

## SC-Database

Software version = 5.81 Data version = 4.62

Experiment list contains 1103 experiments for  
(no ligands specified)

Metal : Sm+++

(no references specified)

(no experimental details specified)

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e- HL Electron (442)  
Electron;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Sm+++	oth	none	25°C	0.0	U				1974JOb	(935) 1
									K(Sm+e=Sm(II))=-25(-1.5V)	

Method:Estimated data

Sm+++	oth	none	25°C	0.0	U				1952LAb	(936) 2
									K(Sm+3e)=-122.4(-2410 mV)	

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AsO4--- H3L Arsenate CAS 7778-39-4 (1557)  
Arsenate;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Sm+++	sol	none	25°C	0.0	C				1992FIa	(1160) 3
									Kso(SmAsO4)=-22.73	

Equilibrium monitored by EDTA and iodine titrations.

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Sm+++	sp	alc/w	25°C	50%	U I			K1=0.27 Klin=-0.89	1973KPe	(2309) 4

Medium: 50% w/w MeOH/H2O, 3 M LiClO4. K1=-0.16(0%); Klin=-0.74(90%)

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Sm+++	gl	NaClO4	25°C	0.70M	C			K1=5.81 K(Sm+HCO3=SmHCO3)=1.29	2004LBb	(3370) 5

Medium: 0.70 m NaClO4. Calculated for I=0, K1=7.46, B2=12.53,  
K(Sm+HCO3=SmHCO3)=2.34, K(Sm+HL=SmL+H)=-2.87, K(Sm+2HL=SmL2+2H)=-8.13

Sm+++	dis	NaClO4	25°C	0.70M	C	I		K1=5.73 B2=10.01	1998LBb	(3371) 6
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Method: H2O/tributylphosphate distribution and ICP-mass spectrometry.

Values calculated for I=0.0 M, K1=7.71, B2=13.09

Sm+++	sol none	25°C	0.0	C				1986FMa (3372)	7
					Kso(Sm2(CO3)3)=-34.41				

Sm+++	sol none	25°C	0.0	C				1986HMa (3373)	8
					Kso(Sm2(CO3)3)=-34.41				

Method: spectrophotometry.

Sm+++	dis oth/un	20°C	2.5M	C				1979DBb (3374)	9
					B4=14.20				

Media: 2.5 M (NH4)2NO3/hexane. Analysis by NAA. By competition with edta;  
K1(Sm(edta))=17.13 recalculated for I=2.5 from J.Am.Chem.Soc.,75 1953,4196

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	con	diox/w	25°C	10%	U I		K1=4.04	1960ATb (3506)	10
Medium: 10% w/w dioxan/H2O. K1=3.75(0%), 4.36(20%)									

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	con	none	25°C	0.00	M		K1=3.80	1972FIa (3686)	11
Sm+++	cal	none	25°C	0.00	M H		K1=3.72	1972SCd (3687)	12
DH(K1)=3.8 kJ mol-1, DS=84.1 J K-1 mol-1									

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	dis	NaCl	25°C	1.0M	C		K1=-0.66	1997HTb (5701)	13
Method: by solvent extraction from 1.0 M NaCl into CHCl3, 0.1 M 1,1,1-trifluoro-4-(2-thienyl)-2,4-pentanedione.									

Sm+++	cal	non-aq	25°C	100%	U H		K1=3.00 B2=4.89	1991ITa (5702)	14
							K3=1.50		
							K4=0.95		

Medium: DMF, 0.2 M Et4NClO4. DH(K1)=13.6 kJ mol-1, DH(K2)=19.8, DH(K3)=15  
DH(K4)=51. DS(K1)=103, DS(K2)=102, DS(K3)=79 J K-1 mol-1

Sm+++	dis	NaClO4	20°C	3.00M	U		K1=0.41 B2=0.25	1982FKb (5703)	15
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Sm+++	sol	NaClO4	25°C	?	U	K1=0.36	1982MAa	(5704)	16
Sm+++	cal	non-aq	25°C	100%	U	K1=2.04	B2=3.36	1980VCa	(5705) 17
Medium: diethylacetamide									
Sm+++	dis	NaClO4	25°C	1.00M	U T	K1=0.13	1975MHa	(5706)	18
Sm+++	sp	alc/w	25°C	50%	U I	K1=0.52	1971KBf	(5707)	19
						Klin=-0.74			
Medium: 50% w/w MeOH/H2O, 3 M LiClO4. K1=-0.02(0%); K1=0.96, Klin=0.09(100%)									
Sm+++	sp	alc/w	25°C	50%	U I	K1=0.54	1971KBg	(5708)	20
						Klin=-0.55			
Medium: 50% v/v EtOH/H2O, 3 M LiClO4. K1=0.97, Klin=0.09(90%)									
Sm+++	sp	none	25°C	0.0	U	K1=-2.03	1970KBe	(5709)	21
						Klin=-2.9			
Sm+++	ISE	NaClO4	25°C	1.0M	U	K1=0.21	1965GSb	(5710)	22
Sm+++	sol	NaClO4	25°C	0.50M	U	K1=-0.46	1962SOa	(5711)	23
Medium: HClO4									
Sm+++	sol	none	25°C	0.0	U		1960ASd	(5712)	24
						Kso(Sm(OH)2Cl)=-17.3			
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F-		HL	Fluoride				CAS 7644-39-3	(201)	
Fluoride;									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	ix	oth/un	25°C	0.02M	C T H		K1=3.61 B2= 5.99	2004LMA	(7176) 25
Medium: 0.025 M HNO3. Applying Pitzer parameters: at I=0, K1=9.60.									
Data for 5 to 45 C. DH(K1)=8.0 kJ mol-1, DH(B2)=18.9.									
Sm+++	ISE	NaClO4	25°C	0.0	C I		K1=4.15	2000LBA	(7177) 26
Method: Fluoride ISE. Values calc. from data for I=0.015-0.70 M NaClO4.									
At I=0.70 M, K1=3.225.									
Sm+++	ix	KNO3	25°C	0.02M	C		K1=3.59 B2= 6.10	1999SBc	(7178) 27
Medium: 0.025 M HNO3. Additional method: ICP-MS.									
Assumed K1(HF) = 3.03, derived from literature values.									
Sm+++	ISE	none	25°C	0.0	C H		K1=3.15 B2=6.95	1989MJa	(7179) 28
						Kso=-16.0			
Also by conductivity and radiometry. DH(Kso)=51.0 kJ mol-1; DS=-135.5.									
Sm+++	ISE	R4N.X	25°C	0.50M	C		K1=3.15 B2=6.95	1989MJb	(7180) 29
Sm+++	cal	NaClO4	25°C	1.00M	C H			1988GBa	(7181) 30

DH(K1)=10.8 kJ mol<sup>-1</sup>; DS(K1)= 95.9 J mol<sup>-1</sup> K<sup>-1</sup>

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Sm+++ ISE NaCl 25°C 1.00M C K1=3.093 1985BBb (7182) 31  
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Sm+++ gl KCl 25°C 1.00M U M 1981KTb (7183) 32  
K(SmEDTA+F)=1.68  
K(Sm(EDTA)F+F)=0.60  
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Sm+++ EMF NaClO4 25°C 1.0M U H K1=3.12 1967WCa (7184) 33  
By calorimetry: DH(K1)=39.3 kJ mol<sup>-1</sup>, DS=191.4 J K<sup>-1</sup> mol<sup>-1</sup>

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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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Sm+++ sol oth/un 25°C 0.0 U 1966FPb (8551) 34  
Kso=-11.19

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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  
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Sm+++ sol oth/un 25°C dil U 1974L0a (8614) 35  
Kso(Sm(H2IO6)(H2O)3)=-9.70

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Mo04-- H2L Molybdate (443)  
Molybdate;

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Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
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Sm+++ con oth/un 25°C .001M U K1=4.85 1968DKc (8757) 36

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Mo12042U----- H8L (2922)  
Uranium-12-molybdate;

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Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
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Sm+++ gl oth/un 20°C 0.10M U 1989SBb (8781) 37  
B(SmHL)=8.13  
B(Sm2L)=8.05  
B(SmH2L)=9.59

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N03- HL Nitrate CAS 7697-37-2 (288)  
Nitrate;

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Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
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Sm+++ cal NaClO4 25°C 2.0M C IH K1=-0.13 1998BMb (9918) 38

DH(K1)=0.2 kJ mol<sup>-1</sup>. From Pitzer extrapolation to I=0.0, K1=0.71,  
DH(K1)=-1.9 kJ mol<sup>-1</sup>

Sm+++ cal NaNO3 25°C 2.0M C H K1=-0.08 1998BMc (9919) 39  
Method: By competition with xylitol.

Sm+++ dis none 25°C 0.0 U K1=2.18 1992MSb (9920) 40

Sm+++ dis R4N.X 17°C 0.0 C T H K1=1.80 1988MSf (9921) 41  
Extraction into tributylphosphate from 0.1-2.74 M NH4NO3 medium.  
At 25 C, K1=1.89; 35 C, K1=1.48; 50 C, K1=1.30. DH(K1)=-38.3 kJ mol<sup>-1</sup>.

Sm+++ sp NaClO4 20°C 4.10M U K1=-0.02 1970ASa (9922) 42

Sm+++ dis NaClO4 25°C 1.0M U K1=0.31 1967KOb (9923) 43

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

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

Sm+++ sp NaClO4 25°C 2.0M C K1=0.22 1978ABc (10257) 44  
Medium pH 5.0. By ion exchange, K1=0.27.

Sm+++ sp NaClO4 25°C 2.0M U K1=4.22 1975EAb (10258) 45

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OH- HL Hydroxide (57)  
Hydroxide;

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

Sm+++ gl NaClO4 25°C 0.0 C IH 2000KBa (12124) 46

\*K1=-7.84  
In 0.7 M NaClO4, \*K1=-8.15. DH(\*K1)=43 kJ mol<sup>-1</sup>.

Sm+++ gl NaClO4 25°C 3.0M C TI 1999CIa (12125) 47

\*K1=-9.05  
K(2Sm+2H2O=Sm2(OH)2+2H)=-14.73  
K(3Sm+5H2O=Sm3(OH)5+5H)=-34.9  
K(5Sm+9H2O=Sm5(OH)9+9H)=-59.03

At 60 C: \*K1=-8.52, \*B(2,2)=-12.77, \*B(3Sm+5H2O)=-30.37

At I=0, 25 C: \*K1=-8.38, \*B(2,2)=-15.37, \*B(5Sm+9H2O)=-58.2

Sm+++ gl NaCl 25°C 0.10M U I 1999FBa (12126) 48

\*B(1,3)=-22.34  
In 0.1 M Me4NCl, \*B(1,3)=-22.78.

Sm+++ gl NaClO4 RT 1.0M C 1983KDe (12127) 49

\*B4=-36.7

Sm+++	gl	NaNO3	25°C	2.0M	U	1983LSb (12128)	50
						*B(1,1)=-8.64	
						*B(2,2)=-14.50	
						*B(3,4)=-26.90	
						*B(4,6)=-39.20	
Sm+++	gl	NaClO4	25°C	1.0M	U	1982NCa (12129)	51
						K(SmOH+H)=8.84	
						K[Sm(OH)2+2H]=15.73	
Sm+++	gl	NaClO4	25°C	1.00M	U	1979KDa (12130)	52
						*K1=-7.5	
						*B2=-15.0	
						*B3=-22.7	
						*B(4,3)=-19.5	
						*Kso=17.5	
Sm+++	EMF	alc/w	20°C	25%	U	1973SPe (12131)	53
						*K1(SmA+H2O=SmAOH+H)=-7.35	
						Medium: ca.25 to 35% w/w MeOH or EtOH/H2O. H3A=NTA	
Sm+++	dis	NaClO4	?	0.10M	U	1971GDb (12132)	54
						*K1=-4.4	
						Medium: LiClO4	
Sm+++	oth	oth/un	rt	10%	U	1967PBb (12133)	55
						Kso=-27.1	
						K(SmL3(s)=SmL3)=-4.9	
						Medium: 10% sea water. Method: Tyndall scattering	
Sm+++	gl	NaClO4	25°C	0.30M	U	1966FKa (12134)	56
						*K1=-8.34	
Sm+++	vlt	none	20°C	0.0	M	1966KAa (12135)	57
						Kso=-25.20	
Sm+++	oth	oth/un	20°C	dil	U	1966OPa (12136)	58
						Kso=-24.2	
						Method: Tyndall scattering	
Sm+++	EMF	none	25°C	0.0	M	1962AEa (12137)	59
						Kso=-23.89	
						Method: H electrode	
Sm+++	sp	none	20°C	0.0	U	1962KBc (12138)	60
						Kso(Sm(OH)3)=-25.2	
						K1(H+OH=H2O)=14.07 assumed. Method:colorimetry	
Sm+++	sol	none	25°C	0.0	U	1960ASd (12139)	61
						Kso(Sm(OH)3)=-25.9 (aged)	

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 Sm+++ gl oth/un 25°C var U 1951MFb (12140) 62  
 Kso(Sm(OH)3)=-22.08  
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Sm+++ gl oth/un 25°C var U 1944MKa (12141) 63  
 Kso(Sm(OH)3)=-21.2  
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Sm+++ sol oth/un 100°C var U 1932ENa (12142) 64  
 Kso=0.90 + y  
 Kso: K(Sm(OH)3(s)=Sm+3OH); y=Kso for Y+++  
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P04--- H3L Phosphate CAS 7664-38-2 (176)  
 Phosphate;  
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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	sol	none	25°C	0.0	M		1997LBd (13323) 65		
							Kso(SmP04)=-26.19		
Calculated from data for 0.10 M HCl04 solution.									

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Sm+++ sol oth/un 25°C 0.0 C I 1993FKb (13324) 66  
 Kso(SmP04)=-27.64  
 In synthetic seawater, Ks(SmP04)=-24.36.  
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Sm+++ sol none 25°C 0.0 C 1991FBa (13325) 67  
 Kso(SmP04)=-25.99  
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 P207---- H4L Pyrophosphate CAS 2466-09-3 (198)  
 Diphosphate; from (HO)2PO.0.PO(OH)2  
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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	KCl	25°C	0.50M	U		1989APd (13646) 68		
							K(Sm+H2L)=4.26		

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Sm+++ kin none 25°C 0.0 U B2=20.16 1967SSo (13647) 69  
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 P3010----- H5L CAS 10380-08-2 (1001)  
 Tripolyphosphate; from (HO)2PO.0.PO(OH).0.PO(OH)2  
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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	KNO3	25°C	0.10M	U	T H	B2=8.7 K(Sm+2HL)=6.5	1974KRa (13900) 70	
K(Sm+2HL)=6.9 and B2=8.9 (35 C), K(Sm+2HL)=6.4 and B2=8.4 (45 C) DH(Sm+2HL)=-11 kJ mol <sup>-1</sup> ; DH(B2)=-28									

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Sm+++ gl NaCl04 30°C 0.30M U K1=7.42 1963KUa (13901) 71  
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Sm+++ gl NaCl04 ? 0.10M U B2=16.98 1962RKa (13902) 72

K(Sm+HL)=4.89  
K(Sm+2HL)=8.66

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	dis	oth/un	25°C	1.0M	C		K1=0.34	1997HTb (15253)	73
Method: by solvent extraction from 1.0 M NaSCN into CHCl3, 0.1 M 1,1,1-trifluoro-4-(2-thienyl)-2,4-pentanedione.									

Sm+++	sp	NaCl04	25°C	1.00M	U	I	K1=0.13    B2=0.26	1993SMb (15254)	74
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Sm+++	sp	NaCl04	?	0.60M	U	T	K1=0.09	1964KSe (15255)	75
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S04--                      H2L      Sulfate                      CAS 7664-93-9    (15)  
Sulfate;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	sol	oth/un	25°C	0.66M	C		K1=1.96	2004SBb (16537)	76
Method: solubility of BaSO4 in 0.117 m SmCl3 solution. Calculated for I=0, K1=3.63.									

Sm+++	kin	NaCl04	25°C	0.50M	U	I	K1=1.88	1974FPb (16538)	77
At I=0.75: K1=1.60									

Sm+++	cal	none	25°C	0.0	U	H		1974FPc (16539)	78
DH(K1)=14.3 kJ mol-1, DS=118.4 J K-1 mol-1. In D20: DH(K1)=15.7, DS=122.9									

Sm+++	con	oth/un	25°C	0.0	U		K1=3.68	1973FPb (16540)	79
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Sm+++	oth	none	25°C	0.0	U		K1=3.66 K1in=0.72	1973FPb (16541)	80
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Method: ultrasonic absorption

Sm+++	con	oth/un	25°C	0.0	U		K1=3.68	1973FPb (16542)	81
Medium:D20									

Sm+++	oth	none	25°C	0.0	U		K1=3.68 K1is=0.73	1973FPb (16543)	82
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Method: ultrasonic absorption. Medium:D20

Sm+++	cal	oth/un	25°C	0.0	U	H		1969FPa (16544)	83
DH(K1)=18.1 kJ mol-1									

Sm+++	cal	oth/un	25°C	0.0	U	H	K1=3.52    B2=5.19	1969IEa (16545)	84
DH(K1)=15.5 kJ mol-1, DH(K2)=8.8, DS(K1)=119.6 J K-1 mol-1, DS(K2)=61.4									



Sm+++ ISE NaClO4 25°C 2.0M U H K1=1.30 B2=1.91 1967CCd (16546) 85  
 By calorimetry: DH(K1)=17.8 kJ mol<sup>-1</sup>, DS=82.3 J K<sup>-1</sup> mol<sup>-1</sup>

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 Sm+++ sp oth/un 25°C 0.0 U K1=3.54 1964BMb (16547) 86  
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Sm+++ con oth/un 25°C 0.0 U K1=3.66 1954SJa (16548) 87  
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S2O3-- H2L Thiosulfate CAS 73686-28-7 (177)  
 Thiosulfate;

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 Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
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Sm+++ con oth/un 32°C var U 1950DUa (16899) 88  
 B(Sm2L3)=11.26

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

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 Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
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Sm+++ gl NaClO4 25°C 1.0M C K1=1.21 B2= 1.52 1981NJa (17646) 89  
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C2H2O3 HL Glyoxylic acid CAS 298-12-4 (1142)  
 Glyoxylic acid; OHC.COOH

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

Sm+++ gl NaClO4 20°C 0.10M U K1=2.55 B2=4.59 1964PSd (18429) 90  
 K3=1.5

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

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 Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
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Sm+++ ix R4N.X 25°C 0.05M C K1=5.51 B2= 9.89 2001SBf (19059) 91  
 K(Sm+HL)=2.35

Medium: 0.05 M NH4NO3. At I=0, K1=6.43, B2=11.08.

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 Sm+++ gl KCl 25°C 1.0M U M 1988KTa (19060) 92  
 K(Sm(edta)+L)=3.25

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 Sm+++ gl KNO3 35°C 0.10M U M K1=6.61 1986RMb (19061) 93  
 B(SmL(cytidine))=9.98

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 Sm+++ sol oth/un 25°C 0.50M U K1=6.62 1970MKe (19062) 94  
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C2H3N3S2 HL CAS 2349-67-9 (6245)  
 2-Amino-5-mercapto-1,3,4-thiadiazole;

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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaClO4	25°C	0.10M	U T H		K1=6.37 B2=11.57 K3=4.18	1983SSb (19257)	95

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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
Sm+++	gl	NaClO4	25°C	1.0M	C		K1=2.00 B2= 3.40	1981NJa (20161)	96
Sm+++	gl	alc/w	25°C	95%	U H		K1=5.14 B2=9.20 B3=11.89 B4=13.00	1967Gwa (20162)	97

Medium:95% MeOH,0.5 M NaClO4. By calorimetry: DH(K1)=11.6 kJ mol<sup>-1</sup>,DS=137.1 J K<sup>-1</sup> mol<sup>-1</sup>; DH(K2)=6.4,DS=99.1; DH(K3)=8.1,DS=78.6; DH(K4)=-1.7,DS=16.7

Sm+++	sp	oth/un	19°C	0.10M	U M		K1=1.95 B2=3.74 B3=5.28	1966GAe (20163)	98
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18-20 C. Ternary complexes with hexamethylenediamine-N,N,N',N'-tetraethanoic acid

Sm+++	gl	oth/un	25°C	0.0	U		K1=2.839 B2=4.80	1964AMa (20164)	99
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Sm+++ cal NaClO4 25°C 2.0M C H 1964GRa (20165) 100  
DH(K1)=6.079 kJ mol<sup>-1</sup>, DS(K1)=59.4 J K<sup>-1</sup> mol<sup>-1</sup>; DH(B2)=12.03, DS(B2)=103;  
DH(B3)=15.79, DS(B3)=128.

Sm+++	gl	NaClO4	20°C	0.10M	U		K1=2.30 B2=3.88	1962KPa (20166)	101
Sm+++	EMF	NaClO4	20°C	2.0M	U		K1=2.01 B2=3.26 B3=3.85 B4=3.8	1958SOa (20167)	102

Method: quinhydrone electrode

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C2H4O2S H2L Thioglycolic CAS 68-11-1 (596)  
Mercaptoethanoic acid; HS.CH2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaClO4	25°C	0.20M	U		K1=6.04 B2=11.51	1996PJa (20364)	103
Sm+++	gl	NaClO4	25°C	0.20M	U M		K1=3.72 K(Sm(EDTA)+L)=3.68	1986LSb (20365)	104
Sm+++	cal	NaClO4	25°C	2.0M	C H			1964GRa (20366)	105

DH(K1)=5.586 kJ mol<sup>-1</sup>, DS(K1)=53.1 J K<sup>-1</sup> mol<sup>-1</sup>; DH(B2)=13.9, DS(B2)=98.3.

Sm+++	gl	NaClO4	20°C	0.10M	U			1964PKa (20367)	106
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K(Sm+HL)=2.11  
K(SmHL+HL)=1.36

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Sm+++      gl   NaCl04   25°C   2.0M U      1962BCa (20368) 107  
K(Sm+HL)=1.81  
K(SmHL+HL)=0.9

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C2H4O3      HL   Glycolic acid      CAS 79-14-1 (33)  
2-Hydroxyethanoic acid; HO.CH2.COOH

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

-----  
Sm+++      gl   NaCl04   25°C   3.0M C      2002TFa (20624) 108  
B(Sm2H-2L6)=-1.83  
B(Sm4H-6L8)=-19.5  
B(Sm4H-7L8)=-28.5

-----  
Sm+++      gl   NaCl04   25°C   0.20M U      K1=6.08    B2=11.71    1996PJ a (20625) 109

-----  
Sm+++      gl   NaCl04   25°C   0.20M U      M    K1=3.92      1986LSb (20626) 110  
K(Sm(EDTA)+L)=3.72

-----  
Sm+++      gl   NaCl04   25°C   0.20M U      M    K1=3.96      1985LSf (20627) 111  
K(Sm(edta)+L)=3.78

-----  
Sm+++      gl   KNO3      32°C   0.10M U      1980PPf (20628) 112  
K(Sm+HL=SmL+H)=-0.87  
\*K(SmL)=-6.01  
K(Sm+2HL=SmL2+2H)=-2.05  
\*K(SmL2)=-5.74

-----  
Sm+++      gl   NaCl04   25°C   0.50M C      T    K1=2.54    B2=4.58    1977C Ma (20629) 113  
B3=5.70  
B4=7.20

-----  
Sm+++      cal   NaCl04   25°C   2.0M C      H      1964GRa (20630) 114  
DH(K1)=-4.347 kJ mol<sup>-1</sup>, DS(K1)=34 J K<sup>-1</sup> mol<sup>-1</sup>; DH(B2)=-10.06, DS(B2)=52.3;  
DH(B3)=-15.42, DS(B3)=59.4; DH(B4)=-20.7, DS(B4)=52.7.

-----  
Sm+++      gl   NaCl04   20°C   0.10M U      K1=2.914    B2=5.01    1964PKb (20631) 115  
B3=6.57

-----  
Sm+++      EMF   NaCl04   20°C   2.0M U      K1=2.56    B2=4.53    1959SO b (20632) 116  
B3=5.9  
B4=6.4  
B5=6.0

Method: quinhydrone electrode

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C2H5NO2      HL   Glycine      CAS 56-40-6 (85)  
2-Aminoethanoic acid; H2N.CH2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaClO4	37°C	0.15M	C	M	2003TKa (21704) 117 K(Sm(edta)+HL)=1.58 K(Sm(edta)+L+2HL)=5.36 K(Sm(edta)+2L+HL)=5.96 K(Sm(edta)+3L)=5.85 K(Sm(enta)+HL)=1.83, K(Sm(enta)+2HL+H2L)=5.55, K(Sm(enta)2+HL)=2.25. K(Sm(ida)+HL)=2.85, K(Sm(ida)2+2HL)=4.68; additional constants.		
Sm+++	gl	NaClO4	25°C	0.20M	U		K1=5.14 B2= 9.48	1996PJa (21705)	118
Sm+++	gl	KNO3	25°C	0.20M	U	M	K1=6.45 K(Sm(phen)+L)=5.92	1990LSb (21706)	119
Sm+++	gl	NaClO4	25°C	0.20M	U		K1=5.14 B2= 9.48	1987PPa (21707)	120
Sm+++	gl	KNO3	35°C	0.10M	U		K(Sm+HL)=3.82	1987RRc (21708)	121
Sm+++	gl	NaClO4	25°C	0.20M	U	M	K1=5.84 K(Sm(EDTA)+L)=4.97	1986LSb (21709)	122
Sm+++	gl	KNO3	35°C	0.10M	U	M	K(Sm+HL)=3.82	1986RMb (21710)	123
							K(Sm+HL+cytidine)=8.51		
Sm+++	gl	NaClO4	25°C	0.20M	U	M	K1=5.84	1985LSe (21711)	124
							K(Sm(edta)+L)=4.97.		
Sm+++	EMF	KCl	25°C	1.0M	U	M	K(SmA+L)=3.56 K(SmA+HL)=3.00 K(SmA+H2L)=3.08	1977GMa (21712)	125

Method: Pt/H2 electrode. H3A is N-hydroxyethyl-1,2-diaminoethane-N,N',N'-triethanoic acid.

