

## SC-Database

Software version = 5.81 Data version = 4.62

Experiment list contains 717 experiments for

(no ligands specified)

Metal : Cs+

(no references specified)

(no experimental details specified)

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e- HL Electron (442)  
Electron;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Cs+	EMF	mixed	25°C	10%	U	I		1974DKb K(Cs+e=Cs/Hg)=-49.24(-2.913V)	(437)	1
Medium: 10% w/w DMSO/H2O; K=-49.04(-2.901V,w=20), -48.53(-2.871V,w=40), -47.72(-2.823V,w=60)										
Cs+	oth	oth/un	25°C	0.0	U	I		1972C0a K(Cs+e=Cs(s))=-49.34(-2.919V)	(438)	2
Method: Estimated. MeOH: -51.83((-3.066V).EtOH: -51.83(-3.066V).BuOH: -50.73(-3.001V).PentOH: -50.36(-2.979V).Me2CO: -50.36(-2.979V)										
Cs+	oth	oth/un	25°C	0.0	U	I		1972C0a K(Cs+e=Cs(s))=-49.34(-2.919V)	(439)	3
Method: Estimated. MeCN: -55.85(-3.304V).HCOOH: -59.89(-3.543V). Also NH3,N2H4										
Cs+	con	non-aq	-65°C	100%	U	T		1972DBa K(Cs + e(solv))=2.71 K(2Cs=Cs2)=1.34	(440)	4
Medium: NH3(liquid). K=2.55, Kd=1.82(-45 C); K=2.41, Kd=2.11(-34 C) Methods: conductivity and magnetic susceptibility										
Cs+	EMF	none	25°C	0.00	U	T		1972MLb K=-32.966 (-1950.2V)	(441)	5
K:Cs+e=Cs(Hg); x(Cs) to 0;K=-34.169(-1.91965V,10 C), -31.854(-1.97922V,40 C), -30.820(-2.00671V,55 C), -29.896(-2.03548V,70 C)										
Cs+	EMF	mixed	25°C	50%	U	I		1971KRb K(Cs+e=Cs(s))=-49.14(-2.907V)	(442)	6
Medium: 50% w/w ethylene glycol/H2O; K=-50.61(-2.994V,w=100)										
Cs+	EMF	none	25°C	0.00	U			1970KGa K(Cs+e=Cs/Hg))=-31.09(-1.839V)	(443)	7
Cs+	con	non-aq	-65°C	100%	U	T		1969DEc K(Cs + e(solv)=Cs)=2.66	(444)	8
Medium: NH3(liquid); K=2.48(-45 C), 2.31(-34 C)										

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 Cs+ EMF non-aq 25°C 100% U 1966LCa (445) 9  
 $K' = -50.49, -2987 \text{ mV}$   
 Medium: CH<sub>3</sub>NHCHO.  $K': \text{Cs} + \text{Cl} + \text{Ag(s)} = \text{Cs(s)} + \text{AgCl(s)}$   
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Cs+ EMF none 25°C 0.0 U T 1939BFa (446) 10  
 $K(\text{Cs+e}) = -49.43(-2923 \text{ mV})$   
 $K = -54.49(0 \text{ C}; -2952), -53.40(5 \text{ C}; -2946 \text{ mV}), -52.35(10 \text{ C}; -2940 \text{ mV}), -51.35(15 \text{ C}; -2935 \text{ mV}), -50.36(20 \text{ C}; -2928 \text{ mV}), -48.46(30 \text{ C}; 2914 \text{ mV})$   
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B04H4- HL Borate CAS 10043-35-3 (991)  
 Borate; B(OH)<sub>4</sub>-  
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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	sp	oth/un	25°C	1.00M	U I		$K_1 = 0.45$	1990RAa (1305)	11

Medium: CsCl. Data at I=0 M and pressures to 2041 atmos.  
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Br- HL Bromide CAS 10035-10-6 (19)  
 Bromide;  
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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	con	non-aq	25°C	100%	U T		$K_1 = 2.57$	1993TAa (1875)	12

Medium: 2-methoxyethanol, -10 to 80 C  
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Cs+	con	diox/w	25°C	?	U		$K_1 = -0.158$	1975MFa (1876)	13
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Data for dioxan/H<sub>2</sub>O solution with a dielectric constant of 78.35  
 Further data available for solutions with varying dielectric constants  
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Cs+	con	none	25°C	0.0	U		$K_1 = -0.84$	1971HPa (1877)	14
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Cs+	con	none	25°C	0.0	U		$K_1 = -0.4$	1971PJa (1878)	15
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Cs+	con	diox/w	25°C	40%	U I		$K_1 = 0.74$	1971TJa (1879)	16
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Medium: 40% w/w dioxan/H<sub>2</sub>O.  $K_1 = 1.75(60\%), 2.42(70\%), 4.03(82.8\%)$   
 In THF/H<sub>2</sub>O:  $K_1 = -0.92(15\%), 0.07(30\%), 0.95(50\%), 2.00(70\%), 2.70(80\%), 3.90(90\%)$   
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Cs+	con	non-aq	25°C	100%	U		$K_1 = 0.39$	1970CDa (1880)	17
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Medium: DMSO  
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Cs+	con	oth/un	25°C	0.0	U		$K_1 = 0.03$	1968HFa (1881)	18
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Cs+	sol	non-aq	25°C	100%	U I		$K_{so} = -0.29$	1967AKa (1882)	19
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Medium: HCONH<sub>2</sub>. In DMF:  $K_{so} = -3.3$   
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Cs+	con	non-aq	25°C	100%	U		$K_1 = 3.36$	1965BFb (1883)	20
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Medium: diaminoethane  
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BrO3- HL Bromate (6017)  
Bromate;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	con	none	25°C	0.0	U		K1=-0.06	1971JBa (2408)	21
Cs+	con	none	25°C	0.0	U		K1=0.00	1969BJa (2409)	22

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	EMF	oth/un	25°C		U		K1=2.72	1969NSa (3562)	23

Assuming K(Cs+Fe(CN)6)=1.30

Cs+	oth	none	25°C	0.0	U		K1=2.85	1966NSa (3563)	24
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Method: transport number  
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C6N6Fe--- H3L Ferricyanide (2491)  
Hexacyanoferrate (III); Fe(III)(CN)6---

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	sol	oth/un	25°C	3.0M	U		K1=0.52	1967RMd (3638)	25

Medium: LiNO3

Cs+	sol	oth/un	25°C	3.0M	U		K1=0.52	1967RMd (3639)	26
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Medium: LiNO3

Cs+	sol	oth/un	25°C	3.0M	U		K1=-0.26	1966MRb (3640)	27
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Medium: LiCl  
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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
Cs+	con	oth/un	25°C	0.00	U		K1=1.71	1976LLa (3702)	28

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	con	mixed	25°C	15%	U	I	K1=-0.03	1974RJa (4718)	29

In 15.1% w/w 1,2-dimethoxyethane/H2O; K1=-0.31(0%), 0.34(30.9%), 0.67(36.7%), 1.04(50.0%), 1.42(60.0%), 2.60(79.9%), 3.06(84.8%). Also in THF and dioxan/H2O

Cs+	con non-aq	25°C	100%	U	I	K1=1.94	1973SAb	(4719)	30
Medium: 29.3% w/w dioxan/MeOH. K1=1.26(0%), 2.70(45.2%), 3.08(52.6%), 3.87(62.3%)									
Cs+	con non-aq	25°C	100%	U		K1=1.7	1971ENa	(4720)	31
Medium: trifluoroethanol. K1=1.63 to 1.88									
Cs+	con non-aq	25°C	100%	U		K1=0.02	1971PGa	(4721)	32
Medium: N-methylformamide									
Cs+	con none	25°C	0.0	U		K1=-0.4	1971PJa	(4722)	33
Cs+	con mixed	25°C	10%	U	I	K1=0.71	1970BKb	(4723)	34
Medium: 10.1% t-butanol/H2O. K1=0.85(14.8%), 1.15(19.7%)									
Cs+	con non-aq	25°C	100%	U		K1=0.48	1970CDa	(4724)	35
Medium: DMSO									
Cs+	con non-aq	25°C	100%	U	I	K1=1.20	1970SAf	(4725)	36
Medium: 9.57% w/w butanol/MeOH. K1=1.27(19.7%), 1.47(39.8%), 1.53(51.4%)									
Cs+	con non-aq	25°C	100%	U	I	K1=2.26	1968PIb	(4726)	37
Medium: 48.1% w/w EtOH/acetone. K1=2.13(65.5%), 2.11(82.7%), 2.14(91.6%), 2.19(100%)									
Cs+	sol non-aq	25°C	100%	U			1967AKa	(4727)	38
						Kso=-0.53			
Medium: formamide. Kso=-4.9 in DMF									
Cs+	oth oth/un	25°C	0.0	U		K1=-0.1	1966MBb	(4728)	39
Cs+	con alc/w	25°C	40%	U	I	K1=0.48	1965HKa	(4729)	40
Medium: 40.4% EtOH. K1=1.26(73.9%), 1.83(91.3%), 2.20(100%)									
Cs+	con alc/w	25°C	100%	U		K1=1.2	1965KHb	(4730)	41
Medium: MeOH									
Cs+	con alc/w	25°C	100%	U		K1=0.95	1965KHb	(4731)	42
Medium: MeOH									
Cs+	con diox/w	25°C	48%	U	I	K1=1.23	1963JFa	(4732)	43
I=0 corr. K1=1.92(64.4% dioxan), 2.35(70.5%), 2.91(75.5%), 3.32(78.8%)									
Cs+	gl diox/w	25°C	70%	U		K1=2.57	1963PGb	(4733)	44
Cs+	oth none	25°C	0.0	U		K1=-0.04	1954GMb	(4734)	45
From activity coefficient, I=0 corr. In CsCl(var) K1=-0.45									
Cs+	oth none	18°C	0.0	U		K1=-0.50	1912NFa	(4735)	46

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Cl03- HL Chlorate CAS 7790-93-4 (971)  
Chlorate;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Cs+	con	none	25°C	0.0	C	I		K1=-0.02	1986SDa (6032)	47

Value derived from data for 0.001-0.05 self medium.

Cl04- HL Perchlorate CAS 7001-90-3 (287)  
Perchlorate;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Cs+	con	none	25°C	0.0	C	I		K1=0.23	1986SDa (6199)	48
Value derived from data for 0.001-0.05 self medium.										
Cs+	gl	non-aq	25°C	100%	U	H		K1=5.78	1981TMb (6200)	49
Medium: Glacial acetic acid. Alternative method: Spectrophotometry. DH(K1)=-13 kJ mol <sup>-1</sup>										
Cs+	con	non-aq	25°C	100%	U			K1=1.55	1978CAa (6201)	50
Medium: Acetonitrile										
Cs+	con	non-aq	25°C	100%	U			K1=1.5	1975YKa (6202)	51
Medium: MeCN										
Cs+	con	non-aq	25°C	100%	U			K1=0.92	1974HPb (6203)	52
Medium: hexamethylphosphotriamide. K1 by Pitts eqn. By Fuoss-Hsia: K1=1.28										
Cs+	con	non-aq	25°C	100%	U			K1=0.35	1973JYa (6204)	53
Medium: propene carbonate;0 corr. K1=0.3 to 0.4										
Cs+	con	alc/w	25°C	100%	U			K1=1.73	1972DAa (6205)	54
Medium: MeOH										
Cs+	con	non-aq	25°C	100%	U			K1=1.01	1971BCa (6206)	55
Medium: tetramethylurea										
Cs+	con	none	25°C	0.0	U			K1=0.23	1971DAa (6207)	56
Cs+	con	non-aq	25°C	100%	U			K1=0.46	1971PGa (6208)	57
Medium: N-methylformamide										
Cs+	con	mixed	25°C	30%	U	I		K1=2.42	1970PPb (6209)	58
Medium: 30.2% w/w acetone/EtOH. K1=2.25(54.7%), 2.24(61.4%), 2.19(74.1%), 2.35(100%)										
Cs+	sol	none	25°C	0.0	U				1969GUb (6210)	59
Kso=-2.38										

Cs+ con alc/w 25°C 100% U I K1=1.52 1968CPb (6211) 60  
Medium: MeOH. In MeCN: K1=1.36. Also values for mixtures

Cs+ dis oth/un 25°C 0.0 U Kd(Cs+L=Cs+L in MeNO2)=-1.74 1968HFb (6212) 61

Cs+ con non-aq 25°C 100% U K1=1.33 1967KHe (6213) 62  
Medium: MeCN

Cs+ con non-aq 25°C 100% U T K1=1.83 1966MWb (6214) 63  
Medium: MeCN, also at 20 C, 30 C

Cs+ con non-aq 25°C 100% U K1=2.16 1962MWa (6215) 64  
Medium: MeCN

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

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

Cs+ sp oth/un 25°C 1.0M U I K1=-0.16 1993MAa (6823) 65  
K1 values over a range of pressures and ionic strengths

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

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

Cs+ sol non-aq 25°C 100% U K1=-0.3 1967CKa (7592) 66  
Medium: MeCN

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

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

Cs+ nmr non-aq 75°C 100% U K1=5.41 1982KPb (7968) 67  
Medium: methylamine

Cs+ con non-aq 25°C 100% U I K1=0.48 1976RMb (7969) 68  
Medium: 1,3-Dimethylethyleneurea. In 1,3-Dimethylpropyleneurea K1=0.14

Cs+ con non-aq 25°C 100% U K1=2.45 1972IWa (7970) 69  
Medium: acetone

Cs+ con alc/w 25°C 93.7M U K1=1.72 1971BPb (7971) 70  
Medium: 93.7% w/w EtOH/H2O

Cs+ con non-aq 25°C 100% U K1=2.79 1971HNb (7972) 71  
Medium: propanol

Cs+	con none	25°C	0.0	U		K1=-0.97	1971HPa	(7973)	72
Cs+	con none	25°C	0.0	U		K1=-0.53	1971PJa	(7974)	73
Cs+	con alc/w	25°C	100%	U	I	K1=0.97	1970BWc	(7975)	74
Medium: MeOH; K1=2.00 in EtOH									
Cs+	con non-aq	25°C	100%	U		K1=0.12	1970CDa	(7976)	75
Medium: DMSO									
Cs+	con non-aq	25°C	100%	U	I	K1=1.15	1969SLa	(7977)	76
In 10% w/w dioxan-DMF. K1=1.54(20%), 1.72(30%), 2.00(40%), 2.07(45%), 2.45(50%), 2.66(55%), 3.04(60%), 3.44(65%), 4.00(70%), 4.60(75%), 5.42(80%)									
Cs+	con oth/un	25°C	0.0	U		K1=-0.03	1968HFa	(7978)	77
Cs+	sol non-aq	25°C	100%	U	I		1967AKa	(7979)	78
						Kso=-0.23			
Medium: H2NCHO. Kso=-1.7(DMF)									
Cs+	dis none	25°C	0.0	U			1967RMe	(7980)	79
						K(Cs+I=Cs(TBP)+I(TBP))=-1.70			
With (i-amylO)2MePO: Kd=-1.48									
Cs+	con non-aq	25°C	100%	U		K1=3.24	1965BFb	(7981)	80
Medium: diaminoethane									
Cs+	con diox/w	25°C	90%	U	I	K1=6.51	1962RSd	(7982)	81
K1=9.95(95.48% dioxan), 12.30(96.92%)									
*****									
I03-		HL	Iodate		CAS 7782-68-5 (1257)				
Iodate;									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	con none	25°C	0.0	U			K1=-0.11	1971JBa	(8507) 82
Cs+	con none	25°C	0.0	U			K1=-0.12	1969BJa	(8508) 83
*****									
I04-		HL	Periodate		CAS 13444-71-8 (6063)				
Periodate;									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	sol oth/un	40°C	0.0	U	T	H		1968KDb	(8599) 84
						Kso(CsI04)=-2.19			
Kso=-3.40(5 C), -2.65(25 C); DHso=54.8 kJ mol-1, DS=157.2 J K-1 mol-1									
*****									
IrCl6---		H3L	(1615)						

Hexachloroiridate;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	gl	oth/un	50°C	0.10M	U		K1=3.15	1978KSb (8621)	85
*****									
NO2-		HL		Nitrite			CAS 7782-77-6	(635)	
Nitrite;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	con	none	25°C	0.0	U		K1=-0.36	1964PSh (9367)	86
*****									
NO3-		HL		Nitrate			CAS 7697-37-2	(288)	
Nitrate;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	con	diox/w	25°C	62%	U	I	K1=4.06	1972SAc (9639)	87
Medium:Dioxan/MeOH. In 29.3% dioxan: K1=1.92. 45.2%: 2.80. 52.6%: 3.28									
Cs+	con	oth/un	25°C	0.0	U		K1=0.03	1971JBa (9640)	88
Cs+	con	oth/un	25°C	0.0	U		K1=0.02	1969BJa (9641)	89
Cs+	con	diox/w	25°C	62%	U	I	K1=1.54	1969SBe (9642)	90
In 55.7% dioxan: K1=1.08. 59.0%: 1.23. 68.4%: 2.06. 71.9%: 2.34. 74.9%: 2.63									
Cs+	oth	oth/un	25°C	0.0	U		K1=0.11	1937ROa (9643)	91
Method: Partial pressure of H2O. K1=0.04 to 0.18									
*****									
OH-		HL		Hydroxide			(57)		
Hydroxide;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	nmr	R4N.X	25°C	3.4M	C		K1=-0.8	2002PLa (11263)	92
NMR Cs-133 under assumption that substitution of Cl for OH does affect chemical shift, which is a rough approximation;Medium: 3.4 M Me4NCl/Me4NOH									
*****									
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
Cs+	gl	none	25°C	0.0	U	T	K1=2.3	1959WOa (13579)	93
K1=2.3(40 C)									
*****									
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
Cs+	gl	none	25°C	0.0	U	T		K1=2.8	1959W0a (13849)	94
K1=2.8(40 C)										
*****										
ReO4-			HL			Perrhenate		(2581)		
Rhenate(VII), Perrhenate;										
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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Cs+	sol	none	25°C	0.0	C				1988HHb (14096)	95
Kso(CsReO4)=-3.40										
Method: perrhenate ion selective electrode.										
*****										
SO4--			H2L			Sulfate		CAS 7664-93-9 (15)		
Sulfate;										
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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Cs+	ISE	R4N.X	25°C	1.0M	C			K1=-0.10	1999CHa (16132)	96
Method: Na ISE. Medium: 1.0 M Me4NCl. Estimated from study of Na-SO4 complexation in 0.50-7.00 M CsCl and 1.0 M Me4NCl.										
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Cs+	gl	NaCl	37°C	0.10M	C	I		K1=0.70	1982DRb (16133)	97
Data for I=0.03-0.50 M NaCl. At I=0.0 M, K1=1.04										
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Cs+	oth	oth/un	25°C	0.50M	U	TI		K1=0.60	1980GAb (16134)	98
Method: Ultrasonic absorption. Medium: Na2SO4										
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Cs+	con	none	25°C	0.0	U				1978FFa (16135)	99
K(Cs+CsSO4)=0.08										
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Cs+	sol	oth/un	25°C	0.70M	C			K1=0.39	1975EWa (16136)	100
Mixed medium of NaCl, KCl, MgCl2, NaClO4, Mg(ClO4)2, Na2SO4, CsCl.										
Method: solubility of gypsum.										
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Cs+	oth	oth/un	25°C	0.28M	U			K1=0.33	1975REa (16137)	101
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Cs+	sp	oth/un	20°C	2.30M	U	M			1971GFa (16138)	102
K(Cs2L+TiOL)=-0.5										
Medium: H2SO4										
*****										
TcO4-			HL					CAS 13568-38-2 (1418)		
Pertechnetiate;										
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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Cs+	con	none	18°C	0.0	U			K1=0.64	1963SKa (17247)	103
*****										

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
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Cs+	gl	R4N.X	20°C	0.10M	U				1963SGd (17378)	104
								K(Cs+H15L10)=2.20		
								K(Cs+H14L10)=3.18		

\*\*\*\*\*  
CH606P2 H4L Medronic acid CAS 1984-15-2 (2384)  
Methanediphosphonic acid; CH2(P03H2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Cs+	gl	R4N.X	25°C	0.50M	U			K1=0.84	1967CIa (18277)	105
								K(Cs+HL)=0.04		

Medium: Me4NCl

\*\*\*\*\*  
C2H402 HL Acetic acid CAS 64-19-7 (36)  
Ethanoic acid; CH3.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Cs+	gl	oth/un	25°C	0.0	M T			K1=0.00	2001RFa (19933)	106
Calculated from data for 0.01 m NaOH/0.02 m HL. Data for 25-175 C.										

Cs+	gl	R4N.X	25°C	0.16M	U I			K1=-0.33	1985RSa (19934)	107
K1=-0.29 (I=0.04); -0.33 (0.25); -0.29 (0.49); -0.18 (1.00)										

Cs+	gl	non-aq	25°C	100%	U H			K1=6.04	1981TMb (19935)	108
Medium: Glacial acetic acid. Alternative method: Spectrophotometry. DH(K1)=-18.0 kJ mol-1										

Cs+	sp	non-aq	25°C	100%	U			K1=6.78	1961PSa (19936)	109
Medium: ethanoic acid										

\*\*\*\*\*  
C2H60 L Ethanol CAS 64-17-5 (1913)  
Ethanol; CH3.CH2.OH

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

Cs+	cal	oth/un	25°C	0.10M	U H				1975BBa (22026)	110
DH=-403.8 kJ mol-1 in H2SO4										

\*\*\*\*\*  
C2H602 L Ethyleneglycol CAS 107-21-1 (924)  
1,2-Dihydroxyethane (Ethane-1,2-diol); HO.CH2.CH2.OH

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

Cs+	nmr	oth/un	20°C	0.0	C			K1=1.36	1989GSc (22142)	111
-----	-----	--------	------	-----	---	--	--	---------	-----------------	-----

Method: 1H and 133Cs pulsed gradient spin-echo nmr. Medium: D2O.

