc/w 25°C 100% U H 1971FCa (107552)1392

Method: micro-calorimetry. Medium: MeOH. DH=-19 kJ mol⁻¹

In EtOH: K1=6.08, DH=-37.2, DS=9.02 J K⁻¹ mol⁻¹

K+ gl alc/w 20°C 100% U K1=>3.9 1968WPa (107553)1393

Medium: MeOH, 1 M KI

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

K+ sp non-aq 25°C 100% C K1=4.32 1996AAe (107577)1394

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-oxyethoxy)ethoxy]]

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

K+ oth non-aq RT 100% C I K1=5.03 2002LAa (107582)1395

K(KL+K)=2.47

B(K2L)=7.5

Method: fluorimetry. Medium: EtOH. In CH3CN, K1=5.03, K(KL+K)=2.3,

B(K2L)=7.33.

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
K+	dis	non-aq	25°C	100%	C				2001SSb (107586)	1396

$$K(K.pic+L(org))=KL.pic)=0.72$$

Distribution of picrate salt into CHCl3/HL.

K: K.pic(aq)+L(org)=KL.pic(org). Data for series of myo-inositol ligands

C56H7208 L CAS 123311-74-0 (6160)

Tetramethyl-t-butylcalix[4]arenetetraketone;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
K+	sp	alc/w	25°C	100%	U I			K1=3.1	1989ACb (107597)	1397

Medium: MeOH. In CH3CN, K1=4.4

C56H72012 L (8751)

Tetramethyl-4-t-Butylcalix[4]arenetetraethanoate;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
K+	EMF	non-aq	25°C	100%	C IH			K1=4.01	1995DGa (107601)	1398

Medium: acetonitrile, 0.05 M Et4NClO4. Competitive method: Ag/Ag+ electrode. DH(K1)=-40.6 kJ mol-1, DS=-59.4. Also data in benzonitrile.

C56H7808 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
K+	sp	non-aq	25°C	100%	C			K1=2.54	1995CUa (107606)	1399

Medium: methanol, 0.01 M Et4NCl.

C56H8008 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
K+	sp	non-aq	25°C	100%	C H			K1=4.51	2004BCb (107613)	1400

Medium: acetonitrile, 0.01 M Et4NClO4. By calorimetry: DH(K1)=-28.3 kJ mol-1, DS(K1)=-8.7 J K-1 mol-1.

C58H78011 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
K+	sp	alc/w	25°C	100%	C			K1=2.6	2001MAa (107622)	1401

Medium: MeOH, 0.01 M Et4NCl.

C58H80O10 L (9264)
5,11,17,23-Tetra-t-butyl-25,27-di(2-methoxyethoxy)-26,28-di(ethylacetate)calix[4]arene;

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

K+ sp non-aq 25°C 100% C H K1=5.06 2004BCb (107631)1402
Medium: acetonitrile, 0.01 M Et4NClO4. DH(K1)=-44.5 kJ mol⁻¹,
DS(K1)=-52.3 J K⁻¹ mol⁻¹.

C60H54N06P3 L (8067)
Tris[2-diphenylphosphoryl]phenoxyethylamine;

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

K+ cal non-aq 25°C 100% U H K1=2.44 B2= 4.49 1998SBb (107638)1403
Medium: MeCN Calorimetric titration of LiNCS. DH(K1)=-16.6 kJ mol⁻¹
DH(B2)=-13.1

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

K+ con non-aq 25°C 100% C H K1=4.35 2002ASc (107649)1404
Medium: acetonitrile. DH(K1)=-42.56 kJ mol⁻¹, DS(K1)=-59.30 J K⁻¹ mol⁻¹.

K+ EMF non-aq 25°C 100% C IH K1=4.04 1995DGa (107650)1405
Medium: acetonitrile, 0.05 M Et4NClO4. Competitive method: Ag/Ag+
electrode. DH(K1)=-45.7 kJ mol⁻¹, DS=-76. Also data for tetrabutyl deriv.

K+ sp alc/w 25°C 100% U I K1=2.4 1989ACb (107651)1406
Medium: MeOH. In CH3CN, K1=4.5

C60H82N2O10 L CAS 155377-20-1 (8806)
5,11,17,23-Tetra-butyl-25,27-bis(carboxymethoxy)-bis[(N,N-diethylaminocarbonyl)methoxy]calix[4]arene

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

K+ gl non-aq 25°C 100% C K1=4.81 2000ABb (107666)1407
B(K2L)=9.10

Medium: MeOH, 0.05 M Et4NClO4.

C60H84N4O8 L CAS 246035-32-5 (2735)
25,27-Bis(N,N-diethylaminocarbonylmethoxy)-26,28-bis(aminocarbonylmethoxy)-t-butylcalix[4]arene;

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

K+ sp non-aq 25°C 100% C K1=<1 1999USa (107679)1408
Medium: MeOH, 0.10 M Et4NCl

C62H84O14 L CAS 135581-11-2 (8630)
9,23-Dioxpentacyclo[23.3.1.13,7.111.15.117.21]dotriacontane, ethanoic acid
derivative;

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

K+ sp non-aq 25°C 100% C K1=3.9 1991ACc (107694)1409
Medium: acetonitrile, 0.01 M Et4NClO4.