\*\*\*\*\*  
C2H6OS HL CAS 60-24-2 (841)  
2-Mercaptoethanol; HS.CH2.CH2.OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaClO4	25°C	0.10M	U	T	K1=6.33	1981SKb (22080)	126
							Temp range 15-35. K1 at 15 = 6.45; K1 at 45 = 6.16		
							*****		
							C2H6OS L DMSO CAS 67-68-5 (329)		
							Dimethylsulfoxide; (CH3)2.SO		

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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 Sm+++ sp non-aq 25°C 100% U 1992MBb (22123) 127  
 K8=1.5  
 K9=0.8  
 K10=0.3

Medium: MeCN. Method: FT-IR and Raman spectroscopy

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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  
 -----

Sm+++ gl NaClO4 22°C 0.10M U 1972MCd (22155) 128  
 K(SmH-1L+H)=7.50

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

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

Sm+++ ISE non-aq 25°C 100% C H K1=1.80 B2=3.0 1992CBa (23230) 129  
 B3=4.3

Medium: DMSO, 0.10 M Et4NClO4. By calorimetry, DH(K1)=-16.1, DH(B2)=-42,  
 DH(B3)=-78 kJ mol<sup>-1</sup>.

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

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

Sm+++ sp oth/un 25°C 0.70M U 1987APa (23395) 130  
 K(Sm+H2L)=5.66

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C3H4O2 HL Acrylic acid CAS 79-10-7 (2044)  
 Propenoic acid; CH2:CH.COOH

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

Sm+++ gl oth/un 25°C ? U M K1=2.23 1998PAa (23994) 131  
 K(SmL+acac)=5.86  
 K(Sm(acac)L+acac)=4.43

Additional method: nmr. Medium not stated.

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C3H4O3 HL Pyruvic acid CAS 127-17-3 (1152)  
 2-Oxopropanoic acid; CH3.CO.COOH

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

Sm+++ nmr NaClO4 25°C 2.00M U H K1=1.53 1980CCa (24071) 132  
 DH=-4.85 kJ mol<sup>-1</sup>. Alternative method: Calorimetry.

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C3H4O4                      H2L      Malonic acid                      CAS 141-82-2    (79)  
Propanedioic acid; CH<sub>2</sub>(COOH)<sub>2</sub>

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaClO4	25°C	0.20M	U	M	K1=4.87 K(Sm(EDTA)+L)=3.70	1986LSb (24547)	133
Sm+++	gl	NaClO4	25°C	0.20M	U	M	K1=4.92 K(Sm(edta)+L)=3.76	1985LSf (24548)	134
Sm+++	gl	NaClO4	25°C	0.20M	U	M	K1=4.87 K(Sm(edta)+L)=3.70	1984LSd (24549)	135
Sm+++	gl	NaClO4	25°C	0.10M	U		K1=4.63	1972DCc (24550)	136
Sm+++	gl	NaClO4	25°C	1.00M	U		K1=3.67    B2=6.07 B(SmHL)=6.51 B(SmHL2)=9.86	1971DGa (24551)	137
Sm+++	ix	NaClO4	25°C	0.15M	U		K(Sm+HL)=1.81 K(SmHL+HL)=1.1	1968KKc (24552)	138
Sm+++	gl	KNO3	25°C	0.10M	U		K1=4.19    B2=6.84	1968PFa (24553)	139

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C3H4O6                      H2L    CAS 560-27-0    (4233)  
Dihydroxypropanedioic acid; HOOC.C(OH)<sub>2</sub>.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	KCl	25°C	0.20M	U		K1=4.06	1973LPb (24632)	140

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C3H5NO2                      HL    (4234)  
Isonitrosoacetone; CH<sub>3</sub>.CO.CH:N.OH, anti-Pyruvic aldehyde oxime

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	diox/w	20°C	50%	U		K1=5.60	1971MAf (24649)	141

Medium: 50% dioxan, 0.1 M NaClO4

\*\*\*\*\*

C3H6N2O2                      L      Methylglyoxime                      CAS 2140-03-6    (2981)  
Methylglyoxime; CH<sub>3</sub>.C(:N.OH).CH:N.OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	diox/w	20°C	50%	U		K1=6.72    B2=12.45	1971MAf (24811)	142

Medium: 50% dioxan, 0.1 M NaClO4

\*\*\*\*\*

C3H6O2                      HL      Propionic acid      CAS 79-09-4    (35)  
 Propanoic acid; CH3.CH2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaClO4	25°C	1.0M	C		K1=1.98    B2= 3.30	1981NJa (25049)	143
Sm+++	gl	NaClO4	25°C	2.0M	U		K1=2.02    B2=3.24	1965CGa (25050)	144
Sm+++	gl	NaClO4	20°C	0.10M	U		K1=2.21    B2=3.70	1964PKa (25051)	145

C3H6O2S                      H2L      Thiolactic acid      CAS 79-42-5    (366)  
 2-Mercaptopropanoic acid; CH3.CH(SH).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaClO4	25°C	0.20M	U		K1=6.69    B2=12.44	1996PJa (25168)	146
Sm+++	gl	NaClO4	25°C	2.00M	U			1968CMa (25169)	147
							K(Sm+HL)=2.06		
Sm+++	gl	NaClO4	31°C	2.0M	U			1963BCb (25170)	148
							K(Sm+HL)=1.83		
							K(SmHL+HL)=0.9		

C3H6O2S                      H2L                      CAS 107-96-0    (437)  
 3-Mercaptopropanoic acid; HS.CH2.CH2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaClO4	25°C	2.00M	U			1968CMa (25225)	149
							K(Sm+HL)=1.74		
Sm+++	gl	NaClO4	31°C	2.0M	U			1963BCb (25226)	150
							K(Sm+HL)=2.19		
							K(SmHL+HL)=1.3		

C3H6O3                      HL                      CAS 81598-26-7    (2521)  
 3-Hydroxypropanoic acid; HO.CH2.CH2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaClO4	25°C	2.00M	U		K1=1.75	1969JCC (25279)	151

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaClO4	25°C	0.20M	U		K1=6.63    B2=12.53	1996PJa (25533)	152

Sm+++	gl	NaClO4	25°C	0.20M	U	M	K1=4.12 K(Sm(EDTA)+L)=3.86	1986LSb (25534)	153
Sm+++	gl	NaClO4	25°C	0.20M	U	M	K1=4.16 K(Sm(edta)+L)=3.92	1985LSf (25535)	154
Sm+++	gl	KNO3	30°C	0.10M	U		K(Sm+HL=SmL+H)=0.29 *K(SmL)=-4.74 K(Sm+2HL=SmL2+2H)=-0.74 *K(SmL2)=-4.13	1983MPc (25536)	155
Sm+++	gl	NaClO4	25°C	0.5M	U		K1=2.63 B3=5.82	B2= 4.66 1981JPa (25537)	156
Additional method: polarimetry									
Sm+++	gl	NaClO4	25°C	0.20M	U		K1=2.50 K3=0.90 K4=0.41	B2=4.54 1964DVa (25538)	157
Sm+++	gl	NaClO4	20°C	0.10M	U		K1=2.88 B3=6.35	B2=5.09 1964PKb (25539)	158
Sm+++	gl	NaClO4	25°C	2.0M	U		K1=2.56 K3=1.32	B2=4.58 1961CCa (25540)	159
*****									
C3H6O3			HL	Methoxyacetic			CAS 625-45-6	(29)	
Methoxyethanoic acid; CH3.O.CH2.COOH									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaClO4	20°C	0.10M	U		K1=2.13 B2=3.39	1964PKa (25607)	160
*****									
C3H7NO2			HL	Alanine			CAS 56-41-7	(86)	
2-Aminopropanoic acid; H2N.CH(CH3).COOH									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaClO4	37°C	0.15M	C	M	K(Sm(edta)+HL)=0.86 K(Sm(edta)+L)=1.08 K(Sm(nta)+HL)=1.68 K(SmH-1(nta)+HL)=2.08  K(Sm(nta)2+HL)=1.84.	2003TKa (26257)	161
Sm+++	gl	NaClO4	25°C	0.20M	U		K1=5.10 B2= 9.19	1996PJa (26258)	162
Sm+++	gl	NaNO3	25°C	0.0	U		K1=5.45	1991ADb (26259)	163
Extrapolated from data for 0.01-0.1 M NaNO3. Data for 35 and 45 C.									



Sm+++	gl	KNO3	25°C	0.20M	U	M	K1=6.75 K(Sm(phen)+L)=6.32	1990LSb (26260)	164
Sm+++	gl	NaClO4	25°C	0.20M	U		K1=5.10 B2= 9.19	1987PPa (26261)	165
Sm+++	gl	NaClO4	25°C	0.20M	U	M	K1=6.68 K(Sm(EDTA)+L)=5.37	1986LSb (26262)	166
Sm+++	gl	NaClO4	25°C	0.20M	U	M	K1=6.68 K(Sm(edta)+L)=5.87.	1985LSe (26263)	167
Sm+++	gl	NaClO4	25°C	0.20M	U	M	K1=6.88 K(Sm(edta)+L)=5.37	1984LSd (26264)	168
Sm+++	sp	R4N.X	25°C	1.00M	U		K1=7.04 B2=11.70 B(Sm2L)=11.20 B(Sm2L2)=15.80	1978SGa (26265)	169
Sm+++	gl	KNO3	25°C	0.10M	U		K1=4.7	1967EMb (26266)	170
*****									
C3H7NO2			HL			B-Alanine	CAS 107-95-9 (575)		
3-Aminopropanoic acid; H2N.CH2.CH2.COOH									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaClO4	37°C	0.15M	C		B(SmHL)=11.71 K(Sm+L=SmH-2(HL))=-1.83	2002TKa (26477)	171
Sm+++	gl	NaClO4	25°C	0.20M	U	M	K1=6.40 K(Sm(EDTA)+L)=4.99	1986LSb (26478)	172
Sm+++	gl	NaClO4	25°C	0.20M	U	M	K1=6.40 K(Sm(edta)+L)=4.99	1984LSd (26479)	173
*****									
C3H7NO2S			H2L			Cysteine	CAS 52-90-4 (96)		
2-Amino-3-mercaptopropanoic acid; H2N.CH(CH2.SH)COOH									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaClO4	37°C	0.15M	C	M	K(Sm(edta)+H2L)=2.36 K(Sm(edta)+HL)=2.26 K(Sm(nta)+L)=2.72 K(Sm(edta)+2HL)=4.06 K(Sm(edta)+L+HL)=5.13, K(Sm(edta)+2L)=5.19, K(Sm(nta)+H2L)=4.97, K(Sm(nta)2+2H2L)=6.8, K(Sm(nta)2+2HL+H2L)=8.6, K(Sm(nta)2+HL)=4.40.	2003TKa (26833)	174
Sm+++	gl	NaClO4	20°C	0.0	U T H		K1=7.300 B2=14.00	1980SDc (26834)	175

Extrapolated from data for I=0.10-1.0 M. Data for 35 and 45 C.

DH(K1)=-17.3 kJ mol<sup>-1</sup>, DS=81 J K<sup>-1</sup> mol<sup>-1</sup>; DH(K2)=-23.0, DS=50.

\*\*\*\*\*

C3H7NO3                      HL      Serine                      CAS 56-45-1    (49)

2-Amino-3-hydroxypropanoic acid; H2N.CH(CH2.OH)COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaClO4	37°C	0.15M	C		B(SmHL)=11.05 K(Sm+L=SmH-2(HL))=-3.7 B(SmH3L3)=31.72 K(Sm+2H+3L=SmH-1(HL)3)=25.65	2002TKa (27173)	176
Sm+++	gl	NaClO4	25°C	0.20M	U		K1=4.89    B2= 8.90	1996PPa (27174)	177
Sm+++	gl	NaNO3	25°C	0.10M	M	I M	K1=5.36 K(Sm(egta)+L)=3.67	1995KDd (27175)	178
Data for 0.15 and 0.05 M NaNO3. At I=0, K1=5.58, K(Sm(egta)+L)=3.96.									

Sm+++      gl    NaClO4    25°C    0.20M    U                      K1=4.92    B2= 8.78    1990PJb (27176) 179

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C3H8O2                      L      Propyleneglycol    CAS 57-55-6    (2025)

Propan-1,2-diol; CH3.CH(OH).CH2(OH)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaClO4	22°C	0.10M	U		K(SmH-1L+H)=7.55	1972Mcd (27684)	180
*****									
C3H8O3		L							
Glycerol                      CAS 56-81-5    (2707)									
Propane-1,2,3-triol; HO.CH2.CH(OH).CH2.OH									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaClO4	22°C	0.10M	U		K(SmH-1L+H)=7.25	1972Mcd (27748)	181

Sm+++      gl    NaCl      25°C    0.10M    U                      1970PKe (27749) 182  
K(SmH-1L+H)=7.25

\*\*\*\*\*

C3H12N09P3                      H6L      NTPA                      CAS 6419-19-8    (2920)

Nitrilotris(methylenephosphonic acid); N(CH2PO3H2)3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	KNO3	25°C	0.10M	U		K1=13.83    B2=23.88 K(Sm+HL)=5.74 K(Sm+2HL)=11.09	2002KAa (28586)	183

Sm+++ gl KNO3 25°C 0.10M C 1991SKb (28587) 184

K(SmL+H)=7.49

K(SmHL+H)=5.36

\*\*\*\*\*

C4H2O4 H2L Squaric acid CAS 2892-51-5 (439)  
3,4-Dihydroxy-3-cyclobutene-1,2-dione;

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

Sm+++ cal NaClO4 25°C 0.10M U H K1=2.81 B2=4.08 19760Ca (28663) 185  
DH(K1)=8.5 kJ mol<sup>-1</sup>, DS=82 J K<sup>-1</sup> mol<sup>-1</sup>; DH(B2)=12.7, DS=121

-----  
Sm+++ gl NaClO4 25°C 0.10M C H K1=2.808 B2= 4.09 19760Cb (28664) 186  
By calorimetry: DH(K1)=8.45 kJ mol<sup>-1</sup>, DS(K1)=82.0 J K<sup>-1</sup> mol<sup>-1</sup>;  
DH(B2)=12.7, DS(B2)=121.

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C4H4N2O5 H2L Thiobarbituric CAS 504-17-6 (4279)  
4,6-Dihydroxy-2-mercaptopyrimidine, 2-thiobarbituric acid;

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

Sm+++ gl oth/un 25°C 0.10M U K1=3.163 1987TSb (28896) 187

\*\*\*\*\*

C4H4N2O3 H2L Barbituric acid CAS 67-52-7 (2818)  
2,4,6-Trihydroxypyrimidine; C4HN2(OH)3

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

Sm+++ gl oth/un 25°C 0.10M U T H K1=4.21 1987TSb (28919) 188  
30 C:K=3.81; 35 C: 3.37. DH=-147 kJ mol<sup>-1</sup>, DS=-414 J K<sup>-1</sup> mol<sup>-1</sup>

\*\*\*\*\*

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

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

Sm+++ gl oth/un 25°C ? U M K1=3.83 1998PAa (29130) 189  
K(SmL+acac)=5.05  
K(Sm(acac)L+acac)=4.01

Additional method: nmr. Medium not stated.

-----  
Sm+++ gl NaClO4 25°C 0.20M U M K1=5.20 1986LSb (29131) 190  
K(Sm(EDTA)+L)=4.60

-----  
Sm+++ gl NaClO4 25°C 0.20M U M K1=5.25 1985LSf (29132) 191  
K(Sm(edta)+L)=4.68

-----  
Sm+++ gl NaClO4 25°C 0.10M U K1=3.82 1973CDc (29133) 192

-----  
Sm+++ gl NaClO4 25°C 1.00M U K1=3.00 B2=4.90 1973DMA (29134) 193

-----  
Sm+++ gl NaClO4 25°C 0.10M U K1=3.82 B2=6.01 1970RFa (29135) 194  
\*\*\*\*\*

C4H4O4 H2L Fumaric acid CAS 110-17-8 (289)  
trans-Butenedioic acid; HOOC.CH:CH.COOH

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

Sm+++ gl NaClO4 25°C 0.10M C K1=2.82 1986LCa (29217) 195  
B(SmHL)=6.22  
K(Sm+HL)=2.14

-----  
Sm+++ gl NaClO4 25°C 0.10M U K1=2.83 1973CDc (29218) 196  
\*\*\*\*\*

C4H4O5 H2L Oxobutanedioic CAS 328-42-7 (1733)  
2-Oxosuccinic acid, Oxalacetic acid; HOOC.CH2.CO.COOH

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

Sm+++ gl NaClO4 25°C 0.50M M K1=3.75 B2=7.41 1991MOa (29281) 197  
\*\*\*\*\*

C4H6O2 HL Methylacrylic (6992)  
2-Methylpropenoic acid; CH2:C(CH3)COOH

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

Sm+++ gl KCl 25°C 0.10M U K1=2.40 1995PAa (29704) 198  
\*\*\*\*\*

C4H6O2 HL Crotonic acid CAS 107-93-7 (2990)  
But-2-enoic acid; CH3.CH:CH.COOH

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

Sm+++ gl NaClO4 25°C 0.20M U M K1=3.96 1986LSb (29724) 199  
K(Sm(EDTA)+L)=3.63

-----  
Sm+++ gl NaClO4 25°C 0.20M U M K1=4.00 1985LSf (29725) 200  
K(Sm(edta)+L)=3.69  
\*\*\*\*\*

C4H6O4 H2L Succinic acid CAS 110-15-6 (112)  
1,4-Butanedioic acid; HOOC.CH2.CH2.COOH

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

Sm+++ gl NaClO4 25°C 0.10M M H K1=3.50 1986CDb (30036) 201  
DH=13.5 kJ mol<sup>-1</sup>, DS=112 J K<sup>-1</sup> mol<sup>-1</sup>

-----  
Sm+++ gl NaClO4 25°C 0.20M U M K1=4.49 1986LSb (30037) 202  
K(Sm(EDTA)+L)=4.01  
-----

Sm+++ gl NaCl04 25°C 0.20M U M K1=4.54 1985LSf (30038) 203  
K(Sm(edta)+L)=4.08

Sm+++ gl NaCl04 25°C 0.20M U M K1=4.49 1984LSd (30039) 204  
K(Sm(edta)+L)=4.01

Sm+++ sol oth/un 25°C 0.50M U K1=4.96 1970MKe (30040) 205

Sm+++ ix NaCl04 25°C 0.15M U 1968KKc (30041) 206  
K(Sm+HL)=2.00  
K(SmHL+HL)=1.4

\*\*\*\*\*

C4H6O4 H2L Me-Malonic Acid CAS 516-15-2 (816)  
Methylpropanedioic acid; HOOC.CH(CH3).COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
Sm+++ gl KCl 25°C 0.20M U K1=4.13 B2=6.31 1975PLa (30136) 207

\*\*\*\*\*

C4H6O4S H2L Thiodiacetic CAS 123-93-3 (140)  
2,2'-Thiodiglycolic acid, Thiodiethanoic acid; HOOC.CH2.S.CH2.COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
Sm+++ gl NaCl04 37°C 0.15M C K1=3.455 B2= 5.72 2003TKa (30230) 208  
B(SmH-1L)=-3.67  
K(Sm+HL)=2.26

Sm+++ gl NaCl04 25°C 1.00M U K1=2.90 B2=4.68 1973DGa (30231) 209  
B(SmHL)=5.59  
B(SmHL2)=7.82

\*\*\*\*\*

C4H6O4S H3L Thiomalic acid CAS 70-49-5 (109)  
2-Mercaptosuccinic acid, 2-Sulfanyl-1,4-butanedioic acid; HOOC.CH(SH).CH2.COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
Sm+++ gl NaCl04 25°C 0.20M U K1=6.24 B2=12.00 1996PJa (30362) 210

Sm+++ gl NaCl04 25°C 0.20M U M K1=4.83 1986LSb (30363) 211  
K(Sm(EDTA)+L)=4.56

\*\*\*\*\*

C4H6O5 H2L Malic acid CAS 617-48-1 (393)  
2-Hydroxybutane-1,4-dioic acid, Hydroxy-succinic acid; HOOC.CH2.CH(OH).COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
Sm+++ gl KCl 25°C 0.1M U K1=4.95 2004SBa (30716) 212  
K(Sm+HL)=2.90  
K(Sm+H-1L)=8.28

Sm+++	gl	KCl	25°C	0.10M	U		K1=5.01 K(Sm+HL)=2.94	2003SBa (30717)	213
Sm+++	gl	NaClO4	25°C	0.20M	U		K1=5.42 B2=10.00	1996PJ a (30718)	214
Sm+++	gl	NaClO4	25°C	0.20M	U	M	K1=4.53 K(Sm(EDTA)+L)=4.11	1986LSb (30719)	215
Sm+++	gl	NaClO4	25°C	0.20M	U	M	K1=4.58 K(Sm(edta)+L)=4.18	1985LSf (30720)	216
Sm+++	gl	KNO3	30°C	0.10M	U	M	K(Sm(EDTA)+L)=2.137	1984AIa (30721)	217
Sm+++	gl	KNO3	20°C	0.10M	U		B(SmHL)=7.62	1980SDa (30722)	218
Sm+++	gl	KNO3	20°C	0.10M	U		K1=4.76 B2=7.82 K(Sm+HL)=2.23	1980SDb (30723)	219
Sm+++	gl	NaClO4	25°C	0.10M	U		K1=4.89 B2=8.16	1970RFa (30724)	220
Sm+++	EMF	NaClO4	25°C	2.00M	U		K1=3.90 B2=6.48	1969JP a (30725)	221
Sm+++	EMF	KCl	25°C	0.20M	U		K1=4.41	1964DAb (30726)	222
*****									
C4H6O5 H2L Diglycolic acid CAS 110-99-6 (243)									
Di(carboxy)methyl ether, 2,2'-Oxydiethanoic acid; HOOC.CH2.O.CH2.COOH									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaClO4	37°C	0.15M	C		K1=5.72 B2=10.53 B3=13.53	2003TKa (30925)	223
Sm+++	gl	KCl	25°C	1.0M	U	M	K(Sm(edta)+L)=2.55	1988KTa (30926)	224
Sm+++	EMF	NaClO4	20°C	1.00M	U	T	K1=5.62 B2=10.01 B3=13.03	1972G0a (30927)	225
K1(5 C)=5.62, B2=10.06, B3=13.09; K1(35 C)=5.61, B2=9.92, B3=12.87; K1(50 C)=5.52, B2=9.79, B3=12.63									
Sm+++	cal	NaClO4	25°C	1.0M	C	H		1963GRd (30928)	226
DH(K1)=-4.385 kJ mol <sup>-1</sup> , DS(K1)=91.2 J K <sup>-1</sup> mol <sup>-1</sup> ; DH(B2)=-12.04, DS(B2)=149; DH(B3)=-17.95, DS(B3)=184.									
Sm+++	EMF	NaClO4	20°C	1.00M	U		K1=5.55 B2=9.89 B3=12.79	1963GTa (30929)	227

Method: quinhydrone electrode

C4H6O6                      H2L      L-Tartaric acid    CAS 87-69-4    (92)  
L-Tartaric acid, L-2,3-Dihydroxybutanedioic acid;  $\text{HOOC} \cdot \text{CH}(\text{OH}) \cdot \text{CH}(\text{OH}) \cdot \text{COOH}$

\*\*\*\*\*

C4H7NO3                      HL                      CAS 543-24-8    (3586)  
N-Acetylglycine; CH<sub>3</sub>.CO.NH.CH<sub>2</sub>.COOH

\*\*\*\*\*

C4H7NO4                      H2L      Aspartic acid      CAS 56-84-8      (21)  
Aminobutanedioic acid; H2N.CH(CH2.COOH).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Sm+++	gl	NaClO4	37°C	0.15M	C			B(SmH2L)=14.89 B(SmHL)=11.84 K(Sm+L=SmH-1(HL))=5.56 K(Sm+L=SmH-2(HL))=-1.80	2002TKa (31936)	234
Sm+++	gl	NaClO4	25°C	0.20M	U			K1=5.89 B2=10.81	1996PJ a (31937)	235
Sm+++	gl	NaClO4	25°C	0.20M	U			K1=5.89 B2=10.81	1996PPa (31938)	236
Sm+++	gl	NaClO4	25°C	0.20M	U			K1=5.89 B2=10.81	1990PJb (31939)	237
Sm+++	gl	NaClO4	25°C	0.20M	U	M		K1=6.16 K(Sm(EDTA)+L)=5.37	1986LSb (31940)	238
Sm+++	gl	NaClO4	30°C	0.10M	U			K1=5.13 B2=9.64	1984YLa (31941)	239
Sm+++	gl	NaClO4	40°C	0.10M	U T			K1=9.45 B2=15.85	1971TSe (31942)	240

Sm+++ gl KCl 25°C 0.10M U K1=5.55 B2=9.72 1968DRb (31943) 241  
 \*\*\*\*\*

C4H7NO4 H2L IDA CAS 142-73-4 (118)  
 Iminodiethanoic acid; HN(CH2.COOH)2

-----  
 Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
 -----  
 Sm+++ gl NaClO4 37°C 0.15M C K1=6.75 B2=12.33 2003TKa (32356) 242  
 B(SmH-2L)=-5.918  
 -----

Sm+++ gl KCl 25°C 1.0M U M 1988Kta (32357) 243  
 K(Sm(edta)+L)=4.29  
 -----

Sm+++ gl NaClO4 25°C 0.20M U M K1=6.86 B2=12.39 1988VSc (32358) 244  
 K(Sm(HEDTA)+L)=5.65  
 K(Sm(CDTA)+L)=4.68  
 K(Sm(DTPA)+L)=4.27  
 -----

Sm+++ gl NaClO4 25°C 0.20M U M K1=6.86 B2=12.39 1987VSb (32359) 245  
 K(Sm(NTA)+L)=5.86  
 K(Sm(edta)+L)=4.47  
 -----

Sm+++ EMF KCl 25°C 1.0M U M 1977GMa (32360) 246  
 K(SmA+L)=4.64  
 K(SmA+H2L)=0.95  
 K(SmA+H3L)=2.39

Method: Pt/H2 electrode. H3A is N-hydroxyethyl-1,2-diaminoethane-N,N',N'-triethanoic acid.