\*\*\*\*\*

C2H8O6P2 H4L CAS 6145-33-1 (3543)

Ethane-1,1-diphosphonic acid; CH3.CH(P03H2)2

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

Cs+ gl R4N.X 25°C 0.50M U K1=1.02 1967CIa (23266) 112  
K(Cs+HL)=0.09

Medium: Me4NCl

\*\*\*\*\*

C2H8O7P2 H4L HEDPA CAS 2809-21-4 (436)

1-Hydroxyethane-1,1-diphosphonic acid; CH3.C(OH)(P03H2)2

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

Cs+ gl R4N.X 25°C 0.50M U K1=1.6 1967CIa (23362) 113  
K(Cs+HL)=0.24

Medium: Me4NCl

\*\*\*\*\*

C2H9N06P2 H4L IDPA CAS 32545-63-4 (1335)

Imino-N,N-bis(methylenephosphonic acid); HN(CH2P03H2)2

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

Cs+ nmr R4N.X 25°C 1.0M C K1=1.0 2003PPa (23452) 114

Method: NMR Cs-133; in 1 M Me4NCl/Me4NOH

\*\*\*\*\*

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  
-----

Cs+ gl R4N.X 25°C 0.50M U K1=1.40 1967CIa (28399) 115  
K(Cs+HL)=0.35

Medium: Me4NCl

\*\*\*\*\*

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

2-Hydroxybutane-1,4-dioic acid, Hydroxy-succinic acid; H00C.CH2.CH(OH).C00H

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

Cs+ ISE oth/un 25°C 0.10M U K1=-0.15 1964RZa (30609) 116

Cs+ gl R4N.X ? 0.28M U K1=-0.1 1963EDa (30610) 117

Medium: Me4NBr

\*\*\*\*\*

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
Cs+	con	non-aq	25°C	100%	U		K1=2.43	1974ESa (34657)	118

Medium: DMSO

\*\*\*\*\*

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
-------	-----	--------	------	------	-----	-------	-------------	-----------	--------

Cs+	gl	diox/w	30°C	75%	U		K1=7.32 B2=11.73	1975MMa (37936)	119
-----	----	--------	------	-----	---	--	------------------	-----------------	-----

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C6H3N3O7		HL	Picric acid				CAS 88-89-1	(593)	
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2,4,6-Trinitrophenol; HO.C6H2(NO2)3

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

Cs+	dis	non-aq	25°C	100%	C		K1=3.06	1999KKb (42102)	120
-----	-----	--------	------	------	---	--	---------	-----------------	-----

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

Cs+	dis	oth/un	25°C	dil	C			1998TKa (42103)	121
-----	-----	--------	------	-----	---	--	--	-----------------	-----

K(CsA+L)=4.49

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

Cs+	con	none	30°C	0.0	U	I M	K1=1.44	1979PSa (42104)	122
-----	-----	------	------	-----	---	-----	---------	-----------------	-----

Cs+	dis	none	25°C	0.00	U	I	K1=2.07	1972Iwc (42105)	123
-----	-----	------	------	------	---	---	---------	-----------------	-----

In nitrobenzene: K1=2.43

Cs+	con	none	25°C	0.00	M		K1=2.07	1971YIa (42106)	124
-----	-----	------	------	------	---	--	---------	-----------------	-----

Cs+	dis	oth/un	25°C	var	U		K1=2.7	1970SSb (42107)	125
-----	-----	--------	------	-----	---	--	--------	-----------------	-----

Method: paper chromatography

\*\*\*\*\*

C6H8O7		H3L	Citric acid				CAS 77-92-9	(95)	
--------	--	-----	-------------	--	--	--	-------------	------	--

2-Hydroxypropane-1,2,3-tricarboxylic acid; HOOCCCH2.CH(OH)(COOH).CH2COOH

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

Cs+	gl	KCl	37°C	0.15M	C		K1=0.47 B2=0.07	1981CDb (46067)	126
-----	----	-----	------	-------	---	--	-----------------	-----------------	-----

Cs+	ISE	oth/un	25°C	0.10M	U		K1=0.32	1964RZa (46068)	127
-----	-----	--------	------	-------	---	--	---------	-----------------	-----

\*\*\*\*\*

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Cs+ sp R4N.X 25°C 0.10M C T K1=0.09 1985HAd (46762) 128  
 \*\*\*\*\*  
 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
-------	-----	--------	------	------	-----	-------	-------------	-----------	--------

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Cs+	gl	R4N.X	25°C	0.10M	U		K1=2.51 B(CsHL)=11.32 B(CsH2L)=17.87 B(Cs2L)=2.94 B(CsHL2)=12.19	1991BSa (51534)	129
-----	----	-------	------	-------	---	--	--	-----------------	-----

\*\*\*\*\*  
 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
-------	-----	--------	------	------	-----	-------	-------------	-----------	--------

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Cs+	con	non-aq	25°C	100%	U		K1=1.80	1989KSa (51769)	130
-----	-----	--------	------	------	---	--	---------	-----------------	-----

Medium: tetrahydrofuran/CHCl3 4:1 (vol)

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Cs+	con	non-aq	25°C	100%	U		K1=1.8	1982YSa (51770)	131
-----	-----	--------	------	------	---	--	--------	-----------------	-----

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

\*\*\*\*\*  
 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
-------	-----	--------	------	------	-----	-------	-------------	-----------	--------

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Cs+	con	alc/w	25°C	100%	U		K1=<-0.3	1980OPa (52214)	132
-----	-----	-------	------	------	---	--	----------	-----------------	-----

Medium: MeOH, 0.1 M Me4NBr

\*\*\*\*\*  
 C8H11O2F3 HL CAS 22767-90-4 (1249)  
 1,1,1-Trifluoro-5,5-dimethyl-2,4-hexanedione; F3C.CO.CH2.CO.CH(CH3)3

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

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Cs+	oth	diox/w	25°C	75%	U		K1=3.10 B2=6.99	1979MMa (61301)	133
-----	-----	--------	------	-----	---	--	-----------------	-----------------	-----

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

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

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Cs+	cal	non-aq	25°C	100%	C H		K1=0.56 B2= 1.16	1996OKa (62664)	134
-----	-----	--------	------	------	-----	--	------------------	-----------------	-----

Medium: DMF, 0.10 M Et4NCl. DH(K1)=-16.7 kJ mol<sup>-1</sup>, DS(K1)=-45 J K<sup>-1</sup> mol<sup>-1</sup>;  
 DH(K2)=5, DS(K2)=28.

---

Cs+	con	non-aq	25°C	100%	U		K1=2.5	1993EVa (62665)	135
-----	-----	--------	------	------	---	--	--------	-----------------	-----

Medium: THF+CHCl3 (4:1 vol)

-----  
Cs+ con non-aq 25°C 100% C K1=1.60 B2= 2.34 1987ZBb (62666) 136  
Medium: MeOH.  
-----

Cs+ vlt non-aq 25°C 100% U K1=1.43 1980MDa (62667) 137  
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  
-----

Cs+ con non-aq 25°C 100% U I K1=1.8 1993EVa (62983) 138  
Medium: THF+CHCl3 4:1(vol). In 100% THF: K1=1.8  
-----

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

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

Cs+ nmr oth/un 20°C 0.0 C K1=3.25 1989GSc (63002) 139  
Method: 1H and 133Cs pulsed gradient spin-echo nmr. Medium: D2O.  
-----

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

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

Cs+ EMF non-aq 25°C 100% U I K1=2.78 1996WPa (63291) 140  
Medium: acetonitrile, 0.05 M NEt4ClO4. In dimethylformamide K1<2  
-----

\*\*\*\*\*  
C8H20O4P2 L CAS 86536-56-3 (2076)  
1,2-Bis(2-dimethylphosphinylmethoxy)ethane; Me2P(O)CH2.O.CH2.CH2.O.CH2.P(O)Me2  
-----

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

Cs+ con non-aq 25°C 100% U K1=2.45 1989KSa (63309) 141  
Medium: tetrahydrofuran/CHCl3 4:1 (vol)  
-----

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

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

Cs+ oth diox/w 25°C 75% U K1=3.54 B2=7.17 1979MMa (66534) 142  
-----

\*\*\*\*\*  
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  
-----

-----  
Cs+ gl diox/w 30°C 75% U K1=4.12 B2=7.80 1975MMA (67743) 143

\*\*\*\*\*

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

-----  
Cs+ con alc/w 25°C 100% U K1=<-0.3 19800Pa (67966) 144

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

-----  
Cs+ con non-aq 22°C 100% U K1=0.90 1981SKd (68121) 145

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

-----  
Cs+ gl none 25°C 0.0 C 1990CDc (68510) 146

Kso(CsH3L)=-18.4

Additional technique: spectrophotometry.

\*\*\*\*\*

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

-----  
Cs+ oth diox/w 25°C 75% U K1=3.52 B2=7.36 1979MMA (71107) 147

\*\*\*\*\*

C10H16N2O8 H4L EDTA CAS 60-00-4 (120)

1,2-Diaminoethane-N,N,N',N'-tetraethanoic acid, Sequestic acid;

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

-----  
Cs+ gl oth/un 25°C 0.32M U T K1=0.15 1965BCa (73685) 148

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

-----  
Cs+ gl R4N.X 25°C 0.10M C T K1=1.06 1991SMa (74710) 149

IUPAC evaluation

Cs+	gl	oth/un	25°C	0.25M	U	H	K1=1.19 B(CsHL)=6.66	1986RSa (74711)	150
-----									
Cs+	gl	oth/un	25°C	0.32M	U		K1=0.9 B2=0.90 K(Cs+HL) < -0.3	1965BCa (74712)	151
Medium: CsCl									
*****									
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
-----									
Cs+	ISE	alc/w	25°C	100%	C	I T	K1=2.69 B2= 4.49	2003ADa (75982)	152
IUPAC Tentative. Medium: 0-0.1 M various. DH(K1)=-32.9 kJ mol-1									
In H2O: K1=0.8, DH(K1)=-5.4									
-----									
Cs+	con	non-aq	25°C	100%	C	H	K1=2.72 B2= 3.83	1999WBa (75983)	153
Medium: N,N-dimethylformamide. By calorimetry: DH(K1)=-19.2 kJ mol-1, DH(K2)=-18.5 kJ mol-1.									
-----									
Cs+	vlt	non-aq	25°C	100%	C	I	K1=3.2	1999WKb (75984)	154
Medium: acetonitrile, 0.10 M Et4NClO4. Also data for TMS, propylene carbonate, acetone, formamide, DMF, DMA, DMSO, MeOH, EtOH.									
-----									
Cs+	nmr	non-aq	RT	100%	U		K1=1.88	1996GMc (75985)	155
Method: 133Cs nmr. Medium: N,N-dimethylformamide									
-----									
Cs+	cal	non-aq	25°C	100%	M	H	K1=3.68	1994BCd (75986)	156
Medium: acetone. DH(K1)=-19.4 kJ mol-1, TDS=1.5									
-----									
Cs+	nmr	non-aq	25°C	100%	U		K1=2.88	1991SKa (75987)	157
Medium: MeCN									
-----									
Cs+	cal	non-aq	25°C	100%	C	H	K1=3.11	1988BUb (75988)	158
Medium: acetonitrile. DH(K1)=-27.7 kJ mol-1, DS(K1)=-33.6 J K-1 mol-1.									
-----									
Cs+	con	non-aq	25°C	100%	C	T	K1=3.1	1988TKa (75989)	159
Medium: MeCN									
-----									
Cs+	ISE	alc/w	25°C	90%	U		K1=2.10	1987KHa (75990)	160
Medium: 90% w/w MeOH/H2O									
-----									
Cs+	con	non-aq	25°C	100%	C	I	K1=2.78 B2= 4.52	1987ZBb (75991)	161
Medium: MeOH. In 70% w/w MeOH/H2O, K1=2.49, K2=1.48.									
-----									
Cs+	cal	alc/w	25°C	100%	U	H T	K1=2.18	1980LIa (75992)	162
Medium: MeOH. DH=-49.0 kJmol-1.									
-----									
Cs+	dis	non-aq	25°C	100%	U		K1=2.6	1980TYa (75993)	163



Medium: propylene carbonate

-----  
Cs+ EMF oth/un 25°C var C T K1=0.79 1979HRa (75994) 164  
Method: ISE based on cation exchange membrane. Medium: aqueous,  
containing 0.06-0.25 m ligand.  
-----

Cs+ cal oth/un 25°C 0.10M U H T K1=0.8 1976ITb (75995) 165  
DH=-5.40 kJ mol<sup>-1</sup>.

\*\*\*\*\*  
C10H22O5 L Tetraglyme CAS 143-24-8 (121)  
2,5,8,11,14-Pentaoxapentadecane; (CH<sub>3</sub>.O.CH<sub>2</sub>.CH<sub>2</sub>.O.CH<sub>2</sub>.CH<sub>2</sub>.)<sub>20</sub>  
-----

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Cs+	dis	non-aq	25°C	100%	C			K1=3.85	1998KSc (76442)	166
Medium: 1,2-dichloroethane.										

-----  
Cs+ con non-aq 25°C 100% U I K1=2.6 1993EVa (76443) 167  
Medium: THF+CHCl<sub>3</sub> 4:1(vol). In 100% THF: K1=2.5  
-----

Cs+ con alc/w 25°C 100% U K1=1.45 1975CJa (76444) 168  
Medium: MeOH

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Cs+	oth	R4N.X	25°C	0.50M	U			K(Cs+H <sub>2</sub> L)=0.71	1971CSb (79272)	169

Method: polarimetry. Medium: Me<sub>4</sub>NOH

\*\*\*\*\*  
C11H20O2 HL Dipivaloylmeth. CAS 1118-71-4 (363)  
2,2,6,6-Tetramethyl-3,5-heptanedione; (CH<sub>3</sub>)<sub>3</sub>C.CO.CH<sub>2</sub>.CO.C(CH<sub>3</sub>)<sub>3</sub>  
-----

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Cs+	gl	diox/w	30°C	75%	U			K1=3.86	1975MMa (79746)	170

\*\*\*\*\*  
C11H22O5 L 16-Crown-5 CAS 55477-28-8 (1592)  
1,4,7,10,13-Pentaoxacyclohexadecane; cyclo(-(O.CH<sub>2</sub>.CH<sub>2</sub>)<sub>5</sub>.CH<sub>2</sub>.CH<sub>2</sub>-)  
-----

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Cs+	dis	none	25°C	0.0	C	M			1989TKc (79851)	171
Method: extraction of metal picrate/L from H <sub>2</sub> O into benzene. K(Cs+HA(org))+L(org)=CsAL(org)+H)=-1.49. HA is picric acid.										

-----  
Cs+ con non-aq 25°C 100% C I K1=2.4 1988TKa (79852) 172  
Medium: MeCN. In propylene carbonate K1=2.2; in MeOH 2.1

\*\*\*\*\*  
 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
Cs+		dis non-aq	25°C	100%	C		K1=4.11	1998KSc (80071)	173

Medium: 1,2-dichloroethane.

Cs+		dis oth/un	25°C	var	U		K1=2.1	1970SSb (80072)	174
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Method: paper chromatography

\*\*\*\*\*  
 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
Cs+		oth R4N.X	25°C	0.50M	U		K(Cs+H2L)=1.0	1973CSa (82289)	175

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
Cs+		con non-aq	25°C	100%	U		K1=2.32	1982YSa (82640)	176

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
Cs+		cal alc/w	25°C	100%	U	H	K1=2.55	1980LIb (82651)	177

Medium: MeOH. DH=-6.36 kJ mol<sup>-1</sup>.

\*\*\*\*\*  
 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
Cs+		oth diox/w	25°C	75%	U		K1=3.57 B2=7.27	1979MMa (82857)	178

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Cs+ gl oth/un 26°C 0.00 U 1976HYa (83111) 179  
B(CsHL2)=9.85

\*\*\*\*\*

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  
-----

Cs+ nmr non-aq RT 100% U K1=0 1996GMc (83134) 180

Method: 133Cs nmr. Medium: N,N-dimethylformamide

-----  
Cs+ nmr non-aq 25°C 100% U K1=1.75 1991SKa (83135) 181

In acetonitrile.

-----  
Cs+ nmr non-aq 25°C 100% U M 1981RPa (83136) 182

K(CsNCS+L)=1.16

Medium: MeNO2. K(CsNCS+L)=0 in DMSO; 0.56 in DMF; 0.61 in acetone;

0.97 in MeCN; 0.96 in propylene carbonate

\*\*\*\*\*

C12H24O4S2 L (6528)

7,10,13,16-Tetraoxa-1,4-dithiacyclooctadecane;

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

Cs+ nmr non-aq 25°C 100% U K1=0.98 1991SKa (83149) 183

In acetonitrile.

\*\*\*\*\*

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  
-----

Cs+ ISE alc/w 25°C 100% C IH T K1=4.6 B2= 6.66 2003ADa (83312) 184

IUPAC Tentative. Medium: 0-0.1 M various. DH(K1)=-47.2 kJ mol-1

In H2O: K1=0.96, DH(K1)=-17. In PC K1=4.50, DH(K1)=-43

-----  
Cs+ dis non-aq 25°C 100% U K1=7.96 B2=10.54 2000KSa (83313) 185

Medium: 1,2-dichloroethane

-----  
Cs+ con non-aq 25°C 100% C T H K1=4.49 2000SSc (83314) 186

Medium: acetonitrile. Data for 15-45 C. DH(K1)=-16 kJ mol-1,

DS(K1)=33 J K-1 mol-1.

-----  
Cs+ cal non-aq 25°C 100% C H K1=3.62 1999WBa (83315) 187

Medium: N,N-dimethylformamide. DH(K1)=-48.4 kJ mol-1.

-----  
Cs+ dis non-aq 25°C 100% C I 1998TKa (83316) 188

K(Cs+A+L(org))=CsAL(org))=5.52

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.

-----  
 Cs+ nmr non-aq RT 100% U K1=3.42 B2= 4.65 1996GMc (83317) 189  
 Method: 133Cs nmr. Medium: N,N-dimethylformamide  
 -----

Cs+ cal alc/w 25°C 80% C H K1=3.40 1995KZa (83318) 190  
 Medium: 80% v/v CH3OH/H2O. DH(K1)=-27.7 kJ mol<sup>-1</sup>, DS(K1)=-28 J K<sup>-1</sup> mol<sup>-1</sup>  
 -----

Cs+ cal non-aq 25°C 100% U IH T K1=4.29 1995OKb (83319) 191  
 Medium: Acetonitrile, 0.1 M Et4NClO4. DH(K1)=-19 kJ mol<sup>-1</sup>  
 IN propylene carbonate K1=4.49, DH(K1)=-44  
 -----

Cs+ cal non-aq 25°C 100% M H K1=4.51 1994BCd (83320) 192  
 Medium: acetone. DH(K1)=-52.8 kJ mol<sup>-1</sup>, TDS=-27.2  
 -----

Cs+ cal non-aq 25°C 100% U H T K1=3.64 199400a (83321) 193  
 Medium: DMF, 0.1 M Et4NClO4. DH(K1)=-50.0 kJ mol<sup>-1</sup>, DS=-98 J K<sup>-1</sup> mol<sup>-1</sup>  
 -----

Cs+ dis non-aq 25°C 100% U B(CsPL)=5.17 1993INa (83322) 194  
 -----

K is the equilibrium constant for extraction of the metal picrate (P) into  
 CH2Cl2. For extraction from D2O, B=5.17.  
 -----

Cs+ con oth/un 25°C 0.05M M K1=4.37 1992BUb (83323) 195  
 K1=4.44 (by calorimetry)  
 -----

Cs+ cal R4N.X 25°C 0.10M C H K1=0.92 19920Ia (83324) 196  
 DH(K1)=-19.3 kJ mol<sup>-1</sup>, DS=-47 J K<sup>-1</sup> mol<sup>-1</sup>  
 -----

Cs+ ix none 25°C 0.0 U I K1=2.9 1991BMb (83325) 197  
 Ligand bound to silica gel. In acetone, K=3.7  
 -----

Cs+ nmr non-aq 25°C 100% U K1=>4 K2=1.37 1991SKa (83326) 198  
 Medium: MeCN  
 -----

Cs+ oth non-aq 25°C 100% C K1=2.63 1989BBh (83327) 199  
 Method: FABMS. Medium: glycerol.  
 -----

Cs+ nmr oth/un 20°C 0.0 C K1=8.35 1989GSc (83328) 200  
 Method: 1H and 133Cs pulsed gradient spin-echo nmr. Medium: D2O.  
 -----

Cs+ cal non-aq 25°C 100% C H K1=5.07 1988BUb (83329) 201  
 Medium: acetonitrile. DH(K1)=-15.6 kJ mol<sup>-1</sup>, DS(K1)=39.6 J K<sup>-1</sup> mol<sup>-1</sup>.  
 -----

Cs+ ISE alc/w 25°C 90% U K1=3.49 1987KHa (83330) 202  
 Medium: 90% w/w MeOH/H2O  
 -----

Cs+ nmr non-aq 25°C 100% U K1=4.03 1985BPa (83331) 203  
 Medium: DMF. In MeCN: K1=4.83  
 -----

Cs+ con alc/w 25°C 100% U K1=4.49 1983LSa (83332) 204  
 -----

Medium: MeOH

-----  
Cs+ nmr oth/un 25°C ? U K1=4.03 1982KPa (83333) 205  
-----

Cs+ cal alc/w 25°C 100% U H T K1=4.79 B2=6.85 1980LIa (83334) 206  
Medium: MeOH. DH(K1)=-47.2 and DH(K2)=-13.9 kJ mol<sup>-1</sup>.  
-----

Cs+ dis non-aq 25°C 100% U K1=4.4 1980TYa (83335) 207  
Medium: propylene carbonate  
-----

Cs+ EMF oth/un 25°C var C T K1=0.98 1979HRa (83336) 208  
Method: ISE based on cation exchange membrane. Medium: aqueous,  
containing 0.06-0.25 m ligand.  
-----

Cs+ nmr non-aq 24°C 100% U T H K1=5.00 B2=6.90 1977MDa (83337) 209  
Medium: pyridine. DH(K2)=-24.2 kJ mol<sup>-1</sup> (25 C). 12 C: K1=6.00, K2=2.10;  
-1 C: 6.00, 2.30; -18 C: 6.00, 2.60; -29 C: 6.00, 2.8; -38 C: 6.70, 3.1  
-----

Cs+ nmr non-aq 25°C 100% U I K2=1.87 1977MPa (83338) 210  
K1>5.7  
Medium: pyridine. K1>5.30, K2=1.53 in acetone; 3.95, 0.38 in DMF; 4.17, 1.04  
in PC; >4.0, 0.57 in MeCN; K1=3.04 in DMSO  
-----

Cs+ cal alc/w 25°C 70% U H K1=2.84 1976ITa (83339) 211  
Medium: 70% w/w MeOH/H<sub>2</sub>O. DH(K1)=-33.8 kJ mol<sup>-1</sup>.  
-----

Cs+ cal oth/un 25°C 0.10M U H T K1=0.99 1976ITb (83340) 212  
DH=-15.9 kJ mol<sup>-1</sup>.  
-----

Cs+ kin none 25°C 0.0 U K1=3.2 1976LFa (83341) 213  
-----

Cs+ ISE alc/w 25°C 100% A K1=4.62 B2=5.92 1971FRa (83342) 214  
Medium: MeOH. In H<sub>2</sub>O: K1=0.8  
-----

\*\*\*\*\*  
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  
-----

Cs+ nmr non-aq RT 100% U K1=0.91 1996GMc (83823) 215  
Method: 133Cs nmr. Medium: N,N-dimethylformamide  
-----

Cs+ cal non-aq 25°C 100% M H K1=1.80 1994BCd (83824) 216  
Medium: acetone. DH(K1)=-23.9 kJ mol<sup>-1</sup>, TDS=-13.7  
-----

Cs+ nmr non-aq 25°C 100% U K1=2.29 1991SKa (83825) 217  
In acetonitrile.  
-----

Cs+ cal non-aq 25°C 100% U H K1=2.69 1986BUb (83826) 218  
In CH<sub>3</sub>CN. DH=-6.0 kJ mol<sup>-1</sup>

-----  
 Cs+ con non-aq 25°C 100% U K1=2.48 1980KMb (83827) 219  
 Medium: MeCN

\*\*\*\*\*  
 C12H26O6 L Pentaglyme CAS 1191-87-3 (2498)  
 2,5,8,11,14,17-Hexaoxaoctadecane; (CH3.O.CH2.CH2.O.CH2.CH2.O.CH2.)2  
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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Cs+	con	non-aq	25°C	100%	U		K1=3.4	1993EVa (83995)	220
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Medium: THF+CHCl3 (4:1 vol). Also data for other solvents

Cs+	cal	oth/un	25°C	0.05M	M		K1=1.76	1992BUb (83996)	221
-----	-----	--------	------	-------	---	--	---------	-----------------	-----

K1=1.72 (by conductivity)

Cs+	con	alc/w	25°C	100%	U		K1=1.85	1975CJa (83997)	222
-----	-----	-------	------	------	---	--	---------	-----------------	-----

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
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Cs+	EMF	non-aq	25°C	100%	C		K1=2.47	1997WVa (84086)	223
-----	-----	--------	------	------	---	--	---------	-----------------	-----

Medium: MeOH, 0.05M Et4NClO4.  
 Method: Ag/Ag+ electrode; by competition with Ag+.

