

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)

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		K(Cs+e=Cs/Hg)=-49.24(-2.913V)	1974DKb (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		K(Cs+e=Cs(s))=-49.34(-2.919V)	1972C0a (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		K(Cs+e=Cs(s))=-49.34(-2.919V)	1972C0a (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		K(Cs + e(solv))=2.71 K(2Cs=Cs2)=1.34	1972DBa (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		K=-32.966 (-1950.2V)	1972MLb (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		K(Cs+e=Cs(s))=-49.14(-2.907V)	1971KRb (442)	6
Medium: 50% w/w ethylene glycol/H2O; K=-50.61(-2.994V,w=100)										
Cs+	EMF	none	25°C	0.00	U			K(Cs+e=Cs/Hg))=-31.09(-1.839V)	1970KGa (443)	7
Cs+	con	non-aq	-65°C	100%	U	T		K(Cs + e(solv)=Cs)=2.66	1969DEc (444)	8
Medium: NH3(liquid); K=2.48(-45 C), 2.31(-34 C)										

 Cs+ EMF non-aq 25°C 100% U 1966LCa (445) 9
 K' = -50.49, -2987 mV
 Medium: CH3NHCHO. K': Cs+ Cl + Ag(s)=Cs(s) + AgCl(s)

Cs+ EMF none 25°C 0.0 U T 1939BFa (446) 10
 K(Cs+e)=-49.43(-2923 mV)
 K=-54.49(0 C;-2952), -53.40(5 C;-2946 mV), -52.35(10 C;-2940 mV), -51.35(15 C;-2935 mV), -50.36(20 C,-2928 mV), -48.46(30 C;2914 mV)

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Cs+	sp	oth/un	25°C	1.00M	U	I		K1=0.45	1990RAa (1305)	11

Medium: CsCl. Data at I=0 M and pressures to 2041 atmos.

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Cs+	con	non-aq	25°C	100%	U	T		K1=2.57	1993TAa (1875)	12

Medium: 2-methoxyethanol, -10 to 80 C

Cs+	con	diox/w	25°C	?	U			K1=-0.158	1975Mfa (1876)	13
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Data for dioxan/H2O solution with a dielectric constant of 78.35
 Further data available for solutions with varying dielectric constants

Cs+	con	none	25°C	0.0	U			K1=-0.84	1971HPa (1877)	14
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Cs+	con	none	25°C	0.0	U			K1=-0.4	1971PJa (1878)	15
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Cs+	con	diox/w	25°C	40%	U	I		K1=0.74	1971TJa (1879)	16
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Medium: 40% w/w dioxan/H2O. K1=1.75(60%), 2.42(70%), 4.03(82.8%)
 In THF/H2O: K1=-0.92(15%),0.07(30%),0.95(50%),2.00(70%),2.70(80%),3.90(90%)

Cs+	con	non-aq	25°C	100%	U			K1=0.39	1970CDa (1880)	17
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Medium: DMSO

Cs+	con	oth/un	25°C	0.0	U			K1=0.03	1968Hfa (1881)	18
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Cs+	sol	non-aq	25°C	100%	U	I		Kso=-0.29	1967AKa (1882)	19
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Medium: HCONH2. In DMF: Kso=-3.3

Cs+	con	non-aq	25°C	100%	U			K1=3.36	1965BFb (1883)	20
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Medium: diaminoethane

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

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
Method: transport number

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
Medium: LiNO3

Cs+ sol oth/un 25°C 3.0M U K1=-0.26 1966MRb (3640) 27
Medium: LiCl

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

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

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
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Medium: Glacial acetic acid. Alternative method: Spectrophotometry.
DH(K1)=-13 kJ mol⁻¹

Cs+	con	non-aq	25°C	100%	U			K1=1.55	1978CAa (6201)	50
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Medium: Acetonitrile

Cs+	con	non-aq	25°C	100%	U			K1=1.5	1975YKa (6202)	51
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Medium: MeCN

Cs+	con	non-aq	25°C	100%	U			K1=0.92	1974HPb (6203)	52
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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
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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
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Medium: MeOH

Cs+	con	non-aq	25°C	100%	U			K1=1.01	1971BCa (6206)	55
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Medium: tetramethylurea

Cs+	con	none	25°C	0.0	U			K1=0.23	1971DAa (6207)	56
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Cs+	con	non-aq	25°C	100%	U			K1=0.46	1971PGa (6208)	57
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Medium: N-methylformamide

Cs+	con	mixed	25°C	30%	U	I		K1=2.42	1970PPb (6209)	58
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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
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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

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

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

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 1971BPa (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

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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
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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%)
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Cs+      con oth/un 25°C  0.0  U      K1=-0.03      1968HFa (7978) 77
-----
Cs+      sol non-aq 25°C 100% U I      Kso=-0.23      1967AKa (7979) 78
Medium: H2NCHO. Kso=-1.7(DMF)
-----
Cs+      dis none  25°C  0.0  U      K(Cs+I=Cs(TBP)+I(TBP))=-1.70      1967RMe (7980) 79
With (i-amylo)2MePO: Kd=-1.48
-----
Cs+      con non-aq 25°C 100% U      K1=3.24      1965BFb (7981) 80
Medium: diaminoethane
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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;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
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Cs+      con none  25°C  0.0  U      K1=-0.11      1971JBa (8507) 82
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Cs+      con none  25°C  0.0  U      K1=-0.12      1969BJa (8508) 83
*****
I04-      HL      Periodate      CAS 13444-71-8 (6063)
Periodate;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Cs+      sol oth/un 40°C  0.0  U T H      Kso(CsI04)=-2.19      1968KDb (8599) 84
Kso=-3.40(5 C), -2.65(25 C); DHso=54.8 kJ mol-1, DS=157.2 J K-1 mol-1
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IrCl6---      H3L      (1615)

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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 1959W0a (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


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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)
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ReO4-     HL      Perrhenate      (2581)
Rhenate(VII), Perrhenate;
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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  0.0  C      Kso(CsReO4)=-3.40      1988HHb (14096) 95
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
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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      K(Cs+CsSO4)=0.08      1978FFa (16135) 99
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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      K(Cs2L+TiOL)=-0.5      1971GFa (16138) 102
Medium: H2SO4
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TcO4-     HL      CAS 13568-38-2 (1418)
Pertechnetiate;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
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Cs+       con none   18°C  0.0  U      K1=0.64      1963SKa (17247) 103
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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