-----  
 Sm+++ cal KNO3 20°C 0.10M U HM 1971GKb (32361) 247  
 K(SmA+L)=4.11

DH(SmA+L)=-17.82 kJ mol<sup>-1</sup>, DS=18.0 J K<sup>-1</sup> mol<sup>-1</sup>. DH(SmAL)=-31.8, DS=298.  
 H4A=EDTA

-----  
 Sm+++ gl KNO3 25°C 0.10M U M K1=6.64 B2=11.88 1962THa (32362) 248  
 Ternary complexes with N-(2-hydroxyethyl)diaminoethane-triethanoic acid  
 \*\*\*\*\*

C4H8N2O2 H2L Dimethylglyoxim CAS 95-45-4 (2032)  
 2,3-Butanedione dioxime, Dimethylglyoxime; CH3.(C:NOH).(C:NOH).CH3

-----  
 Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
 -----  
 Sm+++ gl diox/w 20°C 50% U K1=8.01 B2=14.98 1971MAf (32550) 249  
 Medium: 50% v/v dioxan, 0.1 M NaClO4  
 -----

C4H8N2O3 HL Asparagine CAS 70-47-3 (17)  
 2-Aminobutanedioic acid 4-amide; H2N.CH(CH2.CO.NH2).COOH

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



Sm+++ gl NaClO4 30°C 0.10M U K1=3.94 B2=6.82 1984YLa (32730) 250  
\*\*\*\*\*

C4H8N2O3 HL Gly-Gly CAS 556-50-3 (54)  
Glycyl-glycine; H2N.CH2.CO.NH.CH2.COOH

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

Sm+++ gl NaClO4 30°C 0.10M U T H K1=4.08 B2=6.93 1980SBb (33052) 251  
K3=2.80

DH=-99.92 kJ mol<sup>-1</sup>. Further data available for T=40. Alternative method:  
Conductivity.

\*\*\*\*\*

C4H8N2O4 H2L HDA CAS 19247-05-3 (1025)  
Hydrazine-N,N'-diethanoic acid; HOOC.CH2.NH.NH.CH2.COOH

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

Sm+++ gl KCl 60°C 0.10M U K1=6.43 B2=10.68 1978NBa (33093) 252  
B3=13.64

\*\*\*\*\*

C4H8N2O4 H2L CAS 39156-77-9 (3008)  
Hydrazine-N,N-diethanoic acid; H2N.N(CH2.COOH)2

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

Sm+++ gl KNO3 30°C 0.10M U M 1984AIa (33112) 253  
K(Sm(EDTA)+L)=2.978

-----  
Sm+++ EMF KCl 25°C 0.10M U K1=4.1 B2=7.0 1954VIa (33113) 254  
K3=0.1

\*\*\*\*\*

C4H8O2 HL Isobutyric acid CAS 79-31-2 (573)  
2-Methylpropanoic acid; CH3.CH(CH3).COOH

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

Sm+++ gl NaClO4 25°C 2.00M U H K1=2.00 B2=3.25 1965CGa (33246) 255  
By calorimetry: DH(K1)=11.1 kJ mol<sup>-1</sup>, DS=75.7 J K<sup>-1</sup> mol<sup>-1</sup>; DH(K2)=8.8, DS=53

-----  
Sm+++ gl NaClO4 25°C 0.50M U K1=2.05 B2=3.30 1964SPa (33247) 256

\*\*\*\*\*

C4H8O2S HL CAS 2935-90-2 (1147)  
Methyl-3-mercaptopropionate; HS.CH2.CH2.CO2.CH3

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

Sm+++ gl KNO3 25°C 0.10M U T H K1=2.80 1975SBa (33372) 257  
DH=-33.3 kJ mol<sup>-1</sup> and DS=-28.9 J mol<sup>-1</sup> K<sup>-1</sup>.

Values at 35 and 45 C by conductivity

\*\*\*\*\*

C4H8O2S                      HL                      CAS 627-04-3 (3007)  
S-Ethylthioethanoic acid; CH3.CH2.S.CH2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaClO4	31°C	2.0M	U		K1=1.85    B2=2.75	1963BCb (33413)	258

\*\*\*\*\*

C4H8O3                      HL                      CAS 594-61-6 (81)  
2-Hydroxy-2-methylpropanoic acid; (CH3)2C(OH).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaClO4	25°C	0.20M	U		K1=2.75    B2=4.77 K3=1.40 K4=1.21	1964DVa (33515)	259
Sm+++	EMF	NaClO4	25°C	1.0M	U		K1=2.63    B2=4.76 K3=1.33 K4=1.15	1964EVa (33516)	260

Method: quinhydrone electrode

Sm+++	gl	NaClO4	20°C	0.10M	U		K1=2.993    B2=5.39 B3=6.77	1964PKb (33517)	261
Sm+++	gl	NaClO4	25°C	0.50M	U		K1=2.63    B2=4.60	1964SPa (33518)	262
Sm+++	gl	NaClO4	25°C	2.0M	U		K1=2.75    B2=4.90 K3=1.58	1961CCa (33519)	263

\*\*\*\*\*  
C4H8O4                      HL                      CAS 21620-60-0 (2326)  
2,3-Dihydroxy-2-methylpropanoic acid; HO.CH2.C(OH)(CH3).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	KNO3	25°C	0.10M	C		K1=3.05    B2=5.39 K3=1.64	1975PFb (33685)	264

\*\*\*\*\*

C4H8O5                      HL                      CAS 56309-80-9 (2365)  
2,3-Dihydroxy-2-hydroxymethylpropanoic acid; HO.CH2.C(CH2.OH)(OH).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	EMF	KNO3	25°C	0.10M	U		K1=3.09    B2=5.50 K3=1.90	1976PKb (33711)	265
Sm+++	gl	NaClO4	25°C	0.50M	U		K1=2.86    B2=5.07 B3=6.51	1964SPa (33712)	266

\*\*\*\*\*

C4H9NO2                      HL                      2-Aminobutyric    CAS 2835-81-6 (571)  
2-Aminobutanoic acid; CH3.CH2.CH(NH2).COOH

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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Sm+++      gl  KNO3   25°C 0.10M U T      K1=5.26      1978SSb (33924) 267
*****
C4H9NO3          HL   Threonine          CAS 72-19-5 (48)
2-Amino-3-hydroxybutanoic acid; H2N.CH(CH(OH).CH3)COOH
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Sm+++      gl  NaClO4 25°C 0.20M U      K1=4.98      B2= 9.38 1996PPa (34323) 268
-----
Sm+++      gl  NaClO4 25°C 0.20M U      K1=4.98      B2= 9.38 1990PJB (34324) 269
*****
C4H11O4P          HL                      (4276)
Diethylphosphoric acid; (C2H5O)2.PO.OH
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Sm+++      kin oth/un 25°C      U      K1=1.67      1971MGB (35267) 270
*****
C4H13N3          L   Dien          CAS 111-40-0 (584)
1,4,7-Triazaheptane, 2,2'-Iminobis(ethylamine), diethylenetriamine;
NH2.(CH2)2.NH.(CH2)2.NH2
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Sm+++      EMF NaClO4 25°C 100% C H      K1=5.74      B2=10.31 2000CDa (35813) 271
Medium: DMF, 0.10 M Et4N[CF3SO3]. Method: Ag/Ag+ electrode.
By calorimetry: DH(K1)=-54.8, DH(B2)=-113.6 kJ mol-1.
-----
Sm+++      ISE non-aq 25°C 100% C H      K1=2.78      B2=5.40 1993CCb (35814) 272
Medium: DMSO, 0.1 M Et4NClO4. Method: Ag+ ISE. By calorimetry, DH(K1)=-31.1
kJ mol-1, DS=-51; DH(B2)=-79.6, DS=-164.
*****
C4H14N2O6P2      H2L   EDDPO          CAS 1733-49-9 (2435)
1,2-Diaminoethane-N,N'-bis(methylenephosphonic) acid; (H2O3P.CH2.NH.CH2)2
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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Sm+++      gl  KCl     25°C 0.10M U      K(Sm+HL)=8.43
*****
C5H2O5          H2L   Croconic acid    CAS 488-86-8 (1643)
4,5-Dihydroxycyclopent-4-ene-1,2,3-trione;
-----

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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Sm+++      cal NaClO4 25°C 0.10M U H      K1=3.08      B2=3.83 1978COa (35948) 274
DH(K1)=3.59 kJ mol-1, DS=71.5; DH(K2)=-3.39, DS=-9.61
-----

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C5H4NO2Cl H2L CAS 53223-89-9 (5916)  
5-Chloropyridine-2,3-diol;

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

Sm+++ gl diox/w 35°C 50% U K1=7.82 1984SSd (36036) 275

\*\*\*\*\*

C5H4N2O2 HL CAS 98-97-5 (1879)  
Pyrazine-2-carboxylic acid; cyclo(-CH:CH.N:C(COOH).CH:N-)

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

Sm+++ cal NaClO4 25°C 1.0M C H 1990YKb (36063) 276  
DH(K1)=-0.30 kJ mol-1, DS(K1)=53.6 J K-1 mol-1.

-----  
Sm+++ EMF NaClO4 25°C 1.0M C K1=2.85 B2= 5.22 1983KKb (36064) 277  
B3=7.07

Method: Pt/quinhydrone electrode.

\*\*\*\*\*

C5H4O2S HL 2-Thenoic acid CAS 527-72-0 (2312)  
Thiophene-2-carboxylic acid; C4H3S.COOH

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

Sm+++ gl NaClO4 25°C 0.10M U K1=2.02 B2=3.28 1969RFa (36263) 278

\*\*\*\*\*

C5H4O3 HL 2-Furoic acid CAS 88-14-2 (2492)  
Furan-2-carboxylic acid; C4H3O.COOH

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

Sm+++ gl NaClO4 25°C 0.10M U K1=1.91 B2=3.13 1969RFa (36298) 279

\*\*\*\*\*

C5H4O3 HL CAS 488-93-7 (1166)  
Furan-3-carboxylic acid; C4H3O.COOH

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

Sm+++ cal NaClO4 25°C 2.00M U H K1=1.67 1976YCa (36310) 280  
DH=6.40 kJ mol-1 and DS=53.55 J mol-1 K-1.

\*\*\*\*\*

C5H5NO2 HL CAS 16867-04-2 (2316)  
2,3-Dihydroxypyridine, 3-Hydroxypyridin-2(1H)-one; C5H3N(OH)2

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

Sm+++ gl NaClO4 25°C 0.10M U K1=8.18 1970GDa (36797) 281

\*\*\*\*\*

C5H5O3F3 HL (7056)

2-Oxa-6-trifluorohexa-3,5-dione; CH3.O.CO.CH2.CO.CF3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Sm+++	gl	diox/w	25°C	50%	M	I		K1=5.68 K3=4.25	1994SSa (37070)	282

Medium: 50% dioxan, I=0 corr. At 35 C: K1=5.49, K2=4.93, K3=4.09

\*\*\*\*\*  
C5H6O4                      H2L      Citraconic acid    CAS 498-23-7    (3021)  
Citraconic acid; CH3.C(COOH):CH.COOH

Sm+++	gl	NaClO4	25°C	0.20M	U	M		K1=5.34 K(Sm(EDTA)+L)=4.49	1986LSb (37372)	283
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Sm+++	gl	NaClO4	25°C	0.20M	U	M		K1=5.40 K(Sm(edta)+L)=4.52	1985LSf (37373)	284
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\*\*\*\*\*  
C5H6O4                      H2L      Itaconic acid      CAS 97-65-4    (398)  
Methylenesuccinic acid; HOOCH2.C(:CH2).COOH

Sm+++	gl	KCl	25°C	0.20M	U			K1=3.10 K(Sm+HL)=1.96	1989MFa (37446)	285
-------	----	-----	------	-------	---	--	--	--------------------------	-----------------	-----

Sm+++	gl	NaClO4	25°C	0.20M	U	M		K1=4.47 K(Sm(EDTA)+L)=4.32	1986LSb (37447)	286
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Sm+++	gl	NaClO4	25°C	0.20M	U	M		K1=4.52 K(Sm(edta)+L)=4.35	1985LSf (37448)	287
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Sm+++	sol	oth/un	25°C	1.0M	U			K1=3.78	1984KPf (37449)	288
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in 1.0 M HCl

Sm+++	oth	NaClO4	25°C	1.0M	U			K1=2.07 B(SmHL)=6.48 B(SmH2L2)=12.72	1972STd (37450)	289
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\*\*\*\*\*  
C5H7NO3                      HL                                      (4313)  
Isonitrosoacetylacetone; HO.N:CH.CO.CH2.CO.CH3

Sm+++	gl	diox/w	20°C	50%	U			K1=4.48    B2=7.95	1971MAf (37532)	290
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Medium: 50% v/v dioxan, 0.1 M NaClO4

\*\*\*\*\*  
C5H7NO4                      HL                                      (6083)  
2-Acrylamidoglycolic acid; CH2:CH.CO.NH.CH(OH).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Sm+++	gl	NaNO3	25°C	0.50M	C			K1=2.61 B(SmH-1L)=-3.40 B(Sm2H-3L3)=-8.60	1977DPa (37542)	291
*****										
C5H8N2O3		H2L		(4317)						
Methylacetylglyoxime; CH3.C(:N.OH).C(:N.OH).CO.CH3										
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Sm+++	gl	diox/w	20°C	50%	U			K1=5.59 B2=10.19	1971MAf (37709)	292
*****										
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
Sm+++	gl	KCl	25°C	0.10M	U			K1=5.87 B2=10.50 K3=3.47	1995PAa (38077)	293
Sm+++	gl	diox/w	30°C	75%	U			K1=7.03 B2=12.77 K3=4.26	1979MBc (38078)	294
Sm+++	gl	NaClO4	20°C	0.10M	U	M		K(Sm(EDTA)+L)=3.53	1973TZa (38079)	295
Sm+++	gl	R4N.X	25°C	0.10M	U	M		K(Sm(EDTA)+L)=2.42	1972FGa (38080)	296
Sm+++	gl	alc/w	?	50%	U	I		K1=6.89	1971KOa (38081)	297
Medium: 5-80% MeOH, 0.005 SmCl3, 0.005 HL. K1(5%)=5.81, K1(80%)=8.12										
Sm+++	gl	NaClO4	25°C	2.0M	U			K1=5.32 B2=9.72	1964YCa (38082)	298
Sm+++	gl	oth/un	30°C	0.10M	U			K1=5.59 B2=10.05 K3=2.90	1960GFa (38083)	299
Sm+++	gl	oth/un	30°C	0.0	U			K1=5.9 B2=10.4 K3=3.2	1955IFa (38084)	300
*****										
C5H8O4		H2L		CAS 601-75-2 (479)						
Ethylpropanedioic acid; H00C.CH(C2H5).COOH										
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Sm+++	gl	KCl	25°C	0.20M	U			K1=4.10	1989ZPa (38249)	301
In 70.4% v/v EtOH/H2O: K1 = 6.29										
*****										

C5H8O4                      H2L                      CAS 498-21-5 (2234)

Methylsuccinic acid; HOOC.CH2.CH(CH3).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaCl04	25°C	0.10M	U		K1=3.41    B2=5.05	1970RFa (38268)	302

\*\*\*\*\*

C5H8O4                      H2L                      Glutaric acid                      CAS 110-94-1 (420)

Pentanedioic acid; HOOC.CH2.CH2.CH2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaCl04	25°C	0.10M	M	H	K1=3.24	1986CDb (38354)	303

DH=14.1 kJ mol<sup>-1</sup>, DS=109 J K<sup>-1</sup> mol<sup>-1</sup>

Sm+++	gl	NaCl04	25°C	0.20M	U	M	K1=4.26 K(Sm(EDTA)+L)=3.51	1986LSb (38355)	304
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Sm+++	gl	NaCl04	25°C	0.20M	U	M	K1=4.30 K(Sm(edta)+L)=3.56	1985LSf (38356)	305
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Sm+++	gl	NaCl04	25°C	0.20M	U	M	K1=4.20 K(Sm(edta)+L)=3.51	1984LSd (38357)	306
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Sm+++	sol	oth/un	25°C	0.50M	U		K1=3.68	1970MKe (38358)	307
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C5H8O7                      H2L                      CAS 40120-71-6 (3022)

2,3,4-Trihydroxypentanedioic acid, Trihydroxyglutaric acid; HOOC.(CH(OH))3.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	KCl	24°C	0.20M	U		K1=3.81	1966DDa (38439)	308

\*\*\*\*\*

C5H9NO2                      HL                      Proline                      CAS 147-85-3 (44)

Pyrrolidine-2-carboxylic acid; C4H8N.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaCl04	37°C	0.15M	C	M		2003TKa (38640)	309

K(Sm(edta)+L)=3.4  
K(Sm(nta)+HL)=2.68  
K(Sm(nta)+2HL)=4.56  
K(Sm(nta)2+HL)=2.77

K(Sm(nta)2+2HL)=4.55.

Sm+++	gl	NaCl04	25°C	0.10M	U		B2=5.53	1981ZLa (38641)	310
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C5H9NO3                      HL                      Hydroxyproline                      CAS 51-35-4 (416)

4-Hydroxy-2-pyrrolidinecarboxylic acid; C4H7N(OH)(COOH)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaCl	37°C	0.15M	U		K1=3.44	1997GMa (38750)	311

Sm+++	gl	NaCl04	25°C	0.10M	U		B2=4.95	1981ZLa (38751)	312
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C5H9NO4                      H2L      Glutamic acid      CAS 56-86-0    (22)

2-Aminopentanedioic acid; H2N.CH(CH2.CH2.COOH)COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Sm+++	gl	KCl	30°C	0.10M	U T H		K1=4.087	1978AGb (39124)	313
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Data for 40 C. DH and DS values reported.

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C5H9NO4                      H2L      MIDA                      CAS 4408-64-4    (190)

N-Methyliminodiethanoic acid; CH3.N(CH2.COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Sm+++	gl	KCl	25°C	0.10M	U		K1=6.67    B2=11.90	1980MGc (39279)	314
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B3=15.03

B(Sm+2OH+L)=16.52

Sm+++	gl	KNO3	25°C	0.10M	U		K1=7.05	1977TIa (39280)	315
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C5H10O3                      HL                      CAS 3739-30-8    (3612)

2-Hydroxy-2-methylbutanoic acid, Methylene glycolic acid; CH3.CH2.C(OH)(CH3)COOH

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

Sm+++	gl	KNO3	25°C	0.10M	U		K1=2.80    B2=4.95	1969PCa (40262)	316
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K3=1.51

Sm+++	EMF	NaCl04	25°C	1.0M	U		K1=2.60    B2=4.74	1964EVa (40263)	317
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K3=1.26

K4=1.14

Method: quinhydrone electrode.

\*\*\*\*\*

C5H10O3                      HL                      CAS 617-31-2    (474)

2-Hydroxypentanoic acid; CH3.CH2.CH2.CH(OH).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Sm+++	gl	NaCl04	25°C	1.0M	U		K1=2.40	1968GCa (40286)	318
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C5H10O4                      HL                      CAS 4767-03-7    (4297)

2,2-Bis(hydroxymethyl)propanoic acid; CH3.C(CH2OH)2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Sm+++      gl   NaClO4   25°C   0.10M   U      K1=2.48    B2=4.15    1970RDa (40303) 319  
K3=1.30

\*\*\*\*\*

C5H10O4                      HL                      CAS 19860-56-1 (2327)  
2,3-Dihydroxy-2-methylbutanoic acid; CH3.CH(OH).C(OH)(CH3).COOH

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

Sm+++      gl   KNO3    25°C   0.10M   C      K1=3.14    B2=5.46    1975PFb (40318) 320  
K3=1.45

\*\*\*\*\*

C5H10O5                      L      D-Ribose                      CAS 50-69-1 (512)  
D-Ribose;

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

Sm+++      cal none    25°C   0.0   U    H    K1=1.05      1993MLa (40354) 321  
DH(K1)=-14.2 kJ mol<sup>-1</sup>, TDS=-8.2

\*\*\*\*\*

C5H11NO2                      HL      Valine                      CAS 72-18-4 (43)  
2-Amino-3-methylbutanoic acid; H2N.CH(CH(CH3)2)COOH

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

Sm+++      gl   NaClO4   25°C   0.20M   U      K1=5.24    B2=10.28    1996PPa (40751) 322

Sm+++      gl   KNO3    25°C   0.20M   U    M    K1=6.47      1990LSb (40752) 323  
K(Sm(phen)+L)=5.74

Sm+++      gl   NaClO4   25°C   0.20M   U      K1=5.24    B2=10.28    1990PJb (40753) 324

Sm+++      gl   NaClO4   25°C   0.20M   U    M    K1=6.68      1986LSb (40754) 325  
K(Sm(EDTA)+L)=6.05

Sm+++      gl   NaClO4   25°C   0.20M   U    M    K1=6.68      1985LSe (40755) 326  
K(Sm(edta)+L)=6.05.

Sm+++      gl   KCl      25°C   0.10M   U    T      K1=3.90      1974BFa (40756) 327

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C5H11NO2S                      HL      Methionine                      CAS 63-68-3 (42)  
2-Amino-4-(methylthio)butanoic acid; H2N.CH(CH2.CH2.S.CH3)COOH

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

Sm+++      gl   NaClO4   25°C   0.20M   U      K1=5.04    B2= 9.74    1996PPa (41121) 328

Sm+++      gl   NaNO3    25°C   0.10M   M    I    M    K1=5.44      1995KDD (41122) 329  
K(Sm(egta)+L)=3.78

Data for 0.15 and 0.05 M NaNO3. At I=0, K1=5.74, K(Sm(egta)+L)=3.99.

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Sm+++ gl NaClO4 25°C 0.20M U K1=5.04 B2= 9.74 1990PJb (41123) 330

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C5H12O5 L Xylitol CAS 87-99-0 (2139)

Xylitol; HO.CH2.HCOH.HOCH.HCOH.CH2.OH

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

-----  
Sm+++ cal NaClO4 25°C 2.0M C H K1=1.00 1998BMc (41692) 331

-----  
Sm+++ cal oth/un 25°C ? U H K1=0.91 1994RMb (41693) 332

DH(K1)=-13.7 kJ mol<sup>-1</sup>, TDS=-8.5

\*\*\*\*\*

C6H4O5 H2L Comenic acid CAS 499-78-5 (2544)

3-Hydroxypyran-4-one-6-carboxylic acid;

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

-----  
Sm+++ sp KCl 25°C 0.10M C I K1=6.112 1987PEa (42320) 333

Data for 0.031-0.95 M KCl.

\*\*\*\*\*

C6H5NO2 HL Picolinic acid CAS 98-98-6 (391)

2-Pyridine-carboxylic acid; C5H4N.COOH

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

-----  
Sm+++ gl KNO3 25°C 0.20M U M K1=4.56 1987LSc (42593) 334

K(Sm(nta)+L)=4.52, K(Sm(edta)+L)=4.48.

-----  
Sm+++ gl NaClO4 25°C 0.50M U K1=3.65 B2=6.99 1977GGb (42594) 335  
B3=9.60

-----  
Sm+++ gl KNO3 25°C 0.10M U K1=3.97 B2=7.43 1968PIa (42595) 336  
K3=2.83  
K4=2.20

-----  
Sm+++ gl NaClO4 25°C 2.0M U K1=3.85 B2=6.84 1965YCa (42596) 337

-----  
Sm+++ gl KNO3 25°C 0.10M U K1=4.06 B2=7.40 1964THb (42597) 338  
B3=10.6

\*\*\*\*\*

C6H5NO2 HL Nicotinic acid CAS 59-67-6 (419)

3-Pyridine-carboxylic acid; C5H4N.COOH

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

-----  
Sm+++ gl NaClO4 25°C 0.20M U K1=2.07 1973FDa (42687) 339

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C6H5NO3 H2L CAS 874-24-8 (4356)

3-Hydroxypyridine-2-carboxylic acid; C5H3N.(OH)(COOH)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaClO4	30°C	0.10M	U			1969DNc (42754)	340

K(Sm+HL)=3.54  
K(SmHL+HL)=3.29

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Sm+++	gl	R4N.X	25°C	0.10M	C		K1=1.48	1990CBe (42816)	341
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C6H5NO4	H2L	4-Nitrocatechol	CAS 3316-09-4	(890)
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1,2-Dihydroxy-4-nitrobenzene; O2N.C6H3(OH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Sm+++	gl	NaNO3	25°C	0.0	U	M	K1=9.63	1996KDb (42941)	342
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K(Sm(egta)+L)=5.70

Extrapolated from data for I=0.05-0.15 M NaNO3.

Sm+++	gl	KNO3	25°C	0.10M	U		K1=9.02	B2=15.65	1981BDa (42942)	343
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C6H5NO4	H2L		CAS 3163-07-3	(2711)
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2,4-Dihydroxy-1-nitrobenzene; O2N.C6H3(OH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Sm+++	sp	KCl	25°C	0.10M	M	I	K1=6.22	1989PEa (42959)	344
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C6H5O4Br	L		CAS 40838-32-2	(1084)
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6-Bromo-5-hydroxy-2-(hydroxymethyl)-4H-pyran-4-one;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Sm+++	sp	KCl	25°C	0.10M	U		K1=5.27	1987PLa (43115)	345
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C6H5O4Cl	HL	Chlorokojic aci	(3086)
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3-Chloro-5-hydroxy-2-hydroxymethyl-4-pyrone;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Sm+++	gl	oth/un	30°C	0.10M	U		K1=5.83	B2=10.91	1972DSd (43137)	346
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C6H5O4I	L		(1085)
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6-Iodo-5-hydroxy-2-hydroxymethyl-4H-pyran-4-one;

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

Sm+++ sp KCl 25°C 0.10M U K1=5.31 1987PLa (43157) 347  
 \*\*\*\*\*  
 C6H6N2O2 HL Cupferron CAS 135-20-6 (637)  
 N-Nitrosophenylhydroxylamine; C6H5.N(OH).NO

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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Sm+++ dis NaClO4 25°C 0.10M U K2=4.83 1960RYa (43421) 348  
 K3=3.70

Extraction into hexane

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Sm+++ dis NaClO4 25°C 0.10M U B3=14.25 1954DYa (43422) 349

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

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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Sm+++ gl NaNO3 25°C 0.0 U M K1=9.80 1996KDb (43824) 350  
 K(Sm(egta)+L)=5.76

Extrapolated from data for I=0.05-0.15 M NaNO3.