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Cs+	nmr	none	25°C	0	U	M		1996RSa (84408)	224
-----	-----	------	------	---	---	---	--	-----------------	-----

B(CsTmDOTP)=1.75  
 B(Cs2TmDOTP)=3.37  
 B(Cs3TmDOTP)=4.82  
 B(CsTmDOTPH)=9.18

B(CsTmDOTPH2)=16.02, B(Cs2TmDOTPH)=10.78, B(Cs3TmDOTPH)=12.22  
 mixed-metal complexes in the Cs(I)-Tm(III)-DOTP ternary system

Cs+	gl	R4N.X	25°C	0.10M	M			1990DSa (84409)	225
-----	----	-------	------	-------	---	--	--	-----------------	-----

B(CsH2L)=27.16  
 B(CsH3L)=36.22  
 B(CsH4L)=43.65

Medium: Me4NNO3

\*\*\*\*\*  
 C13H11NO L (6871)  
 Diphenylformamide; HCON(C6H5)2  
 -----

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

-----  
 Cs+ sp non-aq 25°C 100% U T H 1993KPa (85009) 226  
 $K(2CsH-1L=(CsH-1L)^2)=2.20$

Medium: HEF -15 to - 25 C.  $K=2.43(-15C)$   
 $DH=-8.4 \text{ kJ mol}^{-1}$ ;  $DS=16.7$ .

\*\*\*\*\*

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

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

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Cs+	con	non-aq	25°C	100%	C	I	$K1=2.40$	1992TFa (86469)	227
-----	-----	--------	------	------	---	---	-----------	-----------------	-----

Medium: acetonitrile. In propylene carbonate,  $K1=1.61$ .

-----  

Cs+	con	alc/w	25°C	100%	U		$K1=1.73$	1991IOa (86470)	228
-----	-----	-------	------	------	---	--	-----------	-----------------	-----

 Medium: MeOH

\*\*\*\*\*

C13H26O6 L 19-Crown-6 CAS 55471-27-7 (8943)  
 1,4,7,10,13,16-Hexaoxacyclononadecane;

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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Cs+	con	non-aq	25°C	100%	C	I	$K1=3.29$	2000TMB (86494)	229
-----	-----	--------	------	------	---	---	-----------	-----------------	-----

Medium: CH3CN. In other media,  $K1=2.92$  (propylene carbonate), 3.00 (MeOH), 1.89 (DMF), 1.54 (DMSO).

-----  

Cs+	con	oth/un	25°C	dil	C		$K1=0.71$	1999TMA (86495)	230
-----	-----	--------	------	-----	---	--	-----------	-----------------	-----

 Self medium (CsCl).

\*\*\*\*\*

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

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

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Cs+	dis	non-aq	24°C	100%	C			2002MRd (88248)	231
-----	-----	--------	------	------	---	--	--	-----------------	-----

$K(Cs+A+L)=4.65$

Medium: CDCl3. HA is picric acid.

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Cs+	con	non-aq	25°C	100%	C		$K1=3.00$	2000ICa (88249)	232
-----	-----	--------	------	------	---	--	-----------	-----------------	-----

 Medium: nitromethane.

-----  

Cs+	con	non-aq	25°C	100%	C	H	$K1=0.85$	1999WBA (88250)	233
-----	-----	--------	------	------	---	---	-----------	-----------------	-----

 Medium: N,N-dimethylformamide. By calorimetry:  $DH(K1)=-11.2 \text{ kJ mol}^{-1}$ ,  $DH(K2)=-9.8 \text{ kJ mol}^{-1}$ .

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Cs+	vlt	non-aq	25°C	100%	C	I	$K1=3.4$	1999WKB (88251)	234
-----	-----	--------	------	------	---	---	----------	-----------------	-----

 Medium: acetonitrile, 0.10 M Et4NClO4. Also data for TMS, propylene carbonate, acetone, formamide, DMF, DMA, DMSO, MeOH, EtOH.

-----  

Cs+	nmr	non-aq	RT	100%	U		$K1=1.24$	1996GMC (88252)	235
-----	-----	--------	----	------	---	--	-----------	-----------------	-----

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Method:  $^{133}\text{Cs}$  nmr. Medium: N,N-dimethylformamide

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Cs+	oth	oth/un	25°C	0	U	K1=2.30	19940Ua (88253)	236
-----	-----	--------	------	---	---	---------	-----------------	-----

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Cs+	nmr	non-aq	25°C	100%	U	K1=2.11	1991SKa (88254)	237
-----	-----	--------	------	------	---	---------	-----------------	-----

Medium: MeCN

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Cs+	cal	non-aq	25°C	100%	C H	K1=3.43	1988BUb (88255)	238
-----	-----	--------	------	------	-----	---------	-----------------	-----

Medium: acetonitrile.  $\text{DH}(\text{K1}) = -12.5 \text{ kJ mol}^{-1}$ ,  $\text{DS}(\text{K1}) = 23 \text{ J K}^{-1} \text{ mol}^{-1}$ .

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Cs+	con	non-aq	25°C	100%	C I	K1=2.39	1988TKb (88256)	239
-----	-----	--------	------	------	-----	---------	-----------------	-----

Medium: MeCN. In propylene carbonate  $\text{K1} = 2.03$ ; in MeOH 2.15

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Cs+	con	non-aq	25°C	100%	C T H	K1=2.46	1988TMb (88257)	240
-----	-----	--------	------	------	-------	---------	-----------------	-----

Medium: acetonitrile. Data for 15-35 C. Anion: tetraphenylborate.  
 $\text{DH}(\text{K1}) = -32.9 \text{ kJ mol}^{-1}$ ,  $\text{DS}(\text{K1}) = -63.7 \text{ J K}^{-1} \text{ mol}^{-1}$ .

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Cs+	sp	non-aq	22°C	100%	U	K1=4.76	1987CCc (88258)	241
-----	----	--------	------	------	---	---------	-----------------	-----

In deuteriochloroform

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Cs+	ISE	alc/w	25°C	90%	U	K1=2.08	1987KHa (88259)	242
-----	-----	-------	------	-----	---	---------	-----------------	-----

Medium: 90% w/w MeOH/H<sub>2</sub>O

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Cs+	con	non-aq	25°C	100%	C I	K1=2.21	B2= 3.74	1987ZBb (88260)	243
-----	-----	--------	------	------	-----	---------	----------	-----------------	-----

Medium: MeOH. In 70% w/w MeOH/H<sub>2</sub>O,  $\text{K1} = 1.66$ ,  $\text{K2} = 1.02$ .

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Cs+	con	alc/w	25°C	100%	U	K1=1.91	1983LSa (88261)	244
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Cs+	con	non-aq	25°C	100%	U	K1=2.03	1982TAa (88262)	245
-----	-----	--------	------	------	---	---------	-----------------	-----

Medium: propylene carbonate

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Cs+	cal	alc/w	25°C	70%	U H	K1=1.70	1976ITa (88263)	246
-----	-----	-------	------	-----	-----	---------	-----------------	-----

Medium: 70% w/w MeOH/H<sub>2</sub>O.  $\text{DH}(\text{K1}) = -10.2 \text{ kJ mol}^{-1}$ .

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\*\*\*\*\*  
C14H<sub>20</sub>O<sub>5</sub> HL CAS 65112-35-8 (6061)  
3,6,9,12-Tetraoxabicyclo[12.3.1]octadeca-1(18),14,16-trien-18-ol;  
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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Cs+	cal	alc/w	25°C	100%	U H	K1=1.30	1987ZBa (88387)	247
-----	-----	-------	------	------	-----	---------	-----------------	-----

Medium: MeOH.  $\text{DH} = -11.7 \text{ kJ mol}^{-1}$ ;  $\text{DS} = -14.4$ .

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\*\*\*\*\*  
C14H<sub>22</sub>N<sub>2</sub>O<sub>8</sub> H4L CDTA CAS 482-54-2 (200)  
trans-1,2-Diaminocyclohexane-N,N,N',N'-tetraethanoic acid;  
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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Cs+	oth	R4N.X	25°C	0.50M	U			1971CSa (88620)	248
-----	-----	-------	------	-------	---	--	--	-----------------	-----

$\text{K}(\text{Cs} + \text{H}_2\text{L}) = 0.85$

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Method: polarimetry. Medium: Me<sub>4</sub>NOH



\*\*\*\*\*

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

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

Cs+ cal alc/w 25°C 100% U H K1=1.91 1980LIb (90046) 249  
Medium: MeOH. DH=-12.7 kJ mol<sup>-1</sup>.

\*\*\*\*\*

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  
-----

Cs+ gl R4N.X 25°C 0.10M U K1=3.2 1990AFa (90221) 250  
B(CsHL)=12.4

\*\*\*\*\*

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  
-----

Cs+ ISE alc/w 25°C 100% A K1=2.78 B2=4.69 1971FRa (90269) 251  
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  
-----

Cs+ nmr non-aq 25°C 100% C I K1=0.74 1992SLb (90354) 252  
Medium: dimethylacetamide. In N-methylformamide, K1=ca. 0.0.  
Method: 133Cs nmr.

-----  
Cs+ cal alc/w 25°C 100% U H K1=2.50 1986BUd (90355) 253  
In MeOH. DH=-6.5 kJ mol<sup>-1</sup>

-----  
Cs+ EMF non-aq 25°C 100% C K1=<2.0 1979BLb (90356) 254  
Method: Ag electrode; competition with Ag+. Medium: MeOH, 0.05 M  
Me4NClO4.

-----  
Cs+ gl R4N.X 25°C 0.05M C I K1=<2.0 1975LSc (90357) 255  
In 95% MeOH, 0.05 M Me4NBr: K1 < 2

\*\*\*\*\*

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  
-----

Cs+ ISE R4N.X 25°C 0.05M U I K1=<2 1991LSb (90460) 256

Medium: 0.05 M Et4NClO4. In MeCN: K1=5.0; DMF: K1=2.7

\*\*\*\*\*

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  
-----

Cs+ con alc/w 25°C 100% U K1=1.60 1975CJa (90491) 257

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  
-----

Cs+ nmr non-aq 25°C 100% U K1=4.24 1991SKa (90516) 258

In acetonitrile.

-----  
Cs+ cal alc/w 25°C 100% U H K1=5.01 1980LIa (90517) 259

Medium: MeOH. DH=-46.8 kJ mol-1.

-----  
Cs+ ISE alc/w 25°C 100% A K1=5.02 1971FRa (90518) 260

Medium: MeOH

\*\*\*\*\*

C14H30N2O4 L CAS 31255-13-7 (2448)

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

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

Cs+ gl alc/w 25°C 95% C K1=3.85 2004KVa (90576) 261

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

\*\*\*\*\*

C14H30N2O5 L (6722)

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

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

Cs+ ISE non-aq 25°C 100% U K1=2.11 1993RPa (90627) 262

Medium: dimethylformamide, 0.05 M Et4NClO4. By competition with Ag+.

\*\*\*\*\*

C14H30O7 L CAS 1072-40-8 (2499)

2,5,8,11,14,17,20-Heptaoheneicosane; CH3.O.(CH2.CH2.O)6.CH3

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

Cs+ dis non-aq 25°C 100% C K1=5.93 1998KSc (90687) 263

Medium: 1,2-dichloroethane.

-----  
Cs+ con non-aq 25°C 100% U K1=3.9 1993EVa (90688) 264

Medium: THF+CHCl3 (4:1 vol). Also data for other solvents

-----  
Cs+ con alc/w 25°C 100% U K1=2.17 1975CJa (90689) 265  
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  
-----

Cs+ gl diox/w 30°C 75% U K1=3.42 1954FUa (91544) 266  
\*\*\*\*\*

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  
-----

Cs+ cal alc/w 25°C 100% U H K1=1.81 1987ZBa (92248) 267  
Medium: MeOH. DH=-20.0 kJ mol<sup>-1</sup>; DS=-32.6.  
\*\*\*\*\*

C15H24O6 HL CAS 57722-03-9 (2353)  
1-Hydroxy-2-(1,4,7,10,13-pentaoxatridecyl)benzene; HO.C6H4.O(CH2CH2O)4CH3  
-----

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

Cs+ sp alc/w 25°C 100% U K1=3.15 1981EMb (92342) 268  
Medium: MeOH  
\*\*\*\*\*

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

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

Cs+ cal alc/w 25°C 100% U H K1=1.02 1980LIb (92456) 269  
Medium: MeOH. DH=-48.1 kJ mol<sup>-1</sup>.  
\*\*\*\*\*

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  
-----

Cs+ EMF non-aq 25°C 100% U K1=2.29 2001WBa (92573) 270  
Medium: DMF, 0.05 M Et4NClO4. Also data for the 1,4,7-tris((S)-2-hydroxy-2-phenylethyl- derivative (K1=1.62). Competition with Ag+.  
\*\*\*\*\*

C15H36N3O9P3 L CAS 37909-50-5 (2634)  
(N,N-Dimethylamine)methylenetris(phosphonic acid diethyl ester);  
(CH3)2N.C(CH2.PO(OC2H5)2)2  
-----

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

Cs+ con non-aq 22°C 100% U K1=1.51 1981SKd (92602) 271  
Medium: CH3CN

\*\*\*\*\*

C16H2003P2 L CAS 82154-46-9 (2914)  
Dimethylphosphinomethyl-diphenylphosphinomethyl-ether;Me2PO.CH2.O.CH2.PO(C6H5)2

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

Cs+ con non-aq 25°C 100% U K1=1.8 1982YSa (94097) 272  
Medium: tetrahydrofuran+CHCl3 4:1(vol); M is 2,4-dinitrophenolate

\*\*\*\*\*

C16H2206 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  
-----

Cs+ kin alc/w 25°C 100% U K1=1.00 1992CDc (94242) 273  
Medium:MeOH. Data also for other related ligands

\*\*\*\*\*

C16H2405 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  
-----

Cs+ dis non-aq 24°C 100% C 1977MTc (94341) 274  
K(CsA+L)=4.70

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

\*\*\*\*\*

C16H2405 L AN(MOE0)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  
-----

Cs+ dis non-aq 25°C 100% U H 1979KLa (94352) 275  
K(Cs(picrate)+L)=3.70

Medium: CHCl3

\*\*\*\*\*

C16H2406 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  
-----

Cs+ con non-aq 25°C 100% C K1=3.91 2000ICa (94385) 276  
Medium: nitromethane.

-----  
Cs+ dis non-aq 25°C 100% U K1=7.50 B2=10.70 2000KSa (94386) 277  
Medium: 1,2-dichloroethane

-----  
Cs+ oth alc/w 35°C 3.0% C K1=1.11 1999MTd (94387) 278

Method: capillary zone electrophoresis. Medium: 3% v/v EtOH/H<sub>2</sub>O, 0.005 M phosphate buffer, pH 7.0

-----  
Cs+ cal non-aq 25°C 100% C H K1=3.26 1999WBa (94388) 279  
Medium: N,N-dimethylformamide. DH(K1)=-27.2 kJ mol<sup>-1</sup>.  
-----

Cs+ dis oth/un 25°C 0 U K1=3.97 19940Ua (94389) 280  
-----

Cs+ nmr non-aq 25°C 100% U K1=1.80 1991SKa (94390) 281  
Medium: MeCN  
-----

Cs+ sp non-aq 22°C 100% U K1=6.28 1987CCc (94391) 282  
In deuteriochloroform  
-----

Cs+ ISE alc/w 25°C 90% U K1=3.45 1987KHa (94392) 283  
Medium: 90% w/w MeOH/H<sub>2</sub>O  
-----

Cs+ cal non-aq 25°C 100% C H K1=3.95 B2= 6.28 1986ICa (94393) 284  
Medium: MeOH. DH(K1)=-42.30 kJ mol<sup>-1</sup>, DS(K1)=-66.1 J K<sup>-1</sup> mol<sup>-1</sup>;  
DH(K2)=-43, DS(K2)=-101.  
-----

Cs+ sp diox/w 25°C 0.0 U I K1=2.08 1983K0a (94394) 285  
On PVA. In 24.4% w/w dioxan/H<sub>2</sub>O. Data given for 9.7-84.6 w/w mixtures.  
-----

Cs+ sp mixed 25°C 0.0 U I K1=1.86 1983K0a (94395) 286  
On PVA. In 21.9% w/w tetrahydrofuran/H<sub>2</sub>O. Data given for 11.1-86.4 w/w mix  
-----

Cs+ sp alc/w 25°C 100% U K1=3.66 1981EMb (94396) 287  
Medium: MeOH  
-----

Cs+ sp diox/w 25°C 100% U M 1981SSd (94397) 288  
K(Cs(Picrate)+L)=4.82  
-----

Cs+ dis non-aq 25°C 100% C T HM 1975SIc (94398) 289  
K(Cs+A+L(org))=CsAL(org))=3.07  
K(Cs+A+2L(org))=CsAL2(org))=5.6  
K(CsAL+L)=2.5  
-----

Method: Extraction from H<sub>2</sub>O into benzene. HA is picric acid. DH(CsAL(org))  
=-66.9 kJ mol<sup>-1</sup>, DS(CsAL(org))=-166 J K<sup>-1</sup> mol<sup>-1</sup>.  
-----

\*\*\*\*\*

C16H2406 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  
-----

Cs+ cal alc/w 25°C 100% U H K1=2.62 1987ZBa (94471) 290  
Medium: MeOH. DH=-33.5 kJ mol<sup>-1</sup>; DS=-62.1.  
-----

\*\*\*\*\*

C16H24014 H4L CAS 61696-54-6 (6104)  
1,4,7,10,13,16-Hexaoxacyclooctadeca-2,3,11,12-tetracarboxylic acid;  
-----

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	gl	R4N.X	25°C	0.10M	M		K1=3.3 B(CsHL)=8.1	1991FGb (94492)	291
Medium: 0.10 M Et4NN03.									
*****									
C16H25N04		L					(7444)		
1-Aza-4,7,10,13-tetraoxa-1-phenyl-cyclopentadecane;									
Cs+	nmr	alc/w	20°C	100%	C		K1=6.13	1989GSc (94515)	292
Method: 1H and 133Cs pulsed gradient spin-echo nmr. Medium: MeOH									
*****									
C16H26N2012		H4L					(6659)		
1,4,10,13-Tetraoxa-7,16-diaza-2,3,11,12-tetracarboxycyclooctadecane;									
Cs+	gl	R4N.X	25°C	0.10M	U		K1=3.1 B(CsHL)=13.1	1990AFa (94587)	293
*****									
C16H26N2012		H4L					CAS 130190-52-2 (6660)		
1,4,10,13-Tetraoxa-7,16-diaza-2,3,7,16-tetracarboxycyclooctadecane;									
Cs+	gl	R4N.X	25°C	0.10M	U		K1=2.8 B(CsHL)=12.4	1990AFa (94601)	294
*****									
C16H2606		L					CAS 57721-93-4 (2502)		
2,5,8,11,14,17-Hexaoxa-9,10-benzo-octadeca-9-ene; C6H4(0.(CH2.CH2.0)2.CH3)2									
Cs+	con	alc/w	25°C	100%	U		K1=1.66	1975CJa (94629)	295
Medium: MeOH									
*****									
C16H3006		L					CAS 17454-53-4 (5148)		
Cyclohexyl-18-crown-6;									
Cs+	ISE	oth/un	25°C	dil	A I		K1=0.8	1971FRa (95099)	296
In MeOH: K1=4.30, K2=1.52									
*****									
C16H32N205		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
Cs+	cal	non-aq	25°C	100%	C	H		K1=3.5	1999WBa (95189)	297
Medium: N,N-dimethylformamide. DH(K1)=-36.6 kJ mol-1.										
Cs+	cal	non-aq	25°C	100%	M	H		K1=4.54	1994BCd (95190)	298
Medium: acetone. DH(K1)=-40.0 kJ mol-1, TDS=-14.2										
Cs+	nmr	non-aq	25°C	100%	C	I		K1=3.07	1992SLb (95191)	299
Medium: dimethylacetamide. In N-methylformamide, K1=2.4. Method: 133Cs nmr.										
Cs+	cal	non-aq	25°C	100%	U	H		K1=4.68	1986BUb (95192)	300
In CH3CN. DH=-45.8 kJ mol-1										
Cs+	cal	alc/w	25°C	100%	U	H		K1=4.32	1986BUd (95193)	301
In MeOH. DH=-47.4 kJ mol-1										
Cs+	ISE	non-aq	25°C	100%	U	I		K1=3.61	1981CRa (95194)	302
Medium: DMF. In EtOH: 4.77; in DMSO: 3.23; in N-methylpropionamide: 3.87										
Cs+	ISE	non-aq	25°C	100%	U			K1=4.9	1980CRa (95195)	303
Medium: Propylene carbonate										
Cs+	gl	R4N.X	25°C	0.05M	C	I		K1=<2.0	1975LSc (95196)	304
In 95% MeOH: K1=3.90; 100%: 5										
*****										
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
Cs+	con	alc/w	25°C	100%	U			K1=1.57	1991IOa (95382)	305
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
Cs+	ISE	alc/w	25°C	100%	A			K1=4.15	1971FRa (95395)	306
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
Cs+	EMF	alc/w	25°C	100%	U	I		K1=3.46	1994LLa (95413)	307
Medium: MeOH, 0.05M Et4NClO4. Also data for acetonitrile: K=3.77, PC: K=3.6										

DMF: K=2.31 and H2O: K<2. Method: by competition with Ag+.