C62H111N11O12 L CAS 59865-13-3 (9048)
Cyclosporin A;

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

K+ oth non-aq 25°C 100% C K1=<1 2003CGa (107717)1410
Method: CD titration. Medium: acetonitrile.

C63H60N06P3 L (8437)
Tris[2-(diphenylphosphorylmethyl)phenoxyethyl]amine;

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

K+ cal non-aq 25°C 100% U H K1=2.02 B2= 5.01 1998SBb (107719)1411
Medium: MeCN Calorimetric titration of LiNCS. DH(K1)=-12.6 kJ mol⁻¹
DH(B2)=-4.3

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

K+ sp non-aq 25°C 100% C H K1=5.22 1999Lda (107734)1412
B(K2L)=8.05

Medium: acetonitrile, 0.01 M Et4NClO4
By calorimetry, DH(K1)=-10.7 kJ mol⁻¹, DH(K2L)=-23.8 kJ mol⁻¹

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

K+ con non-aq 25°C 100% U K1=3.1 1990EAb (107739)1413
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
K+	sp	non-aq	25°C	100%	C			K1=4.2	1996AAe (107744)	1414
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]arene;										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
K+	oth	non-aq	RT	100%	C	I		K1=4.81 K(KL+K)=2.46 B(K2L)=7.29	2002LAa (107749)	1415

Method: fluorimetry. Medium: EtOH. In CH3CN, K1=4.25, K(KL+K)=2.19, B(K2L)=6.44.

C64H72N4O4P4		L						CAS 104786-07-4	(2065)	
1,4,7,10-Tetra(diphenylphosphinyloxyethyl)-1,4,7,10-tetraazacyclododecane;										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
K+	con	non-aq	25°C	100%	U			K1=5.04	1986STb (107752)	1416
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
K+	sp	non-aq	25°C	100%	C	H		K1=2.69	2004BCb (107761)	1417
Medium: acetonitrile, 0.01 M Et4NClO4. DH(K1)=-8.4 kJ mol ⁻¹ , DS(K1)=23.1 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
K+	sp	alc/w	25°C	100%	U			K1=2.82	1996AAc (107768)	1418
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
K+	sp	non-aq	25°C	100%	C			K1=2.90	2004BCb (107776)	1419

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

K+ EMF non-aq 25°C 100% C IH K1=3.17 1999DCa (107784)1420

Medium: acetonitrile, 0.05 M Bu4NClO4. Method: by competition with Ag+.

By calorimetry: K1=3.10, DH(K1)=-18.47 kJ mol⁻¹, DS(K1)=-1.9 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

K+ cal alc/w 25°C 100% U H 1995ABc (107790)1421

Medium: 100% Methanol. DH(K1)=-32.6 kJ mol⁻¹, DS(K1)=-6 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

K+ sp alc/w 25°C 100% U K1=5.0 1989ACb (107794)1422

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

K+ sp alc/w 25°C 100% U K1=2.7 1992ABb (107798)1423

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

K+ sp non-aq 25°C 100% C K1=2.3 1999USa (107804)1424

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

K+ cal alc/w 25°C 100% U IH 1995ABc (107813)1425
Medium: 100% Methanol. DH(K1)=-42.4 kJ mol⁻¹, DS(K1)=-31 J K⁻¹ mol⁻¹.
In acetonitrile, K1>8.5, DH(K1)=-64 kJ mol⁻¹, DS(K1)=>-52 J K⁻¹ mol⁻¹.

K+ dis non-aq 20°C 100% C M 1988AGa (107814)1426
K(K+A+L(org))=KAL(org))=7.45

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

K+ EMF alc/w 25°C 100% C H K1=6.73 2004MFa (107834)1427
Competitive potentiometry with Ag+. Medium: MeOH, 0.01 M Et₄NCI.
By calorimetry, DH(K1)=-38.1 kJ mol⁻¹, DS(K1)=0 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

K+ con non-aq 25°C 100% U K1=3.95 1985YKa (107846)1428
Medium: EtOH+CHCl₃ 1:1; M is used in nitrophenolate form

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

K+ kin mixed 25°C 0 U K(KX+L)=10.41 1994BHb (107852)1429

Medium: CDCl₃, saturated with H₂O. X=picrate Data also for 2 analogues calixspherands

C75H100O15 L CAS 152495-34-6 (7033)
Penta-tert-butylpentakis(ethoxycarbonylmethoxy)calix[5]arene;

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

K+ EMF alc/w 25°C 100% U K1=5.3 1993BMa (107859)1430
Medium: MeOH, 0.1 M Et₄NCI₀₄.