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Sm+++ gl NaClO4 25°C 0.20M U K1=9.58 1996PJa (43825) 351

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Sm+++ gl NaClO4 25°C 0.20M U M K1=9.20 1986LSb (43826) 352  
 K(Sm(EDTA)+L)=7.45

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Sm+++ gl NaClO4 25°C 0.20M U M K1=9.30 1985LSf (43827) 353  
 K(Sm(edta)+L)=7.98

---

Sm+++ gl NaClO4 28°C 0.20M U M K1=9.20 1982LSa (43828) 354  
 K(Sm(edta)+L)=7.45

---

Sm+++ gl KNO3 25°C 0.05M M I K1=10.36 B2=19.80 1981BDc (43829) 355  
 Also data for I=0.2 and 0.35 M. At I=0, K1=11.00, K2=9.90.

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Sm+++ gl NaClO4 30°C 0.20M U M K1=9.29 1979MSd (43830) 356  
 K(Sm(hedta)+L)=5.94

hedta is N-(hydroxyethyl)diaminoethane-N,N',N'-triethanoic acid.

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Sm+++ gl NaClO4 25°C 0.10M U T K1=10.45 B2=19.66 1979NDa (43831) 357  
 At 45 C, K1=9.62, K2=8.79. Medium ionic strength not stated.

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Sm+++ gl NaClO4 30°C 0.20M U M K1=9.28 1978MSe (43832) 358  
 K(SmL+NTA)=7.00  
 K(SmL+HEDTA)=5.96  
 K(SmL+EDTA)=5.63

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Sm+++ EMF NaCl 25°C 0.10M U K1=11.06 1969PKe (43833) 359

\*\*\*\*\*

C6H6O2                      H2L      Resorcinol                      CAS 108-46-3    (3645)  
1,3-Dihydroxybenzene; HO.C6H4.OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaClO4	25°C	0.20M	U	M	K1=5.95 K(Sm(EDTA)+L)=3.05	1986LSb (43887)	360
Sm+++	gl	NaClO4	25°C	0.20M	U	M	K1=6.01 K(Sm(edta)+L)=3.10	1985LSf (43888)	361
Sm+++	gl	NaClO4	28°C	0.20M	U	M	K1=5.95 K(Sm(edta)+L)=3.05	1982LSa (43889)	362

\*\*\*\*\*

C6H6O2                      H2L      Hydroquinone                      CAS 123-31-9    (3646)  
1,4-Dihydroxybenzene; HO.C6H4.OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaClO4	25°C	0.10M	U	T M	K(Sm(NTA)+L)=5.20 K(Sm(edta)+L)=5.50 K(Sm(hedta)+L)=5.01 K(Sm(cdta)+L)=6.25	1985RMb (43897)	363

Also data for 35 C.

hedta is N-hydroxy-1,2-diaminoethane-N,N',N'-triethanoic acid.

\*\*\*\*\*

C6H6O3                      H3L      Pyrogallol                      CAS 87-66-1    (696)  
1,2,3-Trihydroxybenzene; C6H3(OH)3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaClO4	25°C	0.20M	U		K1=10.15	1996PJb (43979)	364
Sm+++	gl	NaClO4	30°C	0.20M	U	M	K1=10.57 K(Sm(hedta)+L)=5.35	1979MSd (43980)	365

hedta is N-(hydroxyethyl)diaminoethane-N,N',N'-triethanoic acid.

Sm+++	gl	NaClO4	30°C	0.20M	U	M	K1=10.57 K(Sm(NTA)+L)=6.45	1978MSk (43981)	366
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C6H6O3                      H3L      Phloroglucinol                      CAS 6099-90-7    (2525)  
1,3,5-Trihydroxybenzene; C6H3(OH)3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaClO4	25°C	0.20M	U	M	K1=4.20 K(Sm(EDTA)+L)=2.72	1986LSb (44024)	367

Sm+++ gl NaClO4 25°C 0.20M U M K1=4.24 1985LSf (44025) 368  
K(Sm(edta)+L)=2.74

Sm+++ gl NaClO4 28°C 0.20M U M K1=4.20 1982LSa (44026) 369  
K(Sm(edta)+L)=2.70

\*\*\*\*\*

C6H6O3 HL Maltol CAS 118-71-8 (2442)  
3-Hydroxy-2-methyl-4H-pyran-4-one;

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

Sm+++ gl NaClO4 30°C 0.10M U K1=6.51 B2=11.70 1970DSc (44101) 370  
K3=3.73

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C6H6O3 HL Allomaltol CAS 644-46-2 (2688)  
5-Hydroxy-2-methyl-4H-pyran-4-one;

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

Sm+++ sp KCl 25°C 0.11M C I K1=6.152 1987PEa (44128) 371  
Data for 0.031-1.01 M KCl.

\*\*\*\*\*

C6H6O4 HL Kojic acid CAS 501-30-4 (1800)  
5-Hydroxy-2-(hydroxymethyl)-4H-pyran-4-one;

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

Sm+++ sp KCl 25°C 0.10M C I K1=5.939 1987PEa (44242) 372  
Data for 0.005-0.94 M KCl.

Sm+++ gl oth/un 30°C 0.10M U K1=6.03 B2=11.05 1972DSd (44243) 373  
K3=3.94

Sm+++ gl NaClO4 25°C 2.0M U K1=5.38 B2=10.58 1964YCa (44244) 374

\*\*\*\*\*

C6H6O6 H3L cis-Aconitic CAS 585-84-2 (3064)  
cis-1,2,3-Propenetricarboxylic acid, cis-Aconitic acid; HOOC.CH:C(COOH)CH2.COOH

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

Sm+++ gl NaCl 20°C 0.10M U K1=4.29 1986SKb (44302) 375  
K(Sm+HL)=3.33

\*\*\*\*\*

C6H6O8S2 H4L Tiron CAS 149-45-1 (104)  
4,5-Dihydroxybenzene-1,3-disulfonic acid; (HO)2.C6H2(SO3H)2

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

Sm+++ gl KNO3 25°C 0.10M U TIH K1=14.48 B2=27.68 1980BDd (44491) 376  
Data for I=0.05-0.2 M and for I=0.10 M (35 C). Also DH and DS values.

-----  
 Sm+++ gl NaClO4 30°C 0.20M U M K1=14.18 1979MSd (44492) 377  
 K(Sm(hedta)+L)=8.48

hedta is N-(hydroxyethyl)diaminoethane-N,N',N'-triethanoic acid.

-----  
 Sm+++ gl NaClO4 25°C 0.50M C K1=12.37 B2=20.71 1976LAb (44493) 378  
 B(SmHL2)=28.75

-----  
 Sm+++ gl NaClO4 25°C 0.10M U K1=13.92 1970SSi (44494) 379  
 K(Sm+HL)=5.72

\*\*\*\*\*  
 C6H7N L Aniline CAS 62-53-3 (583)  
 Aminobenzene, aniline; C6H5.NH2

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

Sm+++ sp non-aq 25°C 100% U HM 1982KNa (44879) 380  
 K(SmA3+L)=2.29

Medium: CCl4. HA=dipivaloylmethane

\*\*\*\*\*  
 C6H7N3O L Isonicotinic hy CAS 54-85-3 (1267)  
 Pyridine-4-carboxylic acid hydrazide; C5H4N.CO.NH.NH2

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

Sm+++ gl NaClO4 15°C 0.10M U K1=8.85 1980ZMa (45131) 381

\*\*\*\*\*  
 C6H7O3F3 HL (7057)  
 3-Oxa-7-trifluorohepta-4,6-dione; CH3CH2.O.CO.CH2.CO.CF3

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

Sm+++ gl diox/w 25°C 50% M I K1=5.98 B2=11.22 1994SSa (45191) 382  
 K3=4.48

Medium: 50% dioxan, I=0 corr. At 35 C: K1=5.60, K2=5.19, K3=4.31

\*\*\*\*\*  
 C6H8O4 H2L CAS 2583-25-7 (958)  
 2-Allylpropanedioic acid; HOOCH(CH2.CH:CH2).COOH

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

Sm+++ gl KCl 25°C 0.20M U K1=3.79 1989ZPa (45474) 383  
 In 70.4% v/v EtOH/H2O: K1 = 5.89

\*\*\*\*\*  
 C6H8O6 H2L Ascorbic acid CAS 50-81-7 (285)  
 Ascorbic acid (Vitamin C);

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

Sm+++ gl KCl 25°C 0.1M C K1=7.30 2002ESa (45655) 384

$$K(\text{Sm}+\text{HL})=1.65$$

-----  
Sm+++ gl NaClO4 25°C 2.00M U IH 1988HSa (45656) 385

$$K(\text{Sm}+\text{HL})=1.68$$

DH=4.1 kJ mol<sup>-1</sup>, DS=45.9 J K<sup>-1</sup> mol<sup>-1</sup>

\*\*\*\*\*

C6H8O6S H3L CAS 99-68-3 (3692)  
(Carboxymethylthio)butanedioic acid; HOOC.CH(S.CH2.COOH).CH2.COOH

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

-----  
Sm+++ gl NaClO4 25°C 0.10M U TIH K1=4.28 B2=7.60 1986AJc (45713) 386  
DH(K1)=-5.4 kJ mol<sup>-1</sup>, DS=63.9 J K<sup>-1</sup> mol<sup>-1</sup>; DH(K2)=-4.4, DS=46.9

-----  
Sm+++ gl NaClO4 30°C 0.10M U IH K1=4.28 B2=7.60 1983ASa (45714) 387  
DH(K1)=-5.3 kJ mol<sup>-1</sup>, DH(K2)=4.4

\*\*\*\*\*

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

-----  
Sm+++ gl KNO3 25°C 0.10M U M 1975TDa (46249) 388  
B(Sm(IDA)L)=10.5

-----  
Sm+++ dis NaClO4 25°C 0.15M U 1973HHc (46250) 389  
K(Sm+HL+L)=11.14

-----  
Sm+++ gl alc/w 25°C 25% U I K1=8.78 1972BKd (46251) 390  
Medium: EtOH/H2O, 0.05 M (NaCl,NaClO4). 0%, K1=8.04, 50%, K1=9.72

-----  
Sm+++ dis oth/un ? ? U 1970PGb (46252) 391  
K(Sm+OH+H-1L)=18.5  
K(Sm+2OH+H-1L)=24.4

\*\*\*\*\*

C6H8O7 H3L (6770)  
Carboxymethoxysuccinic acid; HOOC.CH2.O.CH(COOH)CH2.COOH

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

-----  
Sm+++ EMF NaClO4 25°C 1.00M U K1=6.11 B2=10.23 1991WPb (46335) 392  
\*\*\*\*\*

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

-----  
Sm+++ gl NaClO4 37°C 0.15M C K1=9.85 B2=17.86 2003TKa (47011) 393  
B(SmH-1L)=4.89

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Sm+++ ISE NaClO4 25°C 0.10M C I K1=11.43 1997LBb (47012) 394  
 Method: Cu ISE and competitive complexation by Cu. Data for 0.1-5.0 M.  
 At I=0.0 M, K1=13.21.

Sm+++ ISE KNO3 25°C 0.10M C K1=11.52 1980NSf (47013) 395  
 Competitive method using Cd ion-selective electrode.

Sm+++ gl KNO3 20°C 1.0M C K2=8.09 1978GHb (47014) 396

Sm+++ gl diox/w 30°C 50% U M K(SmL+A)=5.28 1978SGf (47015) 397

HA=tropolone

Sm+++ gl NaClO4 25°C 0.50M U K1=11.21 1977GGb (47016) 398

Sm+++ EMF KCl 25°C 1.0M U M 1977GMa (47017) 399  
 K(SmA+L)=5.85  
 K(SmA+H2L)=1.81  
 K(SmA+H3L)=1.95  
 K(SmA+H4L)=3.62

Method: Pt/H2 electrode. H3A is N-hydroxyethyl-1,2-diaminoethane-N,N',N'-triethanoic acid.

Sm+++ gl KNO3 20°C 0.10M U M 1974TDa (47018) 400  
 K(SmL+Citrate)=2.7

Sm+++ cal KNO3 20°C 0.10M U HM 1971GKb (47019) 401  
 K(SmA+L)=5.00  
 H4A=EDTA. DH(SmA+L)=-26.07 kJ mol<sup>-1</sup>, DS=6.7 J K<sup>-1</sup> mol<sup>-1</sup>.  
 DH(SmLA)=-40.1 kJ mol<sup>-1</sup>, DS=287 J K<sup>-1</sup> mol<sup>-1</sup>

Sm+++ gl oth/un 20°C 0.20M U 1970VMa (47020) 402  
 B(SmL(OH))=6.17

Sm+++ gl KCl 20°C 0.10M U K1=11.33 B2=20.53 1965ANb (47021) 403

Sm+++ gl KNO3 25°C 0.10M U T H T K1=11.53 B2=20.53 1962MFb (47022) 404  
 15 C: K1=11.53, 9.17; 20 C: 11.51, 9.05; 30 C: 11.55, 8.97; 35 C: 11.52, 8.91;  
 40 C: 11.54, 8.87. DH(K1)=1.7 kJ mol<sup>-1</sup>, DS=226; DH(K2)=-18.3, DS=111

Sm+++ sp oth/un 19°C 0.02M U K1=10.78 B2=20.54 1961AVa (47023) 405

Sm+++ vlt KNO3 20°C 0.10M U 1957NOa (47024) 406  
 K(Sm2L3)=36.7

Sm+++ vlt KNO3 20°C 0.10M U T K1=11.33 1956SGa (47025) 407  
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C6H9N3O2 HL Histidine CAS 71-00-1 (1)  
 2-Amino-3-(4'-imidazolyl)propanoic acid; H2N.CH(CH2.C3H3N2)COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaClO4	37°C	0.15M	C		B(SmH2L)=17.43 B(SmHL)=11.63 B(SmH3L3)=33.42	2002TKa (47611)	408
K(2Sm+6H+4L=Sm2(HL)2(H2L)2)=59.25.									
Sm+++	gl	KNO3	35°C	0.10M	U		K(Sm+HL)=3.85	1987RRc (47612)	409
Sm+++	gl	KNO3	35°C	0.10M	U	M	K(Sm+HL)=3.85	1986RMb (47613)	410
K(Sm+HL+cytidine)=8.63									
Sm+++	gl	NaClO4	37°C	3.00M	U	T	K1=4.37 B2=8.78 B(SmHL)=11.18	1971JWa (47614)	411
Sm+++	gl	NaClO4	25°C	3.00M	U	T	K1=4.46 B2=8.71 B(SmHL)=11.78	1970JWa (47615)	412
*****									
C6H10O2S HL (4370)									
Ethyl thioacetoacetate; CH3.CS.CH2.CO.OCH2.CH3									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	mixed	30°C	75%	U		K1=7.20 B2=13.16 K3=5.52	1970DRa (47967)	413
Medium: 75% acetone, 0.1 M									
*****									
C6H10O3 HL CAS 16841-19-3 (3649)									
1-Hydroxycyclopentanecarboxylic acid; HO.C5H8.CO.OH									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaClO4	25°C	0.10M	U		K1=2.789 B2=4.94 K3=1.50 K4=1.08	1966PRb (47996)	414
*****									
C6H10O3 HL CAS 141-97-9 (3068)									
Ethyl acetoacetate; CH3.CO.CH2.CO2.C2H5									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	mixed	30°C	75%	U		K1=6.40 B2=12.10	1969DRa (48018)	415
Medium: 75% acetone, 0.1 M NaClO4									
*****									
C6H10O4 H2L Adipic acid CAS 124-04-9 (401)									
1,6-Hexanedioic acid; HOOC.(CH2)4.CO.OH									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaClO4	25°C	0.10M	M	H	K1=3.19	1986CDb (48087)	416
DH=15.3 kJ mol <sup>-1</sup> , DS=112 J K <sup>-1</sup> mol <sup>-1</sup>									
Sm+++	sol	oth/un	25°C	0.50M	U		K1=3.77	1970MKe (48088)	417
*****									
C6H10O4S2		H2L					CAS 7244-02-2	(438)	
1,2-Bis(carboxymethylthio)ethane; HOOC.CH2.S.CH2.CH2.S.CH2.COOH									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaClO4	25°C	1.00M	C	H	K1=2.32 B2=3.49	1974GGa (48250)	418
B(SmHL)=5.36									
*****									
C6H10O6		H2L					CAS 23243-68-7	(242)	
1,2-Bis(carboxymethoxy)ethane; HOOC.CH2.O.CH2.CH2.O.CH2.COOH									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	oth	NaClO4	25°C	0.10M	U		K1=5.07	1984AFa (48350)	419
Laser excitation spectroscopy, competition method.									
Sm+++	gl	NaClO4	25°C	1.00M	C	H	K1=5.07 B2=7.98	1974GGa (48351)	420
B3=8.95									
B(SmHL2)=10.33									
*****									
C6H10O8		H2L					Saccharic acid CAS 87-73-0	(1191)	
D-2,3,4,5-Tetrahydroxy-1,6-hexanedioic acid, Glucaric acid; HOOC.(CHOH)4.COOH									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaClO4	25°C	0.10M	U	M	K1=4.56	1997PPb (48487)	421
K(Sm(edta)+L)=4.08									
*****									
C6H11NO5		H2L					HIMDA CAS 93-62-9	(192)	
N-(2-Hydroxyethyl)iminodiethanoic acid; HO.CH2.CH2.N(CH2.COOH)2									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	KNO3	20°C	1.00M	U		K1=8.42 B2=15.91	1974CmD (48788)	422
K(SmL2(OH)+H)=10.62									
Sm+++	oth	NaNO3	20°C	0.10M	U	M	K1=8.8 B2=16.45	1966JMc (48789)	423
Method: paper electrophoresis. Ternary complexes with HEDTA									
Sm+++	vlt	KCl	25°C	0.10M	U		B2=15.74	1965DTa (48790)	424
Sm+++	gl	KNO3	25°C	0.10M	U		K1=9.10 B2=16.87	1963TLA (48791)	425
*****									

C6H12N2O4                      H2L      EDDA                      CAS 5657-17-0 (119)  
 1,2-Diaminoethane-N,N'-diethanoic acid; HOOC.CH2.NH.CH2.CH2.NH.CH2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	R4N.X	25°C	0.10M	C		K1=8.28	1988CCb (49267)	426
Sm+++	gl	NaClO4	25°C	1.00M	C	H	K1=8.26    B2=14.44 B(SmH2L)=17.60	1974GGa (49268)	427

Sm+++	gl	KNO3	25°C	0.10M	U		K1=8.28    B2=14.35	1962THb (49269)	428
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C6H12O3                      HL                      (3662)  
 2-Hydroxy-2-methylpentanoic acid; (Methylpropylglycolic acid)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	EMF	NaClO4	25°C	1.0M	U		K1=2.59    B2=4.71 K3=1.50	1964EVa (49484)	429

Method: quinhydrone electrode.

C6H12O4                      HL                      CAS 1112-33-0 (1246)  
 2,3-Dihydroxy-2,3-dimethylbutanoic acid; (CH3)2.C(OH).C(OH)(CH3).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	KNO3	25°C	0.10M	U		K1=3.52    B2=5.95 K3=1.34	1979PPa (49499)	430

C6H12O7                      HL      Gluconic acid      CAS 526-95-4 (904)  
 D-Gluconic acid, 2,3,4,5,6-Pentahydroxyhexanoic acid; HO.CH2(CHOH)4.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaClO4	25°C	0.20M	U	M	K1=3.54 K(Sm(EDTA)+L)=2.92	1986LSb (49757)	431
Sm+++	gl	NaClO4	25°C	0.20M	U	M	K1=3.58 K(Sm(edta)+L)=2.97	1985LSf (49758)	432

Sm+++	EMF	alc/w	25°C	80%	U		K1=5.51	1966KRb (49759)	433
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Medium: 80% MeOH

Sm+++	gl	KCl	25°C	0.20M	U		K1=2.65    B2=4.88	1963K0c (49760)	434
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C6H13NO2                      HL      Isoleucine                      CAS 73-32-5 (424)  
 2-Amino-3-methylpentanoic acid; CH3.CH2.CH(CH3).CH(NH2).COOH

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

Data for 0.05-0.15 M NaNO<sub>3</sub>. At I=0, K<sub>1</sub>=6.09, K(Sm(egta)+L)=4.27.

\*\*\*\*\*

\*K(SmL)=-8.36  
\*K(Sm(OH)L)=-8.81  
K(Sm(egta)+L)=4.10

\*\*\*\*\*

\*K(SmL)=-8.38  
\*K(Sm(OH)L)=-8.84  
K(Sm(egta)+L)=4.08

\*\*\*\*\*

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

-----  
Sm+++ gl KNO3 20°C 0.10M U K1=5.72 B2=10.30 1982RFa (50403) 444  
-----

Sm+++ gl NaClO4 20°C 0.10M U T K1=6.77 B2=11.53 1981SGd (50404) 445  
Data for 20-40 C. At 30 C: K1=6.51, K2=4.56  
-----

Sm+++ gl KCl 30°C 0.10M U K1=5.54 B2=9.92 1973MSe (50405) 446  
-----

Sm+++ gl alc/w 20°C 50% U I K1=6.84 1970KRa (50406) 447  
Medium: 0-80% MeOH, 0.03 M KCl. K1(0%)=5.74, K1(20%)=6.21, K1(80%)=7.9  
-----

Sm+++ oth NaNO3 20°C 0.10M U K1=7.8 B2=13.80 1966JMc (50407) 448  
Method: paper electrophoresis  
-----

\*\*\*\*\*  
C6H13N3O3 HL Citrulline (579)  
2-Amino-5-ureidovaleric acid; H2N.CO.NH.CH2.CH2.CH2.CH(NH2).COOH  
-----

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

Sm+++ gl NaCl 37°C 0.15M U M K1=3.12 1997GMa (50587) 449  
B(SmHL)=10.50  
B(SmH2AL)=24.50  
-----

Ligand is DL-citrulline. HA is L-hydroxyproline.  
-----

\*\*\*\*\*  
C6H14N2O2 HL Lysine CAS 56-87-1 (41)  
2,6-Diaminohexanoic acid; H2N.(CH2)4.CH(NH2)COOH  
-----

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

Sm+++ gl KNO3 15°C 1.0M U T 1989SSg (50833) 450  
K(Sm+HL)=5.26  
K(SmHL+HL)=2.57  
-----

Also data for 30 C.  
-----

Sm+++ gl NaClO4 20°C 0.10M U T H K1=7.71 B2=14.66 1983SDa (50834) 451  
30 C: K1=7.51, K2=6.85, 40 C: K1=7.18, K2=6.51  
-----

\*\*\*\*\*  
C6H14N4O2 HL Arginine CAS 74-79-3 (40)  
2-Amino-5-guanidopentanoic acid; H2N.CH((CH2)3.NH.C(:NH)(NH2)COOH  
-----

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

Sm+++ gl NaClO4 37°C 0.15M C M 2003TKa (51017) 452  
K(Sm(edta)+HL)=1.88  
K(Sm(edta)+L)=1.9  
K(Sm(nta)+HL)=3.40  
K(SmH-1(nta)+2HL)=7.94  
-----

K(Sm(nta)2+HL)=3.76.  
-----

Sm+++ gl NaClO4 37°C 0.15M C 2002TKa (51018) 453  
-----

B(SmHL)=9.84

K(Sm+L=SmH-1(HL))=5.91

\*\*\*\*\*

C6H18N4 L Tren CAS 4097-89-6 (817)

2,2',2''-Triaminotriethylamine; (H2N.CH2.CH2)3N

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	ISE	non-aq	25°C	100%	C	H	K1=4.28 B2=5.44	1993CCb (52209)	454
Medium: DMSO, 0.1 M Et4NClO4. Method: Ag+ ISE. By calorimetry, DH(K1)=-50.7 kJ mol-1, DS=-88; DH(B2)=-89, DS=-194.									

\*\*\*\*\*

C6H20N2O12P4 H8L EDTPA CAS 1429-50-1 (434)

Ethane-1,2-bis(iminobis(methylenephosphonic acid)); ((H2O3PCH2)2NCH2.)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaCl	37°C	0.15M	C		K1=14.44 K(SmL+H)=7.13 K(SmHL+H)=6.00	1995JWa (52358)	455
Sm+++	gl	NaCl	37°C	0.15M	C		K1=14.44 K(SmL+H)=7.13 K(SmHL+H)=6.00	1995WJa (52359)	456
Sm+++	gl	KNO3	25°C	0.10M	C		K(SmL+H)=7.34 K(SmHL+H)=6.29	1991SKb (52360)	457
Sm+++	gl	KCl	25°C	0.10M	U		K1=22.39 K(Sm+HL)=17.56 K(Sm+H2L)=13.68 K(Sm+H3L)=10.72 K(Sm+H4L)=8.04	1967KDa (52361)	458

K(Sm+H5L)=4

\*\*\*\*\*

C7H4N2O7 H2L CAS 609-99-4 (400)

3,5-Dinitrosalicylic acid; (O2N)2.C6H2(OH).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaNO3	25°C	0.10M	U	I M	K1=5.69 *K(SmL)=-7.34 K(Sm(egta)+L)=4.97	1996KDc (52500)	459
Data for 0.05 and 0.15 M NaNO3. At I=0, K1=6.04, *K(SmL)=-7.54, K(Sm(egta)+L)=5.42.									

Sm+++	gl	oth/un	24°C	0.20M	U		K1=5.14	1972PSd (52501)	460
Medium: LiCl									

\*\*\*\*\*

C7H5NO4                      H2L      Dipicolinic aci    CAS 449-83-2    (418)  
2,6-Pyridinedicarboxylic acid; C5H3N.(COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Sm+++	cal	NaCl04	25°C	0.50M	C	H			1963GRd (52803)	461
DH(K1)=-17.92 kJ mol-1, DS(K1)=108 J K-1 mol-1; DH(B2)=-37.54, DS(B2)=176; DH(B3)=-55.50, DS(B3)=218.										
Sm+++	EMF	oth/un	20°C	0.50M	U			K1=8.86    B2=15.88    K3=5.35	1961GRa (52804)	462

\*\*\*\*\*

C7H5NO4                      HL                      CAS 121-92-6    (490)  
3-Nitrobenzoic acid; O2N.C6H4.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Sm+++	gl	NaCl04	25°C	0.10M	C	H		K1=1.85	1986CLc (52872)	463
DH=5.7 kJ mol-1, DS=54 J K-1 mol-1										

\*\*\*\*\*

C7H5NO4                      HL                      CAS 62-23-7    (489)  
4-Nitrobenzoic acid; O2N.C6H4.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Sm+++	gl	NaCl04	25°C	0.10M	M	H		K1=1.89	1999YKa (52913)	464
By calorimetry: DH(K1)=5.90 kJ mol-1, DS(K1)=56.0 J K-1 mol-1.										