\*\*\*\*\*

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

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

Cs+ ISE non-aq 25°C 100% U K1=3.36 1993RPa (95447) 308  
Medium: dimethylformamide, 0.05 M Et4NClO4. By competition with Ag+.

\*\*\*\*\*

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  
-----

Cs+ con alc/w 25°C 100% U 1975CJa (95484) 309  
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  
-----

Cs+ con non-aq 25°C 100% U K1=4.2 1993EVa (95488) 310  
Medium: THF+CHCl3 (4:1 vol). Also data for other solvents

-----  
Cs+ con alc/w 25°C 100% U K1=2.41 1975CJa (95489) 311  
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  
-----

Cs+ gl non-aq 25°C 100% U K1=1.8 1986STb (95538) 312  
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  
-----

Cs+ EMF non-aq 25°C 100% U I K1=2.90 1996WPa (95570) 313  
Medium: acetonitrile, 0.05 M NEt4ClO4. In propylene carbonate K1=4.04

-----  
Cs+ gl alc/w 25°C 100% C I K1=1.90 1993TCa (95571) 314  
Medium: MeOH, 0.05 M Et4NClO4. In DMF, K1=1.23

\*\*\*\*\*

C17H21O5P L (5732)  
Methyldi(2-methoxyphenoxyethyl)phosphine oxide; Me.PO(CH2.0.C6H4.OMe)2



Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	con	non-aq	25°C	100%	U		K1=1.78	1989TKb (96390)	315
Medium: tetrahydrofuran/CHCl3 4:1 (volume)									
*****									
C17H23NO6		L					(7047)		
5'-(N-Acrylamide)-benzo-15-crown-5; CH2:CH.CO.NH.C14H19O5									
Cs+	sp	non-aq	25°C	100%	U		K1=7.77	1979KMb (96405)	316
Medium: CHCl3									
*****									
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									
Cs+	ISE	none	25°C	0.0	C		K1=1.30	1980WSb (96513)	317
Method: monovalent ion electrode. Also data for the 4'-polyvinylbenzene-derivative: by spectrophotometry, K1=2.48									
*****									
C17H26O6		L					CAS 99159-90-7 (688)		
2,3-Benzo-1,4,7,10,13,16-hexaoxacyclononadeca-2-ene;									
Cs+	sp	non-aq	22°C	100%	U		K1=5.20	1987CCc (96519)	318
In deuterochloroform									
*****									
C17H26O6		L					CAS 65112-34-7 (6059)		
21-Methoxy-3,6,9,12,15-pentaoxabicyclo[15.3.1]heneicosa-1(21),17,19-triene;									
Cs+	cal	alc/w	25°C	100%	U	H	K1=2.76	1987ZBa (96526)	319
Medium: MeOH. DH=-22.8 kJ mol <sup>-1</sup> ; DS=-23.5.									
*****									
C17H34N2O4		L					CAS 142565-14-8 (6562)		
4,7,13,16-Tetraoxa-1,10-diazabicyclo[8.8.5]tricosane;									
Cs+	EMF	non-aq	25°C	100%	C	I	K1=5.16	1993DLb (96741)	320
Medium: propylene carbonate, 0.05 M Et4NClO4. In acetonitrile, K1=4.57.									
Cs+	gl	R4N.X	25°C	0.05M	C	I	K1=3.31	1992CGb (96742)	321
Medium: Et4NClO4. In MeOH: K1=4.8; in DMF K1=2.90									

\*\*\*\*\*  
 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
Cs+	gl	alc/w	25°C	95%	C		K1=1.93	2004KV a (96757)	322

Medium: 95% MeOH/H<sub>2</sub>O, 0.01 M Et<sub>4</sub>NC<sub>10</sub>4.  
 \*\*\*\*\*

C17H35N04 L (1694)  
 N-n-Heptany1-1,4,7,10-tetraoxa-13-azacyclopentadecane;  
 -----

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	ISE	alc/w	25°C	10%	U		K1=2.71	1986HA a (96767)	323

Medium: 10% MeOH/H<sub>2</sub>O  
 \*\*\*\*\*

C18H22O5 L (5737)  
 1,7-Di(2-methoxyphenyl)-1,4,7-trioxaheptane; MeO.C<sub>6</sub>H<sub>4</sub>.O.C<sub>2</sub>H<sub>4</sub>.O.C<sub>2</sub>H<sub>4</sub>.O.C<sub>6</sub>H<sub>4</sub>.OMe  
 -----

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	con	non-aq	25°C	100%	U		K1=1.68	1989TK b (97564)	324

Medium: tetrahydrofuran/CHCl<sub>3</sub> 4:1 (volume)  
 \*\*\*\*\*

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-]isoindole18,20dione;  
 -----

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	sp	non-aq	25°C	100%	C		K1=3.3	20010Y a (97574)	325

Medium: methanol. For the N-propyl derivative, K1=3.4.  
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C18H28N6 L CAS 299416-55-0 (2561)  
 6,6'-Bis(2-methylaminoethylaminomethyl)-2,2'-bipyridyl;  
 -----

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	nmr	non-aq	25°C	100%	U I		K1=3.76	1977ML a (97793)	326

Medium: pyridine. In MeCN: K1=3.55; in acetone: 3.54  
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C18H28O6 L Benzo20-crown-6 (6354)  
 2,3-Benzo-1,5,8,11,14,18-Hexaoxacosa-2-ene;  
 -----

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	sp	non-aq	22°C	100%	U		K1=4.24	1987CC c (97834)	327

In deuteriochloroform  
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C18H28O6 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
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Cs+	con	alc/w	25°C	100%	U		K1=3.38	1983LSa (97840)	328
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Medium: MeOH

C18H28O6 L AN(MOE0E)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
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Cs+	dis	non-aq	25°C	100%	U	H		1979KLa (97845)	329
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K(Cs(picrate)+L)=5.06

Medium: CHCl3

C18H28O7 L Benzo21-crown-7 (6355)

2,3-Benzo-1,4,7,10,13,16,19-Heptaoxaheneicosa-2-ene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Cs+	sp	non-aq	22°C	100%	U		K1=7.21	1987CCc (97855)	330
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In deuteriochloroform

C18H32N2O8 L CAS 24951-52-8 (2560)

Cryptand-2,2,2-dilactam

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Cs+	nmr	non-aq	33°C	100%	U	I	K1=1.96	1977HPa (98132)	331
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Medium: pyridine. In nitromethane: K1=1.67

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
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Cs+	con	alc/w	25°C	100%	U		K1=1.56	1975CJa (98396)	332
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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
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Cs+	gl	alc/w	25°C	95%	M		K1=2.32	1990LNa (98405)	333
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Medium: 95% MeOH, 0.05 M Bu4NBr. For the 12,16-dihydroxy- analogue: K1 < 2

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
Cs+	cal	KCl	25°C	0.10M	U	IH		K1=2.40	1997Zia (98419)	334
DH(K1)=-24.6 kJ mol <sup>-1</sup> , DS=-36.6 J K <sup>-1</sup> mol <sup>-1</sup> . In 95% v/v MeOH/H <sub>2</sub> O: K1=6.35; DH(K1)=-59.5, DS=-78.2										

\*\*\*\*\*

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
Cs+	cal	non-aq	25°C	100%	C	H		K1=2.13	1999WBa (98532)	335
Medium: N,N-dimethylformamide. DH(K1)=-11.2 kJ mol <sup>-1</sup> .										
Cs+	gl	R4N.X	25°C	0.05M	C	H		K1=3.3	1996BCh (98533)	336
Medium: 0.05 M Et4NClO4. By calorimetry: K1=3.4, DH(K1)=-2.4 kJ mol <sup>-1</sup> .										
Cs+	cal	alc/w	25°C	80%	C	H		K1=2.84	1995KZa (98534)	337
Medium: 80% v/v CH <sub>3</sub> OH/H <sub>2</sub> O. DH(K1)=-29.7 kJ mol <sup>-1</sup> , DS(K1)=-45.3 J K <sup>-1</sup> mol <sup>-1</sup>										
Cs+	cal	non-aq	25°C	100%	M	H		K1=3.96	1994BCd (98535)	338
Medium: acetone. DH(K1)=-40.0 kJ mol <sup>-1</sup> , TDS=-17.5										
Cs+	con	oth/un	25°C	0.05M	M			K1=4.04	1992BUb (98536)	339
K1=3.95 (by calorimetry)										
Cs+	nmr	non-aq	25°C	100%	C	I		K1=1.82	1992SLb (98537)	340
Medium: dimethylacetamide. In N-methylformamide, K1=2.35. Method: 133Cs nmr.										
Cs+	cal	non-aq	25°C	100%	U	H		K1=4.83	1986BUb (98538)	341
In CH <sub>3</sub> CN. DH=-44.2 kJ mol <sup>-1</sup>										
Cs+	cal	alc/w	25°C	100%	U	H		K1=3.95	1986BUd (98539)	342
In MeOH. DH=-49.7 kJ mol <sup>-1</sup>										
Cs+	nmr	non-aq	25°C	100%	U			K1=7.55	1986CHc (98540)	343
In CDCl <sub>3</sub> saturated with D <sub>2</sub> O										
Cs+	cal	non-aq	25°C	100%	U	H			1986DGa (98541)	344
DH1 = -51.4 kJ mol <sup>-1</sup> . Medium: nitromethane										
Cs+	nmr	non-aq	32°C	100%	U	I		K1=3.75	1986RPc (98542)	345
Medium: acetone. Additional data for binary acetone-DMSO systems, 0-95% acetone.										
Cs+	nmr	non-aq	32°C	100%	U	I		K1=1.19	1986RPc (98543)	346

Medium: dimethylsulfoxide. Additional data for binary solvent systems  
DMSO-acetonitrile, DMSO-propylenecarbonate.

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Cs+ nmr non-aq 32°C 100% U I K1=4.71 1986RPc (98544) 347

Medium: acetonitrile. Data also in other media  
additional data for binary acetonitrile-dimethylsulfoxide systems

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Cs+ nmr non-aq 32°C 100% U I K1=3.90 1986RPc (98545) 348

Medium: propylene carbonate. Data also in other media  
additional data for binary solvent systems: PC-DMSO and PC-DMF

---

Cs+ cal non-aq 25°C 100% U H 1985DGa (98546) 349

Medium: propylene carbonate. DH1 = -41.3 kJ mol<sup>-1</sup>

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Cs+ cal non-aq 25°C 100% U H 1985DGa (98547) 350

Medium: acetonitrile. DH1 = -43.5 kJ mol<sup>-1</sup>

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Cs+ ISE non-aq 25°C 100% M K1=5.10 1985DGb (98548) 351

Medium: nitromethane

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Cs+ cal non-aq 25°C 100% U H 1984DGa (98549) 352

Medium: N,N-dimethylformamide. DH1=-31.0 kJ mol<sup>-1</sup>; DS1=-63.2 J K<sup>-1</sup> mol<sup>-1</sup>.

---

Cs+ cal non-aq 25°C 100% U H 1984DGa (98550) 353

Medium: DMSO. DH1=-35.6 kJ mol<sup>-1</sup>; DS1=-92.0 J K<sup>-1</sup> mol<sup>-1</sup>

---

Cs+ ISE non-aq 25°C 100% U I K1=4.57 1981CRa (98551) 354

Medium: MeCN. In EtOH: 4.17; in DMF: 2.14; in N-methylpropionamide: 4.4

---

Cs+ ISE non-aq 25°C 100% U K1=4.1 1980CRa (98552) 355

Medium: Propylene carbonate

---

Cs+ con non-aq 25°C 100% U K1=4.54 1980KMb (98553) 356

Medium: MeCN

---

Cs+ EMF oth/un 25°C 0.05M C I K1=<1.4 1978YTa (98554) 357

Method: competition with Tl<sup>+</sup>, using Tl amalgam electrode.

Electrolyte not stated. In DMSO, 0.10 M: K1=1.4

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Cs+ nmr non-aq 25°C 100% U I K1=1.45 1977MLa (98555) 358

Medium: DMSO. In pyridine: K1 > 5; in MeCN: K1=4.57

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Cs+ nmr non-aq 25°C 100% U TIH 1977MPb (98556) 359

Keff=4.0

Medium: propylene carbonate. Keff (40 C)=3.6. Keff=1.8 in DMF, 46 C.

Keff=2.19 in DMF, 25 C. Keff=3.3 in 0.02 M acetone in PC, 52 C

---

Cs+ cal alc/w 25°C 95% C H 1976KLc (98557) 360

Medium: 0.057 M Me4NBr in 95% (v/v) MeOH/H<sub>2</sub>O, pH 10.4.

DH(K1)=-49.8 kJ mol<sup>-1</sup>, DS(K1)=-99 J K<sup>-1</sup> mol<sup>-1</sup>.

-----  
Cs+ gl R4N.X 25°C 0.05M C I K1=<2.0 1975LSc (98558) 361  
In 95% MeOH: K1=3.54; 100%: 4.4

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C18H36O9 L 27-Crown-9 (7043)  
1,4,7,10,13,16,19,22,25-Nonaoxacycloheptacosane;

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

Cs+ cal alc/w 25°C 100% U H K1=3.95 1993ILa (98805) 362  
Medium: MeOH. DH=-36.5 kJ mol<sup>-1</sup>.

\*\*\*\*\*

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  
-----

Cs+ dis non-aq 25°C 100% C K1=7.17 1998KSc (98873) 363  
Medium: 1,2-dichloroethane.

\*\*\*\*\*

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  
-----

Cs+ con non-aq 25°C 100% U K1=2.56 1989TKb (99344) 364  
Medium: tetrahydrofuran/CHCl<sub>3</sub> 4:1 (volume)

\*\*\*\*\*

C19H27NO7 L (7048)  
5'-(N-Acrylamide)-benzo-18-crown-6; CH<sub>2</sub>:CH.CO.NH.C16H23O6

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

Cs+ sp non-aq 25°C 100% U K1=6.42 1979KMb (99393) 365  
Medium: CHCl<sub>3</sub>

\*\*\*\*\*

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  
-----

Cs+ con alc/w 25°C 100% U K1=2.99 1983LSa (99435) 366  
Medium: MeOH

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C19H39NO5 L (1693)  
N-n-Heptyl-1,4,7,10,13-pentaoxa-16-azacyclooctadecane;

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

Cs+ ISE alc/w 25°C 10% U K1=3.53 1986HAa (99477) 367

Medium: 10% MeOH/H<sub>2</sub>O

\*\*\*\*\*

C19H39N3O5 L CAS 60598-00-7 (1537)  
4-Methyl-1,4,10-triaza-7,13,16,21,24-pentaoxa-bicyclo[8,8,8]hexacosane;

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

Cs+ gl R4N.X 25°C 0.10M U K1=2 1978LMa (99490) 368

\*\*\*\*\*

C20H22O6 L (6834)  
1,8-Bis(2-Formyphenoxy)-3,6-dioxaoctane; (CH<sub>2</sub>.O.CH<sub>2</sub>.CH<sub>2</sub>.O.C<sub>6</sub>H<sub>4</sub>.CH<sub>3</sub>)<sub>2</sub>

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

Cs+ con non-aq 25°C 100% U K1=1.3 1993Eva (99930) 369

Medium: THF+CHCl<sub>3</sub> (4:1 vol)

\*\*\*\*\*

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  
-----

Cs+ oth oth/un 25°C 0.05M C I K1=0.98 2002KTa (100094) 370

Method: capillary electrophoresis. Medium: 0.03-0.06 M CsCl.

In CH<sub>3</sub>CN, K1=3.037.

-----  
Cs+ dis non-aq 24°C 100% C 2002MRd (100095) 371

K(Cs+A+L)=5.61

Medium: CDCl<sub>3</sub>. HA is picric acid.

-----  
Cs+ con non-aq 25°C 100% C K1=3.2 2000ICa (100096) 372

Medium: nitromethane.

-----  
Cs+ con non-aq 25°C 100% C T H K1=3.34 2000SSc (100097) 373

Medium: acetonitrile. Data for 15-45 C. DH(K1)=-15 kJ mol<sup>-1</sup>,

DS(K1)=14 J K<sup>-1</sup> mol<sup>-1</sup>.

-----  
Cs+ dis oth/un 25°C 0.06M C 2000YYa (100098) 374

K(CsL+A)=0.24

K(Cs+L(org)+A=C<sub>s</sub>LA(org))=4.25

Method: extraction of metal picrate (0.06 M, pH 12) into dichloromethane/  
ligand solution. HA: picric acid. Data for many additional solvents.

-----  
Cs+ oth alc/w 35°C 3.0% C K1=0.83 1999MTd (100099) 375

Method: capillary zone electrophoresis. Medium: 3% v/v EtOH/H<sub>2</sub>O, 0.005 M  
phosphate buffer, pH 7.0

-----  
Cs+ dis non-aq 25°C 100% U K1=6.55 B2= 9.95 1998KSb (100100) 376

Medium: 1,2-dichloroethane  
-----

Cs+	oth	oth/un	25°C	0.04M	C	K1=0.94	1998Tia	(100101)	377
Method: capillary electrophoresis.									
Medium: 0.005 M phosphate buffer, pH 7.1, 0.04 M MCl.									
Cs+	nmr	non-aq	RT	100%	U	K1=1.63	1996GMc	(100102)	378
Method: 133Cs nmr. Medium: N,N-dimethylformamide									
Cs+	dis	oth/un	25°C	0	U	K1=3.57	19940Ua	(100103)	379
Cs+	dis	non-aq	23°C	100%	C	K1=4.5	1992HGb	(100104)	380
						K(Cs+A+L(org))=CsAL(org))=5.19			
						K(Cs+A+2L(org))=CsAL2(org))=7.3			
Extraction of metal chloride (A) from aqueous solution into nitrobenzene/0.01M Bu4NB(Ph)4. Peak potential voltammetry and distribution of 137Cs.									
Cs+	nmr	non-aq	25°C	100%	U	K1=1.97	1991SKa	(100105)	381
Medium: MeCN									
Cs+	cal	non-aq	25°C	100%	C H		1988Bub	(100106)	382
Medium: acetonitrile. DH(K1)=-8.4 kJ mol-1, DS(K1)=40 J K-1 mol-1.									
Cs+	con	non-aq	25°C	100%	U	K1=3.3	1986STb	(100107)	383
Medium: THF:CHCl3 4:1 v/v. Metal as 2,4-dinitrophenolate									
Cs+	con	non-aq	25°C	100%	U	K1=3.49	1985YKa	(100108)	384
Medium: EtOH+CHCl3 1:1; M is used in nitrophenolate form									
Cs+	con	mixed	25°C	?	U	K1=4.84	1984MPa	(100109)	385
Medium: 60%(vol) isopropanol+ 20% H2O + 20% CHCl3									
Cs+	vlt	non-aq	25°C	100%	U I	K1=3.50	1978HKc	(100110)	386
Medium: CH3CN, 0.05M Bu4NClO4									
Cs+	nmr	non-aq	25°C	100%	U I	K1=3.84 B2=6.20	1977MPa	(100111)	387
Medium: pyridine. K1=1.48 in DMF; 1.34 in DMSO; 1.54 in MeCN; 3.0 in acetone; 3.0 in PC									
Cs+	nmr	non-aq	29°C	100%	U	K1=2.35	1977SZa	(100112)	388
Medium: DMF									
Cs+	sol	none	25°C	0.0	U I	K1=0.83	1975SNa	(100113)	389
Cs+	ISE	alc/w	25°C	100%	A	K1=3.55 B2=6.47	1971FRa	(100114)	390
Medium: MeOH									
*****									
C20H24O6 L CAS 72011-24-6 (8872)									
2,3:5,6-Dibenzo-1,4,7,10,13,16-hexaoxacyclooctadeca-2,5-diene;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Cs+ dis non-aq 23°C 100% C K1=4.0 1992HGb (100260) 391  
 $K(\text{Cs}+\text{A}+\text{L}(\text{org})=\text{CsAL}(\text{org}))=5.43$   
 $K(\text{Cs}+\text{A}+2\text{L}(\text{org})=\text{CsAL}_2(\text{org}))=7.8$

Extraction of metal chloride (A) from aqueous solution into nitrobenzene/  
 0.01M Bu4NB(Ph)4. Peak potential voltammetry and distribution of 137Cs.