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(PO3H2)2

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

Cs+ gl R4N.X 25°C 0.50M U K1=0.84 1967CIa (18277) 105
K(Cs+HL)=0.04

Medium: Me4NCl

C2H4O2 HL Acetic acid CAS 64-19-7 (36)
Ethanoic acid; CH3.COOH

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

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

C2H6O 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

C2H6O2 L Ethyleneglycol CAS 107-21-1 (924)
1,2-Dihydroxyethane (Ethane-1,2-diol); HO.CH2.CH2.OH

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

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

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

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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
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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
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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; HOOCCH2.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)	
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;

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

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

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

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

Cs+ con non-aq 25°C 100% U K1=1.80 1989KSa (51769) 130
 Medium: tetrahydrofuran/CHCl3 4:1 (vol)

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

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

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

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

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-)

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

Cs+ cal non-aq 25°C 100% C H K1=0.56 B2= 1.16 19960Ka (62664) 134
 Medium: DMF, 0.10 M Et4NCl. DH(K1)=-16.7 kJ mol⁻¹, DS(K1)=-45 J K⁻¹ mol⁻¹;
 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, Sequestric 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

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Cs+      gl  oth/un 25°C 0.25M U  H   K1=1.19      1986RSa (74711) 150
                B(CsHL)=6.66
-----
Cs+      gl  oth/un 25°C 0.32M U           K1=0.9   B2=0.90   1965BCa (74712) 151
                K(Cs+HL) < -0.3
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 a/c/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 a/c/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 a/c/w 25°C 100% U H T K1=2.18      1980LIa (75992) 162
Medium: MeOH. DH=-49.0 kJ mol-1.
-----
Cs+      dis non-aq 25°C 100% U           K1=2.6      1980TYa (75993) 163

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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⁻¹.

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

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

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+CHCl₃ 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+H₂L)=0.71 1971CSb (79272) 169
Method: polarimetry. Medium: Me₄NOH

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

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

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.CH₂.CH₂)₅.CH₂.CH₂-)

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 H₂O 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
 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⁻¹.

 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

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⁻¹, DS(K1)=-28 J K⁻¹ mol⁻¹

Cs+ cal non-aq 25°C 100% U IH T K1=4.29 19950Kb (83319) 191
Medium: Acetonitrile, 0.1 M Et4NClO4. DH(K1)=-19 kJ mol⁻¹
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⁻¹, 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⁻¹, DS=-98 J K⁻¹ mol⁻¹

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⁻¹, DS=-47 J K⁻¹ mol⁻¹

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⁻¹, DS(K1)=39.6 J K⁻¹ mol⁻¹.

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 ⁻¹ .											
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 ⁻¹ (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 ₂ O. DH(K1)=-33.8 kJ mol ⁻¹ .											
Cs+	cal	oth/un	25°C	0.10M	U	H	T	K1=0.99		1976ITb (83340)	212
DH=-15.9 kJ mol ⁻¹ .											
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 ₂ O: K1=0.8											

C ₁₂ H ₂₆ N ₂ O ₄ 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: ¹³³ Cs 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 ⁻¹ , 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 ₃ CN. DH=-6.0 kJ mol ⁻¹											

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

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

Cs+ con non-aq 25°C 100% U K1=3.4 1993EVa (83995) 220
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

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

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 kJ mol⁻¹; DS=16.7.

C13H26O5 L (6410)

15,15-Dimethyl-1,4,7,10,13-pentaoxacyclohexadecane;

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

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;

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

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;

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

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

K(Cs+A+L)=4.65

Medium: CDCl3. HA is picric acid.

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 kJ mol⁻¹, DH(K2)=-9.8 kJ mol⁻¹.

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

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

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

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

Cs+ cal non-aq 25°C 100% C H K1=3.43 1988BUb (88255) 238
Medium: acetonitrile. DH(K1)=-12.5 kJ mol⁻¹, DS(K1)=23 J K⁻¹ mol⁻¹.

Cs+ con non-aq 25°C 100% C I K1=2.39 1988TKb (88256) 239
Medium: MeCN. In propylene carbonate K1=2.03; in MeOH 2.15

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.
DH(K1)=-32.9 kJ mol⁻¹, DS(K1)=-63.7 J K⁻¹ mol⁻¹.

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

Cs+ ISE alc/w 25°C 90% U K1=2.08 1987KHa (88259) 242
Medium: 90% w/w MeOH/H₂O

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/H₂O, K1=1.66, K2=1.02.

Cs+ con alc/w 25°C 100% U K1=1.91 1983LSa (88261) 244

Cs+ con non-aq 25°C 100% U K1=2.03 1982TAa (88262) 245
Medium: propylene carbonate

Cs+ cal alc/w 25°C 70% U H K1=1.70 1976ITa (88263) 246
Medium: 70% w/w MeOH/H₂O. DH(K1)=-10.2 kJ mol⁻¹.

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

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

Cs+ cal alc/w 25°C 100% U H K1=1.30 1987ZBa (88387) 247
Medium: MeOH. DH=-11.7 kJ mol⁻¹; DS=-14.4.

C14H22N2O8 H4L CDTA CAS 482-54-2 (200)
trans-1,2-Diaminocyclohexane-N,N,N',N'-tetraethanoic acid;

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

Cs+ oth R4N.X 25°C 0.50M U K(Cs+H2L)=0.85 1971CSa (88620) 248

Method: polarimetry. Medium: Me₄NOH

 C14H24O8S L CAS 63689-67-8 (2274)
 1,4,7,10,13,16-Hexaoxa-19-thia-cycloheptadecane-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⁻¹.

 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⁻¹

 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

C15H1202 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

C15H2205 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⁻¹; DS=-32.6.

C15H2406 HL CAS 57722-03-9 (2353)
1-Hydroxy-2-(1,4,7,10,13-pentaoxatridecyl)benzene; HO.C6H4.0(CH2CH2O)4CH3

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

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

C15H2608 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⁻¹.

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

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

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+.

C15H36N09P3 L CAS 37909-50-5 (2634)
(N,N-Dimethylamine)methylenetris(phosphonic acid diethyl ester);
(CH3)2N.C(CH2.PO(OC2H5)2)2

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

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 K(CsA+L)=4.70 1977MTc (94341) 274

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(MOEO)2E CAS 60232-72-6 (2246)
18-Methoxy-16-methyl-3,6,9,12-tetraoxabicyclo[12.3.1]octadeca-1(18),14,16-triene;

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

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

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/H₂O, 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⁻¹.

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/H₂O

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⁻¹, DS(K1)=-66.1 J K⁻¹ mol⁻¹;
 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/H₂O. 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/H₂O. 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 H₂O into benzene. HA is picric acid. DH(CsAL(org))
 =-66.9 kJ mol⁻¹, DS(CsAL(org))=-166 J K⁻¹ mol⁻¹.