\*\*\*\*\*

C7H5O2F                      HL                      CAS 445-29-4    (5711)  
3-Fluorobenzoic acid; F.C6H4.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Sm+++	gl	NaCl04	25°C	0.10M	C	H		K1=1.95	1986CLc (53241)	465
DH=6.1 kJ mol-1, DS=58 J K-1 mol-1										

\*\*\*\*\*

C7H5O2F                      HL                      CAS 456-22-4    (5710)  
4-Fluorobenzoic acid; F.C6H4.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Sm+++	gl	NaCl04	25°C	0.10M	C	H		K1=2.12	1986CLc (53261)	466
DH=8.0 kJ mol-1, DS=67 J K-1 mol-1										

\*\*\*\*\*

C7H5O6BrS                      H2L                      (1626)  
3-Bromo-5-sulfosalicylic acid; Br.C6H2(OH)(COOH).SO3H

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Sm+++	gl	NaCl04	25°C	0.10M	C	H    T			1993ALa (53375)	467



B(1,1,1)=12.48  
 B(1,0,1)=7.39  
 B(1,0,2)=12.39  
 B(1,-1,1)=-0.35

B(p,q,r); pSm+qH+rL=(Sm)pHqLr. B(1,-2,1)=-8.18.

\*\*\*\*\*

C7H6O5 HL Thiotropolone CAS 1073-38-7 (8477)  
 2-Mercapto-2,4,6-cycloheptatrien-1-one;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	diox/w	30°C	50%	M	I	K1=5.31 B2=10.01 K3=3.91	1978SSi (53548)	468

Medium: 50% v/v dioxane/H2O, 0.10 M NaClO4. Data for 0.005 and 0.2 M NaClO4.

\*\*\*\*\*

C7H6O2 HL Tropolone CAS 533-75-5 (3129)  
 2-Hydroxycyclohepta-2,4,6-trien-1-one;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	KNO3	25°C	0.10M	U		K1=6.91 B2=12.59 K3=4.60	1969CMb (53691)	469

\*\*\*\*\*

C7H6O2 HL Benzoic Acid CAS 65-85-0 (462)  
 Benzenecarboxylic acid; C6H5.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	cal	NaClO4	25°C	0.10M	U	H	K1=2.21 B2=3.92	1982CBc (53855)	470

DH1= 7.6 kJ mol<sup>-1</sup> DS1= 68 J K<sup>-1</sup> mol<sup>-1</sup>

\*\*\*\*\*

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaClO4	25°C	0.1M	C	H		1996HYa (54292)	471

By calorimetry: DH(K1)=0.98 kJ mol<sup>-1</sup>, DH(B2)=3.91 J K<sup>-1</sup> mol<sup>-1</sup>

Sm+++	gl	NaNO3	25°C	0.10M	U	I M	K1=8.48 *K(SmL)=-7.86 K(Sm(egta)+L)=5.83	1996KDc (54293)	472
-------	----	-------	------	-------	---	-----	--	-----------------	-----

Data for 0.05 and 0.15 M NaNO3. At I=0, K1=8.82, \*K(SmL)=-8.02, K(Sm(egta)+L)=5.09.

Sm+++	gl	NaClO4	25°C	0.10M	C	T	K(Sm+HL)=2.06 K(SmHL+HL)=1.76	1989HMa (54294)	473
-------	----	--------	------	-------	---	---	----------------------------------	-----------------	-----

Sm+++ gl alc/w 25°C 40% U M T K1=7.99 1986LSb (54295) 474  
K(Sm(EDTA)+L)=7.75

Medium: 40% v/v EtOH/H2O, 0.2 M NaClO4

Sm+++ gl NaClO4 25°C 0.20M U M K1=8.07 1985LSf (54296) 475  
K(Sm(edta)+L)=7.79

Sm+++ ix mixed 20°C 50% U 1976TRa (54297) 476  
K(Sm+HL)=2.57  
K(Sm+2HL)=4.33  
K(Sm+3HL)=6.40

Medium: 50% v/v acetone/H2O, 0.25 M NaClO4

Sm+++ gl alc/w 25°C 100% U K1=5.75 B2=10.42 1973BPd (54298) 477  
K3=3.24

Medium: 99.9% MeOH, 0.1 M NaCl

\*\*\*\*\*  
C7H6O3 H2L CAS 99-06-9 (1370)  
3-Hydroxybenzoic acid; HO.C6H4.COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
Sm+++ gl NaClO4 25°C 0.10M C H 1988LLa (54388) 478  
K(Sm+HL)=2.15

DH=7.33 kJ mol<sup>-1</sup>, DS=65.6 J K<sup>-1</sup> mol<sup>-1</sup>

\*\*\*\*\*  
C7H6O3 H2L CAS 99-96-7 (1371)  
4-Hydroxybenzoic acid; HO.C6H4.COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
Sm+++ gl NaClO4 25°C 0.10M M H K1=1.93 1999YKa (54431) 479  
By calorimetry: DH(K1)=7.82 kJ mol<sup>-1</sup>, DS(K1)=60.0 J K<sup>-1</sup> mol<sup>-1</sup>.

Sm+++ gl NaClO4 25°C 0.10M C H 1988LLa (54432) 480  
K(Sm+HL)=2.42

DH=7.57 kJ mol<sup>-1</sup>, DS=71.6 J K<sup>-1</sup> mol<sup>-1</sup>

\*\*\*\*\*  
C7H6O4 H3L Resorcylic acid CAS 89-86-1 (876)  
2,4-Dihydroxybenzoic acid, b-Resorcylic acid; C6H3(OH)2.COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
Sm+++ gl NaClO4 25°C 0.20M U M T K1=6.58 1986LSb (54540) 481  
K(Sm(EDTA)+L)=4.47

Sm+++ gl NaClO4 25°C 0.20M U M K1=6.58 1985LSd (54541) 482  
K(Sm(edta)+L)=4.47  
B(Sm(edta)L)=17.30

Sm+++ gl NaClO4 25°C 0.20M U M K1=6.65 1985LSf (54542) 483  
K(Sm(edta)+L)=4.51

\*\*\*\*\*

C7H6O4 H3L Protocatechuic CAS 99-50-3 (875)  
3,4-Dihydroxybenzoic acid; C6H3(OH)2.COOH

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

Sm+++ gl NaClO4 25°C 0.20M U K1=10.48 1996PJ a (54698) 484

Sm+++ gl NaClO4 25°C 0.20M U M K1=8.63 1986LSb (54699) 485  
K(Sm(EDTA)+L)=5.07

Sm+++ gl NaClO4 25°C 0.20M U M K1=8.65 1985LSd (54700) 486  
K(Sm(edta)+L)=5.07  
B(Sm(edta)L)=17.90

Sm+++ gl NaClO4 25°C 0.20M U M K1=8.72 1985LSf (54701) 487  
K(Sm(edta)+L)=5.15

\*\*\*\*\*

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

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

Sm+++ gl NaClO4 30°C 0.20M U M K1=12.48 1979MSd (54764) 488  
K(Sm(hedta)+L)=5.85

hedta is N-(hydroxyethyl)diaminoethane-N,N',N'-triethanoic acid.

Sm+++ gl NaClO4 30°C 0.20M U M K1=12.48 1978MSk (54765) 489  
K(Sm(NTA)+L)=6.70

\*\*\*\*\*

C7H6O5S H2L CAS 632-25-7 (4436)  
2-Carboxybenzenesulfonic acid; H00C.C6H4.SO3H

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

Sm+++ gl KCl 25°C 0.20M U K1=2.5 1973DPa (54782) 490

\*\*\*\*\*

C7H6O6S H3L CAS 5965-83-3 (399)  
5-Sulfosalicylic acid, 2-Hydroxy-5-sulfobenzoic; H03S.C6H3(OH).COOH

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

Sm+++ gl NaClO4 25°C 1.0M C K1=6.34 B2=12.02 1983NCa (55045) 491

Sm+++ gl KNO3 20°C 0.10M U T K1=7.99 1982DBa (55046) 492

Sm+++ gl NaClO4 20°C 1.0M U K1=6.77 B2=12.56 1972CBb (55047) 493

-----

Sm+++ sp NaClO4 20°C 0.10M U K1=7.65 B2=13.58 1968KTb (55048) 494  
K(Sm+HL)=2.23

\*\*\*\*\*

C7H6O9S2 H3L CAS 56507-30-3 (2659)

3,5-Disulfosalicylic acid; (HO3S)2.C6H2(OH).COOH

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

Sm+++ gl NaClO4 25°C 0.50M C T K1=8.20 B2=13.54 1976LAc (55101) 495

\*\*\*\*\*

C7H7NOS HL (2034)

N-Thioformyl-N-phenylhydroxylamine; H(C:S)N(C6H5)OH

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

Sm+++ gl diox/w 30°C 70% U K1=7.87 B2=13.94 1981MBb (55156) 496

K3=4.34

\*\*\*\*\*

C7H7NO2 HL Anthranilic CAS 118-92-3 (1589)

2-Aminobenzoic acid, Anthranilic acid; H2N.C6H4.COOH

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

Sm+++ gl NaNO3 25°C 0.10M M I M K1=3.97 1995KDc (55257) 497

K(Sm(egta)+L)=3.76

Data for 0.05 and 0.15 M NaNO3. At I=0, K1=4.31, K(Sm(egta)+L)=4.10.

-----  
Sm+++ gl NaClO4 25°C 0.10M C K1=2.44 B2=4.78 1989HMa (55258) 498

-----  
Sm+++ gl alc/w 25°C 0.20M U M K1=3.36 1986LSb (55259) 499

K(Sm(EDTA)+L)=3.21

-----  
Sm+++ gl NaClO4 25°C 0.10M U H K1=4.23 1982KYc (55260) 500

By calorimetry, DH(K1)=4.14 kJ mol<sup>-1</sup>, DS(K1)=94.89 J K<sup>-1</sup> mol<sup>-1</sup>.

-----  
Sm+++ gl non-aq 25°C 100% U K1=6.94 B2=12.36 1970BBh (55261) 501

K3=3.26

K4=2.55

Medium: MeOH, 0.1 M NaCl

\*\*\*\*\*

C7H7NO2 HL CAS 150-13-0 (1376)

4-Aminobenzoic acid; H2N.C6H4.COOH

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

Sm+++ gl NaClO4 25°C 0.10M M H K1=2.26 1999YKa (55392) 502

By calorimetry: DH(K1)=7.53 kJ mol<sup>-1</sup>, DS(K1)=68.5 J K<sup>-1</sup> mol<sup>-1</sup>.

-----  
Sm+++ gl KCl 25°C 0.20M U K1=2.47 1977EBa (55393) 503

\*\*\*\*\*

C7H7NO2                      HL                      CAS 495-18-1 (184)  
Benzohydroxamic acid; C6H5.CO.NH.OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	diox/w	35°C	50%	A		K1=9.95    B2=18.41 K3=7.46	1977AKa (55515)	504

\*\*\*\*\*  
C7H7NO3                      H2L                      CAS 89-73-6 (204)  
2-Hydroxybenzohydroxamic acid (salicylhydroxamic acid); HO.C6H4.CO.NHOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	mixed	25°C	75%	U			1970SEa (55609)	505
							K(Sm+HL)=7.20 K(SmHL+HL)=6.77 K(Sm(HL)2+HL)=5.01		

Medium: 75% acetone, 0.1 M NaClO4

\*\*\*\*\*  
C7H7NO5S                      H2L                      CAS 3577-63-7 (3181)  
5-Sulfoanthranilic acid; (5-sulfo-2-aminobenzoic acid)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaNO3	25°C	0.10M	M	I M	K1=3.81 K(Sm(egta)+L)=3.35	1995KDc (55680)	506

Data for 0.05 and 0.15 M NaNO3. At I=0, K1=4.19, K(Sm(egta)+L)=3.59.

\*\*\*\*\*  
C7H7NO6S                      H3L                      CAS 6201-86-1 (7899)  
3-Amino-5-sulfosalicylic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	KCl	25°C	0.20M	M	T H	K1=8.14 K(Sm+OH+L)=15.24	1991BPb (55694)	507

DH(K1)=-84 kJ mol<sup>-1</sup>, DS(K1)=-126 J K<sup>-1</sup> mol<sup>-1</sup>. DH(Sm(OH)L)=-205,  
DS(Sm(OH)L)=-396. Also data for 35, 45 and 55 C.

\*\*\*\*\*  
C7H8O2                      H2L    Methylcatechol    CAS 452-86-8 (525)  
1,2-Dihydroxy-4-methylbenzene; CH3.C6H3(OH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaNO3	25°C	0.0	U	M	K1=9.88 K(Sm(egta)+L)=5.87	1996KDb (56077)	508

Extrapolated from data for I=0.05-0.15 M NaNO3.

\*\*\*\*\*  
C7H8O4                      HL    Methyl kojic    CAS 1506-07-8 (2686)  
3-Hydroxy-6-(hydroxymethyl)-2-methyl-4H-pyran-4-one;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	sp	KCl	25°C	0.10M	M	I	K1=6.30	1986PLb (56133)	509
*****									
C7H8O5		HL					CAS 2029-29-4	(2687)	
3-Hydroxy-2,6-bis(hydroxymethyl)-4H-pyran-4-one;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	sp	KCl	25°C	0.10M	M	I	K1=5.99	1986PLb (56152)	510
*****									
C7H11NO4		H2L					CAS 499-82-1	(3163)	
Piperidine-2,6-dicarboxylic acid; C5H9N(COOH)2									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	KNO3	25°C	0.10M	U		K1=6.13 B2=11.43	1963THb (56812)	511
*****									
C7H11NO6		H3L					(2926)		
2-Aminobutanoic-N-propane-1,3-dioic acid; HOOCH(C2H5)NH.CH(COOH)2									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	KNO3	25°C	0.1M	U		K1=8.94	1982KKc (56851)	512
*****									
C7H11NO6		H3L		MNTA			(1026)		
Nitrilo(2-propanoic)-diethanoic acid; HOOCH(CH3).N(CH2.COOH)2									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	KNO3	20°C	0.10M	U		K1=12.18 B2=21.43	1974RMg (56916)	513
*****									
C7H12N2O3		HL		Gly-Pro			CAS 704-15-4	(257)	
Glycyl-proline; H2N.CH2.CO.NC4H7.COOH									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	KNO3	25°C	0.15M	M	T H	K1=3.80	1983SKb (57129)	514
Data for 35 and 45 C. At 35 C, DH(K1)=23 kJ mol <sup>-1</sup> , DS(K1)=150 J K <sup>-1</sup> mol <sup>-1</sup> .									
*****									
C7H12O3		HL					CAS 609-69-8	(3731)	
2-Hydroxycyclohexanecarboxylic acid; HO.C6H10.COOH									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaClO4	25°C	1.0M	U		K1=2.18 B2=3.91	1967STd (57267)	515
*****									
C7H12O3		HL					(4422)		
3-Methyl ethylacetoacetate; CH3.CO.CH(CH3).CO.OCH2.CH3									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Sm+++	gl	mixed	30°C	75%	U		K1=8.05	1971DRb (57278)	516
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Medium: 75% acetone, 0.1 M

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C7H12O4	H2L						CAS 510-20-3 (482)		
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Diethylpropanedioic acid (Diethylmalonic acid); HOOC.C(C2H5)2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Sm+++	gl	KNO3	25°C	0.10M	U		K1=4.33 B2=6.92	1968PFa (57371)	517
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C7H12O6	HL	Quinic acid					CAS 77-95-2 (2578)		
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1,3,4,5-Tetrahydroxycyclohexane-1-carboxylic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Sm+++	gl	NaCl	20°C	0.10M	U		K1=2.84	1977SSc (57410)	518
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Sm+++	EMF	NaCl04	25°C	1.0M	U		K1=2.66 B2=4.65 K3=1.43 K4=0.72	19670Ta (57411)	519
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Method: quinhydrone electrode

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C7H13NO6	H2L						CAS 32013-58-4 (6079)		
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N-(2,3-Dihydroxypropyl)iminodiethanoic acid; HO.CH2.CH(OH).CH2.N(CH2.COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Sm+++	gl	KNO3	20°C	0.10M	U		K1=8.50 B2=16.02	1980RPa (57619)	520
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C7H14N2O3	HL	Gly-Val					CAS 7963-21-9 (973)		
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Glycyl-valine; H2N.CH2.CO.NH.CH(CH(CH3)2).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Sm+++	gl	KNO3	30°C	0.15M	U T H		K1=3.91	1980SKe (57757)	521
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Data for 20 and 40 C. DH(K1)=16.9 kJ mol<sup>-1</sup>, DS(K1)=131 J K<sup>-1</sup> mol<sup>-1</sup>.

Ligand is glycyl-DL-valine.

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C7H14O3	HL						CAS 63204-98-9 (3738)		
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2-Hydroxy-2,4-dimethylpentanoic acid; (CH3)2.CH.CH2.C(CH3)(OH).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Sm+++	EMF	NaCl04	25°C	1.0M	U		K1=2.71 B2=4.90	1965TVa (57866)	522
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K3=1.48

K4=1.02

Method: quinhydrone electrode

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C7H14O3 HL CAS 65311-45-1 (6266)  
3-Hydroxy-3,4-dimethyl-pentanoic acid; CH3.CH2.C(OH)(CH3).CH(CH3).COOH

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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaClO4	25°C	0.10M	C		K1=2.44 B2=4.17	1976SPa (57879)	523

\*\*\*\*\*

C7H15NO4 HL CAS 41244-51-3 (4459)  
N,N-Bis(2'-hydroxyethyl)alanine; (HO.CH2.CH2)2.N.CH(CH3)COOH

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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	KNO3	20°C	0.10M	U		K1=5.36 B2=9.75	1982RFa (57942)	524

\*\*\*\*\*

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

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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	sp	KNO3	12°C	0.10M	U		K(Sm+H2L)=4.20	1965GEa (58532)	525

\*\*\*\*\*

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

---

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	cal	non-aq	25°C	100%	C H			2004MIa (58676)	526

Method: calorimetric titration. Medium: chloroform. DH(SmL3+A)=7.0 kJ mol-1, DS=81 J K-1 mol-1; DH(SmL3+2A)=7.8, DS=134. HA is benzoic acid.

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Sm+++	gl	alc/w	22°C	80%	U		K1=6.41 B2=11.93 K3=4.20	1995MTa (58677)	527
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Medium: 0.1 M NaClO4 in 80% (v/v) EtOH/H2O.

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C8H6O4 H2L Phthalic acid CAS 88-99-3 (113)  
Benzene-1,2-dicarboxylic acid; C6H4(COOH)2

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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaNO3	25°C	0.10M	M I M		K1=4.64 K(Sm(egta)+L)=4.25	1995KDb (59009)	528

Data for 0.05 and 0.15 M NaNO3. At I=0, K1=4.96, K(Sm(egta)+L)=4.58.

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Sm+++	gl	alc/w	25°C	40%	U M		K1=5.04 K(Sm(EDTA)+L)=4.18	1986LSb (59010)	529
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Medium: 40% v/v EtOH/H2O, 0.2 M NaClO4

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Sm+++	gl	NaClO4	25°C	0.20M	U M		K1=5.09 K(Sm(edta)+L)=4.21	1985LSf (59011)	530
-------	----	--------	------	-------	-----	--	----------------------------	-----------------	-----



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Sm+++ gl NaClO4 30°C 0.10M U K1=4.99 B2=8.37 1966KPb (59012) 531

\*\*\*\*\*

C8H6O4 H2L Isophthalic aci CAS 212-91-5 (1619)

Benzene-1,3-dicarboxylic acid; C6H4(COOH)2

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

-----  
Sm+++ cal NaClO4 25°C 0.10M U H K1=2.82 1982CBc (59060) 532

DH= 10.71 kJ mol<sup>-1</sup>, DS= 90 J K<sup>-1</sup> mol<sup>-1</sup>

\*\*\*\*\*

C8H7NO2 HL CAS 532-54-7 (4363)

Isonitrosoacetophenone, Phenylglyoxal 2-oxime;

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

-----  
Sm+++ gl diox/w 20°C 50% U K1=6.02 B2=11.50 1971MAf (59107) 533

Medium: 50% v/v dioxan, 0.1 M NaClO4

\*\*\*\*\*

C8H7O2Cl HL CAS 1450-74-4 (6325)

2-Hydroxy-5-chloro-acetophenone; Cl(HO)C6H3.CO.CH3

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

-----  
Sm+++ gl alc/w 25°C 20% M I K1=5.97 1994KDa (59222) 534

Medium: 20% v/v EtOH/H2O, 0.10 M NaNO3. Also data for 0.05 and 0.15 M

NaNO3. At I=0 (20% v/v), K1=6.19, \*K(SmL)=-8.78, \*K(Sm(OH)L)=-8.96.

\*\*\*\*\*

C8H8N2O2 HL Phenylglyoxime (3222)

Phenylglyoxime; C6H5.C(:N.OH).CH:N.OH

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

-----  
Sm+++ gl diox/w 20°C 50% U K1=6.88 B2=12.94 1971MAf (59342) 535

Medium: 50% dioxan, 0.1 M NaClO4

\*\*\*\*\*

C8H8N4O5 L (6097)

2-Acetylpyridinethiosemicarbazone; C5H4N.CO.CH:N.NH.CS.NH2

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

-----  
Sm+++ gl alc/w 25°C 75% C I K1=7.66 B2=14.91 1988GSa (59412) 536

In 75%(v/v) ethanol/water; 0.1 M NaClO4. I=0.2 M: K1=7.60, K2=7.15;

I=0.05 M: K1=7.79, K2=7.34; I=0.02 M: K1=7.95, K2=7.50

\*\*\*\*\*

C8H8O2 HL 2-Acetylphenol CAS 118-93-4 (1888)

2-Hydroxyacetophenone; HO.C6H4.CO.CH3

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

Sm+++ gl alc/w 25°C 20% M I K1=6.44 1994KDa (59470) 537  
 Medium: 20% v/v EtOH/H2O, 0.10 M NaNO3. Also data for 0.05 and 0.15 M  
 NaNO3. At I=0 (20% v/v), K1=6.73, \*K(SmL)=-8.70, \*K(Sm(OH)L)=-9.25.

\*\*\*\*\*

C8H8O2 HL Phenylacetic CAS 103-82-2 (1361)  
 Phenylethanoic acid; C6H5.CH2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Sm+++	gl	NaClO4	25°C	0.1M	C	H	K1=2.13	1996HYa (59562)	538
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By calorimetry: DH(K1)=9.99 kJ mol-1

Sm+++	gl	NaClO4	25°C	0.10M	C	H	K1=2.13	1990HYa (59563)	539
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By calorimetry: DH(K1)=10.0 J K-1 mol-1

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C8H8O2 HL CAS 583-80-2 (3191)  
 beta-Methyltropone;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Sm+++	sp	alc/w	?	3%	U		K1=7.07	1967GDb (59604)	540
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Medium: 3% EtOH, 0.2 M NaClO4

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C8H8O3 H2L CAS 490-78-8 (6324)  
 2,5-Dihydroxyacetophenone; (HO)2C6H3.CO.CH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Sm+++	gl	alc/w	25°C	20%	M	I		1994KDa (59683)	541
-------	----	-------	------	-----	---	---	--	-----------------	-----

K(Sm+HL)=6.27

Medium: 20% v/v EtOH/H2O, 0.10 M NaNO3. Also data for 0.05 and 0.15 M  
 NaNO3. At I=0 (20% v/v), K1=6.57, \*K(SmHL)=-8.61, \*K(Sm(OH)HL)=-9.04.

\*\*\*\*\*

C8H8O3 HL o-Anisic acid CAS 579-75-9 (2337)  
 2-Methoxybenzoic acid; CH3O.C6H4.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Sm+++	gl	NaClO4	25°C	0.10M	M	H	K1=2.10	1988CLb (59749)	542
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DH=6.85 kJ mol-1, DS=63 J K-1 mol-1

Sm+++	gl	alc/w	25°C	42%	U		K1=2.8	1983PMa (59750)	543
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Sm+++	gl	diox/w	30°C	76%	M		K1=6.48	1978PMa (59751)	544
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Medium: 76% v/v dioxane/H2O, 0.10 M NaClO4.