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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
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Cs+ dis non-aq 23°C 100% C K1=2.7 1992HGb (100266) 392  
 Extraction of metal chloride (A) from aqueous solution into nitrobenzene/  
 0.01M Bu4NB(Ph)4. Peak potential voltammetry and distribution of 137Cs.

\*\*\*\*\*

C20H2606 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
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Cs+ dis non-aq 25°C 100% U H 1979KLa (100345) 393  
 $K(\text{Cs}(\text{picrate})+\text{L})=6.10$

Medium: CHCl3

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C20H31N204F L CAS 173417-87-3 (6461)  
 26-Fluoro-4,7,13,16-tetraoxa-1,10-diazatricyclo[8.8.7.1,20,24]hexacosa-20,22,24(26)-triene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Cs+ EMF non-aq 25°C 100% C H K1=4.70 1999BHa (100439) 394  
 Medium: MeOH, 0.05 M Et4NClO4. By calorimetry  $\text{DH}(\text{K1})=-43.7 \text{ kJ mol}^{-1}$ .  
 Method: by competition with Ag+, using Ag/Ag+ electrode.

\*\*\*\*\*

C20H32N204 L CAS 61696-66-0 (6497)  
 4,7,13,16-Tetraoxa-1,10-diazatricyclo[8.8.7.1,20,24]hexacosa-20,22,24(26)-triene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Cs+ EMF non-aq 25°C 100% C H K1=4.76 1999BHa (100456) 395  
 Medium: MeOH, 0.05 M Et4NClO4. By calorimetry  $\text{DH}(\text{K1})=-44.2 \text{ kJ mol}^{-1}$ .  
 Method: by competition with Ag+, using Ag/Ag+ electrode.

\*\*\*\*\*

C20H3207 L AN(MOE0EO)2E (2248)  
 24-Methoxy-22-methyl-3,6,9,12,15,18-hexaoxabicyclo[18.3.1]-tetracosa-1(24),20,22-triene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Cs+ dis non-aq 25°C 100% U H 1979KLa (100490) 396

$$K(\text{Cs}(\text{picrate})+\text{L})=5.81$$

Medium: CHCl<sub>3</sub>

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	sp	non-aq	22°C	100%	U		K1=6.24	1987CCc (100495)	397

In deuteriochloroform

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C20H33NO6 L CAS 105495-12-3 (1692)  
N-(2-(2-Phenylloxy)ethoxy)ethyl-1,4,7,10-tetraoxa-13-azacyclopentadecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	ISE	alc/w	25°C	10%	U		K1=3.15	1986HAa (100500)	398

Medium: 10% MeOH/H<sub>2</sub>O

\*\*\*\*\*

C20H34O8 L (2504)  
2,5,8,11,14,17,20,23-Octaoxa-12,13-benzotetracos-12-ene; C<sub>6</sub>H<sub>4</sub>(O.(CH<sub>2</sub>.CH<sub>2</sub>.O)<sub>3</sub>.CH<sub>3</sub>)<sub>2</sub>

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	con	alc/w	25°C	100%	U		K1=2.29	1975CJa (100524)	399

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
Cs+	dis	non-aq	25°C	100%	U		K1=8.58 B2=10.26	2000KSa (100633)	400

Medium: 1,2-dichloroethane

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	con	non-aq	25°C	100%	C T H		K1=>5.5	2000SSc (100634)	401

Medium: acetonitrile. Data for 15-45 C. DH(K1)=-19 kJ mol<sup>-1</sup>, DS(K1)=35 J K<sup>-1</sup> mol<sup>-1</sup>.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	nmr	non-aq	RT	100%	U		K1=2.91	1996GMc (100635)	402

Method: 133Cs nmr. Medium: N,N-dimethylformamide

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	dis	non-aq	25°C	100%	U		K(Cs(pic)+L)=Cs(pic),L)=6.52	1995BSa (100636)	403

Medium:CHCl<sub>3</sub>. Data for host-guest associations; pic: picrate. L is a cis-syn-cis and cis-anti-cis mixture. Also data for syn-L (K=6.65) and anti-L(6.31)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	nmr	non-aq	25°C	100%	U		K1=3.59	1991SKa (100637)	404

In acetonitrile.

Cs+ cal non-aq 25°C 100% C H K1=5.40 1988Bub (100638) 405  
Medium: acetonitrile. DH(K1)=-23.7 kJ mol<sup>-1</sup>, DS(K1)=23 J K<sup>-1</sup> mol<sup>-1</sup>.

Cs+ con none 25°C 0.0 C T H K1=4.06 1988Tmc (100639) 406  
Data for 15-35 C. DH(K1)=-50.1 kJ mol<sup>-1</sup>, DS(K1)=-89.7 J K<sup>-1</sup> mol<sup>-1</sup>.  
Anion is tetraphenyl borate.

Cs+ dis non-aq 25°C 100% U H 1979KLa (100640) 407  
K(Cs(picrate)+L)=6.25  
Medium: CHCl<sub>3</sub>

Cs+ nmr non-aq 25°C 100% U I 1977MPa (100641) 408  
K1>5.0  
Medium: pyridine. K1=2.04 in DMSO; >4.0 in MeCN; 4.0 in PC; 3.45 in DMF;  
>4 in acetone

Cs+ ISE oth/un 25°C dil A K1=0.9 1971FRa (100642) 409  
Isomer B. In MeOH: K1=3.49. For isomer A: K1=1.25; in MeOH: K1=4.61, B2=5.20

Cs+ cal oth/un 40°C 0.0 U T K1=0.96 1971INa (100643) 410  
K1(10 C)=1.00, K1(25 C)=0.96

Cs+ cal oth/un ? 0.01M U K1=1.07 1969IRa (100644) 411  
Data for isomer A

\*\*\*\*\*  
C20H38N206 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
Cs+	cal	alc/w	25°C	80%	C H	K1=2.96	1995KZa (100738)	412	
Medium: 80% v/v CH <sub>3</sub> OH/H <sub>2</sub> O. DH(K1)=-48.9 kJ mol <sup>-1</sup> , DS(K1)=-107 J K <sup>-1</sup> mol <sup>-1</sup>									
*****									
C20H38O8	L					CAS 118787-30-7	(5290)		
Cyclohexyl-24-crown-8;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	ISE	oth/un	25°C	dil	A	K1=1.9	1971FRa (100757)	413	
*****									
C20H40N204	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
Cs+	gl	non-aq	25°C	100%	C I	K1=3.13	1992LSc (100774)	414	
Medium: MeCN, 0.05 M Et <sub>4</sub> NClO <sub>4</sub> . In DMF K1=2.0; in H <sub>2</sub> O K1<2									
*****									
C20H40N206	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
Cs+	gl	alc/w	25°C	95%	M		K1=3.71	1990LNa (100784)	415
Medium: 95% MeOH, 0.05 M Bu4NBr. For the 12,19-dihydroxy- analogue: K1 < 2									
*****									
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
Cs+	gl	alc/w	25°C	95%	M		K1=2.86	1990LNa (100793)	416
Medium: 95% MeOH, 0.05 M Bu4NBr. For the 9,19-dihydroxy- analogue: K1=2.74									
*****									
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
Cs+	cal	alc/w	25°C	80%	C	H	K1=2.04	1995KZa (100800)	417
Medium: 80% v/v CH3OH/H2O. DH(K1)=-51.8 kJ mol <sup>-1</sup> , DS(K1)=-136 J K <sup>-1</sup> mol <sup>-1</sup>									
*****									
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
Cs+	ISE	alc/w	25°C	95%	C		K1=7.0	1977LSc (100809)	418
Medium: 95% (w/w) MeOH/H2O, 0.1 M Et4NBr.									
Cs+	cal	R4N.X	25°C	0.06M	C	H		1976KLc (100810)	419
Medium: 0.057 M Me4NBr. Method: flow microcalorimetry.									
DH(K1)=-22.6 kJ mol <sup>-1</sup> , DS(K1)=-41 J K <sup>-1</sup> mol <sup>-1</sup> .									
Cs+	gl	R4N.X	25°C	0.05M	C	I	K1=2.0	1975LSc (100811)	420
In 95% MeOH: K1=7.0									
*****									
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
Cs+	cal	alc/w	25°C	100%	U	H	K1=4.15	1993ILa (100850)	421
Medium: MeOH. DH=-46.9 kJ mol <sup>-1</sup> .									
*****									
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

Cs+ gl R4N.X 25°C 0.10M U K1=<2 1978LMa (100886) 422  
In CH3OH, K1<2

\*\*\*\*\*

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  
-----

Cs+ dis non-aq 25°C 100% C K1=2.14 1999KKb (100900) 423

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  
-----

Cs+ EMF non-aq 25°C 100% C I K1=3.10 1997DMd (100926) 424

Method: Ag electrode; competitive titration. Medium: acetonitrile, 0.05 M  
Et4NClO4. Also data for PC (K1=4.1), MeOH (3.2), DMF (3.41), 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  
-----

Cs+ gl non-aq 25°C 100% U I K1=3.55 1996SDa (100938) 425

Medium: MeCN, 0.05 M Et4NClO4. In MeOH: K1=2.5, DMF: 2.28

-----  
Cs+ gl R4N.X 25°C 0.10M C K1=<2.0 1993SFb (100939) 426

Medium: 0.1 M Et4NClO4.

\*\*\*\*\*

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  
-----

Cs+ con alc/w 25°C 100% U K1=<-0.3 1980Pa (101257) 427

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  
-----

Cs+ gl alc/w 25°C 80% M H K1=2.70 1985AEb (101264) 428

Medium: 80% w/w MeOH/H2O, pH=11. By calorimetry: DH(K1)=-4.69 kJ mol<sup>-1</sup>,  
DS(K1)=36.2 J K<sup>-1</sup> mol<sup>-1</sup>.

\*\*\*\*\*

C21H31O7P3 L CAS 82154-48-1 (2916)

Methyl di((2-dimethylphosphinylmethoxy)phenoxy)methyl)phosphine oxide;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Cs+		con non-aq	25°C	100%	U			K1=2.79	1982YSa (101418)	429
Medium: tetrahydrofuran+CHCl3 4:1(vol); M is 2,4-dinitrophenolate L=CH3P(O)[CH2OC6H4OCH2P(O)(CH3)2]2										

C21H42N4O6S L CAS 503465-05-2 (9248)  
4,12,18,21,26,29-Hexaoxa-1,7,9,15-tetraazabicyclo[13.8.8]hentriacontane-8-thione;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Cs+		gl alc/w	25°C	95%	C			K1=3.60	2004KVa (101462)	430
Medium: 95% MeOH/H2O, 0.01 M Et4NClO4.										

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
Cs+		sp oth/un	25°C	0.10M	U			K1=1.27	1980NTa (101918)	431
At pH 12.35 in Li4(EDTA)										

C22H26N4O12 L CAS 74044-87-4 (2796)  
4'-Picrylaminobenzo-18-crown-6

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Cs+		sp oth/un	25°C	0.10M	U			K1=1.36 K(Cs+HL)=1.08	1980NTa (101990)	432
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
Cs+		con non-aq	25°C	100%	C			K1=2.70 B2= 4.80	2000ICa (101996)	433
Medium: nitromethane.										

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Cs+		oth alc/w	35°C	3.0%	C			K1=1.45	1999MTd (102039)	434
Method: capillary zone electrophoresis. Medium: 3% v/v EtOH/H2O, 0.005 M phosphate buffer, pH 7.0										

Cs+ dis oth/un 25°C 0 U K1=4.27 19940Ua (102040) 435

Cs+ con non-aq 25°C 100% U K1=5.0 1993EVa (102041) 436  
Medium: THF+CHCl3 (4:1 vol)

Cs+ cal non-aq 25°C 100% C H K1=4.25 1986ICa (102042) 437  
Medium: MeOH. DH(K1)=-44.10 kJ mol<sup>-1</sup>, DS(K1)=-66.4 J K<sup>-1</sup> mol<sup>-1</sup>.

Cs+ ISE alc/w 25°C 100% A K1=4.20 B2=6.10 1971FRa (102043) 438  
Medium: MeOH

\*\*\*\*\*  
C22H28O7 L CAS 133560-78-8 (8962)  
2,3:17,18-Dibenzo-1,4,7,10,13,16,19-heptaoxacycloheicosa-2,17-diene,  
Dibenzo[21]crown-7;

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

Cs+ sp non-aq 25°C 100% C K1=<2 2002YEB (102063) 439  
Method: steady state fluorescence spectroscopy. Medium: acetonitrile.

\*\*\*\*\*  
C22H30O4P2 L CAS 470454-09-2 (8993)  
4,10-Dibenzyl-1,7-dioxa-4,10-diphosphacyclododecan-4,10-dioxide;

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

Cs+ dis non-aq 24°C 100% C 2002MRd (102129) 440  
K(Cs+A+L)=4.28

Medium: CDCl3. HA is picric acid.

\*\*\*\*\*  
C22H32O7P2 L (2078)  
1,5-Bis(2-(dimethylphosphinylmethoxy)phenoxy)-3-oxapentane;

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

Cs+ con non-aq 25°C 100% U K1=3.11 1989KSA (102205) 441  
Medium: tetrahydrofuran/CHCl3 4:1 (vol)

\*\*\*\*\*  
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]hexacos-5-ene;

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

Cs+ gl R4N.X 25°C 0.05M U H K1=2.4 1998DBa (102268) 442  
Medium: 0.05 M Et4NClO4. By calorimetry: DH(K1)=-1.8 kJ mol<sup>-1</sup>,

Cs+ nmr non-aq 25°C 100% C I K1=1.47 1992SLb (102269) 443  
Medium: dimethylacetamide. In N-methylformamide, K1=1.75.  
Method: 133Cs nmr.

Cs+ gl oth/un 25°C 0.02M U H K1=2.99 1980CKa (102270) 444

DH=-31.8 kJ mol<sup>-1</sup>. Alternative method, calorimetry

-----  
Cs+ nmr alc/w 25°C 100% U H K1=2.9 1980KDa (102271) 445  
Medium: MeOH. DH=-4.1 kJ mol<sup>-1</sup>.

\*\*\*\*\*

C22H36O9 L Benzo-27-Crown9 CAS 63144-76-3 (2842)

2,3-Benzo-1,4,7,10,13,16,19,22,25-nonanoxacycloheptacos-2-ene;

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

Cs+ sp non-aq 22°C 100% U K1=5.73 1987CCc (102298) 446

In deuteriochloroform

\*\*\*\*\*

C22H37NO7 L CAS 105495-13-4 (1691)

N-(2-(2-Phenyloxy)ethoxy)ethyl-1,4,7,10,13-pentaoxa-16-azacyclooctadecane;

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

Cs+ ISE alc/w 25°C 10% U K1=3.23 1986HAa (102304) 447

Medium: 10% MeOH/H<sub>2</sub>O

\*\*\*\*\*

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  
-----

Cs+ nmr non-aq 24°C 100% U M 1981BEb (102369) 448

K(Cs(picrate)+L)=6.9

Medium: CDCl<sub>3</sub>

\*\*\*\*\*

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  
-----

Cs+ nmr non-aq 25°C 100% U K1=>4 K2=1.98 1991SKa (102377) 449

In acetonitrile.

-----  
Cs+ ISE alc/w 25°C 100% A K1=1.9 1971FRa (102378) 450

Medium: MeOH

\*\*\*\*\*

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  
-----

Cs+ gl alc/w 25°C 95% M K1=4.05 1990LNa (102414) 451

Medium: 95% MeOH, 0.05 M Bu<sub>4</sub>NBr. For the 12,22-dihydroxy- analogue: K1 < 2

\*\*\*\*\*



C22H44N2O8 L Cryptand 4,2,2 (7304)  
1,10-Diaza-4,7,13,16,21,24,27,30-octaoxabicyclo[8,8,14]dotricontane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	cal	alc/w	25°C	95%	U	H	K1=>5.5	1997Zia (102420)	452
Medium: 95% v/v MeOH/H2O, 0.1 M. DH(K1)=-46.4 kJ mol-1, DS>-56.4 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
Cs+	gl	alc/w	25°C	100%	C	I	K1=6	1975LSc (102427)	453
Medium: MeOH									
*****									

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	gl	alc/w	25°C	95%	C		K1=2.67	2004KVa (102437)	454
Medium: 95% MeOH/H2O, 0.01 M Et4NClO4.									
*****									

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
Cs+	gl	alc/w	25°C	100%	U		K1=3.3	1978LMa (102485)	455
Medium: MeOH									
*****									

C24H20B- HL CAS 4358-26-3 (2489)  
Tetraphenylborate;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	sol	alc/w	25°C	50%	C	I		1983BWb (102890)	456
							Kso(CsB(C6H5)4)=-7.48		
Method: spectrophotometry. Data for 20-100% MeOH/H2O									
*****									

Cs+	nmr	non-aq	25°C	100%	U		K1=4.11	1982KPb (102891)	457
Medium: methylamine									
*****									

Cs+	con	non-aq	25°C	100%	U		K1=1.28	1978CAa (102892)	458
Medium: Acetonitrile									
*****									

Cs+	con	non-aq	25°C	100%	U		K1=1.3	1975YKa (102893)	459
Medium: MeCN									

\*\*\*\*\*

C24H24N2O4 L (5741)  
1,10-Di(8-quinolyl)-1,4,7,10-tetraoxadecane; C9H6N.O.C2H4.O.C2H4.O.C2H4.O.C9H6N

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Cs+ con non-aq 25°C 100% U K1=4.2 1989BEa (102936) 460  
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  
-----  
Cs+ dis non-aq 23°C 100% C K1=3.7 1992HGb (102951) 461  
K(Cs+A+L(org))=CsAL(org))=5.28  
K(Cs+A+2L(org))=CsAL2(org))=8.2

Extraction of metal chloride (A) from aqueous solution into nitrobenzene/  
0.01M Bu4NB(Ph)4. Peak potential voltammetry and distribution of 137Cs.

\*\*\*\*\*

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  
-----  
Cs+ dis non-aq 23°C 100% C K1=3.6 1992HGb (102957) 462  
K(Cs+A+L(org))=CsAL(org))=4.71  
K(Cs+A+2L(org))=CsAL2(org))=6.4

Extraction of metal chloride (A) from aqueous solution into nitrobenzene/  
0.01M Bu4NB(Ph)4. Peak potential voltammetry and distribution of 137Cs.

\*\*\*\*\*

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

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Cs+ dis non-aq 25°C 100% U H 1979KLa (103069) 463  
K(Cs(picrate)+L)=5.71

Medium: CHCl3

\*\*\*\*\*

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

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Cs+ dis non-aq 25°C 100% U H 1979KLa (103075) 464  
K(Cs(picrate)+L)=3.28

Medium: CHCl3

\*\*\*\*\*

C24H32O6 L DP(OEEO)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
Cs+	dis	non-aq	25°C	100%	U	H		1979KLa (103081)	465
							K(Cs(picrate)+L)=4.71		

Medium: CHCl3

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	oth	oth/un	25°C	0.05M	C		K1=0.95	2002KLa (103113)	466
Method: capillary electrophoresis. Medium: 0.03-0.06 M CsCl. In CH3CN, K1=3.900.									

Cs+	sp	non-aq	25°C	100%	C		K1=3.10	2002Yeb (103114)	467
Method: steady state fluorescence spectroscopy. Medium: acetonitrile.									

Cs+	con	non-aq	25°C	100%	C T H		K1=4.08	2000SSc (103115)	468
Medium: acetonitrile. Data for 15-45 C. DH(K1)=-27 kJ mol <sup>-1</sup> , DS(K1)=-13 J K <sup>-1</sup> mol <sup>-1</sup> .									

Cs+	oth	alc/w	35°C	3.0%	C		K1=1.15	1999MTd (103116)	469
Method: capillary zone electrophoresis. Medium: 3% v/v EtOH/H2O, 0.005 M phosphate buffer, pH 7.0.									

Cs+	nmr	non-aq	RT	100%	U		K1=2.21	1996GMc (103117)	470
Method: 133Cs nmr. Medium: N,N-dimethylformamide									

Cs+	dis	oth/un	25°C	0	U		K1=3.76	1994OUa (103118)	471
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Cs+	con	non-aq	25°C	100%	U		K1=5.1	1993Eva (103119)	472
Medium: THF+CHCl3 (4:1 vol)									

Cs+	nmr	non-aq	25°C	100%	U		K1=3.68	1991SKa (103120)	473
In acetonitrile.									

Cs+	vlt	non-aq	25°C	100%	U		K1=8.5	1990SPa (103121)	474
Medium: 1,2-dichloroethane									

Cs+	cal	non-aq	25°C	100%	C H		K1=3.85	1986ICa (103122)	475
Medium: MeOH. DH(K1)=-37.9 kJ mol <sup>-1</sup> , DS(K1)=-53.4 J K <sup>-1</sup> mol <sup>-1</sup> .									

Cs+	nmr	non-aq	30°C	100%	U TIH		K1=3.94	1986RPb (103123)	476
In CH3CN. At 75 C, K1=3.19; 50 C, K1=3.57; 5 C. K1=4.50.									

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Cs+ nmr non-aq 20°C 100% U TIH K1=2.32 1986RPb (103124) 477  
 In DMF. At 50 C, K1=1.89; 40 C, K1=2.02; 30 C, K1=2.15; 0 C, K1=2.44  
 Also in 61.5% DMF/38.5% CH3CN and 22.7%/77.3% mixtures.

Cs+ dis non-aq 35°C 100% U I K1=3.4 1980TYb (103125) 478  
 Medium: propylene carbonate

Cs+ cal alc/w 25°C 70% U H K1=2.48 1976ITa (103126) 479  
 Medium: 70% w/w MeOH/H2O. DH(K1)=-37.4 kJ mol-1

Cs+ ISE alc/w 25°C 100% A K1=3.78 1971FRa (103127) 480  
 Medium: MeOH

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
Cs+	dis	non-aq	24°C	100%	C			K(Cs+A+L)=4.65	2002MRd (103230)	481

Medium: CDCl3. HA is picric acid.

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
Cs+	con	non-aq	25°C	100%	U			K1=3.1	1989EVa (103294)	482

Medium: tetrahydrofuran/CHCl3 4:1 (volume)

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
Cs+	cal	alc/w	25°C	80%	C			K1=<2	1995KZa (103353)	483

Medium: 80% v/v CH3OH/H2O.