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
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Cs+	cal	alc/w	25°C	100%	U	H		K1=2.62	1987ZBa (94471)	290
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Medium: MeOH. DH=-33.5 kJ mol⁻¹; 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 1991FGb (94492) 291
B(CsHL)=8.1

Medium: 0.10 M Et4NNO3.

C16H25NO4 L (7444)
1-Aza-4,7,10,13-tetraoxa-1-phenyl-cyclopentadecane;

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

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

C16H26N2O12 H4L (6659)
1,4,10,13-Tetraoxa-7,16-diaza-2,3,11,12-tetracarboxycyclooctadecane;

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

Cs+ gl R4N.X 25°C 0.10M U K1=3.1 1990AFa (94587) 293
B(CsHL)=13.1

C16H26N2O12 H4L CAS 130190-52-2 (6660)
1,4,10,13-Tetraoxa-7,16-diaza-2,3,7,16-tetracarboxycyclooctadecane;

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

Cs+ gl R4N.X 25°C 0.10M U K1=2.8 1990AFa (94601) 294
B(CsHL)=12.4

C16H26O6 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

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

Cs+ con alc/w 25°C 100% U K1=1.66 1975CJa (94629) 295
Medium: MeOH

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

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

Cs+ ISE oth/un 25°C dil A I K1=0.8 1971FRa (95099) 296
In MeOH: K1=4.30, K2=1.52

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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-Octaoxacyclotetradecane;										
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 Et4NC1O4. 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-methoxyphenoxy)methylphosphine oxide; Me.PO(CH2.0.C6H4.OMe)2


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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=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
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
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
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
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;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Cs+        sp non-aq 22°C 100% U      K1=5.20      1987CCc (96519) 318
In deuteriochloroform
*****
C17H26O6          L                      CAS 65112-34-7 (6059)
21-Methoxy-3,6,9,12,15-pentaoxabicyclo[15.3.1]heneicosa-1(21),17,19-triene;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Cs+        cal alc/w 25°C 100% U H      K1=2.76      1987ZBa (96526) 319
Medium: MeOH. DH=-22.8 kJ mol-1; DS=-23.5.
*****
C17H34N2O4          L                      CAS 142565-14-8 (6562)
4,7,13,16-Tetraoxa-1,10-diazabicyclo[8.8.5]tricosane;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
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.
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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
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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/H2O, 0.01 M Et4NC1O4.

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

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

Cs+ ISE alc/w 25°C 10% U K1=2.71 1986HA a (96767) 323
Medium: 10% MeOH/H2O

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

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

Cs+ con non-aq 25°C 100% U K1=1.68 1989TK b (97564) 324
Medium: tetrahydrofuran/CHCl3 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.

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

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

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

Cs+ con alc/w 25°C 100% U K1=3.38 1983LSa (97840) 328

Medium: MeOH

C18H28O6 L AN(MOEOE)20 CAS 60232-73-7 (2247)
21-Methoxy-19-methyl-3,6,9,12,15-pentaoxabicyclo[15.3.1]heneicos-1(21),17,19-triene
;

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

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

Medium: CHCl3

C18H28O7 L Benzo21-crown-7 (6355)
2,3-Benzo-1,4,7,10,13,16,19-Heptaoxaheneicos-2-ene;

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

Cs+ sp non-aq 22°C 100% U K1=7.21 1987CCc (97855) 330

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

Cs+ nmr non-aq 33°C 100% U I K1=1.96 1977HPa (98132) 331

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

Cs+ con alc/w 25°C 100% U K1=1.56 1975CJa (98396) 332

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

Cs+ gl alc/w 25°C 95% M K1=2.32 1990LNa (98405) 333

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⁻¹, DS=-36.6 J K⁻¹ mol⁻¹. In 95% v/v MeOH/H₂O: 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⁻¹.

Cs+	gl	R4N.X	25°C	0.05M	C	H		K1=3.3	1996BCh (98533)	336
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Medium: 0.05 M Et4NClO4. By calorimetry: K1=3.4, DH(K1)=-2.4 kJ mol⁻¹.

Cs+	cal	alc/w	25°C	80%	C	H		K1=2.84	1995KZa (98534)	337
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Medium: 80% v/v CH₃OH/H₂O. DH(K1)=-29.7 kJ mol⁻¹, DS(K1)=-45.3 J K⁻¹ mol⁻¹

Cs+	cal	non-aq	25°C	100%	M	H		K1=3.96	1994BCd (98535)	338
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Medium: acetone. DH(K1)=-40.0 kJ mol⁻¹, TDS=-17.5

Cs+	con	oth/un	25°C	0.05M	M			K1=4.04	1992BUb (98536)	339
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K1=3.95 (by calorimetry)

Cs+	nmr	non-aq	25°C	100%	C	I		K1=1.82	1992SLb (98537)	340
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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
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In CH₃CN. DH=-44.2 kJ mol⁻¹

Cs+	cal	alc/w	25°C	100%	U	H		K1=3.95	1986BUd (98539)	342
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In MeOH. DH=-49.7 kJ mol⁻¹

Cs+	nmr	non-aq	25°C	100%	U			K1=7.55	1986CHc (98540)	343
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In CDCl₃ saturated with D₂O

Cs+	cal	non-aq	25°C	100%	U	H			1986DGa (98541)	344
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DH1 = -51.4 kJ mol⁻¹. Medium: nitromethane

Cs+	nmr	non-aq	32°C	100%	U	I		K1=3.75	1986RPc (98542)	345
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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
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Medium: dimethylsulfoxide. Additional data for binary solvent systems
DMSO-acetonitrile, DMSO-propylenecarbonate.

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

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⁻¹

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

Medium: acetonitrile. DH1 = -43.5 kJ mol⁻¹

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

Medium: nitromethane

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

Medium: N,N-dimethylformamide. DH1=-31.0 kJ mol⁻¹; DS1=-63.2 J K⁻¹ mol⁻¹.

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

Medium: DMSO. DH1=-35.6 kJ mol⁻¹; DS1=-92.0 J K⁻¹ mol⁻¹

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⁺, using Tl amalgam electrode.

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

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

Cs+ nmr non-aq 25°C 100% U TIH Keff=4.0 1977MPb (98556) 359

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/H₂O, pH 10.4.

DH(K1)=-49.8 kJ mol⁻¹, DS(K1)=-99 J K⁻¹ mol⁻¹.