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C8H8O3 HL Mandelic Acid CAS 611-72-3 (80)  
 2-Phenyl-2-hydroxyethanoic acid; C6H5.CH(OH).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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-----  
Sm+++ cal alc/w 25°C 60% U H 1996YLa (59870) 545  
K(SmL+Phen)=2.68

Medium: 60% v/v MeOH/H2O. Phen: 1,10-phenanthroline.  
DH=-11.7 kJ mol<sup>-1</sup>, DS=12 J K<sup>-1</sup> mol<sup>-1</sup>.  
-----

Sm+++ gl NaClO4 25°C 0.10M C K1=2.90 B2=4.75 1989HMa (59871) 546  
-----

Sm+++ gl NaClO4 25°C 2.0M U T K1=2.47 1972DCb (59872) 547  
-----

Sm+++ gl NaClO4 25°C 1.0M U K1=2.56 B2=4.57 1970Gnd (59873) 548  
K3=1.37  
-----

Sm+++ gl KNO3 25°C 1.0M U I K1=2.23 B2=4.23 1967PNb (59874) 549  
At I=0.1: K1=2.56, K2=1.67  
-----

Sm+++ gl NaClO4 25°C 1.0M U K1=2.56 B2=4.32 1966TVa (59875) 550  
K3=1.42  
K4=1.26  
-----

\*\*\*\*\*  
C8H8O3 HL m-Anisic acid CAS 586-38-9 (2804)  
3-Methoxybenzoic acid; CH3O.C6H4.COOH  
-----

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

Sm+++ gl NaClO4 25°C 0.10M M H K1=2.24 1988CLb (59918) 551  
DH=8.25 kJ mol<sup>-1</sup>, DS=71 J K<sup>-1</sup> mol<sup>-1</sup>  
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\*\*\*\*\*  
C8H8O3 HL CAS 148-52-8 (3193)  
3-Methoxysalicylaldehyde; CH3O.C6H3(OH).CHO  
-----

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

Sm+++ gl NaNO3 25°C 0.10M M I M K1=4.634 1995Kdd (59932) 552  
K(Sm(egta)+L)=3.355  
-----

Data for 0.15 and 0.05 M NaNO3. At I=0, K1=4.902, K(Sm(egta)+L)=3.681.  
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\*\*\*\*\*  
C8H8O3 HL p-Anisic acid CAS 100-09-4 (1373)  
4-Methoxybenzoic acid; CH3O.C6H4.COOH  
-----

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

Sm+++ gl NaClO4 25°C 0.10M M H K1=2.24 1988CLb (59962) 553  
DH=9.01 kJ mol<sup>-1</sup>, DS=73 J K<sup>-1</sup> mol<sup>-1</sup>  
-----

Sm+++ gl diox/w 30°C 76% M K1=6.21 1978PMa (59963) 554  
Medium: 76% v/v dioxane/H2O, 0.10 M NaClO4.  
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\*\*\*\*\*  
C8H8O4 HL CAS 520-45-6 (4478)  
3-Acetyl-2-hydroxy-6-methylpyran-4-one, Dehydroethanoic acid;  
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Sm+++      gl  diox/w 35°C  50%  U          K1=4.48  B2=8.20  1971MAa (60097) 555
Medium: 50% dioxan, 0.1 M NaClO4
*****
C8H9NO2          HL                      CAS 4389-45-1 (3226)
3-Methyl-2-aminobenzoic acid; CH3.C6H3(NH2).COOH
-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Sm+++      gl  NaNO3  25°C 0.10M M I M    K1=5.24          1995KDC (60236) 556
                                K(Sm(egta)+L)=5.04
Data for 0.05 and 0.15 M NaNO3. At I=0, K1=5.49, K(Sm(egta)+L)=5.18.
*****
C8H9NO2          HL                      CAS 5330-97-2 (6248)
Phenylacetohydroxamic acid; C6H5.CH2.CO.NH.OH
-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Sm+++      gl  KNO3   30°C 0.10M C M    K1=5.99  B2=11.64  1987RSc (60354) 557
                                K3=4.80
                                K(Sm(hedta)+L)=4.48
hedta is N-hydroxyethyldiaminoethane-N,N',N'-triethanoic acid.
-----
Sm+++      gl  KNO3   20°C 0.10M M T    K1=6.05  B2=11.77  1986RSc (60355) 558
                                K3=4.88
Data for 20-50 C. At 30 C, K1=5.99, K2=5.65, K3=4.80.
*****
C8H9NO4          H2L                      (4520)
Dehydroethanoic acid oxime;
-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Sm+++      gl  diox/w 35°C  50%  U          K(Sm+HL)=4.40
                                K(Sm+2HL)=7.97
Medium: 50% dioxan, 0.1 M NaClO4
*****
C8H9N3O2          L                      CAS 7254-31-4 (1266)
Acylnicotinoyl hydrazide; C5H4N.CO.NH.NH.CO.CH3
-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Sm+++      gl  NaClO4 25°C 0.10M U          K1=13.75 B2=25.00 1980ZMa (60572) 560
*****
C8H10N6O2S2       H2L                      (2746)
2,5-Dihydroxybenzoquinone bis-thiosemicarbazone;
-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
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-----  
Sm+++ gl diox/w 30°C 50% C TIH K1=4.80 B2=8.64 1989GDa (60819) 561  
DH(K1)=-79.8 kJ mol<sup>-1</sup>

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C8H10O4 L CAS 34241-51-5 (5701)  
3-Acetyl-6-methylhydropyrane-2,4-dione;

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

Sm+++ gl alc/w 22°C 20% U K1=4.30 B2=7.84 1988ZTa (60854) 562  
K3=3.00

\*\*\*\*\*

C8H10O5 H2L CAS 145-73-7 (138)  
7-Oxa-bicyclo[2.2.1]-heptan-2,3-dicarboxylic acid;

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

Sm+++ gl KCl 30°C 0.10M C K1=6.01 B2=10.29 1996SZa (60875) 563  
For the -5-en-2-exo isomer, K1=6.22, B2=10.90.

\*\*\*\*\*

C8H11NO8 H4L CAS 7408-20-0 (2608)  
Amino-di(butanedioic acid);HN(CH(COOH)CH2.COOH)2

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

Sm+++ gl KCl 25°C 0.10M U K1=10.86 B2=18.06 1979BEb (61215) 564  
B(SmHL)=15.46

\*\*\*\*\*

C8H11NO9P2 H5L CAS 147608-63-7 (8924)  
[(2-Hydroxy-5-nitro-1,3-phenylene)bis(methylene)]bisphosphonic acid;

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

Sm+++ gl NaClO4 25°C 0.10M U K1=12.7 2002BBh (61235) 565  
B(SmHL)=20.3  
B(SmH2L)=25.17  
B(SmH3L)=27.6  
B(SmH-1L)=1.8

B(SmH-2L)=-10.2. By spectrophotometry, K1=12.07, B(SmHL)=19.84, B(SmH2L)=  
24.03, B(SmH3L)=28.01, B(SmH-1L)=1.24, B(SmH-2L)=-7.2.

\*\*\*\*\*

C8H11O4P H2L (4536)  
(alpha-Hydroxy-alpha-methylbenzyl)phosphonic acid;

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

Sm+++ gl NaCl 25°C 0.10M U 1973BSg (61313) 566  
K(Sm+HL)=2.18

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C8H11O7ClP2 H5L CAS 147608-64-8 (8925)

[(5-Chloro-2-hydroxy-1,3-phenylene)bis(methylene)]bisphosphonic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Sm+++	gl	NaClO4	25°C	0.10M	U			K1=12.62 B(SmHL)=20.11 B(SmH2L)=24.42 B(SmH-1L)=3.91 B(SmH-2L)=-6.8	2002BBh (61319)	567
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C8H12N2O3                      H2L      Barbitol                      CAS 57-44-3    (2744)  
5,5-Diethylbarbituric acid, Veronal, Barbitone;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Sm+++	gl	oth/un	25°C	0.10M	U			K1=2.974	1987TSb (61442)	568
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C8H12N2O8                      H4L                      CAS 35039-85-1    (4537)  
1,2-Diaminoethane-N,N'-dimalonic acid; (HOOC)2.CH.NH.CH2.CH2.NH.CH(COOH)2

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

Sm+++	gl	KNO3	20°C	0.10M	U			K1=12.58    B2=16.79	1975DPa (61521)	569
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Sm+++	vlt	KNO3	25°C	0.10M	U			K1=10.97	1972GBd (61522)	570
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C8H12O2                      HL                      CAS 874-23-7    (3203)  
2-Acetylcyclohexanone;

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

Sm+++	gl	mixed	25°C	75%	U			K1=8.92    B2=16.99 K3=8.16	1971DRa (61677)	571
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Medium: 75% acetone, 0.1 M NaClO4

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

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

Sm+++	gl	oth/un	30°C	0.10M	U			K1=2.86    B2=5.45	1975DSa (61691)	572
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C8H12O4                      H2L                      CAS 1076-97-9    (2224)  
Cyclohexane-1,4-dicarboxylic acid; C6H10.(COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Sm+++	gl	NaClO4	25°C	0.10M	M	H		K1=4.42	1986CDb (61715)	573
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DH=15.3 kJ mol<sup>-1</sup>, DS=136 J K<sup>-1</sup> mol<sup>-1</sup>

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C8H13NO6 H3L (3835)  
2-Amino-2-carboxypropane-N,N-diethanoic acid; HOOCC(CH3)2N(CH2COOH)2

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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	KNO3	20°C	0.10M	U		K1=9.42 B2=16.51	1974RMg (61768)	574

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C8H13NO6 H3L (5681)  
2-Aminobutanoic-N,N-diethanoic acid; CH3CH2CH(COOH)N(CH2COOH)2

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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	KNO3	20°C	0.10M	U		K1=11.13 B2=19.57	1974RMg (61794)	575

\*\*\*\*\*

C8H14O3 HL CAS 607-97-6 (4489)  
3-Ethylethylacetoacetate; CH3.CO.CH(C2H5).CO.OC2H5

---

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	mixed	30°C	75%	U		K1=8.79	1971DRb (62082)	576

Medium: 75% acetone, 0.1 M

\*\*\*\*\*

C8H16O3 HL CAS 58888-84-9 (3807)  
2-Hydroxy-2-propylpentanoic acid; CH3.CH2.CH2.C(OH)(CH2.CH2.CH3).COOH

---

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	EMF	NaClO4	25°C	1.0M	U		K1=2.65 B2=4.82	1965TVa (62637)	577

Method: quinhydrone electrode

\*\*\*\*\*

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
Sm+++	ISE	non-aq	25°C	100%	U		K1=5.17 B2=6.76	1982MDa (62725)	578

Medium: propylene carbonate

\*\*\*\*\*

C8H18N2O10P2 H6L EDDADPO CAS 2310-83-0 (2436)  
1,2-Diaminoethane-N,N'-diethanoic-N,N'-dimethylphosphonic acid;  
(-CH2.N(CH2.COOH)(CH2.PO3H2))2

---

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	KCl	25°C	0.10M	U			1965DKb (62904)	579

K(Sm+HL)=17.8  
K(Sm+H2L)=9.6

\*\*\*\*\*

C8H18O4 L Triglyme CAS 112-49-2 (2358)  
1,2-Bis(methoxyethoxy)ethane; CH3O.C2H4O.CH2.CH2.OC2H4.OCH3

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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Sm+++      gl  non-aq 25°C 100% C          K1=4.25      1989BPa (62996) 580
Medium: anhydrous propylene carbonate, 0.1 M Et4NClO4
*****
C8H22N2O6P2      H4L                      CAS 13516-59-1 (3850)
2,2'-(Ethylenedi-imino)bis(propylphosphonic acid);
-----

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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Sm+++      gl  KCl    25°C 0.10M U          K1=12.56      1965DKb (63344) 581
                                K(Sm+HL)=6.20
*****
C9H5NOI2      HL                      CAS 83-73-8 (3280)
5,7-Di-iodo-8-hydroxyquinoline;
-----

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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Sm+++      gl  diox/w 35°C 75% U          K1=6.95      B2=12.85      1971MAb (63570) 582
                                K3=5.15
Medium: 75% v/v dioxan, 0.1 M NaClO4
*****
C9H5NO4      HL                      CAS 22308-86-7 (4607)
3-Nitroso-4-hydroxycoumarin (oximidobenzotetronic acid);
-----

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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Sm+++      sp  diox/w 20°C 50% U          K1=2.59      B2=4.20      1977MBb (63614) 583
*****
C9H6NO4BrS      H2L                      CAS 3062-37-1 (3889)
7-Bromo-8-hydroxyquinoline-5-sulfonic acid;
-----

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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Sm+++      gl  NaClO4 25°C 0.10M U          K1=5.30      B2=9.87      1973MAa (63703) 584
                                K3=4.2
*****
C9H6NO4IS      H2L      Ferron          CAS 547-91-1 (275)
7-Iodo-8-hydroxyquinoline-5-sulfonic acid; (HO)(HO3S)C9H4NI
-----

```

```

-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Sm+++      gl  NaClO4 25°C 0.10M U I      K1=5.37      B2=10.29      1987BCd (63827) 585
                                B3=14.47
Data also in 42% MeOH, 51.1% EtOH and 61.2% dioxan
-----