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

K+ sp non-aq 25°C 100% U K1=5.1 1989ACb (107869)1431
Medium: CH3CN

C76H98N2O16 L CAS 170514-24-6 (7124)

25,27-Bis((4-benzo-15-crown-5)aminocarbonylmethoxy)calix[4]arene;

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

K+ nmr non-aq RT 100% U 1995BDa (107875)1432

K(KL(PF6)+Cl)=3.54

K(KL(PF6)+NO3)=3.11

K(KL(PF6)+HSO4)=3.75

K(KL(PF6)+H2PO4) > 4

Medium: CD3CN

C77H82O9 L CAS 253317-20-3 (9288)

p-Tert-butylldihomooxalix[4]arene tetraphenyketone;

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

K+ sp alc/w 25°C 100% C I K1=4.0 1999MAb (107893)1433

Medium: MeOH, 0.01 M Et4NCl. In acetonitrile, K1=3.4.

C78H90O10P2 L CAS 160638-26-6 (9130)

5,11,17,23-Tetra-t-butyl-bis(diethylcarbamoylethoxy)-bis(diphenylphosphinoylethoxy)calix[4]arene

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

K+ sp alc/w 20°C 100% C K1=3.69 2003YVa (107899)1434

Medium: 100% EtOH, 0.01 M Et4NBr. Ligand is cone isomer. For paco isomer, K=4.21. 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

K+ dis non-aq 25°C 100% U 1995FDa (107904)1435

K=4.12

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

K+ sp non-aq 25°C 100% C I K1=5.15 2000AAa (107911)1436

Medium: methanol, 0.01 M Et4NCl. Also data for acetonitrile, 0.01 M Et4NCl and for the pentaethyl ester.

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

K+ EMF alc/w 25°C 100% U K1=6.1 1993BMa (107916)1437

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

K+ sp mixed 25°C 50% C K1=5.7 2001JDa (107921)1438
K(KL+K)=2.7

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

K+ ISE NaCl rt 0.01M C K1=<2 2003MGa (107927)1439

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

K+ ISE NaCl rt 0.01M C K1=<3 2003MGa (107935)1440

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

K+ cal non-aq 25°C 100% C K1=6.14 1997DZa (107940)1441

Medium: benzonitrile. DH(K1)=-47.68 kJ mol⁻¹, DS(K1)=-42.4 J K⁻¹ mol⁻¹.

K+ sp non-aq 25°C 100% U I K1=5.1 1989ACb (107941)1442

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

K+ EMF non-aq 25°C 100% C I K1=5.29 2000AAa (107950)1443
Medium: methanol, 0.01 M Et4NCl. Method: by competition with Ag+.
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

K+ dis non-aq 25°C 100% U 1995FDa (107965)1444
K=4.01
Medium: CDCl3. Method: by H2O/CDCl3 extraction of picrate salt.
K: MA(org)+L(org)=MLA(org) where A=picrate.

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

K+ dis non-aq 25°C 100% U 1995FDa (107977)1445
K=4.60
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

K+ dis non-aq 25°C 100% U 1995FDa (107982)1446
K=5.76
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

K+ ISE NaCl rt 0.01M C K1=6.7 2003MGa (107991)1447
Method: segmented sandwich membrane ISE.
Phosphonic acid diethyl ester derivative: K1=10.2

C120H192O24 L CAS 175349-58-3 (7495)
C-Undecylcalix[4]resorcinarene octa-alpha-(tert-butyl ethanoate);

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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
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K+         dis non-aq 25°C 100% U                               1995FDa (108008)1448
                                         K=4.65
Medium: CDCl3. Method: by H2O/CDCl3 extraction of picrate salt.
K: MA(org)+L(org)=MLA(org) where A=picrate.
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C120H200N8O16          L          CAS 169888-21-5 (7490)
C-Undecylcalix[4]resorcinarene octa-alpha-(N,N-diethyl acetamide);
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
K+         dis non-aq 25°C 100% U                               1995FDa (108019)1449
                                         K=5.73
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
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
K+         gl  alc/w  25°C 100% U          K1=3.0          1989ABb (108075)1450
Medium: MeOH
*****
Polymer          Enniatin A          CAS 2303-13-1 (4176)
Enniatin A
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
K+         gl  alc/w  20°C 100% U          K1=3.08         1968WPa (108164)1451
Medium: MeOH, 1 M KI
*****
Polymer          Myosin A          (3529)
Myosin A;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
K+         EMF oth/un 5°C   ?  U T      K1=2.9   B2=5.20   1957LSa (108261)1452
For Myocin B, 5 C: K1=2.9, K2=2.3; 27 C: K1=2.9, K2=1.7
*****
Polymer          (4181)
Phosphatidic acid;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
K+         gl  oth/un 24°C 0.10M U          K1=0.9          1966AKa (108270)1453
*****
Polymer          (4204)
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Pyruvate kinase;

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

K+ sp R4N.X 25°C 0.10M U K'=0.92 1966SSc (108403)1454

Medium: Me4NCl. See reference for definitions

Polymer (1966)
poly(Benzo-1,4,7,10,13,16-hexaoxacyclooctadecane)

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

K+ sp non-aq 25°C 100% U K1=8.39 1979KMb (108425)1455

Medium: CHCl3

Polymer (1965)
poly(Benzo-1,4,7,10,13-pentaoxacyclopentadecane)

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

K+ sp non-aq 25°C 100% U K1=10.3 1979KMb (108429)1456

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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