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

C18H3609 L 27-Crown-9 (7043)
1,4,7,10,13,16,19,22,25-Nonaoxacycloheptacosane;

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

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

C18H3809 L Glyme-9 CAS 25990-94-7 (7806)
2,5,8,11,14,17,20,23,26-Nonaoxaheptacosane;

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

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

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

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

Cs+ con non-aq 25°C 100% U K1=2.56 1989TKb (99344) 364
Medium: tetrahydrofuran/CHCl₃ 4:1 (volume)

C19H27N07 L (7048)
5'-(N-Acrylamide)-benzo-18-crown-6; CH₂:CH.CO.NH.C16H2306

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: CHCl₃

C19H3006 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

C19H39N05 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/H2O

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

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

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; (CH2.0.CH2.CH2.0.C6H4.CH0)2

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+CHCl3 (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 CH3CN, K1=3.037.

Cs+ dis non-aq 24°C 100% C K(Cs+A+L)=5.61 2002MRd (100095) 371

Medium: CDCl3. 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⁻¹,

DS(K1)=14 J K⁻¹ mol⁻¹.

Cs+ dis oth/un 25°C 0.06M C K(CsL+A)=0.24 2000YYa (100098) 374

K(Cs+L(org)+A=CsLA(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/H2O, 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	

Cs+ dis non-aq 23°C 100% C K1=4.0 1992HGb (100260) 391
 K(Cs+A+L(org)=CsAL(org))=5.43
 K(Cs+A+2L(org)=CsAL2(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.

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

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

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

Medium: CHCl3

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

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

Cs+ EMF non-aq 25°C 100% C H K1=4.70 1999BHa (100439) 394
 Medium: MeOH, 0.05 M Et4NClO4. By calorimetry DH(K1)=-43.7 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]hexacos-20,22,24(26)-triene;

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

Cs+ EMF non-aq 25°C 100% C H K1=4.76 1999BHa (100456) 395
 Medium: MeOH, 0.05 M Et4NClO4. By calorimetry DH(K1)=-44.2 kJ mol-1.
 Method: by competition with Ag+, using Ag/Ag+ electrode.

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

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

Cs+ dis non-aq 25°C 100% U H 1979KLa (100490) 396

K(Cs(picrate)+L)=5.81

Medium: CHCl3

C20H32O8 L Benzo24-crown-8 (6356)

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

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

Cs+ sp non-aq 22°C 100% U K1=6.24 1987CCc (100495) 397

In deuteriochloroform

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/H2O

C20H34O8 L (2504)

2,5,8,11,14,17,20,23-Octaoxa-12,13-benzotetracos-12-ene; C6H4(O.(CH2.CH2.O)3.CH3)2

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

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⁻¹,

DS(K1)=35 J K⁻¹ mol⁻¹.

Cs+ nmr non-aq RT 100% U K1=2.91 1996GMc (100635) 402

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

Cs+ dis non-aq 25°C 100% U 1995BSa (100636) 403

K(Cs(pic)+L)=Cs(pic),L)=6.52

Medium:CHCl3. Data for host-guest associations; pic: picrate. L is a cis-syn-cis and cis-anti-cis mixture. Also data for syn-L (K=6.65) and anti-L(6.31)

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⁻¹, DS(K1)=23 J K⁻¹ mol⁻¹.

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⁻¹, DS(K1)=-89.7 J K⁻¹ mol⁻¹.
Anion is tetraphenyl borate.

Cs+ dis non-aq 25°C 100% U H K(Cs(picrate)+L)=6.25 1979KLa (100640) 407
Medium: CHCl₃

Cs+ nmr non-aq 25°C 100% U I K1>5.0 1977MPa (100641) 408
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

C20H38N2O6 L CAS 178822-46-3 (8615)
6-Methylene-4,8,14,17,22,25-hexaoxa-1,11-diazabicyclo[9.8.8]heptacosane;

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

Cs+ cal alc/w 25°C 80% C H K1=2.96 1995KZa (100738) 412
Medium: 80% v/v CH₃OH/H₂O. DH(K1)=-48.9 kJ mol⁻¹, DS(K1)=-107 J K⁻¹ mol⁻¹

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

C20H40N2O4 L (6625)
1,10-Diaza-4,7,13,16-tetraoxabicyclo[8.8.8]hexacosane;

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

Cs+ gl non-aq 25°C 100% C I K1=3.13 1992LSc (100774) 414
Medium: MeCN, 0.05 M Et₄NClO₄. In DMF K1=2.0; in H₂O K1<2

C20H40N2O6 L Cryptand 2,2,2H (6606)
1,10-Diaza-4,7,14,17,23,26-Hexaoxabicyclo[10.8.8]octacosane;

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

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-1, DS(K1)=-136 J K-1 mol-1

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

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

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-1, DS(K1)=-41 J K-1 mol-1.

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-1.

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.CH2.0)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⁻¹,
DS(K1)=36.2 J K⁻¹ mol⁻¹.

C21H31O7P3 L CAS 82154-48-1 (2916)

Methyl di((2-dimethylphosphinylmethoxy)phenoxy)methyl)phosphineoxide;

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 2004KV a (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 1980NTa (101990) 432
K(Cs+HL)=1.08

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-heptaoxacycloheneicosane-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⁻¹, DS(K1)=-66.4 J K⁻¹ mol⁻¹.

 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-heptaoxacycloheptacosane-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-dioxo-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		K(Cs+A+L)=4.28	2002MRd (102129)	440

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]hexacosane-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⁻¹,

Cs+	nmr	non-aq	25°C	100%	C	I	K1=1.47	1992SLb (102269)	443
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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
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DH=-31.8 kJ mol⁻¹. 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⁻¹.

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/H2O

C22H40O6 L CAS 76993-47-0 (2340)
2,5,8,11,14,17-Hexaoxatricyclo[22.4.0.0(18,23)]octacosane (trans-cis-trans isomer)

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

Cs+ nmr non-aq 24°C 100% U M 1981BEb (102369) 448
K(Cs(picrate)+L)=6.9

Medium: CDCl₃

C22H40O7 L (6596)
2,3,11,12,-Dicyclohexano-1,4,7,10,13,16,19-heptaoxacycloheneicosane;
dicyclohexyl-21-crown-7;

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

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 Bu₄NBr. 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-quinoly1)-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(MOEO)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(MOEO)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

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⁻¹,
DS(K1)=-13 J K⁻¹ mol⁻¹.

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 19940Ua (103118) 471

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⁻¹, DS(K1)=-53.4 J K⁻¹ mol⁻¹.

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.

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

Cs+ con alc/w 25°C 100% U K1=2.66 1975CJa (103394) 485
Medium: MeOH

C24H4405 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

C24H4408 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

C24H48N209 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

C24H48N209 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

C24H48N406 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.

C24H48N606S2 L CAS 503465-10-9 (9242)
9,12,23,26,31,34-Hexaoxa-1,4,6,15,17,20-hexaazabicyclo[18.8.8]hexatricontane-5,16-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/H2O, 0.01 M Et4NClO4.