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-----
Sm+++      gl  oth/un 20°C 0.10M U          K1=5.93      1977SKd (63828) 586
*****
C9H6N3OC1S      HL                      CAS 27004-41-7 (216)
-----

```



2-(2'-Thiazolylazo)-4-chlorophenol; C3H2NS.N:N.C6H3(Cl).OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Sm+++	gl	KNO3	25°C	0.10M	U			K1=7.77	1974KSa (63930)	587
*****										
C9H6O6		H3L							CAS 569-51-7 (1621)	
1,2,3-Benzenetricarboxylic acid; C6H3.(COOH)3										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Sm+++	gl	NaClO4	25°C	0.10M	U	H		K1=5.08 K(Sm+HL)=2.75	1994CRa (63976)	588
DH(K1)=17.9 kJ mol-1; DS=157 J K-1 mol-1										
*****										
C9H7N		L							CAS 91-22-5 (1538)	
Quinoline;										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Sm+++	gl	NaClO4	25°C	0.5M	M	H		K1=3.67	1991KBb (64067)	589
By calorimetry: DH(K1)=2.26 kJ mol-1, DS(K1)=77.9 J K-1 mol-1.										
*****										
C9H7NO		HL							CAS 148-24-3 (504)	
8-Hydroxyquinoline (8-quinolinol);										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Sm+++	sol	none	RT	0.0	U				1981FCa (64343)	590
Kso(SmL3)=-30.80										
Method: spectrophotometry.										

Sm+++	gl	oth/un	20°C	0.10M	U			K1=7.03	1977SKd (64344)	591
-------	----	--------	------	-------	---	--	--	---------	-----------------	-----

Sm+++	gl	diox/w	30°C	50%	U			K1=9.05	B2=17.31	1970GMB (64345)	592
-------	----	--------	------	-----	---	--	--	---------	----------	-----------------	-----

Medium: 50% dioxan, 0.3 M NaClO4

Sm+++	dis	NaClO4	25°C	0.10M	U				1960RYa (64346)	593
-------	-----	--------	------	-------	---	--	--	--	-----------------	-----

K2K3=12.07

Sm+++	dis	NaClO4	25°C	0.10M	U			K1=6.84 B3=19.50	1954DYa (64347)	594
-------	-----	--------	------	-------	---	--	--	---------------------	-----------------	-----

\*\*\*\*\*

C9H7NO2		HL							CAS 1127-45-3 (4614)	
---------	--	----	--	--	--	--	--	--	----------------------	--

8-Hydroxyquinoline-N-oxide;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Sm+++	gl	diox/w	30°C	50%	U			K1=7.12	1970GMB (64411)	595
Medium: 50% dioxan, 0.3 M NaClO4										

\*\*\*\*\*

C9H7N04S                      H2L      Sulfoxine                      CAS 84-88-8    (448)  
8-Hydroxyquinoline-5-sulfonic acid;

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

Sm+++            cal KNO3    20°C 0.10M U    HM                      1971GKb (64578) 596

K(SmA+L)=4.35

DH(SmA+L)=-23.82 kJ mol<sup>-1</sup>, DS=1.67 J K<sup>-1</sup> mol<sup>-1</sup>

DH(SmAL): DH=-37.83, DS=281.7. H4A=EDTA

-----  
Sm+++            gl    oth/un 25°C 0.0 U    H            K1=6.58    B2=12.28    1958F0b (64579) 597

K3=4.76

DH(K1)=-12.1, DH(K2)=-15.1, DH(K3)=-15.9; DS(K1)=84, DS(K2)=59, DS(K3)=38

DS=38

\*\*\*\*\*

C9H7N3O2S                      H2L      TAR                      CAS 2246-46-0    (707)  
4-(2'-Thiazolylazo)-resorcinol; C3H2NS.N:N.C6H3(OH)2

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

Sm+++            sp    NaNO3    25°C 0.10M C                      K1=8.10                      19850Hb (64726) 598

K(Sm+HL)=4.71

K(SmL+H)=6.05

\*\*\*\*\*

C9H8O4                      H2L                      CAS 97652-17-0    (3855)  
3-Carboxy-4-methyltropolone;

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

Sm+++            sp    NaClO4    ?    0.20M U                      K1=7.99                      1967GDc (64953) 599

K(SmHL)=10.36

-----  
Sm+++            gl    NaClO4    25°C 0.20M U                      K1=7.98    B2=14.40    1966GDa (64954) 600

K3=3.78

\*\*\*\*\*

C9H8O4                      H2L                      CAS 15872-28-3    (8407)  
Bicyclo[2.2.1]hepta-2,5-diene-2,3-dicarboxylic acid;

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

Sm+++            gl    KCl            30°C 0.10M U                      K1=4.21                      1996SZa (64981) 601

\*\*\*\*\*

C9H9O2Br                      HL                      CAS 56609-15-5    (1417)  
3-Bromo-2-hydroxy-5-methyl-acetophenone; CH3.CO.C6H2(OH)(Br)CH3

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

Sm+++            gl    diox/w 27°C 0.10M U                      K1=4.64                      1982LMa (65165) 602

\*\*\*\*\*

C9H10O2                      HL      Benzylacetic      CAS 501-52-0    (1362)  
3-Phenylpropanoic acid; C6H5.CH2.CH2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Sm+++	gl	NaClO4	25°C	0.1M	C	H		K1=2.19    B2= 3.75	1996HYa (65373)	603
By calorimetry: DH(K1)=9.47 kJ mol-1, DH(B2)=18.16 J K-1 mol-1										

Sm+++	gl	NaClO4	25°C	0.10M	C	H		K1=2.19    B2=3.75	1990HYa (65374)	604
By calorimetry: DH(K1)=9.5 J K-1 mol-1, DH(K2)=8.7										

\*\*\*\*\*  
C9H10O3                      HL      Atrolactic acid    CAS 940-31-8    (3859)  
2-Hydroxy-2-phenylpropanoic acid; CH3.C(OH)(C6H5).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Sm+++	gl	NaClO4	25°C	1.0M	U			K1=2.57    B2=4.46	1966TVa (65444)	605
								K3=1.54		
								K4=1.31		

\*\*\*\*\*  
C9H10O3                      HL                      CAS 1878-49-5    (1600)  
2-Phenyl-2-methoxyethanoic acid; C6H5.CH(OCH3)COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Sm+++	gl	NaClO4	25°C	0.10M	C			K1=2.24    B2=3.64	1989HMa (65466)	606

\*\*\*\*\*  
C9H10O3                      HL      Tropic acid      CAS 529-64-6    (1601)  
2-Phenyl-3-hydroxypropanoic acid; HO.CH2.CH(COOH)C6H5

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Sm+++	gl	NaClO4	25°C	0.10M	C			K1=2.24    B2=4.11	1989HMa (65480)	607

\*\*\*\*\*  
C9H10O4                      HL                      CAS 1521-38-6    (8489)  
2,3-Dimethoxybenzoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Sm+++	gl	diox/w	25°C	76%	M			K1=5.89	1978PMa (65534)	608
Medium: 76% v/v dioxane/H2O, 0.10 M NaClO4.										

\*\*\*\*\*  
C9H10O4                      HL                      CAS 91-52-1    (8490)  
2,4-Dimethoxybenzoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Sm+++	gl	diox/w	25°C	76%	M			K1=6.88	1978PMa (65541)	609
Medium: 76% v/v dioxane/H2O, 0.10 M NaClO4.										

\*\*\*\*\*

C9H10O4                      HL                      CAS 1466-76-8 (8491)  
2,6-Dimethoxybenzoic acid;

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

Sm+++            gl    diox/w 25°C 76% M            K1=6.00            1978PMa (65548) 610  
Medium: 76% v/v dioxane/H2O, 0.10 M NaClO4.

\*\*\*\*\*

C9H10O4                      H2L                      (7232)  
Bicyclo[2.2.1]hept-5-en-2-endo,3-cis-dicarboxylic acid;

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

Sm+++            gl    KCl      30°C 0.10M C            K1=4.17    B2=7.07    1996SZa (65577) 611  
For the -2,5-dien-2-exo isomer, K1=4.21.

\*\*\*\*\*

C9H10O4                      H2L                      CAS 3853-88-1 (5687)  
endo-cis-Bicyclo-[2,2,1]-5-hepten-2,3-dicarboxylic acid;

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

Sm+++            gl    NaClO4 24°C 0.10M U            K1=4.50            1986ZBa (65592) 612  
K(Sm+HL)=1.84

\*\*\*\*\*

C9H10O5                      H2L                      CAS 54384-22-4 (8406)  
1-Methyl-(exo,exo)-7-oxabicyclo[2.2.1]hept-5-ene-2,3-dicarboxylic acid;

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

Sm+++            gl    KCl      30°C 0.10M U            K1=5.18    B2= 8.02    1996SZa (65609) 613

\*\*\*\*\*

C9H10O5                      H2L                      (7233)  
1-Methyl-7-oxa-bicyclo[2.2.1]hept-5-en-2-exo,3-cis-dicarboxylic acid;

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

Sm+++            gl    KCl      30°C 0.10M C            K1=5.18    B2=8.02    1996SZa (65624) 614

\*\*\*\*\*

C9H10O8                      H4L                      CAS 3724-52-5 (1264)  
cis-1,2,3,4-Cyclopentanetetracarboxylic acid; C5H6.(COOH)4

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

Sm+++            gl    NaClO4 30°C 0.20M U T            K1=10.15            1979NSb (65649) 615  
K1=10.28 when T=40.  
K1=10.40 when T=50.

\*\*\*\*\*

C9H11NO2                      HL            Phenylalanine    CAS 63-91-2 (2)  
2-Amino-3-phenylpropanoic acid; H2N.CH(CH2.C6H5)COOH

-----

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaCl04	37°C	0.15M	C			2002TKa (65971)	616
							B(SmHL)=11.49 K(Sm+2L=SmH-2(HL)2)=7.95		

Sm+++	gl	NaCl	25°C	0.15M	U	H	K1=3.46	1992ZNa (65972)	617
By calorimetry: DH(K1)=1.18 kJ mol <sup>-1</sup> , DS(K1)=70.20 J K <sup>-1</sup> mol <sup>-1</sup> .									

Sm+++	gl	NaNO3	25°C	0.0	U		K1=4.77	1991ADb (65973)	618
Extrapolated from data for 0.01-0.1 M NaNO3. Data for 35 and 45 C.									

\*\*\*\*\*

C9H11NO3                      H2L      Tyrosine                      CAS 60-18-4 (4)  
 2-Amino-3-(4-hydroxyphenyl)propanoic acid; HO.C6H4.CH2.CH(NH2).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	KNO3	25°C	0.10M	U	T H		1976SAd (66241)	619
							K(Sm+HL)=4.71 K(SmHL+HL)=4.13		

\*\*\*\*\*

C9H11N3O2S                      HL                      CAS 51146-75-9 (6170)  
 N-(2-Hydroxy-3-methoxybenzylidene)thiosemicarbazide; CH3O(OH)C6H3.CH:N.CS.NH.NH2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	diox/w	30°C	75%	U		K1=7.26	1988MKd (66511)	620
*****									
C9H11N3O3						HL	CAS 58336-41-7 (6169)		
N-(2-Hydroxy-3-methoxybenzylidene)semicarbazide; CH3O(OH)C6H3.CH:N.CO.NH.NH2									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	diox/w	30°C	75%	U		K1=10.26	1988MKd (66518)	621
*****									
C9H12N2O10						H5L	CAS 80921-06-8 (2924)		
2,3-Diaminopropanoic-N,N'-di-1,3-propanedioic acid; (HOOC)2CH.NH.CH(COOH).CH2.NH.CH(COOH)2									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	ISE	KNO3	25°C	0.10M	U		K1=11.79	1983KBd (66745)	622
Hg-electrode.									
*****									
C9H13NO6						H3L	(3881)		
2,6-Dicarboxypiperidyl-N-ethanoic acid;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	KNO3	25°C	0.10M	U		K1=10.59    B2=18.36	1968TKe (66893)	623

\*\*\*\*\*

C9H13N3O5                      L      Cytidine                      CAS 65-46-3    (2152)  
Cytidine, Cytosine-1-beta-D-ribofuranoside;

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

Sm+++            gl    KNO3    35°C 0.10M U            M    K1=3.10                      1986RMb (67080) 624  
K(Sm+L+HGly)=8.41, K(Sm+L+HHis)=8.54, K(Sm+L+oxalate)=9.89

\*\*\*\*\*

C9H14O7P2                      H5L                      CAS 147608-61-5    (7128)  
Hydroxy-4-methylbenzene-2,6-di(methylphosphonic acid);

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

Sm+++            gl    NaClO4 25°C 0.10M U                      K1=12.8                      2002BBh (67371) 625  
B(SmHL)=21.3  
B(SmH2L)=27.3  
B(SmH3L)=30.1  
B(SmH-1L)=2.2

B(SmH-2L)=-9.7.

\*\*\*\*\*

C9H15NO6                      H3L                      (7177)  
2-Aminopentanoic-N,N-diethanoic acid; C3H7C(COOH)N(CH2COOH)2

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

Sm+++            gl    KNO3    20°C 0.10M U                      K1=10.87    B2=19.07    1974RMg (67413) 626

\*\*\*\*\*

C9H16N2O6                      H3L            MEDTA                      CAS 40423-02-7    (5717)  
N-Methyldiaminoethane-N,N',N'-triethanoic acid; HOOC.CH2.N(CH3)CH2.CH2.N(CH2.COOH)2

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

Sm+++            cal NaClO4 25°C 0.50M M    IH            K1=12.42                      1986RCa (67644) 627  
DH=-14.1 kJ mol<sup>-1</sup>, DS=191 J K<sup>-1</sup> mol<sup>-1</sup>

\*\*\*\*\*

C9H16O4                      H2L                      CAS 1636-27-7    (485)  
Dipropylpropanedioic acid (Di-n-propylmalonic acid);

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

Sm+++            gl    KNO3    25°C 0.10M U                      K1=4.38    B2=7.34    1968PFa (67778) 628

\*\*\*\*\*

C9H28N3O15P5                      10L            DTPPH                      CAS 15827-60-8    (2921)  
Diethylenetriamine-N,N,N',N'',N''-penta(methylphosphonic acid);  
H2O3PCH2.N(CH2CH2.N(CH2PO3H2)2)2    H

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

Sm+++            gl    NaClO4 25°C 0.10M M                      1987ZGa (68412) 629

K(Sm+H2L)=8.64

-----  
Sm+++ gl oth/un 25°C 0.10M U 1984ZGa (68413) 630

K(Sm+H2L)=10.33

K(Sm+H3L)=7.69

K(Sm+H4L)=6.68

K(Sm+H5L)=5.98

\*\*\*\*\*  
C10H5O2F7S L (6996)

1-(2-Thienyl)-3-heptafluoropropylpropane-1,3-dione; C3F7.C(0)CH2C(0)C4H3S  
-----

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

Sm+++ gl alc/w 22°C 80% U K1=6.18 B2=11.81 1995MTa (68433) 631

K3=4.96

Medium: 0.1 M NaClO4 in 80% (v/v) EtOH/H2O.

\*\*\*\*\*  
C10H6O3 HL CAS 481-39-0 (3295)

5-Hydroxy-1,4-naphthoquinone;  
-----

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

Sm+++ gl diox/w 25°C 50% C T H K1=7.79 B2=15.48 1992SAa (68480) 632

K3=6.50

At 35 C: K1=7.68, K2=6.70, K3=5.63; DH(K1)=-19.4 kJ mol<sup>-1</sup>

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

Sm+++ gl NaClO4 25°C 0.10M U H K1=4.81 1994CRa (68528) 633

K(Sm+HL)=3.74

DH(K1)=16.7 kJ mol<sup>-1</sup>, DS=148 J K<sup>-1</sup> mol<sup>-1</sup>; DH(Sm+HL)=9.0, DS=102

\*\*\*\*\*  
C10H7NO2 HL CAS 131-91-9 (2668)

1-Nitroso-2-naphthol, alpha-Nitroso-beta-naphthol;  
-----

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

Sm+++ sp KCl 25°C 0.10M M I K1=4.62 1976PEa (68592) 634

\*\*\*\*\*  
C10H7NO2 HL Quinaldic acid CAS 93-10-7 (2209)

Quinoline-2-carboxylic acid;  
-----

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

Sm+++ gl NaClO4 30°C 0.10M U K1=2.64 B2=5.09 1969DNc (68720) 635

\*\*\*\*\*  
C10H7NO2 HL CAS 86-59-9 (873)

Quinoline-8-carboxylic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaClO4	30°C	0.10M	U		K1=2.64	1969DNc (68771)	636
*****									
C10H7NO5S			H2L				CAS 14090-74-5	(2676)	
1-Nitroso-2-hydroxynaphthalene-7-sulfonic acid;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	KCl	25°C	0.10M	M		K1=4.60 B2=8.29	1979LSb (68818)	637
*****									
C10H7NO5S			H2L				(4766)		
1-Nitroso-2-hydroxynaphthalene-6-sulfonic acid;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	sp	KCl	25°C	0.10M	C		K1=4.69	1973PMb (68854)	638
*****									
C10H7NO5S			H2L				CAS 3682-32-4	(1812)	
2-Nitroso-1-hydroxynaphthalene-4-sulfonic acid;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	KCl	25°C	0.10M	U	I	K1=3.48	1967MAi (68894)	639
K1=4.57(I=0) *****									
C10H7NO5S			H2L				CAS 31005-79-9	(1814)	
2-Nitroso-1-hydroxynaphthalene-8-sulfonic acid;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	sp	KCl	25°C	0.10M	M		K1=5.65	1978PPb (68951)	640
*****									
C10H7NO8S2			H3L			Nitroso-R acid	CAS 525-05-3	(1811)	
1-Nitroso-2-hydroxynaphthalene-3,6-disulfonic acid;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	oth/un	25°C	0.10M	U		K1=4.63 B2=8.00	1990ATa (69029)	641
*****									
Sm+++	gl	KCl	25°C	0.10M	U		K1=5.15	1968MAe (69030)	642
*****									
C10H7NO8S2			H3L				CAS 52664-45-6	(1627)	
2-Nitroso-1-hydroxynaphthalene-4,6-disulfonic acid;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaCl	25°C	0.10M	U		K1=3.886 B2=10.27	1974SAa (69054)	643



C10H7N08S2	H3L	CAS 50332-99-3	(1628)
2-Nitroso-1-hydroxynaphthalene-4,7-disulfonic acid;			

C10H7N5O5                      HL                      CAS 102964-51-2    (6212)  
5-(2'-Nitrophenylazo)barbituric acid;

C10H7O2F3 HL CAS 326-06-7 (196)  
3-Benzoyl-1,1,1-trifluoroacetone; CF3.CO.CH2.CO.C6H5

Medium: 0.1 M NaClO<sub>4</sub> in 80% (v/v) EtOH/H<sub>2</sub>O.

C10H8N2 L 2,2'-Bipyridyl CAS 366-18-7 (25)  
2,2'-Bipyridine; (C5H4N)2

Sm+++ sp non-aq 25°C 100% C T K1=2.72 2005SYa (69644) 648  
In ethylacetate; At 50 C K1=2.54

C10H8N4O3 HL CAS 43168-60-1 (6209)  
5-Phenylazobarbituric acid;

C10H8O2                      H2L                      CAS 92-44-4    (1658)  
2,3-Dihydroxynaphthalene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Sm+++	gl	NaClO4	20°C	0.10M	U	M			1973Pac (69778)	651

K(SmA+L)=6.81, H4A=EDTA

\*\*\*\*\*

C10H8O5S H3L DHNSA (877)

2,3-Dihydroxynaphthalene-6-sulfonic acid;

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

Sm+++ gl NaClO4 30°C 0.20M U M K1=9.68 1979MSd (69860) 652

K(Sm(hedta)+L)=6.56

hedta is N-(hydroxyethyl)diaminoethane-N,N',N'-triethanoic acid.

-----  
Sm+++ gl NaClO4 30°C 0.20M U M K1=9.73 1978MSl (69861) 653

K(Sm(edta)+L)=6.32

-----  
Sm+++ gl NaClO4 25°C 0.50M C K1=9.82 B2=17.15 1976LAd (69862) 654

B(SmHL)=15.4

B(SmHL2)=24.43

\*\*\*\*\*

C10H8O8S2 H4L Chromotropic ac CAS 148-25-4 (1875)

1,8-Dihydroxynaphthalene-3,6-disulfonic acid;

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

Sm+++ gl NaClO4 20°C 0.10M M T H K1=8.55 1978AKb (69966) 655

Data for 40 C. DH(K1)=-23.9 kJ mol<sup>-1</sup>, DS(K1)=71 J K<sup>-1</sup> mol<sup>-1</sup>.

-----  
Sm+++ gl KCl 25°C 0.10M M I 1974MLa (69967) 656

K(Sm+HL)=2.26

\*\*\*\*\*

C10H9NO4S H2L CAS 29021-67-8 (3926)

2-Methyl-8-hydroxyquinoline-5-sulfonic acid;

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

Sm+++ gl NaClO4 30°C 0.10M U TI K1=5.15 B2=9.92 1988BCd (70202) 657

B3=13.61

in 42.5% MeOH-water: K1=6.29, B2=11.76, B3=16.28

51.8% EtOH-water: K1=6.64, B2=12.31, B3=16.75

\*\*\*\*\*

C10H9N3OS HL CAS 60321-26-8 (4671)

2-(2-Thiazolylazo)methylphenol; C3H2NS.N:N.C6H3(CH3)OH

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

Sm+++ sp diox/w 25°C 10% U K1=9.41 B2=17.95 1973KSd (70366) 658

Medium: 10% dioxan, 0.1 M KNO3

\*\*\*\*\*

C10H9N3O2S HL CAS 3012-52-0 (217)

2-(2'-Thiazolylazo)-4-methoxyphenol; CH3O.C6H3(OH).N:N.C3H2N2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	sp	KNO3	25°C	0.10M	U		K1=8.98	1974KSa (70404)	659
*****									
C10H9O2Br		HL					CAS 4023-81-8	(1182)	
4-Bromo-1-phenyl-1,3-butanedione; Br.C6H4.CO.CH2.CO.CH3									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	diox/w	30°C	75%	U		K1=7.28 K3=4.35	B2=13.36 1979MBc (70439)	660
*****									
C10H9O2F		HL					CAS 29681-98-9	(307)	
1-(4-Fluorophenyl)butane-1,3-dione; F.C6H4.CO.CH2.CO.CH3									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	diox/w	30°C	75%	U		K1=7.34 K3=4.50	B2=13.62 1979MBc (70452)	661
*****									
C10H10O5		HL					CAS 13522-48-0	(4722)	
3-Mercapto-1-phenylbut-2-en-1-one; C6H5.CO.CH:CH.C(SH).CH3									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	mixed	30°C	75%	U		K1=4.03 K3=3.11	B2=7.58 1969DNb (70640)	662
Medium: 75% acetone, 0.1 M NaClO4									
*****									
C10H10O2		HL					Benzoylacetone CAS 93-91-4	(197)	
1-Phenylbutane-1,3-dione; C6H5.CO.CH2.CO.CH3									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	diox/w	30°C	75%	U		K1=7.45 K3=4.28	B2=13.45 1979MBc (70769)	663
-----									
Sm+++	gl	alc/w	25°C	80%	U		K1=8.03 K3=4.30	B2=14.31 1967DZa (70770)	664
Medium: 80% MeOH, 0.1 M NaCl									

Sm+++	gl	alc/w	24°C	80%	U		K1=8.03 K3 = 4.30	B2=14.31 1967DZb (70771)	665
Medium: 80% v/v MeOH/H2O, 0.1 M NaCl									
*****									
C10H10O6		H2L					CAS 5411-14-3	(2394)	
1,2-Phenylenedioxodiethanoic acid; C6H4(O.CH2.CO.OH)2									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Sm+++ gl NaClO4 25°C 0.10M M K1=4.57 B2=7.48 1977HCb (70859) 666  
\*\*\*\*\*

C10H11NOS L (2831)

Acetothioacetanilide; CH3.CO.CH2.CS.NH.C6H5

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

Sm+++ gl diox/w 25°C 50% U K1=5.01 B2=9.30 1986NBa (70885) 667  
\*\*\*\*\*

C10H11NO2 L CAS 102-01-2 (250)

Acetoacetanilide; CH3.CO.CH2.CO.NH.C6H5

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

Sm+++ gl diox/w 25°C 50% U K1=5.77 1986NBa (70914) 668  
\*\*\*\*\*

C10H11NO3 HL (1960)

N-Hydroxyacetoacetanilide; CH3.CO.CH2.CO.N(OH).C6H5

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

Sm+++ gl diox/w 20°C 82% U K1=6.69 B2=12.93 1979KSb (70944) 669  
K3=5.82  
\*\*\*\*\*

C10H11N5O L CAS 105507-56-0 (8131)

N-Methylisatin-beta-amidinohydrazone;

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

Sm+++ gl diox/w 30°C 50% C TIH K1=5.19 B2= 9.39 1986SGc (71095) 670

Medium: 50% v/v dioxan/H2O, 0.10 M NaClO4. Data for 0.02-0.20 M NaClO4  
and 30-50 C. DH(K1)=65.1 kJ mol<sup>-1</sup>, DS=314 J K<sup>-1</sup> mol<sup>-1</sup>; DH(K2)=62.2, DS=286  
\*\*\*\*\*

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  
-----

Sm+++ dis R4N.X 25°C 0.10M U 1970SBa (71115) 671

B3=18.4

B(SmL3(OH))=24.2

Medium: Et4NC1O4

\*\*\*\*\*  
C10H12N2O4 H2L CAS 16598-05-3 (967)

2-Pyridylmethyliminodiethanoic acid; C5H4N.CH2.N(CH2.COOH)2

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

Sm+++ gl KNO3 25°C 0.10M U K1=8.92 B2=16.88 1964THa (71273) 672  
\*\*\*\*\*

C10H12N4O5                      HL      Inosine                      CAS 58-63-9    (2344)  
Hypoxanthine-9-beta-D-ribofuranoside;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	KNO3	35°C	0.10M	U	M	K1=4.39 B(Sm(gly)L)=10.22 B(Sm(his)L)=10.89	1987RRc (71405)	673

\*\*\*\*\*  
C10H12N4O6                      H2L      Xanthosine                      CAS 5968-90-1    (1176)  
3,9-Dihydro-9-ribofuranosyl-1H-purine-2,6-dione;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	KNO3	35°C	0.10M	U	M	K(Sm+HA+HL)=5.28 K(Sm+HB+HL)=5.95 K(Sm+HL)=4.52	1987RRc (71500)	674

HA=glycine, HB=histidine.

\*\*\*\*\*  
C10H12O2                      HL                      CAS 1946-74-3    (202)  
3-Isopropyltropolone;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	diox/w	30°C	50%	U	M	K1=7.78    B2=15.00 K3=5.62 K(Sm(NTA)+L)=6.09	1980SGa (71603)	675
Sm+++	gl	alc/w	24°C	80%	U		K1=8.7    B2=15.99 K3=6.0 K4=4.6	1968DZb (71604)	676

Medium: 80% MeOH, 0.1 M NaCl

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	sp	alc/w	?	3%	U		K1=7.04	1967GDb (71605)	677

Medium: 3% EtOH, 0.2 M NaClO4

\*\*\*\*\*  
C10H12O4                      HL                      CAS 5936-18-9    (2743)  
2-Hydroxy-3,4-dimethoxyacetophenone; (HO)(CH3)2C6H2.CO.CH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	diox/w	15°C	50%	C T H		K1=7.98    B2=15.14	1987GBa (71657)	678

K1(35, 40, 50 C) = 7.72, 7.48, 7.40 respectively. DH(K1)=-31.8 kJ mol<sup>-1</sup>

\*\*\*\*\*  
C10H12O5                      HL                      CAS 490-64-2    (8492)  
2,4,5-Trimethoxybenzoic acid;

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

Sm+++ gl diox/w 25°C 76% M K1=6.62 1978PMa (71676) 679  
 Medium: 76% v/v dioxane/H2O, 0.10 M NaClO4.

\*\*\*\*\*

C10H12O5 HL CAS 570-02-5 (8493)  
 2,4,6-Trimethoxybenzoic acid;

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

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Sm+++ gl diox/w 25°C 76% M K1=5.97 1978PMa (71683) 680  
 Medium: 76% v/v dioxane/H2O, 0.10 M NaClO4.

\*\*\*\*\*

C10H16N2O8 H4L EDDS CAS 52759-67-8 (1100)  
 1,2-Diaminoethane-N,N'-di-1,4-butanedioic acid; (CH2.NH.CH(COOH)CH2.COOH)2

---

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

---

Sm+++ gl KCl 25°C 0.10M U K1=13.08 1980MMe (73178) 681  
 K(Sm+HL)=6.27

---

Sm+++ gl KNO3 20°C 0.10M U K1=13.77 1975DPa (73179) 682

---

Sm+++ gl KNO3 30°C 0.10M U K1=8.68 1972STc (73180) 683

---

Sm+++ vlt KNO3 25°C 0.10M U K1=13.46 1971BGb (73181) 684

\*\*\*\*\*

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

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

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Sm+++ gl KNO3 25°C 0.50M U M 2005TPa (74142) 685  
 K(Sm(OH)L+H)=9.84  
 K(SmL+gly)=3.05  
 K(SmL+ida)=5.22  
 K(SmL(OH)gly+H)=6.43

K(SmL+nta)=4.82

Hgly- glycine;H2ida - IDA;H3nta- NTA, also data for mixed ligand complexes

---

Sm+++ gl NaClO4 37°C 0.15M C K1=16.1 2003TKa (74143) 686  
 K(Sm+HL)=8.37  
 B(SmH-1L)=5.5

---

Sm+++ cal NaClO4 25°C 0.10M C H 1987YJa (74144) 687  
 DH(K1)=-13.7 kJ mol-1, DS(K1)=270 J K-1 mol-1.

---

Sm+++ gl KCl 25°C 1.0M U 1984BKc (74145) 688  
 K(SmL+H)=1.49

---

Sm+++ gl NaNO3 25°C 0.50M U I K1=16.92 1984KKb (74146) 689

---

Sm+++	gl	NaClO4	25°C	0.20M	U	K1=12.83	1984LSd (74147)	690
Sm+++	gl	NaClO4	28°C	0.20M	U	K1=11.02	1982LSa (74148)	691
Sm+++	gl	NaClO4	20°C	0.02M	U M	K(SmL+PO4)=3.60	1982MPd (74149)	692
Sm+++	vlt	KNO3	20°C	0.10M	U	K1=17.30	1978NLb (74150)	693
Sm+++	gl	NaClO4	25°C	0.50M	U	K1=16.72	1977GGb (74151)	694
Sm+++	sp	none	25°C	0.0	C	K1=14.33	1977HAa (74152)	695
Medium not reported.								
Sm+++	gl	KCl	25°C	1.00M	U	K2=3.65 K(SmL+HL)=2.49 K(2SmL+L)=6.66	1976BKa (74153)	696
Sm+++	gl	KCl	25°C	1.0M	U	K(SmL+H)=2.03	1976GMb (74154)	697
Sm+++	sp	KCl	25°C	0.10M	U	K2=3.65 K(2SmL+L)=6.66 K(SmL+HL)=2.49	1975BKa (74155)	698
Sm+++	EMF	KCl	25°C	0.10M	U T	K(SmL+H)=1.69	1974BKb (74156)	699
Sm+++	gl	KCl	25°C	1.0M	C	K2=3.65 K(SmL+HL)=2.49 K(2SmL+L=Sm2L3)=6.66	1974BKe (74157)	700
Sm+++	gl	KNO3	20°C	0.10M	U M	K(SmL+Citrate)=2.8	1974TDa (74158)	701
Sm+++	gl	KNO3	25°C	0.10M	U T M	K(SmL+HA)=3.35 K(SmL+A)=5.10 K(SmL+HA)(2 C)=3.80, K(35 C)=3.41, K(45 C)=3.28, K(SmL+A)(2 C)=5.20, K(35 C)=5.17, K(45 C)=4.98, H5A=tripolyphosphoric acid	1973TRb (74159)	702
Sm+++	gl	KNO3	25°C	0.10M	U T M	K(SmL+A)=4.9 K(2 C)=4.8, K(35 C)=4.7, K(45 C)=4.6, H4A=adenosine triphosphate	1973TRb (74160)	703
Sm+++	cal	KNO3	20°C	0.10M	U	K(SmL(H2O)x=SmL(H2O)x-1+H2O)=-0.7	1971GKb (74161)	704
Sm+++	gl	NaClO4	25°C	0.10M	U M	K(SmL+A)=6.69, H4A=tiron	1969AIb (74162)	705

-----  
 Sm+++ dis oth/un 25°C ? U K1=16.81 1969PJ a (74163) 706  
 Method: paper electrophoresis. Medium: pH=1.86  
 -----

Sm+++ sp oth/un 19°C 0.04M U K1=16.34 B2=22.83 1963GAc (74164) 707  
 K(Sm+HL)=8.18  
 K(Sm+H4L)=2.58  
 K(Sm+H3L)=3.62  
 K(SmL+HL)=2.31  
 -----

Sm+++ con oth/un 25°C ? U K1=16.43 1961TSb (74165) 708  
 K(SmL+H)=2.22  
 -----

Sm+++ ix KCl 25°C 0.10M U H K1=16.53 1959BD b (74166) 709  
 DH(K1)=-3.4 kJ mol<sup>-1</sup>, DS=305 J K<sup>-1</sup> mol<sup>-1</sup>  
 -----

Sm+++ gl oth/un 20°C 0.01M U K1=16.97 1955WSa (74167) 710  
 Polarography also used  
 -----

Sm+++ gl KCl 20°C 0.10M U I T K1=16.9 1954SGa (74168) 711  
 By polarography, 0.1 M KNO<sub>3</sub>, K1=16.7 or 17.14  
 -----

Sm+++ gl KCl 20°C 0.10M U I T K1=16.55 1953WSa (74169) 712  
 By polarography, 0.1 M KNO<sub>3</sub>, K1=16.3  
 -----

Sm+++ gl KCl 20°C 0.10M U K1=17.2 1952VIa (74170) 713  
 \*\*\*\*\*  
 C10H16N5O13P3 H4L ATP CAS 56-65-5 (403)  
 Adenosine-5'-triphosphoric acid;  
 -----

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Sm+++	gl	NaCl04	20°C	0.20M	U	T H		K1=7.22 B2=11.05 K(Sm(nta)+L)=4.19 K(Sm(edta)+L)=4.04	1993VL a (74816)	714

Data for 30, 40 C. DH(K1)=16.3 kJ mol<sup>-1</sup>, DS(K1)=194 J K<sup>-1</sup> mol<sup>-1</sup>. DH(K2)=23.9, DS(K2)=155; DH(Sm(nta)+L)=19.2, DS=146; DH(Sm(edta)+L)=13.4, DS=123.  
 -----

Sm+++ gl KCl 25°C 0.10M U K1=6.71 B2=10.53 1988SSd (74817) 715  
 K(Sm+HL)=4.51  
 -----

Sm+++ kin oth/un 25°C 0.05M C K1=6.66 1983MCc (74818) 716  
 Method: inhibition of the hexokinase reaction, pH 8.0 (0.05 M TAPS).  
 -----

Sm+++ gl KNO<sub>3</sub> 35°C 0.10M U M 1972TRc (74819) 717  
 K(Sm(EDTA)+L)=4.7  
 -----

\*\*\*\*\*  
 C10H16O2 HL CAS 100563-25-5 (4706)  
 2-Butanoylcyclohexanone; CH<sub>3</sub>.CH<sub>2</sub>.CH<sub>2</sub>.CO.C<sub>6</sub>H<sub>9</sub>O  
 -----



Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	oth/un	30°C	0.10M	U		K1=9.69 K3=8.44	B2=18.48 1972DSe (74925)	718

\*\*\*\*\*

C10H17N2O10P                      H5L                      CAS 69219-70-1 (7961)  
Bis{[bis(carboxymethyl)amino]methyl}phosphinic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaCl	25°C	0.16M	C		K1=15.60 K(Sm+HL)=9.30 K(SmL+H)=2.97 B(SmHL)=18.57	2001XRa (75026)	719

\*\*\*\*\*

C10H17N3O6S                      H3L                      Glutathione                      CAS 70-18-8 (333)  
Glutamyl-cysteinyl-glycine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaClO4	25°C	0.10M	U	TIH	K1=7.100	2003GSb (75143)	720

Values for 0.05-0.2 M NaClO4, 15-45 C and 10-30% MeOH/H2O, 20% EtOH/H2O, 20% DMF/H2O. At I=0, K1=8.240. DH(K1)=-25.6 kJ mol<sup>-1</sup>, DS(K1)=-72.

\*\*\*\*\*

C10H18N2O7                      H3L                      HEDTA                      CAS 150-39-0 (392)  
N-(Hydroxyethyl)diaminoethane-N,N',N'-triethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaClO4	25°C	0.50M	U		K1=14.85	1977GGb (75491)	721
Sm+++	EMF	KCl	25°C	1.0M	U		K2=3.66 K(SmL+HL)=1.97 K(SmL+H4L)=2.07	1977GMa (75492)	722

Method: Pt/H2 electrode.

Sm+++	EMF	KCl	25°C	1.0M	U	M		1977GMa (75493)	723
							K(Sm(edta)+L)=3.51 K(Sm(edta)+HL)=2.06 K(Sm(edta)+H2L)=1.82		

Method: Pt/H2 electrode.

Sm+++	gl	NaClO4	20°C	0.10M	U			1974PJa (75494)	724
							K(SmL+A)=3.54 K(SmL+B)=3.64		

HA=pentane-2,4-dione, B=1-phenylbutane-1,3-dione

Sm+++	gl	NaClO4	25°C	1.0M	U		K2=2.89 K(SmL+HL)=1.94 K(SmL+H2L)=0.66	1973NMa (75495)	725
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$$K(SmL+H3L)=1.68$$

Sm+++      gl   oth/un   20°C      ?   U      1971MNa (75496) 726

$$K(SmL+H3L)=0.06$$
$$K(SmL+H_2L)=0.62$$
$$K(SmL+HL)=1.92$$
$$K(SmL+L)=3.36$$

Sm+++      gl    KNO3    25°C 0.10M U    M    1963TLb (75497) 727

$$K(SmL+A)=4.57$$
$$K(SmL+B)=4.49$$
$$K(SmL+C)=3.02$$

H2A=iminodiethanoic acid, H2B=hydroxyethyliminodiethanoic acid,  
H2C=diaminoethane-N,N'-diethanoic acid

Sm+++ EMF oth/un 20°C 0.10M U K1=15.64 1962PMa (75498) 728

Sm+++      g1   KNO3   15°C 0.10M U T H      K1=15.44      1961MFb (75499) 729

K1=15.39(20 °C), 15.28(25 °C), 15.21(30 °C), 15.23(35 °C), 15.16(40 °C)

$$DH(K1) = -17.0 \text{ kJ mol}^{-1} (25 \text{ } ^\circ\text{C}), DS = 228 \text{ J K}^{-1} \text{ mol}^{-1}$$

Sm+++      gl    KNO3    25°C 0.10M U      K1=15.17      1956SPa (75500) 730

By polarography  $K_1=15.3$

\*\*\*\*\*

C10H19N3O4	HL	Leu-Gly-Gly	CAS 1187-50-4 (1230)
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Leucyl-glycyl-glycine;  $\text{H}_2\text{N}.\text{CH}(\text{CH}_2.\text{CH}(\text{CH}_3)_2).\text{CO}.\text{NH}.\text{CH}_2.\text{CO}.\text{NH}.\text{CH}_2.\text{COOH}$

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

Sm+++      gl   KNO3   25°C 0.10M U T H      K1=3.44      1981SGf (75696) 731

Data for 35 and 45 C.  $\Delta H(K1)=3.6 \text{ kJ mol}^{-1}$ ,  $\Delta S(K1)=78 \text{ J K}^{-1} \text{ mol}^{-1}$ .

\*\*\*\*\*

C10H20N2O4                      H2L                      CAS 58534-57-9    (2113)

Hexamethylenediamine-N,N-diethanoic acid;  $\text{H}_2\text{N}(\text{CH}_2)_6.\text{N}(\text{CH}_2.\text{COOH})_2$

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

Sm+++      gl    KNO3    25°C 0.10M U      1977Tia (75777) 732

$$K(S_m+HL)=7.07$$

\*\*\*\*\*

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

1,4,7,10,13-Pentaoxacyclopentadecane; cyclo(-(O.CH<sub>2</sub>.CH<sub>2</sub>)<sub>5</sub>-)

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

Sm+++ cal non-aq 25°C 100% U H K1=2.81 1993LLa (76126) 733

Medium: MeCN.  $\Delta H(K1) = -45.7 \text{ kJ mol}^{-1}$ .

Sm+++      dis non-aq 25°C 100%   U      B2=8.27      1990NIa (76127) 734

B2=extraction eq.constant:  $M+3P+2(S)=ML_2P_3(S)$ ; solvent(S)=CH<sub>2</sub>Cl<sub>2</sub>, P=picrate

-----  
Sm+++ gl non-aq 25°C 100% C K1=7.34 B2=9.28 1989BP a (76128) 735  
Medium: anhydrous propylene carbonate, 0.1 M Et4NClO4  
-----

Sm+++ ISE non-aq 25°C 100% C K1=6.11 1983ANb (76129) 736  
The equilibration took 7-12 days. Medium: PC, 0.10 M Et4NClO4  
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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  
-----

Sm+++ ISE non-aq 25°C 100% C K1=5.03 1986BD a (76472) 737  
Medium: propylene carbonate, 0.1 M Et4NClO4  
-----

\*\*\*\*\*  
C11H8O3 H2L CAS 86-48-6 (1129)  
1-Hydroxy-2-naphthoic acid;  
-----

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

Sm+++ gl alc/w 25°C 50% U T M 1985RMb (77018) 738  
K(Sm(nta)+L)=5.00  
K(Sm(edta)+L)=6.00  
K(Sm(hedta)+L)=4.90  
K(Sm(cdta)+L)=6.30  
Medium: 0.1 M NaClO4 in 50% v/v EtOH/H2O. Also data for 35 C.  
hedta is N-hydroxy-1,2-diaminoethane-N,N',N'-triethanoic acid.  
-----

Sm+++ gl diox/w 25°C 75% U K1=5.22 1975DJ a (77019) 739  
\*\*\*\*\*

C11H8O3 L CAS 1133-72-8 (2614)  
2-Aceto-1,3-indandione;  
-----

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

Sm+++ gl diox/w 30°C 75% U T K1=4.09 B2=8.07 1984AP a (77043) 740  
-----

Sm+++ gl mixed 22°C 60% U K1=4.06 B2=7.74 1979JM a (77044) 741  
K3=3.30  
Medium: 60% acetone/H2O  
-----

\*\*\*\*\*  
C11H8O3 H2L CAS 2083-08-1 (1131)  
2-Hydroxy-1-naphthoic acid;  
-----

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

Sm+++ gl diox/w 25°C 75% U K1=5.90 1975DJ a (77065) 742  
-----

\*\*\*\*\*  
C11H8O3 HL CAS 483-35-6 (3347)  
2-Hydroxy-3-methyl-1,4-naphthoquinone;  
-----

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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Sm+++      gl  diox/w 35°C  75%  M      K1=5.26  B2=9.21  1986SSc (77078) 743
*****
C11H8O3      H2L      CAS 92-70-6 (1130)
2-Hydroxy-3-naphthoic acid (3-Hydroxy-2-naphthoic acid);
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Sm+++      gl  alc/w  25°C  50%  U T  M      1985RMb (77132) 744
                                K(Sm(nta)+L)=4.82
                                K(Sm(edta)+L)=5.90
                                K(Sm(hedta)+L)=4.98
                                K(Sm(cdta)+L)=6.20

```

Medium: 0.1 M NaClO<sub>4</sub> in 50% v/v EtOH/H<sub>2</sub>O. Also data for 35 C.  
hedta is N-hydroxy-1,2-diaminoethane-N,N',N'-triethanoic acid.