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
Cs+	sp	non-aq	22°C	100%	U			K1=5.99	1987CCc (103393)	484

In deuteriochloroform

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Cs+	con	alc/w	25°C	100%	U			K1=2.66	1975CJa (103394)	485

Medium: MeOH

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	nmr	non-aq	24°C	100%	U	M		1981BEb (103408)	486

K(Cs(picrate)+L)=5.2

Medium: CDC13

\*\*\*\*\*  
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
Cs+	nmr	non-aq	RT	100%	U		K1=2.89 B2= 4.30	1996GMc (103428)	487

Method: 133Cs nmr. Medium: N,N-dimethylformamide

\*\*\*\*\*  
C24H48N2O9 L BOA15C5 CAS 31255-19-3 (6119)  
3-Oxa-1,5-bis-(1-aza-4,7,10,13-tetraoxacyclopentadecyl)pentane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	ISE	alc/w	25°C	90%	U		K1=3.66 B2=6.80	1988HKA (103457)	488

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
Cs+	gl	alc/w	25°C	100%	C	I	K1=5.9	1975LSc (103463)	489

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
Cs+	gl	R4N.X	25°C	0.10M	U		K1=3.4	1981GLa (103481)	490
Cs+	kin	non-aq	25°C	100%	C		K1=<6.0	1977LSc (103482)	491

Medium: 0.10 M Et4NBr in MeOH.

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	gl	alc/w	25°C	95%	C		K1=2.54	2004KVa (103504)	492

Medium: 95% MeOH/H<sub>2</sub>O, 0.01 M Et<sub>4</sub>NClO<sub>4</sub>.

\*\*\*\*\*

C24H<sub>48</sub>O<sub>12</sub> 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  
-----  
Cs+ cal alc/w 25°C 100% U H K<sub>1</sub>=3.98 1993ILa (103519) 493  
Medium: MeOH. DH=-45.6 kJ mol<sup>-1</sup>.

\*\*\*\*\*

C24H<sub>72</sub>O<sub>12</sub>Si<sub>12</sub> L CAS 18919-94-3 (1287)  
Tetracosamethyl-cyclododecasiloxane; ((CH<sub>3</sub>)<sub>2</sub>SiO)<sub>12</sub>

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Cs+ con alc/w 25°C 100% U K<sub>1</sub>=0.12 1980OPa (103590) 494  
Medium: MeOH, 0.1 M Me<sub>4</sub>NBr

\*\*\*\*\*

C<sub>25</sub>H<sub>22</sub>O<sub>2</sub>P<sub>2</sub> L CAS 207-21-8 (2099)  
Methylenebis(diphenylphosphine oxide); Ph<sub>2</sub>P(O)CH<sub>2</sub>P(O)Ph<sub>2</sub>

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Cs+ con non-aq 25°C 100% U K<sub>1</sub>=2.9 1984YKa (103627) 495  
Medium: tetrahydrofuran + CHCl<sub>3</sub> 4:1, Cs as 2,4-dinitrophenolate

\*\*\*\*\*

C<sub>25</sub>H<sub>37</sub>N<sub>2</sub>O<sub>7</sub>P 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  
-----  
Cs+ dis non-aq 20°C 100% C K(CsP+L)=4.57 1998DDc (103756) 496  
Medium: CHCl<sub>3</sub>. P is picrate.

\*\*\*\*\*

C<sub>25</sub>H<sub>40</sub>O<sub>12</sub> L CAS 239470-22-5 (8948)  
4'-Carboxybenzo-30-crown-10;

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Cs+ con non-aq 25°C 100% C T H K<sub>1</sub>=4.63 1999RGa (103774) 497  
Medium: acetonitrile. Data for 5-35 C. DH(K<sub>1</sub>)=-42.3 kJ mol<sup>-1</sup>, DS(K<sub>1</sub>)=-53 J K<sup>-1</sup> mol<sup>-1</sup>.

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C<sub>25</sub>H<sub>50</sub>N<sub>2</sub>O<sub>8</sub> L BCA15C<sub>5</sub> 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  
-----

Cs+ ISE alc/w 25°C 90% U K1=3.07 B2=6.85 1988HKa (103828) 498  
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  
-----

Cs+ gl R4N.X 25°C 0.10M U K1=2.8 1981GLa (103834) 499

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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  
-----

Cs+ gl alc/w 25°C 95% C K1=4.49 2004KV a (103843) 500

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

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C26H24O2P2 L (6648)

Bis(diphenylphosphinyl)ethane; (C6H5)2PO.CH2CH2.PO(C6H5)2

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

Cs+ con non-aq 25°C 100% U K1=1.4 1990EAb (103910) 501

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  
-----

Cs+ con non-aq 25°C C K1=2.1 1999TEa (103915) 502

In: tetrahydrofurane/CHCl3 4:1 v/v

-----  
Cs+ oth non-aq 25°C 100% U K1=2.1 1995TEa (103916) 503

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

Metal ion is used as 2,4-dinitrophenolate.

\*\*\*\*\*

C26H36N2O6 L DiBzCryptand222 (746)

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

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

Cs+ cal non-aq 25°C 100% U IH 1988DSa (104129) 504

Medium: MeCN. DH(K1)=-42.8 kJ mol<sup>-1</sup>. Also data in propylene carbonate, and dimethylsulphoxide

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Cs+ ISE non-aq 25°C 100% U M K1=3.46 1987DSa (104130) 505

Medium: acetonitrile

\*\*\*\*\*

C26H3609 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  
-----  
Cs+ sp non-aq 25°C 100% C K1=3.07 2002Yeb (104162) 506  
Method: steady state fluorescence spectroscopy. Medium: acetonitrile.

\*\*\*\*\*

C26H3609 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  
-----  
Cs+ cal non-aq 25°C 100% C H K1=3.67 1986ICa (104167) 507  
Medium: MeOH. DH(K1)=-41.97 kJ mol<sup>-1</sup>, DS(K1)=-71 J K<sup>-1</sup> mol<sup>-1</sup>.

-----  
Cs+ nmr non-aq 20°C 100% U TIH K1=2.33 1986RPb (104168) 508  
In DMF. At 40 C, K1=2.05; 30 C, K1=2.20; 10 C, K1=2.58; 0 C, K1=2.78;  
-10 C, K1=2.89

-----  
Cs+ nmr non-aq 20°C 100% U TIH K1=2.50 1986RPb (104169) 509  
In 86.04 % DMF, 13.96 % CH<sub>3</sub>CN. At 40 C, K1=2.17; 30 C, K1=2.28; 10C, K1=2.64  
, 0 C, K1=2.79; -10 C, K1=2.96. Data also in 61.5% DMF and 22.7% DMF

-----  
Cs+ nmr non-aq 30°C 100% U TIH K1=3.89 1986RPb (104170) 510  
In CH<sub>3</sub>CN. At 77 C, K1=3.09; 45 C, K1=3.63; 9 C, K1=4.24, and other temps.

-----  
Cs+ cal alc/w 25°C 70% U H K1=1.42 1976ITa (104171) 511  
Medium: 70% w/w MeOH/H<sub>2</sub>O. DH(K1)=-25.7 kJ mol<sup>-1</sup>

\*\*\*\*\*

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  
-----  
Cs+ dis non-aq 24°C 100% C K(Cs+A+L)=5.34 2002MRd (104211) 512

Medium: CDCl<sub>3</sub>. HA is picric acid.

\*\*\*\*\*

C26H3808 L (2507)  
2,5,8,11,16,19,22,25-Octaoxa-12,13:14,15-dibenzoheptacos-12,14-diene;

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Cs+ con alc/w 25°C 100% U K1=1.43 1975CJa (104218) 513  
Medium: MeOH

\*\*\*\*\*



C26H40O11P2 L (5727)  
 1,7-Bis(2-(diethoxyphosphinylmethoxy)phenyl)-1,4,7-trioxahепtane;2(EtO)2PO.CH2OC6H4  
 C2H4OC2H4)2O

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	con	non-aq	25°C	100%	U		K1=3.6	1989EVa (104242)	514

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
Cs+	dis	none	25°C	dil	C		K1=8.10 K(Cs+A+L(org))=CsAL(org))=5.83	1987BBf (104278)	515

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
Cs+	cal	alc/w	25°C	100%	U	H	K1=2.55	1987BUb (104294)	516

In MeOH. DH=-3.3 kJ mol<sup>-1</sup>

\*\*\*\*\*  
 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
Cs+	nmr	non-aq	24°C	100%	U	M	K(Cs(picrate)+L)=5.9	1981BEb (104308)	517

Medium: CDCl3

\*\*\*\*\*  
 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
Cs+	gl	R4N.X	25°C	0.10M	U		K1=<2	1981GLa (104327)	518

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	gl	alc/w	25°C	95%	C		K1=3.51	2004KVa (104338)	519

Medium: 95% MeOH/H2O, 0.01 M Et4NC104.

\*\*\*\*\*

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

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Cs+ gl alc/w 25°C 95% C K1=1.76 2004KVa (104348) 520  
Medium: 95% MeOH/H2O, 0.01 M Et4NClO4.

\*\*\*\*\*

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  
-----  
Cs+ con non-aq 25°C 100% U K1=1.3 1990EAb (104400) 521  
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  
-----  
Cs+ oth non-aq 25°C 100% U K1=2.2 1995TEa (104405) 522  
Medium: tetrahydrofuran:CHCl3 4:1 (v/v).  
Metal ion is used as 2,4-dinitrophenolate.

\*\*\*\*\*

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  
-----  
Cs+ con non-aq 25°C 100% U K1=3.9 1989BEa (104674) 523  
Medium: tetrahydrofuran/CHCl3 4:1 (volume)

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C28H24O6 L TetBz18-Crown-6 CAS 99700-20-6 (6070)  
2,3:8,9:11,12:14,15-Tetrabenzo-1,4,7,10,13,16-hexaoxacyclooctadeca-2,8,11,14-tetraene

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Cs+ dis non-aq 23°C 100% C K1=3.0 1992HGb (104680) 524  
K(Cs+A+L(org))=CsAL(org))=4.12  
K(Cs+A+2L(org))=CsAL2(org))=5.8

Extraction of metal chloride (A) from aqueous solution into nitrobenzene/  
0.01M Bu4NB(Ph)4. Peak potential voltammetry and distribution of 137Cs.

\*\*\*\*\*

C28H2406 L CAS 72011-26-8 (8874)  
 2,3:8,9:11,12:17,18-Tetrabenzo-1,4,7,10,13,16-hexaoxacyclooctadeca-2,8,11,17-tetraene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	dis	non-aq	23°C	100%	C		K1=2.5	1992HGb (104685)	525

Extraction of metal chloride (A) from aqueous solution into nitrobenzene/  
 0.01M Bu4NB(Ph)4. Peak potential voltammetry and distribution of 137Cs.

\*\*\*\*\*  
 C28H2803P2 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
Cs+	con	non-aq	25°C	100%	U		K1=3.7	1993EVa (104708)	526

Medium: THF+CHCl3 (4:1 vol)

Cs+	con	non-aq	25°C	100%	U		K1=1.9	1992BEa (104709)	527
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Medium: THF+CHCl3 (4:1 vol)

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 C28H2804P2 L (7891)  
 1,6-Bis(diphenylphosphinyl)-2,5-dioxohexane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	con	non-aq	25°C		C		K1=2.7	1999TEa (104720)	528

In: tetrahydrofuran/CHCl3 4:1 v/v

\*\*\*\*\*  
 C28H30N202P2 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
Cs+	con	non-aq	25°C	100%	U		K1=2.4	1984YKa (104725)	529

Medium: tetrahydrofuran + CHCl3 4:1, Cs as 2,4-dinitrophenolate

\*\*\*\*\*  
 C28H32N206 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
Cs+	con	non-aq	25°C	100%	U		K1=4.9	1989BEa (104748)	530

Medium: tetrahydrofuran/CHCl3 4:1 (volume)

\*\*\*\*\*  
 C28H4006 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
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Cs+ con alc/w 25°C 100% U I M 1979BDa (104836) 531

K(CsCl+L)=3.54

Medium: MeOH. In DMSO: K(CsClO4+L)=3.31. In MeCN: K(CsBPh4+L)=3.37

\*\*\*\*\*

C28H40O8 L AN(MOE0EOM)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  
-----

Cs+ dis non-aq 25°C 100% U H 1979KLa (104855) 532

K(Cs(picrate)+L)=3.79

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  
-----

Cs+ con non-aq 25°C 100% C T H K1=4.20 2000SSc (104875) 533

Medium: acetonitrile. Data for 15-45 C. DH(K1)=-38 kJ mol<sup>-1</sup>,  
DS(K1)=-49 J K<sup>-1</sup> mol<sup>-1</sup>.

-----  
Cs+ nmr non-aq RT 100% U K1=1.79 1996GMc (104876) 534

Method: 133Cs nmr. Medium: N,N-dimethylformamide

-----  
Cs+ dis oth/un 25°C 0 U K1=4.11 19940Ua (104877) 535

-----  
Cs+ con non-aq 25°C 100% U I K1=4.92 1991ASb (104878) 536

Medium: 1,2-dichlorethane. In nitromethane: K1=4.56; in MeCN: K=3.81;  
in acetone: K=3.70

-----  
Cs+ vlt non-aq 25°C 100% U K1=9.4 1990SPa (104879) 537

Medium: 1,2-dichloroethane

-----  
Cs+ nmr alc/w 30°C 100% U TIH K1=4.18 1979SPc (104880) 538

Medium: MeOH, DH(K1)=-53.2 kJ mol<sup>-1</sup>. In py: K=4.41, DH=-33.2. In CH3CN, K=3.39, DH=-21.5. In CH3NO2: K=4.30, DH=-33.3. In acetone: K=4.04, DH=-56.4

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Cs+ nmr non-aq 20°C 100% U K1=4.23 1976LCa (104881) 539

Medium: acetone

\*\*\*\*\*

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  
-----

Cs+ con non-aq 25°C 100% U K1=4.2 1989EVa (104944) 540

Medium: tetrahydrofuran/CHCl3 4:1 (volume)

\*\*\*\*\*

C28H47NO11 L (1689)  
N-(2-(2-(4'-Benzo-15-crown-5)-oxyethoxy)ethyl-1,4,7,10-tetraoxa-13-azacyclopentadecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	ISE	alc/w	25°C	10%	U		K1=3.23	1986HAa (104967)	541

Medium: 10% MeOH/H2O

\*\*\*\*\*  
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
Cs+	nmr	non-aq	24°C	100%	U	M		1981BEb (105008)	542

K(Cs(picrate)+L)=3.5

Medium: CDCl3

\*\*\*\*\*  
C28H52O6 L (5352)  
Di(t-butylcyclohexyl)-18-crown-6

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	oth	oth/un	25°C	dil	U		K1=0.9	1970MSa (105014)	543

\*\*\*\*\*

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
Cs+	ISE	alc/w	25°C	90%	U		K1=3.66 B2=6.80	1988HKA (105032)	544

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
Cs+	gl	alc/w	25°C	95%	C		K1=3.48	2004KVa (105039)	545

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]dotetratricontane-5,22-dithio

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	gl	alc/w	25°C	95%	C		K1=1.70	2004KVa (105049)	546

Medium: 95% MeOH/H<sub>2</sub>O, 0.01 M Et<sub>4</sub>NClO<sub>4</sub>.

\*\*\*\*\*

C29H30O3P2 L CAS 176849-77-7 (7160)

1,6-Bis(diphenylphosphinyl)-2-oxohexane;

---

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Cs+	oth	non-aq	25°C	100%	U			K1=2.0	1995TEa (105078)	547

Medium: tetrahydrofurane:CHCl<sub>3</sub> 4:1 (v/v).

Metal ion is used as 2,4-dinitrophenolate.

\*\*\*\*\*

C29H30O3P2 L CAS 176849-78-8 (7161)

1,6-Bis(diphenylphosphinyl)-3-oxohexane;

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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Cs+	oth	non-aq	25°C	100%	U			K1=2.0	1995TEa (105083)	548

Medium: tetrahydrofurane:CHCl<sub>3</sub> 4:1 (v/v).

Metal ion is used as 2,4-dinitrophenolate.

\*\*\*\*\*

C29H30O4P2 L (7897)

1,7-Bis(diphenylphosphinyl)-2,6-dioxoheptane;

---

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Cs+	con	non-aq	25°C		C			K1=2.7	1999TEa (105088)	549

In: tetrahydrofurane/CHCl<sub>3</sub> 4:1 v/v

\*\*\*\*\*

C29H35NO5 L CAS 201154-06-5 (7825)

N-(1-Pyrenylmethyl)-1,4,7,10,13-pentaoxa-16-azacyclooctadecane;

---

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Cs+	sp	mixed	25°C	90%	C				1997KKa (105099)	550

K(CsSCN+L)=3.67

Method: fluorescence emission. Medium: MeOH/CHCl<sub>3</sub> (9:1 v/v).

\*\*\*\*\*

C29H40N2O6Cl2 L CAS 181706-77-4 (8627)

3,18-Dichlorooctahydro-5H,16H-6,15-(ethanoxyethanoxyethano)-dibenzotetraoxaazacycloheneicosine;

---

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Cs+	cal	non-aq	25°C	100%	C	H		K1=2.90	1998ZBc (105136)	551

Medium: MeOH. DH(K<sub>1</sub>)=-19.5 kJ mol<sup>-1</sup>, DS(K<sub>1</sub>)=-9.90 J K<sup>-1</sup> mol<sup>-1</sup>.

\*\*\*\*\*

C29H58N2O10 L BCA18C6 CAS 74776-87-7 (6117)

1,5-Bis-(1-aza-4,7,10,13,16-pentaoxacyclooctadecyl)pentane;

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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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-----  
Cs+ ISE alc/w 25°C 90% U K1=3.36 B2=6.73 1988HKA (105169) 552  
Medium: 90% w/w MeOH/H2O

\*\*\*\*\*  
C30H30N2O010 L CAS 259886-49-2 (8959)  
Cucurbit[5]uril;  
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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Cs+ sol none 25°C dil C K1=0.90 2001BCf (105215) 553  
Method: dissolution of ligand in a 0.002-0.02 M CsX solution; spectrophoto  
metric measurement.

\*\*\*\*\*  
C30H32O4P2 L (6816)  
1,8-Bis(diphenylphosphinyl)-3,6-dioxaoctane;  
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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Cs+ con non-aq 25°C 100% U K1=2.2 1992BEa (105226) 554  
Medium: THF+CHCl3 (4:1 vol)

\*\*\*\*\*  
C30H32O5P2 L (7892)  
1,9-Bis(diphenylphosphinyl)-2,5,8-trioxononane;  
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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Cs+ con non-aq 25°C C K1=3.2 1999TEa (105234) 555  
In: tetrahydrofuran/CHCl3 4:1 v/v

\*\*\*\*\*  
C30H34N2O2P2 L CAS 68743-31-3 (2066)  
Diaminoethane-N,N'-di-2-ethyldiphenylphosphine oxide; (CH2.NH.C2H4.P(O)(C6H5)2)2  
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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Cs+ con non-aq 25°C 100% U K1=2.1 1986STb (105239) 556  
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;  
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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Cs+ sp non-aq 25°C 100% U K1=3.3 1996AAb (105252) 557  
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
Cs+	dis	non-aq	25°C	100%	U	H		1979KLa (105259)	558
K(Cs(picrate)+L)=6.57									
Medium: CHCl <sub>3</sub>									
*****									
C30H38N2O4		L					(5828)		
Trimethoxyphenylcryptand 3,1.									
25,26,27-Trimethoxy-5,10,15-trimethyl-22-oxa-1,19-diazatetra-									
Cs+	nmr	non-aq	25°C	100%	U		K1=<5.24	1986CHc (105271)	559
In CDCl <sub>3</sub>									
*****									
C30H42O10P4		L					CAS 97910-31-1 (2083)		
Tris-((2-(dimethylphosphinylmethoxy)phenoxy)methyl)phosphine oxide;									
Cs+	con	non-aq	25°C	100%	U		K1=3.04	1989KSa (105300)	560
Medium: tetrahydrofuran/CHCl <sub>3</sub> 4:1 (vol)									
*****									
C30H48O13P2		L					CAS 112120-14-6 (5729)		
1,13-Bis(2-(diethoxyphosphinylmethoxy)phenyl)-1,4,7,10,13-pentaoxatridecane;									
Cs+	con	non-aq	25°C	100%	U		K1=4.6	1989EVa (105342)	561
Medium: tetrahydrofuran/CHCl <sub>3</sub> 4:1 (volume)									
*****									
C31H34O4P2		L					(7157)		
1,9-Bis(diphenylphosphinyl)-3,7-dioxononane;									
Cs+	oth	non-aq	25°C	100%	U		K1=1.8	1995TEa (105524)	562
Medium: THF:CHCl <sub>3</sub> 4:1 v/v. Cs as 2,4-dinitrophenolate. Also other similar ligands									
*****									
C32H29O3P3		L					CAS 21851-89-8 (2640)		
P,P,P',P'',P'''-Pentaphenyldimethylenetri(phosphineoxide); (Ph <sub>2</sub> P(O)CH <sub>2</sub> ) <sub>2</sub> P(O)Ph									
Cs+	sp	non-aq	25°C	100%	U	M		1981SPb (105581)	563
K(CsI+L)=1.30									
Medium: CH <sub>3</sub> CN									
*****									



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
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Cs+	con	non-aq	25°C	100%	U			K1=2.8	1992BEa (105644)	564
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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
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Cs+	con	non-aq	25°C		C			K1=3.7	1999TEa (105649)	565
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In: tetrahydrofuran/CHCl3 4:1 v/v

C32H38N4O6Cl2 HL CAS 172033-56-6 (8675)

2,2'-[1,4,10,13-Tetraoxa-7,16-diazacyclooctadecane-7,16-diylbis(methylene)]bis[5-Cl-8-quinolinol]

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Cs+	cal	non-aq	25°C	100%	C	H			1995ZBa (105678)	566
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K(Cs+HL)=2.70

Medium: methanol. DH(K)=-36.9 kJ mol<sup>-1</sup>, DS(K)=-72.2 J K<sup>-1</sup> mol<sup>-1</sup>.