C24H48O12 L 36-Crown-12 (7046)
1,4,7,10,13,16,19,22,25,28,31,34-Dodecaoxacyclohexatriacontane;

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

Cs+ cal alc/w 25°C 100% U H K1=3.98 1993ILa (103519) 493
Medium: MeOH. DH=-45.6 kJ mol⁻¹.

C24H72O12Si12 L CAS 18919-94-3 (1287)
Tetracosamethyl-cyclododecasiloxane; ((CH3)2SiO)12

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

Cs+ con alc/w 25°C 100% U K1=0.12 1980Pa (103590) 494
Medium: MeOH, 0.1 M Me4NBr

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

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

Cs+ con non-aq 25°C 100% U K1=2.9 1984YKa (103627) 495
Medium: tetrahydrofuran + CHCl3 4:1, Cs as 2,4-dinitrophenolate

C25H37N2O7P L CAS 202407-79-2 (8035)
26,27-Dimethoxy-3,7,24-triMe-11,14,17,20-tetraoxa-2,4-diaza-phosphatricycloheptacosahexaeneoxide;

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

Cs+ dis non-aq 20°C 100% C K(CsP+L)=4.57 1998DDc (103756) 496

Medium: CHCl3. P is picrate.

C25H40O12 L CAS 239470-22-5 (8948)
4'-Carboxybenzo-30-crown-10;

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

Cs+ con non-aq 25°C 100% C T H K1=4.63 1999RGa (103774) 497
Medium: acetonitrile. Data for 5-35 C. DH(K1)=-42.3 kJ mol⁻¹, DS(K1)=-53 J K⁻¹ mol⁻¹.

C25H50N2O8 L BCA15C5 CAS 71972-29-7 (6116)
1,5-Bis-(1-aza-4,7,10,13-tetraoxacyclopentadecyl)pentane;

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

Cs+ ISE a/c/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

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 a/c/w 25°C 95% C K1=4.49 2004KVa (103843) 500

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

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⁻¹. Also data in propylene carbonate, and dimethylsulphoxide

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⁻¹, DS(K1)=-71 J K⁻¹ mol⁻¹.

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 % CH3CN. 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 CH3CN. 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/H2O. DH(K1)=-25.7 kJ mol⁻¹

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: CDCl3. 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-trioxahseptane;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 1987BBf (104278) 515
K(Cs+A+L(org))=CsAL(org))=5.83

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⁻¹

C26H48O6 L (2342)
19,21,26,28-Tetramethyl-2,5,8,11,14,17-hexaoxatricyclo[22.4.0.0(18,23)]octacosane;

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

Cs+ nmr non-aq 24°C 100% U M K1=5.9 1981BEb (104308) 517
K(Cs(picrate)+L)=5.9

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 2004KV a (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]nonatricontane-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)

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

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

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
 Medium: THF+CHCl3 (4:1 vol)

 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

 C28H30N2O2P2 L CAS 68745-29-9 (5707)
 N,N'-Bis(diphenylphosphinylmethyl)-1,2-diaminoethane; ((C6H5)2PO.CH2.NH.CH2-)2

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

 Cs+ con non-aq 25°C 100% U K1=2.4 1984YKa (104725) 529
 Medium: tetrahydrofuran + CHCl3 4:1, Cs as 2,4-dinitrophenolate

 C28H32N2O6 L (5743)
 1,16-Di(8-quinolyl)-1,4,7,10,13,16-hexaoxahexadecane; C9H6N.O.(C2H4O)5.C9H6N

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

 Cs+ con non-aq 25°C 100% U K1=4.9 1989BEa (104748) 530
 Medium: tetrahydrofuran/CHCl3 4:1 (volume)

 C28H40O6 L CAS 29471-17-8 (1262)
 2,3:11,12-Bis(4'-tert-butylbenzo)-1,4,7,10,13,16-hexaoxacyclooctadecane;

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

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(MOEOEOM)2AN (2243)

29,30-Dimethoxy-13,27-dimethyl-3,6,9,17,20,23-hexaoxatricyclo-triconta-1,11,13,15,25,27-hexaene;

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

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⁻¹, DS(K1)=-49 J K⁻¹ mol⁻¹.

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-dichloroethane. 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⁻¹. 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

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 a/c/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 K(Cs(picrate)+L)=3.5 1981BEb (105008) 542
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 a/c/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 a/c/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 a/c/w 25°C 95% C K1=1.70 2004KVa (105049) 546

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

C29H3003P2 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:CHCl3 4:1 (v/v).

Metal ion is used as 2,4-dinitrophenolate.

C29H3003P2 L CAS 176849-78-8 (7161)

1,6-Bis(diphenylphosphinyl)-3-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 (105083) 548

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

Metal ion is used as 2,4-dinitrophenolate.

C29H3004P2 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/CHCl3 4:1 v/v

C29H35N05 L CAS 201154-06-5 (7825)

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

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

Cs+ sp mixed 25°C 90% C 1997Kka (105099) 550

K(CsSCN+L)=3.67

Method: fluorescence emission. Medium: MeOH/CHCl3 (9:1 v/v).

C29H40N206Cl2 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(K1)=-19.5 kJ mol⁻¹, DS(K1)=-9.90 J K⁻¹ mol⁻¹.

C29H58N2010 L BCA18C6 CAS 74776-87-7 (6117)

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

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

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;

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

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;

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

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;

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

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

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

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;

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

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 K(Cs(picrate)+L)=6.57 1979KLa (105259) 558

Medium: CHCl3

C30H38N2O4 L (5828)
Trimethoxyphenylcryptand 3,1.
25,26,27-Trimethoxy-5,10,15-trimethyl-22-oxa-1,19-diazatetra-

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

Cs+ nmr non-aq 25°C 100% U K1=<5.24 1986CHc (105271) 559
In CDCl3

C30H42O10P4 L CAS 97910-31-1 (2083)
Tris-((2-(dimethylphosphinylmethoxy)phenoxy)methyl)phosphine oxide;

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

Cs+ con non-aq 25°C 100% U K1=3.04 1989Ksa (105300) 560
Medium: tetrahydrofuran/CHCl3 4:1 (vol)

C30H48O13P2 L CAS 112120-14-6 (5729)
1,13-Bis(2-(diethoxyphosphinylmethoxy)phenyl)-1,4,7,10,13-pentaoxatridecane;

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

Cs+ con non-aq 25°C 100% U K1=4.6 1989Eva (105342) 561
Medium: tetrahydrofuran/CHCl3 4:1 (volume)

C31H34O4P2 L (7157)
1,9-Bis(diphenylphosphinyl)-3,7-dioxononane;

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

Cs+ oth non-aq 25°C 100% U K1=1.8 1995TEa (105524) 562
Medium: THF:CHCl3 4:1 v/v. Cs as 2,4-dinitrophenolate. Also other si
milar ligands

C32H29O3P3 L CAS 21851-89-8 (2640)
P,P,P',P'',P'''-Pentaphenyldimethylenetri(phosphineoxide); (Ph2P(O)CH2)2P(O)Ph

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

Cs+ sp non-aq 25°C 100% U M K(CsI+L)=1.30 1981SPb (105581) 563

Medium: CH3CN

C32H36O5P2 L CAS 137728-07-5 (6837)
1,11-Bis(diphenylphosphinyl)-3,6,9-trioxaundecane;

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

Cs+ con non-aq 25°C 100% U K1=2.8 1992BEa (105644) 564
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

Cs+ con non-aq 25°C C K1=3.7 1999TEa (105649) 565
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

Cs+ cal non-aq 25°C 100% C H K(Cs+HL)=2.70 1995ZBa (105678) 566
Medium: methanol. DH(K)=-36.9 kJ mol⁻¹, DS(K)=-72.2 J K⁻¹ mol⁻¹.

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

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

C32H46N2O8Cl2 L CAS 181706-75-2 (8626)
3,18-Dichlorododecahydro-5H,16H-6,15-(ethanoxyethanoxyethano)dibenzo-hexaoxadiazacyclohexacosine;

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

Cs+ cal non-aq 25°C 100% C H K1=3.94 1998ZBc (105786) 568
Medium: MeOH. DH(K1)=-47.5 kJ mol⁻¹, DS(K1)=-83.9 J K⁻¹ mol⁻¹.

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

Cs+ con non-aq 25°C 100% U K1=4.8 1989Eva (105822) 569

Medium: tetrahydrofuran/CHCl3 4:1 (volume)

C32H55NO13 L CAS 105495-11-2 (1690)
N-(2-(2-(4'-Benzo-18-crown-6)-oxyethoxy)ethyl-1,4,7,10,13-pentaoxa-16-azacyclooctadecane);

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

Cs+ ISE a/c/w 25°C 10% U K1=3.21 B2=6.27 1986HAa (105831) 570
Medium: 10% MeOH/H2O

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

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

Cs+ ISE a/c/w 25°C 95% C K1=4.4 1977LSc (105849) 571
K(CsL+Cs)=3.0

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

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

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

Cs+ cal a/c/w 25°C 100% U H 1986BUd (105861) 572
In MeOH. DH=-21.7 kJ mol⁻¹

C33H41N3O6Cl2 L CAS 181706-78-5 (8628)
3,18-Dichlorohexahydro(ethanoxyethanoxyethano)-23,27-nitrilodibenzotetraoxadiazacyclopentacosine;

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

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

C33H46N2O12 L (7049)
1,4-Diaza-1,4-di(5'-benzo-15-crown-5)-hepta-2,6-dione; CH2(CH2CONH.C14H19O5)2

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

Cs+ sp non-aq 25°C 100% U K1=7.03 1979KMb (105980) 574
Medium: CHCl3

C34H38O12P2 L (6906)
1,2:10,11:15,16:24,25-Tetrabenzo-13,27-di(methylphospha)-3,6,9,12,14,17,20,23,27,28-10-crown-28

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	oth	non-aq	22°C	100%	U		K1=0.3	1978YSa (106038)	575
Medium: 1:1 v/v EtOH+CHCl3. 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+CHCl3 (4:1 vol)									

C34H40O7P2		L					(7894)		
1,15-Bis(diphenylphosphinyl)-2,5,8,11,14-pentaoxopentadecane;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	con	non-aq	25°C		C		K1=4.2	1999TEa (106049)	577
In: tetrahydrofurane/CHCl3 4:1 v/v									

C34H42N2O6Cl2		L					CAS 181706-79-6	(8629)	
3,18-Dichlorooctahydro-5H,16H-6,15-(ethanoxyethanoxyethano)tribenzotetraoxadiazacyc lodococine;									

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 ⁻¹ , DS(K1)=-28.4 J K ⁻¹ mol ⁻¹ .									

C34H44N2O5		L					CAS 101671-92-5	(5825)	
Trimethoxyphenylcryptand 3,1,1. 30,31,32-Trimethoxy-5,10,15-trimethyl-22,27-dioxo-1,9-diaza....									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Cs+	nmr	non-aq	25°C	100%	U		K1=7.63	1986CHc (106067)	579
Medium: CDCl3									

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	K(Cs+HL)=3.44	1988PJa (106097)	580
Medium: MeOH. DH = -14.4 kJ mol ⁻¹ ; DS = 19									

C34H54O8		H2L					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⁻¹; DS = 16

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

Medium: MeOH

C34H68N4O8 L CAS 49811-34-9 (8578)
10,13,25,28,33,36,41,44-Octaoxa-1,7,16,22-tetraazatricyclo[20.8.8.87,16]hexatetraco
ntane;

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

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

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

C36H30O3Si3 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

C36H3604P2 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)

C36H3606P2 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)

C36H4004S2 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

C36H4006 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

C36H4006 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

C36H4407P2 L (5725)
1,17-Di(diphenylphosphinyl))-3,6,9,12,15-pentaoxaseptadecane;
Ph2PO.C2H4(O.C2H4)4OC2H4POPh2

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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=3.7      1992BEa (106333) 595
Medium: THF+CHCl3 (4:1 vol)
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C36H4408P2          L                      (7895)
1,18-Bis(diphenylphosphinyl)-hexaoxooctadecane;
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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=4.7      1999TEa (106343) 596
In: tetrahydrofuran/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-
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Cs+        nmr non-aq 25°C 100% U          K1=12.009   1986CHc (106377) 597
In CDCl3
*****
C36H52014P2        L                      (5739)
3,4:12,13:21,22-Tribenzo-1,24-di(diethoxyphosphinyl)-2,5,8,11,14,17,20,23-octaoxate
tricosatriene;
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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=4.7      1989BEa (106395) 598
Medium: tetrahydrofuran/CHCl3 4:1 (volume)
*****
C36H54010          L                      CAS 86116-04-3 (5647)
1,8-Bis(4'-(2,3-benzo-1,4,7,10,13-pentaoxacyclopentadecane))-octane;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Cs+        ISE alc/w 25°C 90% U          K1=2.62    B2=3.01    1987KHa (106417) 599
90% w/w MeOH/H2O. Also data for the 1,4,7,10-tetraoxadecane-bridged
ligand: K1=2.89; K2=0.74.
*****
C36H5606          L                      CAS 54535-81-8 (1263)
2,3:11,12-Bis(3',5'-di-tert-butylbenzo)-1,4,7,10,13,16-hexaoxacyclooctadecane;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Cs+        con alc/w 25°C 100% U I M          K(CsCl+L)=3.17 1979BDa (106435) 600
Medium: MeOH. In DMSO: K(CsClO4+L)=3.13. In MeCN: K(CsBPh4+L)=3.43
*****

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

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

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⁻¹, DS(K1)=-95 J K⁻¹ mol⁻¹.