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
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Cs+	con	non-aq	25°C	100%	U			K1=4.2	1989BEa (105775)	567
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Medium: tetrahydrofuran/CHCl3 4:1 (volume)

C32H46N2O8Cl2 L CAS 181706-75-2 (8626)

3,18-Dichlorododecahydro-5H,16H-6,15-(ethanoxyethanoxyethano)dibenzohexaoxadiazacyclohexacosine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Cs+	cal	non-aq	25°C	100%	C	H		K1=3.94	1998ZBc (105786)	568
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Medium: MeOH. DH(K1)=-47.5 kJ mol<sup>-1</sup>, DS(K1)=-83.9 J K<sup>-1</sup> mol<sup>-1</sup>.

C32H52O14P2 L CAS 112120-15-7 (5730)

1,13-Bis(2-(diethoxyphosphinylmethoxy)phenyl)-1,4,7,10,13,16-hexaoxahexadecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Cs+	con	non-aq	25°C	100%	U			K1=4.8	1989Eva (105822)	569
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Medium: tetrahydrofuran/CHCl<sub>3</sub> 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;

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Cs+ ISE alc/w 25°C 10% U K1=3.21 B2=6.27 1986HAa (105831) 570  
Medium: 10% MeOH/H<sub>2</sub>O

\*\*\*\*\*

C32H64N4O10 L CAS 42133-16-4 (8579)  
4,10,13,19,25,28,33,36,41,44-Decaoxa-1,7,16,22-tetraazatricyclo[20.8.8.87,16]hexate tracontane;

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Cs+ ISE alc/w 25°C 95% C K1=4.4 1977LSc (105849) 571  
K(CsL+Cs)=3.0

Medium: 95% (w/w) MeOH/H<sub>2</sub>O, 0.1 M Et<sub>4</sub>NBr.

\*\*\*\*\*

C32H66N2O4 L 22DD Kryptofix CAS 79495-97-9 (6655)  
1,10-Didecyl-1,10-diaza-4,7,13,16-tetraoxacyclooctadecane;

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Cs+ cal alc/w 25°C 100% U H 1986BUd (105861) 572  
In MeOH. DH=-21.7 kJ mol<sup>-1</sup>

\*\*\*\*\*

C33H41N3O6Cl<sub>2</sub> 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  
-----  
Cs+ cal non-aq 25°C 100% C H K1=3.58 1998ZBc (105926) 573  
Medium: MeOH. DH(K1)=-26.5 kJ mol<sup>-1</sup>, DS(K1)=-20.4 J K<sup>-1</sup> mol<sup>-1</sup>.

\*\*\*\*\*

C33H46N2O12 L (7049)  
1,4-Diaza-1,4-di(5'-benzo-15-crown-5)-hepta-2,6-dione; CH<sub>2</sub>(CH<sub>2</sub>CONH.C<sub>14</sub>H<sub>19</sub>O<sub>5</sub>)<sub>2</sub>

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Cs+ sp non-aq 25°C 100% U K1=7.03 1979KMb (105980) 574  
Medium: CHCl<sub>3</sub>

\*\*\*\*\*

C34H38O12P<sub>2</sub> 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
Cs+	oth	non-aq	22°C	100%	U		K1=0.3	1978YSa (106038)	575

Medium: 1:1 v/v EtOH+CHCl<sub>3</sub>. Cs as acetate salt

\*\*\*\*\*

C34H40O6P2 L CAS 137728-08-6 (6838)

1,14-Bis(diphenylphosphinyl)-3,5,8,11-tetraoxatetradecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	con	non-aq	25°C	100%	U		K1=3.7	1992BEa (106042)	576

Medium: THF+CHCl<sub>3</sub> (4:1 vol)

\*\*\*\*\*

C34H40O7P2 L (7894)

1,15-Bis(diphenylphosphinyl)-2,5,8,11,14-pentaoxopentadecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	con	non-aq	25°C		C		K1=4.2	1999TEa (106049)	577

In: tetrahydrofuran/CHCl<sub>3</sub> 4:1 v/v

\*\*\*\*\*

C34H42N2O6Cl2 L CAS 181706-79-6 (8629)

3,18-Dichlorooctahydro-5H,16H-6,15-(ethanoxyethanoxyethano)tribenzotetraoxadiazacyc  
lodocosine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	cal	non-aq	25°C	100%	C	H	K1=3.72	1998ZBc (106057)	578

Medium: MeOH. DH(K1)=-29.7 kJ mol<sup>-1</sup>, DS(K1)=-28.4 J K<sup>-1</sup> mol<sup>-1</sup>.

\*\*\*\*\*

C34H44N2O5 L CAS 101671-92-5 (5825)

Trimethoxyphenylcryptand 3,1,1.

30,31,32-Trimethoxy-5,10,15-trimethyl-22,27-dioxo-1,9-diaza....

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	nmr	non-aq	25°C	100%	U		K1=7.63	1986CHc (106067)	579

Medium: CDCl<sub>3</sub>

\*\*\*\*\*

C34H53O8Br H2L CAS 38784-08-6 (2336)

5-Bromolasalocid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	gl	alc/w	25°C	100%	M	H		1988PJ a (106097)	580

K(Cs+HL)=3.44

Medium: MeOH. DH = -14.4 kJ mol<sup>-1</sup>; DS = 19

\*\*\*\*\*

C34H54O8 H2L Lasalocid CAS 25999-20-6 (2335)

Lasalocid acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	nmr	non-aq	20°C	100%	C		K(Cs+HL)=2.0	1998MLa (106128)	581

Medium: CD3OD. Method: 13C nmr.

Cs+	dis	oth/un	25°C	0.0	U		K1=1.0	1992LPb (106129)	582
Cs+	gl	alc/w	25°C	100%	M	H	K(Cs+HL)=3.5	1988PJa (106130)	583

Medium: MeOH. DH = -15.1 kJ mol<sup>-1</sup>; DS = 16

Cs+	gl	alc/w	25°C	100%	U		K(Cs+2HL)=3.36	1982BDc (106131)	584
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Medium: MeOH

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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
Cs+	ISE	alc/w	25°C	95%	C		K1=3.5 K(CsL+Cs)=2.5	1977LSc (106180)	585

Medium: 95% (w/w) MeOH/H2O, 0.1 M Et4NBr.

\*\*\*\*\*

C36H3003Si3 L CAS 512-63-0 (1285)  
Hexaphenyl-cyclotrisiloxane; ((C6H5)2SiO)3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	con	alc/w	25°C	100%	U		K1=<-0.3	19800Pa (106215)	586

Medium: MeOH, 0.1 M Me4NBr

\*\*\*\*\*

C36H32N2O6 L (5744)  
5,6:11,12-Dibenzo-1,16-di(8-quinolyl)-1,4,7,10,13,16-hexaoxahexadecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	con	non-aq	25°C	100%	U		K1=4.9	1989BEa (106218)	587

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
Cs+	sol	none	25°C	dil	C		K1=2.52	2001BCf (106256)	588

Method: dissolution of ligand in a 0.002-0.02 M CsX solution;

spectrophotometric measurement.

-----  
Cs+ sol none 25°C 0.0 U K1=9.64 1992BCa (106257) 589  
\*\*\*\*\*

C36H36O4P2 L (2073)  
3-t-Butyl-1,2-dihydroxybenzene bis(diphenylphosphinylmethyl) ether  
-----

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

Cs+ con non-aq 25°C 100% U K1=2.48 1989KSa (106279) 590  
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  
-----

Cs+ con non-aq 25°C 100% U K1=3.30 1989KSa (106283) 591  
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  
-----

Cs+ dis non-aq 25°C 100% U H 1979KLa (106293) 592  
K(Cs(picrate)+L)=2.9  
Medium: CHCl3  
\*\*\*\*\*

C36H40O6 L ANANAN(MOM)2ANAN 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  
-----

Cs+ dis non-aq 25°C 100% U H 1979KLa (106299) 593  
K(Cs(picrate)+L)=3.94  
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  
-----

Cs+ dis non-aq 25°C 100% U H 1979KLa (106305) 594  
K(Cs(picrate)+L)=2.85  
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
Cs+	con	non-aq	25°C	100%	U		K1=3.7	1992BEa (106333)	595
Medium: THF+CHCl3 (4:1 vol)									
*****									
C36H44O8P2		L					(7895)		
1,18-Bis(diphenylphosphinyl)-hexaoxooctadecane;									
Cs+	con	non-aq	25°C		C		K1=4.7	1999TEa (106343)	596
In: tetrahydrofurane/CHCl3 4:1 v/v									
*****									
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-									
Cs+	nmr	non-aq	25°C	100%	U		K1=12.009	1986CHc (106377)	597
In CDCl3									
*****									
C36H52O14P2		L					(5739)		
3,4:12,13:21,22-Tribenzo-1,24-di(diethoxyphosphinyl)-2,5,8,11,14,17,20,23-octaoxate									
tracosatriene;									
Cs+	con	non-aq	25°C	100%	U		K1=4.7	1989BEa (106395)	598
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;									
Cs+	ISE	alc/w	25°C	90%	U		K1=2.62 B2=3.01	1987KH a (106417)	599
90% w/w MeOH/H2O. Also data for the 1,4,7,10-tetraoxadecane-bridged									
ligand: K1=2.89; K2=0.74.									
*****									
C36H56O6		L					CAS 54535-81-8	(1263)	
2,3:11,12-Bis(3',5'-di-tert-butylbenzo)-1,4,7,10,13,16-hexaoxacyclooctadecane;									
Cs+	con	alc/w	25°C	100%	U	I M		1979BDa (106435)	600
K(CsCl+L)=3.17									
Medium: MeOH. In DMSO: K(CsClO4+L)=3.13. In MeCN: K(CsBPh4+L)=3.43									
*****									

C36H62O11 HL Monensin CAS 17090-79-8 (737)  
 Monensin, 1,6-dioxaspiro[4,5]decane derivative;

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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Cs+ con non-aq 25°C 100% C H K1=1.3 1997PBb (106492) 601  
 Medium: acetonitrile. Additional method: potentiometry with ISE.  
 By calorimetry, DH(K1)=-36 kJ mol<sup>-1</sup>, DS(K1)=-95 J K<sup>-1</sup> mol<sup>-1</sup>.

---

Cs+ vlt non-aq 25°C 100% C I K1=6.2 1997WRa (106493) 602  
 Method: cyclic voltammetry. Medium: acetonitrile, 0.05 M Et4NClO4.  
 In DMSO, K1=3.3; in acetone, K1=5.5.

---

Cs+ vlt non-aq 23°C 100% U I K1=6.2 1994FRa (106494) 603  
 Medium: MeCN. In PrCN: K1=5.6; acetone: 5.5; DMF: 5.4; Me-pyrrol.: 4.3;  
 NN-DMA: 3.9; DMSO: 3.3; Di-Et-formamide: 3.3; Di-Et-acetamide: 3.1; PC: 5.6

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Cs+ ISE alc/w 25°C 100% M K1=3.59 1984CTa (106495) 604  
 Medium: MeOH

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Cs+ ISE non-aq 25°C 100% M K1=4.64 1984CTa (106496) 605  
 Medium: N,N-dimethylformamide. In DMSO K1=3.24

---

Cs+ ISE alc/w 25°C 100% U K1=5.18 1984CTb (106497) 606  
 Medium: EtOH

---

Cs+ gl alc/w 25°C 100% U K1=3.75 1978HPa (106498) 607  
 \*\*\*\*\*

C37H54N2O14 L (7050)  
 1,4-Diaza-1,4-di(5'-benzo-18-crown-6)-hepta-2,6-dione; CH2(CH2CONH.C16H23O6)2

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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Cs+ sp non-aq 25°C 100% U K1=8.54 1979KMb (106631) 608  
 Medium: CHCl3

\*\*\*\*\*

C38H32O3P2 L (6804)  
 1,3-Bis(2-Diphenylphosphinylphenyl)-2-oxapropane; O(CH2.C6H4(PO.(C6H5)2)

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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Cs+ con non-aq 25°C 100% U K1=2.7 1993BEb (106641) 609  
 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

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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Cs+ con non-aq 25°C 100% U K1=2.9 1991EBa (106647) 610  
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
Cs+	con	non-aq	25°C	100%	U		K1=3.4	1993EVa (106658)	611
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
Cs+	con	non-aq	25°C	100%	U		K1=4.4	1992BEa (106679)	612
Medium: THF+CHCl3 (4:1 vol)									

\*\*\*\*\*  
C38H48O9P2 L (7896)  
1,21-Bis(diphenylphosphinyl)-2,5,8,11,14,17,20-heptaoheneeicosane;  
-----

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	con	non-aq	25°C		C		K1=4.8	1999TEa (106684)	613
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
Cs+	nmr	non-aq	25°C	100%	U		K1=15.91	1986CHc (106689)	614
In CDCl3									

\*\*\*\*\*  
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
Cs+	sp	non-aq	25°C	100%	C		K1=4.7 K(CsL+L)=1.7	20010Ya (106720)	615

Medium: methanol. For the 1,4-butanediyl derivative, K1=4.6, K(CsL+L)=2.0.  
\*\*\*\*\*  
C40H36O4P2 L (6805)  
1,6-Bis(2-Diphenylphosphinylphenyl)-2,5-dioxahexane; (CH2.O.CH2.C6H4(PO(6H5)2)2  
-----



Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	con	non-aq	25°C	100%	U		K1=2.4	1993BEb (106732)	616
Medium: THF+CHCl3 4:1(vol)									
*****									
C40H3605P2		L					CAS 86341-96-0 (5724)		
1,7-Di(2-diphenylphosphinyl)phenyl-1,4,7-trioxaheptane;Ph2PO.C6H4.O.C2H4.O.C2H4.O.C6H4.POPh2									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	con	non-aq	25°C	100%	U		K1=3.6	1991EBa (106744)	617
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									
*****									
C40H4404P2		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
Cs+	con	non-aq	25°C	100%	U		K1=2.27	1989KSa (106763)	618
Medium: tetrahydrofuran/CHCl3 4:1 (vol)									
*****									
C40H4608		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
Cs+	sp	non-aq	25°C	100%	C H		K1=4.2	1995CUa (106775)	619
Medium: methanol, 0.01 M Et4NCl. By calorimetry: DH(K1)=-23 kJ mol <sup>-1</sup> , DS(K1)=2 J K <sup>-1</sup> mol <sup>-1</sup> .									
*****									
C40H4808		L					AN2DP(OEOEO)2E (2235)		
3,4,5,6-Bis(3-methyl-5-(2-methoxy-5-methylbenzo))-2,7,10,13,16,19-hexaoxacyclodocosane-3,5-diene;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	dis	non-aq	25°C	100%	U H			1979KLa (106793)	620
K(Cs(picrate)+L)=5.49									
Medium: CHCl3									
*****									
C40H50N20010		L					CAS 143902-45-8 (8935)		
Decamethylcucurbit[5]uril;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	cal	mixed	25°C	50%	C H		K1=1.57	2000ZKb (106805)	621
Medium: 50% v/v formic acid/H2O. DH(K1)=-18.4 kJ mol <sup>-1</sup> , DS(K1)=-32 J K <sup>-1</sup> mol <sup>-1</sup> .									

\*\*\*\*\*

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  
-----  
Cs+ ISE non-aq 25°C 100% C K1=3.47 1998WLC (106821) 622  
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-octa-  
xatetracosane;

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Cs+ con non-aq 25°C 100% U K1=4.8 1989BEa (106826) 623  
Medium: tetrahydrofuran/CHCl3 4:1 (volume)

\*\*\*\*\*

C40H62O12 L CAS 86116-05-4 (5648)  
1,8-Bis(4'-(2,3-benzo-1,4,7,10,13,16-hexaoxacyclooctadecane))-octane;

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Cs+ ISE alc/w 25°C 90% U K1=4.07 B2=4.57 1987KHa (106834) 624  
90% w/w MeOH/H2O. Also data for the 1,4,7,10-tetraoxadecane-bridged  
ligand: K1=4.20; K2=0.67.

\*\*\*\*\*

C40H64O12 L Nonactin CAS 6833-84-7 (4179)  
Nonactin

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Cs+ sp non-aq 25°C 100% C K1=3.18 1977CEb (106838) 625  
Method: temperature jump relaxation. Medium: MeOH.

-----  
Cs+ vlt non-aq 22°C 100% U K1=2.59 1974RKd (106839) 626  
Medium: 0.025 NBu4ClO4 in CH3CN

-----  
Cs+ oth alc/w 30°C 100% U K1=2.86 1973ZFa (106840) 627  
Method: vapour pressure osmometry. Medium: methanol.

-----  
Cs+ nmr non-aq 17°C 100% U K1=4.0 1970PCa (106841) 628  
Medium: CsClO4 in acetone. With 0.5 mol fraction water, K1=2.6

\*\*\*\*\*

C41H42O6 L CAS 151832-07-4 (6874)  
9-(Dimethylethyl)-29,30,31,32,33-pentamethoxy-23-oxahexacyclotritriacontapentadecan-  
e;

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

Cs+ dis non-aq 25°C 100% U 1993HSa (106869) 629  
K(Cs(picrate)+L)=5.52

Medium: CDCl3

\*\*\*\*\*

C41H66O12 L Monactin CAS 7182-54-9 (4180)  
Monactin

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

Cs+ sp non-aq 25°C 100% C K1=3.30 1977CEb (106885) 630  
Method: temperature jump relaxation. Medium: MeOH.

-----  
Cs+ oth alc/w 30°C 100% U K1=3.04 1973ZFa (106886) 631  
Method: vapour pressure osmometry. Medium: MeOH

\*\*\*\*\*

C42H40O4P2 L (7153)  
1,2-Bis(2-(2-(diphenylphosphinyl)ethyl)phenoxy)ethane

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

Cs+ oth non-aq 25°C 100% U K1=1.8 1995TEa (106910) 632  
Medium: THF:CHCl3 4:1 v/v. Cs 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  
-----

Cs+ con non-aq 25°C 100% U K1=2.3 1993BEb (106915) 633  
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  
-----

Cs+ con non-aq 25°C 100% U K1=2.8 1993BEb (106923) 634  
Medium: THF+CHCl3 4:1(vol)

-----  
Cs+ con non-aq 25°C 100% U K1=2.21 1989KSa (106924) 635  
Medium: tetrahydrofuran/CHCl3 4:1 (vol)

\*\*\*\*\*

C42H40O7P2 L CAS 95651-36-8 (2079)  
1,7-Di(2-(diphenylphosphinylmethoxy)phenyl)-1,4,7-trioxaheptane;  
(Ph2PO.CH2.O.C6H4.O.C2H4)2O

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

Cs+ con non-aq 25°C 100% U K1=3.50 1989KSa (106933) 636  
Medium: tetrahydrofuran/CHCl3 4:1 (vol)

-----  
Cs+ con non-aq 25°C 100% U K1=3.50 1989TKb (106934) 637  
Medium: tetrahydrofuran/CHCl3 4:1 (volume)

\*\*\*\*\*

C42H5007 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  
-----  
Cs+ sp non-aq 25°C 100% C K1=4.8 2000PBa (106948) 638  
Medium: MeOH.

-----  
Cs+ dis non-aq 22°C 100% C M 1996CPa (106949) 639  
K(CsA+L(org))=CsAL(org))=6.87  
Medium: CHCl3 saturated with H2O. Method: extraction of CsA into CHCl3/L  
solution. HA is picric acid. For the cone conformation, K=<4.

\*\*\*\*\*

C42H68012 L CAS 20261-85-2 (5373)  
Dinactin;

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Cs+ sp non-aq 25°C 100% C K1=3.62 1977CEb (106978) 640  
Method: temperature jump relaxation. Medium: MeOH.

-----  
Cs+ oth alc/w 30°C 100% U K1=3.23 1973ZFa (106979) 641  
Method: vapour pressure osmometry. Medium: MeOH

\*\*\*\*\*

C43H4204P2 L (7156)  
1,3-Bis((2-diphenylphosphinyl)phenoxy)propane;

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Cs+ oth non-aq 25°C 100% U K1=1.8 1995TEa (106998) 642  
Medium: THF:CHCl3 4:1 v/v. Cs as 2,4-dinitrophenolate. Also other si  
milar ligands

\*\*\*\*\*

C43H4206P2 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  
-----  
Cs+ con non-aq 25°C 100% U K1=1.30 1989TKb (107003) 643  
Medium: tetrahydrofuran/CHCl3 4:1 (volume)

\*\*\*\*\*

C43H70012 L CAS 7561-71-9 (5374)  
Trinactin;

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

-----  
Cs+ oth alc/w 30°C 100% U K1=3.34 1973ZFa (107030) 644  
Method: vapour pressure osmometry. Medium: MeOH

\*\*\*\*\*

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  
-----

Cs+ con non-aq 25°C 100% U K1=1.9 1993BEb (107089) 645  
Medium: THF+CHCl3 4:1(vol)

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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  
-----

Cs+ con non-aq 25°C 100% U K1=3.7 1993BEb (107108) 646  
Medium: THF+CHCl3 4:1(vol)

\*\*\*\*\*

C44H44O5P2 L (5733)  
1,7-Di(2-(diphenylphosphinylethyl)phenyl)-1,4,7-trioxaheptane;  
(Ph2PO.C2H2.C6H4.OC2H4)2O

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

Cs+ oth non-aq 25°C 100% U K1=1.7 1995TEa (107116) 647  
Medium: THF:CHCl3 4:1 v/v. Cs as 2,4-dinitrophenolate

\*\*\*\*\*

C44H50N2O6 L (9016)  
4,13-Bis[2-(9-anthryloxy)ethyl]-4,13-diaza-18-crown-6;

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

Cs+ sp non-aq 20°C 100% C K1=3.42 2002MTb (107135) 648  
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  
-----

Cs+ gl non-aq 25°C 100% C K1=3.1 2000ABb (107142) 649  
B(Cs2L)=7.50

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
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Cs+ sp non-aq 25°C 100% C K1=1.9 1999USa (107157) 650  
Medium: MeOH, 0.10 M Et4NCl

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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
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Cs+ sp non-aq 25°C 100% C IH K1=5.4 1996AAe (107163) 651  
Medium: acetonitrile. By calorimetry, DH(K1)= -40.5 kJ mol<sup>-1</sup>, DS(K1)=-32  
J K<sup>-1</sup> mol<sup>-1</sup>. In 100% MeOH, K1=5.1, DH(K1)=-44, DS(K1)=-50.