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

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

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 a/c/w 25°C 100% U K1=5.18 1984CTb (106497) 606
Medium: EtOH

Cs+ gl a/c/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

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

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)

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

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

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

Cs+ con non-aq 25°C 100% U K1=2.9 1991EBa (106647) 610
Medium: THF+CHCl3 4:1(vol)

C38H4006P2 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

C38H4808P2 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)

C38H4809P2 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 20010Ya (106720) 615
K(CsL+L)=1.7

Medium: methanol. For the 1,4-butanediyl derivative, K1=4.6, K(CsL+L)=2.0.

C40H3604P2 L (6805)
1,6-Bis(2-Diphenylphosphinylphenyl)-2,5-dioxahexane; (CH2.0.CH2.C6H4(PO(6H5)2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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-trioxahptane;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 ⁻¹ , DS(K1)=2 J K ⁻¹ mol ⁻¹ .										

C40H4808			L					AN2DP(OEOEO)2E	(2235)	
3,4,5,6-Bis(3-methyl-5-(2-methoxy-5-methylbenzo))-2,7,10,13,16,19-hexaoxacyclodocosa-3,5-diene;										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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 ⁻¹ , DS(K1)=-32 J K ⁻¹ mol ⁻¹ .										

 C40H52N4O4 L CAS 205066-94-0 (8760)
 Tetraphenyl-1,4,7,10-tetraazacyclododecane-1,4,7,10-tetraethanol;

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

 Cs+ ISE non-aq 25°C 100% C K1=3.47 1998Wlc (106821) 622
 Medium: DMF, 0.05 M Et4NC104.

 C40H52O14P2 L CAS 127832-94-4 (5740)
 2,3:9,10:15,16:21-Tetrabenzo-1,24-di(diethoxyphosphinyl)-2,5,8,11,14,17,20,23-octaoxatetracosane;

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

 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 NBu4Cl04 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: CsCl04 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-oxahexacyclotritriacontapentadecane;

 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-trioxahptane;
(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)

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;

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

Cs+ sp non-aq 25°C 100% C K1=1.9 1999USa (107157) 650
Medium: MeOH, 0.10 M Et4NCl

C44H52O10 L CAS 163317-54-2 (9089)
1,3-Calix[4]-bis-crown-5;

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

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⁻¹, DS(K1)=-32
J K⁻¹ mol⁻¹. 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.

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.

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

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⁻¹, DS(K1)=-52 J K⁻¹ mol⁻¹.

C44H56O4 H4L (7294)
4-Tert-butyl-calix[4]arene;

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

Cs+ nmr non-aq 20°C 100% U K1=2.2 1996ABa (107185) 655
Medium: acetone

C45H39O3P3 L CAS 73218-92-5 (5679)
1,3,5-Tris(diphenylphosphinylmethyl)-benzene; C6H3(CH2.PO(C6H5)2)3

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

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;

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;

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;

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

Cs+ sp mixed 25°C 90% C 1997KKa (107248) 659
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;

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

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;

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)

C48H4408P2 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)

C48H5008P2 L (6808)
1,18-Bis(2-Diphenylphosphinylphenyl)-2,5,8,11,14,17-hexaoxanadecane;

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)

C48H54010P4 L CAS 97910-30-0 (2084)
Tris((2-(diphenylphosphinylmethoxy)ethoxy)methyl)phosphine oxide;

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

Cs+ con non-aq 25°C 100% U K1=3.84 1989Ksa (107386) 665
Medium: tetrahydrofuran/CHCl3 4:1 (vol)

C48H6008 H2L R-Bu-Calixarene CAS 147513-53-9 (6705)
4-tert-Butylcalix[4]arenedicarboxylic acid;

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

Cs+ gl alc/w 25°C 100% C K1=4.21 1993ABb (107400) 666
B(Cs2L)=8.05

Medium: MeOH, 0.01 M Et4NClO4. Data also for di-tert-butyl ester

C48H60012 L CAS 157769-14-7 (9090)
1,3-Calix[4]-bis-crown-6;

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

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.

C48H60016 H4L (8251)
5,11,17,23-Tetrahydroxycalix[4]arene-bis(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          K1=5.79      2001PCa (107414) 668
Medium: methanol
*****
C48H64O8          L          CAS 354800-65-0 (8253)
1,6,11,16-Tetra-t-butyl-2,5,7,10,12,15,17,20-octaoxa-1,6,11,16(1,2)-tetrabenzenacyc
loicosaphane;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Cs+        dis non-aq 25°C 100% C          K1=10.9      2001LSa (107425) 669
          K(CsL+NO3)=2.93
          K(CsL+ClO4)=2.92
          K'(Cs+L+NO3=C(L)NO3)=0.54
          K'(Cs+L+ClO4=C(L)ClO4)=3.67
Medium: 1,2-dichloroethane. K': Cs(aq)+L(org)+NO3(aq)=Cs(L)NO3(org).
*****
C49H60O14          HL          CAS 317810-09-6 (8840)
5-Carboxycalix[4]arene-bis(crown-6-ether) 1,3-alternate;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Cs+        dis non-aq 25°C 100% U          K(Cs+HL(org)=CsL(org)+H)=-4.15
          2002TTb (107450) 670
Method: extraction from H2O into CHCl3.
*****
C50H60NO15F3S      HL          CAS 317810-10-9 (8841)
5-N-(Trifluoromethylsulfonyl)carbamoylecalix[4]arene-bis(crown-6-ether)
1,3-alternate;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Cs+        dis non-aq 25°C 100% U          K(Cs+HL(org)=CsL(org)+H)=1.63
          2002TTb (107457) 671
Method: extraction from H2O into CHCl3.
Data for related N-(X-sulfonyl)-derivatives.
*****
C52H64O12          H4L      R-Bu-Calixarene CAS 113215-72-8 (6704)
5,11,17,23-Tetra-(t-butyl)-25,26,27,28-tetrakis[(hydroxycarbonyl)methoxy]calix[4]ar
ene;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Cs+        gl alc/w 25°C 100% C          K1=6.2      1993ABb (107488) 672
          B(CsHL)=17.2
          B(CsH2L)=27.3
          B(CsH3L)=35.9
In methanol; 0.01 M (CH3CH2)4NC1O4
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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

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.