\*\*\*\*\*

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
-------	-----	--------	------	------	-----	-------	----	----------	-----------	--------

Cs+ sp non-aq 25°C 100% C K1=6.19 2000Pba (107169) 652  
Medium: MeOH.

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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
-------	-----	--------	------	------	-----	-------	----	----------	-----------	--------

Cs+ EMF non-aq 25°C 100% C K1=6.4 1995CUa (107174) 653  
Medium: methanol, 0.01 M Et4NClO4. Method: Ag-competitive potentiometry.

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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
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Cs+ EMF non-aq 25°C 100% C H K1=6.1 1995CUa (107180) 654  
Medium: methanol, 0.01 M Et4NClO4. Method: Ag-competitive potentiometry.  
By calorimetry, DH(K1)=-50.2 kJ mol<sup>-1</sup>, DS(K1)=-52 J K<sup>-1</sup> mol<sup>-1</sup>.

\*\*\*\*\*

C44H56O4 H4L (7294)  
4-Tert-butyl-calix[4]arene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Cs+ nmr non-aq 20°C 100% U K1=2.2 1996ABa (107185) 655  
Medium: acetone

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C45H39O3P3	L	CAS 73218-92-5 (5679)
1,3,5-Tris(diphenylphosphinylmethyl)-benzene; C6H3(CH2.PO(C6H5)2)3		

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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Cs+        con non-aq 25°C 100% U      K1=3.3      1984YKa (107211) 656
Medium: tetrahydrofuran + CHCl3 4:1, Cs as 2,4-dinitrophenolate
*****
C45H48N3O3P3      L      CAS 90179-28-5 (5682)
N,N',N''-tris(Diphenylphosphinylmethyl)-1,4,7-triazacyclononane;
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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Cs+        con non-aq 25°C 100% U      K1=2.2      1984YKa (107224) 657
Medium: tetrahydrofuran + CHCl3 4:1, Cs as 2,4-dinitrophenolate
*****
C46H40O6P2      L      (6814)
1,2-Bis((2-(2-diphenylphosphinyl)phenoxy)ethoxy)benzene;
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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Cs+        con non-aq 25°C 100% U      K1=3.7      1991EBa (107239) 658
Solvent : Tetrahydrofurane + CHCl3 4:1(vol)
*****
C46H46N2O4      L      CAS 185118-12-1 (7824)
N,N'-Bis(1-pyrenylmethyl)-1,4,10,13-tetraoxa-7,16-diazacyclooctadecane;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Cs+        sp mixed 25°C 90% C      K(CsSCN+L)=2.07
Method: fluorescence emission. Medium: MeOH/CHCl3 (9:1 v/v).
*****
C46H46O7P2      L      (6807)
1,15-Bis(2-Diphenylphosphinylphenyl)-2,5,8,11,14-pentaoxapentadecane;
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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Cs+        con non-aq 25°C 100% U      K1=3.9      1993BEb (107258) 660
Medium: THF+CHCl3 4:1(vol)
*****
C46H48O6P2      L      (7155)
1,8-Bis(2-(2-(diphenylphosphinyl)ethyl)phenoxy)-3,6-dioxyoctane
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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Cs+        oth non-aq 25°C 100% U      K1=2.2      1995TEa (107269) 661
Medium: THF:CHCl3 4:1 v/v. Cs as 2,4-dinitrophenolate. Also other si
milar ligands
*****
C46H48O9P2      L      CAS 95651-38-0 (2082)
1,5-Bis(2-(2-(diphenylphosphinylmethoxy)ethoxy)phenoxy)-3-oxapentane;
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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	con	non-aq	25°C	100%	U		K1=4.45	1989KSa (107278)	662
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
Cs+	con	non-aq	25°C	100%	U		K1=3.96	1989KSa (107359)	663
Medium: tetrahydrofuran/CHCl3 4:1 (vol)									
*****									
C48H50O8P2		L					(6808)		
1,18-Bis(2-Diphenylphosphinylphenyl)-2,5,8,11,14,17-hexaoxanodecane;									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	con	non-aq	25°C	100%	U		K1=4.3	1993BEb (107363)	664
Medium: THF+CHCl3 4:1(vol)									
*****									
C48H54O10P4		L					CAS 97910-30-0	(2084)	
Tris((2-(diphenylphosphinylmethoxy)ethoxy)methyl)phosphine oxide;									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	con	non-aq	25°C	100%	U		K1=3.84	1989KSa (107386)	665
Medium: tetrahydrofuran/CHCl3 4:1 (vol)									
*****									
C48H60O8		H2L					R-Bu-Calixarene CAS 147513-53-9	(6705)	
4-tert-Butylcalix[4]arenedicarboxylic acid;									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	gl	alc/w	25°C	100%	C		K1=4.21 B(Cs2L)=8.05	1993ABb (107400)	666
Medium: MeOH, 0.01 M Et4NClO4. Data also for di-tert-butyl ester									
*****									
C48H60O12		L					CAS 157769-14-7	(9090)	
1,3-Calix[4]-bis-crown-6;									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	sp	non-aq	25°C	100%	C	IH	K1=4.9	1996AAe (107409)	667
Medium: acetonitrile. By calorimetry, DH(K1)=-29.7 kJ mol-1, DS(K1)=-6 J K-1 mol-1. In 100% MeOH, K1=4.8, DH(K1)=-56.2, DS(K1)=-98.									
*****									
C48H60O16		H4L					(8251)		
5,11,17,23-Tetrahydroxycalix[4]arene-bis(crown-6);									



Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Cs+	sp	non-aq	25°C	100%	C		K1=5.79	2001PCa (107414)	668
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Medium: methanol

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C48H64O8		L					CAS 354800-65-0	(8253)	
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1,6,11,16-Tetra-t-butyl-2,5,7,10,12,15,17,20-octaoxa-1,6,11,16(1,2)-tetrabenzenacycloicosaphane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Cs+	dis	non-aq	25°C	100%	C		K1=10.9	2001LSa (107425)	669
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K(CsL+N03)=2.93  
K(CsL+C104)=2.92  
K'(Cs+L+N03=Cs(L)N03)=0.54  
K'(Cs+L+C104=Cs(L)C104)=3.67

Medium: 1,2-dichloroethane. K': Cs(aq)+L(org)+N03(aq)=Cs(L)N03(org).  
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C49H60O14		HL					CAS 317810-09-6	(8840)	
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5-Carboxycalix[4]arene-bis(crown-6-ether) 1,3-alternate;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Cs+	dis	non-aq	25°C	100%	U			2002TTb (107450)	670
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K(Cs+HL(org)=CsL(org)+H)=-4.15

Method: extraction from H2O into CHCl3.  
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C50H60N015F3S		HL					CAS 317810-10-9	(8841)	
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5-N-(Trifluoromethylsulfonyl)carbamoylcalix[4]arene-bis(crown-6-ether)  
1,3-alternate;

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

Cs+	dis	non-aq	25°C	100%	U			2002TTb (107457)	671
-----	-----	--------	------	------	---	--	--	------------------	-----

K(Cs+HL(org)=CsL(org)+H)=1.63

Method: extraction from H2O into CHCl3.  
Data for related N-(X-sulfonyl)-derivatives.  
\*\*\*\*\*

C52H64O12		H4L					R-Bu-Calixarene CAS 113215-72-8	(6704)	
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5,11,17,23-Tetra-(t-butyl)-25,26,27,28-tetrakis[(hydroxycarbonyl)methoxy]calix[4]arene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Cs+	gl	alc/w	25°C	100%	C		K1=6.2	1993ABb (107488)	672
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B(CsHL)=17.2  
B(CsH2L)=27.3  
B(CsH3L)=35.9

In methanol; 0.01 M (CH3CH2)4NC104

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C52H68N4O8 L (4823)  
25,27-Bis(N,N-diethylaminocarbonylmethoxy)-26,28-bis(N-butylaminocarbonylmethoxy)calix[4]arene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	sp	non-aq	25°C	100%	C		K1=<1	1999USa (107506)	673

Medium: MeOH, 0.10 M Et4NCl

\*\*\*\*\*

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
Cs+	dis	non-aq	22°C	100%	U		K1=5.67	1996SCa (107540)	674

Medium: CHCl3 saturated with H2O

Data also for other substituted t-butylcalix[4]arene-crown-5 analogues

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C54H90N6O18 L Valinomycin CAS 2001-95-8 (2142)  
Valinomycin, Potassium Ionophore

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	dis	non-aq	22°C	100%	C	M		1996CPa (107547)	675

K(CsA+L(org))=CsAL(org))=8.97

Medium: CHCl3 saturated with H2O. Method: extraction of CsA into CHCl3/L solution. HA is picric acid.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	sp	alc/w	25°C	100%	U		K1=3.90	1972FEb (107548)	676

Medium: methanol/0.1M tetrabutyl-ammonium-perchlorate

\*\*\*\*\*

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
Cs+	sp	non-aq	25°C	100%	C	H	K1=4.9	1996AAe (107576)	677

Medium: acetonitrile. By calorimetry, DH(K1)=-11.4 kJ mol<sup>-1</sup>, DS(K1)=57 J K<sup>-1</sup> mol<sup>-1</sup>.

\*\*\*\*\*

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]]-26,28-bis[2-(2-oxyethoxy)ethoxy]calix[4]arene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	oth	non-aq	RT	100%	C	I	K1=6.9 K(CsL+Cs)=3.91 B(Cs2L)=10.8	2002LAa (107581)	678

Method: fluorimetry. Medium: EtOH. In CH<sub>3</sub>CN, K<sub>1</sub>=5.77, K(CsL+Cs)=3.36, B(Cs<sub>2</sub>L)=9.1.

\*\*\*\*\*

C<sub>56</sub>H<sub>64</sub>O<sub>10</sub> 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
Cs+	dis	non-aq	25°C	100%	C				2001SSb (107585)	679
									KCs.pic+L(org)=CsL.pic)=0.85	

Distribution of picrate salt into CHCl<sub>3</sub>/HL.

K: Cs.pic(aq)+L(org)=CsL.pic(org). Data for series of myo-inositol ligands

\*\*\*\*\*

C<sub>56</sub>H<sub>72</sub>O<sub>8</sub> L CAS 123311-74-0 (6160)  
Tetramethyl-t-butylcalix[4]arenetetraketone;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Cs+	sp	alc/w	25°C	100%	U	I		K <sub>1</sub> =3.1	1989ACb (107596)	680
Medium: MeOH. In CH <sub>3</sub> CN, K <sub>1</sub> =3.7										

\*\*\*\*\*

C<sub>56</sub>H<sub>78</sub>O<sub>8</sub> 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
Cs+	sp	non-aq	25°C	100%	C	H		K <sub>1</sub> =4.6	1995CUa (107605)	681
Medium: methanol, 0.01 M Et <sub>4</sub> NCl. By calorimetry: DH(K <sub>1</sub> )=-36 kJ mol <sup>-1</sup> , DS(K <sub>1</sub> )=-30 J K <sup>-1</sup> mol <sup>-1</sup> .										

\*\*\*\*\*

C<sub>58</sub>H<sub>78</sub>O<sub>11</sub> 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
Cs+	sp	alc/w	25°C	100%	C			K <sub>1</sub> =3.0	2001MAa (107621)	682
Medium: MeOH, 0.01 M Et <sub>4</sub> NCl.										

\*\*\*\*\*

C<sub>58</sub>H<sub>80</sub>O<sub>10</sub> 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
Cs+	sp	non-aq	25°C	100%	C	H		K <sub>1</sub> =3.19	2004BCb (107630)	683
Medium: acetonitrile, 0.01 M Et <sub>4</sub> NCl <sub>04</sub> . DH(K <sub>1</sub> )=-6.7 kJ mol <sup>-1</sup> , DS(K <sub>1</sub> )=38.4 J K <sup>-1</sup> mol <sup>-1</sup> .										

\*\*\*\*\*

C<sub>60</sub>H<sub>80</sub>O<sub>12</sub> L CAS 97600-39-0 (6158)

Tetraethyl-4-t-butylcalix[4]arenetetraethanoate;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Cs+	sp	alc/w	25°C	100%	U	I		K1=2.7	1989ACb (107648)	684
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Medium: MeOH. In CH<sub>3</sub>CN, K1=2.8

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C60H82N2O10 L CAS 155377-20-1 (8806)  
5,11,17,23-Tetra-butyl-25,27-bis(carboxymethoxy)-bis[(N,N-diethylaminocarbonyl)methoxy]calix[4]ar

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Cs+	gl	non-aq	25°C	100%	C			K1=3.2 B(Cs2L)=8.35	2000ABb (107665)	685
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Medium: MeOH, 0.05 M Et<sub>4</sub>NClO<sub>4</sub>.

\*\*\*\*\*

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
-------	-----	--------	------	------	-----	-------	----	----------	-----------	--------

Cs+	sp	non-aq	25°C	100%	C			K1=<1	1999USa (107678)	686
-----	----	--------	------	------	---	--	--	-------	------------------	-----

Medium: MeOH, 0.10 M Et<sub>4</sub>NCl

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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
-------	-----	--------	------	------	-----	-------	----	----------	-----------	--------

Cs+	sp	non-aq	25°C	100%	C			K1=4.0	1991ACc (107692)	687
-----	----	--------	------	------	---	--	--	--------	------------------	-----

Medium: acetonitrile, 0.01 M Et<sub>4</sub>NClO<sub>4</sub>.

\*\*\*\*\*

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
-------	-----	--------	------	------	-----	-------	----	----------	-----------	--------

Cs+	sp	non-aq	25°C	100%	C	H		K1=6.3 B(Cs2L)=10.1	1999Lda (107733)	688
-----	----	--------	------	------	---	---	--	------------------------	------------------	-----

Medium: acetonitrile, 0.01 M Et<sub>4</sub>NClO<sub>4</sub>.

By calorimetry, DH(K1)=-29.0 kJ mol<sup>-1</sup>, DH(Cs2L)=-54.0 kJ mol<sup>-1</sup>

\*\*\*\*\*

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
-------	-----	--------	------	------	-----	-------	----	----------	-----------	--------

Cs+ con non-aq 25°C 100% U K1=2.2 1990EAb (107738) 689  
Medium: THF+CHCl3 4:1(vol). Metal as 2,4-dinitrophenolate

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C64H64O12 L CAS 162898-44-4 (9092)

1,3-Calix[4]-bis-naphtho-crown-6;

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

Cs+ sp non-aq 25°C 100% C H K1=4.9 1996AAe (107743) 690

Medium: acetonitrile. By calorimetry, DH(K1)=-11 kJ mol<sup>-1</sup>, DS(K1)=57

J K-1 mol<sup>-1</sup>.

\*\*\*\*\*

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  
-----

Cs+ oth non-aq RT 100% C I K1=6.68 2002LAa (107748) 691

K(CsL+Cs)=3.81

B(Cs2L)=10.0

Method: fluorimetry. Medium: EtOH. In CH3CN, K1=6.0, K(CsL+Cs)=4.3,

B(Cs2L)=10.3.

\*\*\*\*\*

C64H72N4O4P4 L CAS 104786-07-4 (2065)

1,4,7,10-Tetra(diphenylphosphinylolethyl)-1,4,7,10-tetraazacyclododecane;

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

Cs+ con non-aq 25°C 100% U K1=3.6 1986STb (107751) 692

Medium: THF:CHCl3 4:1 v/v. M as 2,4-dinitrophenolate

\*\*\*\*\*

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  
-----

Cs+ sp alc/w 25°C 100% U H K1=3.16 1996AAc (107767) 693

Medium MeOH, 0.1 M Et4NCl. DH(K1)=-10.9 kJ mol<sup>-1</sup>; DS=24 J K<sup>-1</sup> mol<sup>-1</sup>.

Data also for the crown-5 and crown-6 analogues

\*\*\*\*\*

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  
-----

Cs+ sp non-aq 25°C 100% C K1=<1 1999USa (107803) 694

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
Cs+	cal	alc/w	25°C	100%	U	IH			1995ABc (107811)	695

Medium: 100% Methanol. DH(K1)=-9 kJ mol<sup>-1</sup>, DS(K1)=17 J K<sup>-1</sup> mol<sup>-1</sup>.  
In acetonitrile, K1=3.5, DH(K1)=-26 kJ mol<sup>-1</sup>, DS(K1)=-20 J K<sup>-1</sup> mol<sup>-1</sup>.

Cs+	dis	non-aq	20°C	100%	C	M			1988AGa (107812)	696
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K(Cs+A+L(org)=CsAL(org))=7.23  
Method: extraction of metal picrate into CHCl<sub>3</sub>/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
Cs+	sp	alc/w	25°C	100%	C			K1=4.36	2004MFa (107832)	697

Medium: MeOH, 0.01 M Et<sub>4</sub>NCl.

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
Cs+	con	non-aq	25°C	100%	U			K1=3.47	1985YKa (107845)	698

Medium: EtOH+CHCl<sub>3</sub> 1:1; M is used in nitrophenolate form

C75H100O15 L CAS 152495-34-6 (7033)  
Penta-tert-butylpentakis(ethoxycarbonylmethyloxy)calix[5]arene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Cs+	EMF	alc/w	25°C	100%	U			K1=5.5	1993BMa (107858)	699

Medium: MeOH, 0.1 M Et<sub>4</sub>NClO<sub>4</sub>.

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
Cs+	sp	non-aq	25°C	100%	U			K1=5.6	1989ACb (107868)	700

Medium: CH<sub>3</sub>CN

C77H82O9 L CAS 253317-20-3 (9288)  
p-Tert-butyldihomooxacalix[4]arene tetraphenylketone;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Cs+ sp alc/w 25°C 100% C I K1=2.2 1999MAb (107892) 701  
Medium: MeOH, 0.01 M Et4NCl. In acetonitrile, K1=4.1.

\*\*\*\*\*

C78H90O10P2 L CAS 160638-26-6 (9130)  
5,11,17,23-Tetra-t-butyl-bis(diethylcarbamoylmethoxy)-bis(diphenylphosphinoylmethox  
y)calix[4]aren

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

Cs+ sp alc/w 20°C 100% C K1=2.66 2003YVa (107898) 702  
Medium: 100% EtOH, 0.01 M Et4NBr. Ligand is cone isomer. For paco isomer,  
K=2.61. 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  
-----

Cs+ dis non-aq 25°C 100% U K=4.04 1995FDa (107903) 703

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  
-----

Cs+ sp non-aq 25°C 100% C I K1=5.26 2000AAa (107910) 704  
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  
-----

Cs+ EMF alc/w 25°C 100% U K1=5.3 1993BMa (107915) 705  
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  
-----

Cs+ sp mixed 25°C 50% C K1=6.9 2001JDa (107920) 706  
K(CsL+Cs)=4.0

Medium: 50% v/v CH2Cl2/MeOH, 0.01 M benzyl(trimethyl)ammonium hydroxide.

Method: fluorescence spectroscopy.

\*\*\*\*\*

C90H120018 L CAS 92003-62-8 (6159)

Hexaethyl-4-t-butylcalix[6]arenehexaethanoate;

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Cs+ sp non-aq 25°C 100% U I K1=4.3 1989ACb (107939) 707  
Medium: CH3CN

\*\*\*\*\*

C90H130015 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  
-----  
Cs+ sp non-aq 25°C 100% C I K1=5.55 2000AAa (107949) 708  
Medium: methanol, 0.01 M Et4NCl. By potentiometry, K1=5.45.

Also data for acetonitrile, 0.01 M Et4NCl04 and for the pentaethyl ester.

\*\*\*\*\*

C96H144024 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  
-----  
Cs+ dis non-aq 25°C 100% U K=4.09 1995FDa (107964) 709

Medium: CDCl3. Method: by H2O/CDCl3 extraction of picrate salt.

K: MA(org)+L(org)=MLA(org) where A=picrate.

\*\*\*\*\*

C104H160024 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  
-----  
Cs+ dis non-aq 25°C 100% U K=4.63 1995FDa (107976) 710

Medium: CDCl3. Method: by H2O/CDCl3 extraction of picrate salt.

K: MA(org)+L(org)=MLA(org) where A=picrate.

\*\*\*\*\*

C104H168N8016 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  
-----  
Cs+ dis non-aq 25°C 100% U K=5.43 1995FDa (107981) 711

Medium: CDCl3. Method: by H2O/CDCl3 extraction of picrate salt.

K: MA(org)+L(org)=MLA(org) where A=picrate.

\*\*\*\*\*



C120H192024 L CAS 175349-58-3 (7495)  
C-Undecylcalix[4]resorcinarene octa-alpha-(tert-butyl ethanoate);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Cs+	dis	non-aq	25°C	100%	U				1995FDa (108007)	712
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K=4.53

Medium: CDCl3. Method: by H2O/CDCl3 extraction of picrate salt.

K: MA(org)+L(org)=MLA(org) where A=picrate.

\*\*\*\*\*

C120H200N8016 L CAS 169888-21-5 (7490)  
C-Undecylcalix[4]resorcinarene octa-alpha-(N,N-diethyl acetamide);

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

Cs+	dis	non-aq	25°C	100%	U				1995FDa (108018)	713
-----	-----	--------	------	------	---	--	--	--	------------------	-----

K=5.50

Medium: CDCl3. Method: by H2O/CDCl3 extraction of picrate salt.

K: MA(org)+L(org)=MLA(org) where A=picrate.

\*\*\*\*\*

Polymer PEG 400 (6647)  
Polyethylene glycol 400;

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

Cs+	nmr	oth/un	20°C	0.0	C			K1=2.77	1989GSc (108335)	714
-----	-----	--------	------	-----	---	--	--	---------	------------------	-----

Method: 1H and 133Cs pulsed gradient spin-echo nmr. Medium: D2O.

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Polymer (4204)  
Pyruvate kinase;

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

Cs+	sp	R4N.X	25°C	0.10M	U				1966SSc (108402)	715
-----	----	-------	------	-------	---	--	--	--	------------------	-----

K'=1.36

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
-------	-----	--------	------	------	-----	-------	----	----------	-----------	--------

Cs+	sp	non-aq	25°C	100%	U			K1=7.80	1979KMb (108424)	716
-----	----	--------	------	------	---	--	--	---------	------------------	-----

Medium: CHCl3

\*\*\*\*\*

Polymer (1965)  
poly(Benzo-1,4,7,10,13-pentaoxacyclopentadecane)

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

Cs+ sp non-aq 25°C 100% U K1=7.62 1979Kmb (108428) 717  
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

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