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⁻¹, DS(K1)=57 J K⁻¹ mol⁻¹.

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]]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 2002LAa (107581) 678
K(CsL+Cs)=3.91
B(Cs2L)=10.8

Method: fluorimetry. Medium: EtOH. In CH3CN, K1=5.77, K(CsL+Cs)=3.36, B(Cs2L)=9.1.

C56H64010 L CAS 405108-40-9 (8249)
1,2-Di-O-[2-(2-benzyloxyethoxy)ethyl]-3,4,5,6-tetra-O-benzyl-myoinositol;

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 CHCl3/HL.

K: Cs.pic(aq)+L(org)=CsL.pic(org). Data for series of myo-inositol ligands

C56H7208 L CAS 123311-74-0 (6160)
Tetramethyl-t-butylcalix[4]arenetetraetone;

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

Cs+ sp alc/w 25°C 100% U I K1=3.1 1989ACb (107596) 680
Medium: MeOH. In CH3CN, K1=3.7

C56H7808 L CAS 122356-76-7 (8681)
Tetra-tert-butyl-1,3-dimethoxycalix[4]arene-crown-6;

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

Cs+ sp non-aq 25°C 100% C H K1=4.6 1995CUa (107605) 681
Medium: methanol, 0.01 M Et4NCl. By calorimetry: DH(K1)=-36 kJ mol-1,
DS(K1)=-30 J K-1 mol-1.

C58H78011 HL CAS 465527-74-6 (9287)
7,13,19,25-Tetra-t-butyl-28-methoxy-27,29,30-triethylacetate-2,3-dihomo-3-oxacalix[4]arene;

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

Cs+ sp alc/w 25°C 100% C K1=3.0 2001MAa (107621) 682
Medium: MeOH, 0.01 M Et4NCl.

C58H80010 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 K1=3.19 2004BCb (107630) 683
Medium: acetonitrile, 0.01 M Et4NCl04. DH(K1)=-6.7 kJ mol-1,
DS(K1)=38.4 J K-1 mol-1.

C60H80012 L CAS 97600-39-0 (6158)

Tetraethyl-4-t-butylcalix[4]arenetetraethanoate;

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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Cs+        sp alc/w 25°C 100% U I      K1=2.7        1989ACb (107648) 684
Medium: MeOH. In CH3CN, 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
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Cs+        gl non-aq 25°C 100% C          K1=3.2        2000ABb (107665) 685
B(Cs2L)=8.35
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Medium: MeOH, 0.05 M Et4NClO4.
*****
C60H84N4O8          L          CAS 246035-32-5 (2735)
25,27-Bis(N,N-diethylaminocarbonylmethoxy)-26,28-bis(aminocarbonylmethoxy)-t-butylcalix[4]arene;
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-----
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 Et4NCl
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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;
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-----
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 Et4NClO4.
```

```
*****
C64H60O12          L          CAS 211870-40-5 (4258)
Calix[4]arene-bis(dibenzo)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=6.3        1999LDa (107733) 688
B(Cs2L)=10.1
```

```
Medium: acetonitrile, 0.01 M Et4NClO4.
By calorimetry, DH(K1)=-29.0 kJ mol-1, DH(Cs2L)=-54.0 kJ mol-1
*****
C64H62O6P4          L          (6813)
1,2-Bis(4,5-di(diphenylphosphinyl)-pent-1-oxy)benzene;
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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 1990EAb (107738) 689
Medium: THF+CHCl3 4:1(vol). Metal as 2,4-dinitrophenolate

C64H64O12 L CAS 162898-44-4 (9092)

1,3-Calix[4]-bis-naphtho-crown-6;

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

Cs+ sp non-aq 25°C 100% C H K1=4.9 1996AAe (107743) 690

Medium: acetonitrile. By calorimetry, DH(K1)=-11 kJ mol⁻¹, DS(K1)=57

J K-1 mol⁻¹.

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⁻¹; DS=24 J K-1 mol⁻¹.

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⁻¹, DS(K1)=17 J K⁻¹ mol⁻¹.
In acetonitrile, K1=3.5, DH(K1)=-26 kJ mol⁻¹, DS(K1)=-20 J K⁻¹ mol⁻¹.

Cs+ dis non-aq 20°C 100% C M 1988AGa (107812) 696
K(Cs+A+L(org))=CsAL(org))=7.23
Method: extraction of metal picrate into CHCl₃/L solution. HA is picric acid.

C69H102N4O9 L CAS 116352-85-3 (9286)
para-t-Butyldihomooxacalix[4]arene tetra(diethyl)amide;

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

Cs+ sp alc/w 25°C 100% C K1=4.36 2004MFa (107832) 697
Medium: MeOH, 0.01 M Et₄NCl.

C72H68O10P4 L CAS 88928-02-3 (5680)
Tetrakis-4',5',4",5"- (diphenylphosphinylmethyl)-2,3:11,12-dibenzo-18-crown-6;

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

Cs+ con non-aq 25°C 100% U K1=3.47 1985YKa (107845) 698
Medium: EtOH+CHCl₃ 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 Et₄NClO₄.

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: CH₃CN

C77H82O9 L CAS 253317-20-3 (9288)
p-Tert-butyl-dihomooxacalix[4]arene tetraphenylketone;

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

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(diphenylphosphinoylmethoxy)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.

C90H120O18 L CAS 92003-62-8 (6159)

Hexaethyl-4-t-butylcalix[6]arenehexaethanoate;

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

Cs+ sp non-aq 25°C 100% U I K1=4.3 1989ACb (107939) 707
Medium: CH3CN

C90H130O15 L CAS 269057-78-5 (3334)

5,11,17,23,29-Penta-tert-octylcalix[5]arene-31,32,33,34,35-pentaethanoate
pentamethyl ester;

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

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 Et4NClO4 and for the pentaethyl ester.

C96H144O24 L CAS 169888-22-6 (7534)

C-Undecylcalix[4]resorcinarene octa-alpha-(methyl ethanoate);

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

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.

C104H160O24 L CAS 175349-60-7 (7494)

C-Heptylcalix[4]resorcinarene octa-alpha-(tert-butyl ethanoate);

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

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.

C104H168N8O16 L CAS 175349-61-8 (7483)

C-Heptylcalix[4]resorcinarene octa-alpha-(N,N-diethyl acetamide);

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

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

Cs+ dis non-aq 25°C 100% U 1995FDa (108007) 712

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.

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

END