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-----
Sm+++      gl  diox/w 25°C  75%  U      K1=5.31      1975DJa (77133) 745
*****
C11H8O4      HL      CAS 7555-37-5 (4812)
3-Acetyl-4-hydroxycoumarin
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Sm+++      gl  diox/w 35°C  50%  U      K1=3.78  B2=6.62  1971MAa (77185) 746
Medium: 50% dioxan, 0.01 M NaClO4
*****
C11H8O4      HL      CAS 6724-42-1 (6183)
8-Formyl-7-hydroxy-4-methyl-2H-1-benzopyran-2-one; CH0.C9H30(:O)(CH3)(OH)
-----

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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Sm+++      gl  diox/w 30°C  50%  U TI  M      K1=5.45  B2=9.83  1985ECa (77207) 747
                                K3=3.13
20 C: K1=5.76, K2=4.38, K3=3.46; 40C: K1=5.16, K2=3.84, K3=2.82
*****
C11H8O6S      H3L      CAS 66695-90-7 (1996)
1-Hydroxy-4-sulfo-2-naphthoic acid;
-----

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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Sm+++      gl  NaClO4 25°C  0.10M C      K1=8.28  B2=14.31  1979LAb (77233) 748
                                K(Sm+HL)=2.21
*****
C11H8O6S      H3L      CAS 15509-36-1 (2658)
3-Hydroxy-7-sulfo-2-naphthoic acid;
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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----

```

Sm+++ gl NaClO4 25°C 0.10M C K1=7.44 1976MLb (77255) 749  
K(Sm+HL)=2.31

\*\*\*\*\*

C11H8O9S2 H4L CAS 67097-84-1 (1995)

1-Hydroxy-4,7-disulfo-2-naphthoic acid;

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

Sm+++ cal NaClO4 25°C 0.10M C H K1=8.49 B2=14.2 1986LLc (77286) 750  
K(Sm+HL)=2.25

DH(Sm+HL)=2.9 kJ mol<sup>-1</sup>, DS=53 J K<sup>-1</sup> mol<sup>-1</sup>

\*\*\*\*\*

C11H9N04 H2L CAS 4321-82-7 (4829)

3-Acetyl-4-hydroxycoumarin oxime;

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

Sm+++ gl diox/w 35°C 50% U 1971MAa (77428) 751

K(Sm+HL)=3.62

K(Sm+2HL)=6.39

Medium: 50% dioxan, 0.01 M NaClO4

\*\*\*\*\*

C11H9N3O2 H2L PAR CAS 1141-59-9 (636)

4-(2'-Pyridylazo)-1,3-dihydroxybenzene; C5H4N.N:N.C6H3(OH)2

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

Sm+++ sp NaNO3 25°C 0.10M C K1=10.25 19840Ha (77579) 752

K(Sm+HL)=4.28

\*K(SmHL)=-6.33

Medium pH 4.8-6.3.

-----  
Sm+++ sp KCl 20°C 0.10M U 1971EKa (77580) 753

K(Sm+HL)=3.49

-----  
Sm+++ sp NaClO4 20°C 0.10M U K1=10.1 1967SNb (77581) 754

K(Sm+HL)=11.4

\*\*\*\*\*

C11H9N3O3 HL HNQS CAS 62331-38-8 (6194)

2-Hydroxy-1,4-naphthoquinone monosemicarbazone; C10H5(OH)(O):N.NH.CO.NH2

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

Sm+++ gl diox/w 35°C 75% U TI K1=5.00 B2=8.48 1987SSb (77614) 755

At I=0.1 M. At 35 C, I=0.05, K1=5.28, K2=4.27; I=0.01, K1=5.65, K2=4.77,

At 40 C, I=0.1 M, K1=4.62, K2=3.90; at 45 C, I=0.1 M, K1=4.57, K2=3.83

\*\*\*\*\*

C11H10N4O4 HL CAS 92265-26-4 (6210)

5-(2'-Methoxyphenylazo)barbituric acid;

-----

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	diox/w	25°C	75%	U		K1=5.39 B2=10.35	1986MIa (77748)	756
*****									
C11H12N2O2		HL					CAS 103314-23-4	(6182)	
2-(N-2-Pyrrolidimino)benzoic acid; C4H7N:N.C6H4.COOH									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaClO4	25°C	0.10M	U	TIH	B2=12.86	1986GSb (78022)	757
35 C: B2=13.24; 45 C:B2=13.35. DH(B2)=-40.7 kJ mol-1, DS=121 J K-1 mol-1									
*****									
C11H12N2O2		HL				Tryptophan	CAS 73-22-3	(3)	
2-Amino-3-(3-indolyl)propanoic acid; H2N.CH(CH2.C8H6N)COOH									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	KCl	25°C	0.10M	U	T H	K1=4.75	1976BFc (78233)	758
For 55C K1= 4.15									
*****									
C11H12N2O5S		HL					CAS 56475-09-3	(8410)	
3-(4'-Sulfophenylhydrazo)-pentane-2,4-dione;									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	oth/un	30°C	0.10M	U		B2=21.78	1985EEb (78327)	759
Medium: not stated. For 3'-sulfophenylhydrazo-, B2=21.91; for 2'-sulfo-phenylhydrazo-, B2=24.03; for 4'-methyl-2'-sulfophenylhydrazo-, B2=23.01.									
*****									
C11H12O2		HL					CAS 4023-79-4	(305)	
1-(4-Methylphenyl)butane-1,3-dione; CH3.C6H4.CO.CH2.CO.CH3									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	diox/w	30°C	75%	U		K1=7.54 B2=13.75	1979MBc (78377)	760
K3=4.34									
*****									
C11H12O3		HL					CAS 94-02-0	(3351)	
Ethyl benzoylacetate; C6H5.CO.CH2.CO2.C2H5									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	mixed	25°C	75%	U		K1=8.40 B2=15.38	1971DRa (78404)	761
Medium: 75% acetone, 0.1 M NaClO4									
*****									
C11H13NO3		H2L					CAS 63467-38-9	(1961)	
4-Methyl-N-hydroxyacetoacetanilide; CH3.CO.CH2.CO.N(OH).C6H4.CH3									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo

Sm+++ gl diox/w 20°C 82% U K1=7.16 B2=13.57 1979KSb (78501) 762  
K3=6.14

\*\*\*\*\*

C11H13NO3 H2L CAS 67777-63-3 (8480)

N-[1-(2-Hydroxyphenyl)ethylidene]-beta-alanine;

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

Sm+++ gl NaClO4 25°C 0.10M U TI K1=9.11 B2=16.24 1978MSj (78529) 763

Also data for 30 and 35 C and 0.01 and 0.05 M NaClO4.

\*\*\*\*\*

C11H13NO4 L CAS 15658-60-3 (4587)

Diethyl 2,6-pyridinedicarboxylate; Dipicolinic acid diethyl ester;

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

Sm+++ sp non-aq 20°C 100% C K1=6.9 B2=13.30 1997RPa (78537) 764

B3=17.0

Medium: acetonitrile.

\*\*\*\*\*

C11H13NO4S HL CAS 58943-48-9 (1411)

N-Acetylacetylidene-orthanilic acid; HO3S.C6H4.N:C(CH3).CH2.CO.CH3

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

Sm+++ EMF NaClO4 25°C 0.10M U K1=18.40 1982MSc (78596) 765

\*\*\*\*\*

C11H13NO5 H3L HBIDA CAS 7372-13-6 (1603)

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

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

Sm+++ gl KNO3 25°C 0.10M C K1=13.08 B2=23.16 1989YSa (78638) 766

K(Sm+HL)=5.77

K(Sm+2HL)=12.32

-----  
Sm+++ gl KNO3 20°C 0.10M U K1=13.62 B2=23.68 1983MSc (78639) 767

\*\*\*\*\*

C11H14N2O4 H2L (1880)

N-(6-Methyl-2-pyridylmethyl)iminodiethanoic acid; CH3C5H3NCH2N(CH2COOH)2

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

Sm+++ gl KNO3 25°C 0.10M U K1=6.57 B2=11.05 1964THa (78892) 768

\*\*\*\*\*

C11H15NO5 HL CAS 1429-25-0 (2696)

3-Hydroxy-6-(hydroxymethyl)-2-(4-morpholinylmethyl)-4H-pyran-4-one;

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

Sm+++ sp KCl 25°C 0.10M M I 1986POa (79053) 769  
B(SmHL)=11.54

\*\*\*\*\*

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  
-----

Sm+++ vlt KNO3 20°C 0.10M U K1=13.38 1981NSc (79332) 770  
-----

Sm+++ EMF KNO3 25°C 0.10M U K1=15.83 1980KBc (79333) 771  
-----

Sm+++ vlt KNO3 20°C 0.10M U K1=17.84 1978NLb (79334) 772  
-----

Sm+++ vlt KNO3 20°C 0.10M U K1=17.97 1964ICb (79335) 773  
-----

\*\*\*\*\*

C11H18N2O8 H4L CAS 38539-29-0 (2573)

1,3-Diaminopropane-N,N'-di(1,4-butanedioic acid)

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

Sm+++ gl KNO3 25°C 0.10M U K1=9.82 1976GKd (79372) 774  
-----

\*\*\*\*\*

C11H18N2O8 H4L CAS 4408-81-5 (923)

1,3-Diaminopropane-N,N,N',N'-tetraethanoic acid; ((HOOCH<sub>2</sub>)<sub>2</sub>NCH<sub>2</sub>)<sub>2</sub>CH<sub>2</sub>

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

Sm+++ ix KNO3 20°C 0.10M U H K1=13.14 1971AWa (79467) 775  
DH=23.6 kJ mol<sup>-1</sup>, DS=331.9 J K<sup>-1</sup> mol<sup>-1</sup>. Polarography also used  
-----

Sm+++ ix oth/un 20°C 0.10M U H 1971AWa (79468) 776  
DH=23.1 kJ mol<sup>-1</sup>, DS=329.8 J K<sup>-1</sup> mol<sup>-1</sup>. Medium: KClO<sub>4</sub>. Polarography also used  
-----

Sm+++ gl KNO3 20°C 0.10M U K1=13.21 1964LAa (79469) 777  
Also K1=13.08. By polarography: K1=13.12  
-----

\*\*\*\*\*

C11H18N2O9 H4L HDPTA CAS 3148-72-9 (431)

1,3-Diamino-2-hydroxypropane-N,N,N',N'-tetraethanoic acid;

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

Sm+++ gl KNO3 25°C 0.10M M K1=13.66 1986PLc (79572) 778  
-----

\*\*\*\*\*

C11H18N2O9 H4L CAS 668-21-1 (2562)

2-Hydroxy-1,3-diaminopropane-N,N'-di(1,4-butanedioic) acid

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

Sm+++ gl KNO3 25°C 0.10M U K1=11.06 1976GKd (79603) 779



C11H18O2                      HL                      CAS 40072-58-3 (4820)  
2-(3'-Methylbutanoyl)cyclohexanone (2-isovaleryl cyclohexanone);

Medium: 75% acetone

C11H18O2                      HL                      CAS 5601-52-5 (4821)  
2-Butanoyl-6-methylcyclohexanone (2-butyril-6-methylcyclohexanone);

C11H18O9 H3L CAS 64020-00-4 (8225)  
1,1,1-Tris(carboxymethoxymethyl)ethane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Sm+++	gl	R4N.X	25°C	0.10M	C			K1=6.8	2001V5a (79676)	782
Medium: 0.10 M Me4NCl. Also data for N-ethyl-, N-phenyl-, N-NH2-, N,N-dibenzyl- and N-CH2OCH2COOH- derivatives.										

C11H20O4                      H2L                      CAS 2283-16-1    (2854)  
2,2-Dibutylpropanedioic acid; H<sub>2</sub>OC.C(C<sub>4</sub>H<sub>9</sub>)<sub>2</sub>.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	KNO3	25°C	0.10M	U		K1=4.43	1968PFa (79771)	783

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
Sm+++	cal	non-aq	25°C	100%	U	H	K1=4.14	1993LLa (79873)	784	
Medium: MeCN. DH(K1)=-24.0 kJ mol <sup>-1</sup> .										

C12H7O2F7 L (6994)  
1-Heptafluoropropyl-3-phenylpropane-1,3-dione; C3F7.CO.CH2.CO.C6H5

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Sm+++	gl	alc/w	22°C	80%	U			K1=6.35 K3=5.46	B2=12.09	1995MTa (80190) 785

Medium: 0.1 M NaClO<sub>4</sub> in 80% (v/v) EtOH/H<sub>2</sub>O.

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C12H8N2 L Phenanthroline CAS 66-71-7 (144)  
1,10-Phenanthroline;

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
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Sm+++ dis non-aq 25°C 100% C HM 1998YHa (80514) 786  
K(SmA3+L)=7.62

Method: solvent extraction from 0.10 M NaClO4 into CHCl3. HA is  
1-(2-thienyl)-4,4,4-trifluoro-1,3-butanedione. DH(SmA3+L)=9 kJ mol<sup>-1</sup>.

\*\*\*\*\*

C12H10N6O4S H2L CAS 77327-19-6 (8343)  
2-[4-Amino-3-(1,2,4-triazolylazo)]naphthol-4-sulphonic acid;

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Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
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Sm+++ gl NaClO4 30°C 0.10M U T H B2=12.57 1982GMb (80787) 787  
B3=17.89

Data for 40 and 50 C. Also DH and DS values.

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C12H11N3OS HL (6787)  
2-Hydroxy-1-naphthaldehyde thiosemicarbazone;

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

Sm+++ gl diox/w 20°C 75% U I K1=7.43 B2=13.80 1992SSc (80895) 788  
Medium: 75% v/v dioxan/H2O; 0.1 M NaClO4

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C12H11N3O2 HL CAS 50536-09-5 (6323)  
2-Hydroxy-1-naphthaldehyde-semicarbazone; HO.C10H6.CH:N.NH.CO.NH2

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

Sm+++ gl diox/w 20°C 75% U I K1=8.960 B2=16.148 1992SSc (80924) 789  
Medium: 75% v/v dioxan/H2O; 0.1 M NaClO4

\*\*\*\*\*

C12H12NO3Cl HL (1055)  
2-Chloro-4-dimethylamino-benzylidenepyruvic acid; (CH3)2N.C6H3Cl.CH:CH.CO.CO0H

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

Sm+++ sp NaClO4 25°C 0.50M U K1=2.219 1987MSa (80974) 790

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C12H12N2O3 HL Nalidixic acid CAS 389-08-2 (1401)  
1-Ethyl-1,4-dihydro-7-methyl-4-oxo-1,8-naphthyridine-3-carboxylic acid;

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

Sm+++ gl alc/w 22°C 0.1M U K1=6.50 B2=12.18 2000TBb (81081) 791  
K3=4.45

Medium: 0.1 M NaClO4 in 70% v/v EtOH/H2O

\*\*\*\*\*

C12H13NO3 HL (1054)  
4-Dimethylamino-benzylidenepyruvic acid; (CH3)2N.C6H4.CH:CH.CO.COOH

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

Sm+++ sp NaClO4 25°C 0.50M U K1=2.313 1987MSa (81204) 792

\*\*\*\*\*

C12H16O7S HL CAS 204931-01-1 (7817)  
2,3-Benzo-1,4,7,10-tetraoxacyclododeca-2-ene-4'-sulfonic acid;

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

Sm+++ dis R4N.X 25°C 0.12M C K1=2.20 1998SUa (81701) 793

Medium: 0.12 M Et4NBr.

Method:solvent extraction into cyclohexane/di(2-ethylhexyl)phosphoric acid

\*\*\*\*\*

C12H17NO4 HL (2695)  
3-Hydroxy-6-(hydroxymethyl)-2-(1-piperidinylmethyl)-4H-pyran-4-one;

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

Sm+++ sp KCl 25°C 0.10M M I 1986POa (81718) 794

B(SmHL)=14.05

\*\*\*\*\*

C12H18N2O5S H2L CAS 80459-15-0 (1595)  
2-Nitroso-5-(N-propyl-3-sulfopropylamino)phenol;

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

Sm+++ gl KNO3 25°C 0.10M C K1=5.86 1988YSa (81819) 795

\*\*\*\*\*

C12H18N2O8 H2L CAS 93031-52-8 (5829)  
1,4-Dioxa-7,10-diazacyclododecane-5,12-dione-7,10-diethanoic acid;

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

Sm+++ gl R4N.X 25°C 0.10M C K1=6.13 1988CCb (81843) 796

\*\*\*\*\*

C12H18N2O8 H4L CAS 76079-31-7 (2587)  
trans-1,2-Diaminocyclohexane-N,N'-di(propanedioic acid)

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

Sm+++ EMF KNO3 25°C 0.10M U K1=13.83 1985SGa (81877) 797

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Sm+++ EMF KNO3 25°C 0.10M U K1=15.63 B2=20.23 1980Sgb (81878) 798

\*\*\*\*\*

C12H20N2O8 H4L CAS 1798-13-6 (4935)

1,2-Diaminobutane-N,N,N',N'-tetraethanoic acid;  
(HOOC.CH2)2N.CH2.CH(C2H5).N(CH2.COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	vlt	KNO3	20°C	0.10M	U		K1=18.25	1968NLa (82033)	799
*****									
C12H20N2O8		H4L					CAS 40623-42-5	(1101)	
1,2-Diaminoethane-N,N'-di(2-pentane-1,5-dioic acid); (CH2NHCH(COOH)CH2CH2COOH)2									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	KNO3	20°C	0.10M	U		K1=8.30	1975DPa (82095)	800
Sm+++	gl	KNO3	25°C	0.10M	U		K1=7.82	1973GBd (82096)	801
Sm+++	gl	KNO3	30°C	0.10M	U		K1=8.22	1972STc (82097)	802
*****									

C12H20N2O8 H4L CAS 61368-60-3 (3389)  
1,2-Diaminoethane-N,N'-diethanoic-N,N'-di-2-propanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	vlt	KNO3	20°C	0.10M	U		K1=16.59	1976NKa (82143)	803
*****									
C12H20N2O8		H4L					CAS 40623-42-5	(3388)	
1,2-Diaminoethane-N,N'-diethanoic-N,N'-dipropanoic acid;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaClO4	25°C	0.10M	U	IH	K1=12.86 B(Sm+HL)=6.16	1988RNa (82177)	804
DH(K1)=1.85 kJ mol <sup>-1</sup> , DH(Sm+HL)=32.4, DS(K1)=252 J K <sup>-1</sup> mol <sup>-1</sup>									

Sm+++	vlt	R4N.X	30°C	0.01M	C		K1=15.20	1981GMh (82178)	805
Method: polarography, using Cd as indicator ion. Medium: 0.01 M Et4NBr.									
*****									
C12H20N2O8		H4L					CAS 2458-58-4	(922)	
1,4-Diaminobutane-N,N,N',N'-tetraethanoic acid; (HOOC.CH2)2N.(CH2)4.N(CH2.COOH)2									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaClO4	25°C	0.50M	M	H	K1=9.52 K(SmL+H)=6.92 K(SmHL+H)=5.52	1985CBa (82234)	806

DH(K1)=27.2 kJ mol<sup>-1</sup>, DS=273 J K<sup>-1</sup> mol<sup>-1</sup> (by calorimetry)

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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
Sm+++	sp	NaClO4	20°C	0.10M	U		K1=18.22	1971ISa (82330)	807
Sm+++	vlt	oth/un	20°C	0.10M	U		K1=18.32	1966DMa (82331)	808
Sm+++	vlt	KNO3	20°C	0.10M	U		K1=18.32	1966NSb (82332)	809
*****									
C12H20N2O8		H4L					CAS 22968-57-6	(3992)	
meso-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
Sm+++	sp	NaClO4	20°C	0.10M	U		K1=16.74	1971ISa (82417)	810
Sm+++	vlt	oth/un	20°C	0.10M	U		K1=16.47	1966DMa (82418)	811
*****									
C12H20N2O8S		H4L		TEDTA			CAS 923-74-0	(3394)	
2,2'-Thiobis(ethyliminodiethanoic acid); S(CH2.CH2.N(CH2.COOH)2)2									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	KNO3	25°C	0.10M	C		K1=14.76	1985TPa (82473)	812
*****									
C12H20N2O9		H4L		EEDTA			CAS 923-73-9	(2112)	
Oxa-bis(ethyleneimino)diethanoic acid; ((HOOC.CH2)2N.CH2.CH2)2O									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	EMF	KNO3	20°C	0.10M	U		K1=18.19	1962MMc (82562)	813
*****									
C12H20O8N2		H4L					(6908)		
2-Methyl-1,2-diaminopropane-N,N,N'N'-tetraethanoic acid; (HOOC.CH2)2N.CH2.C(CH3)2.N(CH2.COOH)2									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	vlt	KNO3	20°C	0.10M	C		K1=17.04	1978NLa (82680)	814
*****									
C12H21NO6		H3L					(7209)		
1-Carboxy-1-aminoheptane-N,N-diethanoic acid; HOOC.CH(C6H13)N(CH2.COOH)2									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	alc/w	20°C	40%	U		K1=10.93	1985LBc (82704)	815
Medium: 40% v/v MeOH/H2O, 0.1 M KNO3									
*****									
C12H24N4O4		H2L					(7343)		

1,4,7,10-Tetraazacyclododecane-1,7-bis(ethanoic acid);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	R4N.X	25°C	0.10M	C		K1=12.93	1998CCb (83092)	816
*****									
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
Sm+++	dis	R4N.X	25°C	0.12M	C		K1=0.79	1998SUa (83617)	817
Medium: 0.12 M Et4NBr.									
Method:solvent extraction into cyclohexane/di(2-ethylhexyl)phosphoric acid									

Sm+++	dis	non-aq	25°C	100%	U			1993INa (83618)	818
							B(SmPL)=6.57		
							B(SmPL2)=8.68		

K is the equilibrium constant for extraction of the metal picrate (P) into CH2Cl2. For extraction from D2O, B=7.03 and 9.17.

Sm+++	cal	alc/w	25°C	100%	U	H	K1=2.03	1993LLa (83619)	819
Medium: MeOH. DH(K1)=15.4 kJ mol <sup>-1</sup> .									

Sm+++	dis	non-aq	25°C	100%	U		B2=8.68	1990NIa (83620)	820
B2=extraction eq.constant: M+3P+2(S)=ML2P3(S); solvent(S)=CH2Cl2, P=picrate									

Sm+++	gl	non-aq	25°C	100%	C		K1=8.23	1989BP a (83621)	821
Medium: anhydrous propylene carbonate, 0.1 M Et4NClO4									

Sm+++	ISE	non-aq	25°C	100%	C		K1=8.10	1983ANb (83622)	822
The equilibration took 7-12 days. Medium: PC, 0.10 M Et4NClO4									

Sm+++	cal	alc/w	25°C	100%	U	H	K1=2.03	1977ILb (83623)	823
Medium: Methanol. DH=15.4 kJ mol <sup>-1</sup> .									

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	ISE	non-aq	25°C	100%	U	H	K1=9.9	1990MGa (83892)	824
In acetonitrile, 0.1 M Et4NClO4. DH=-105 kJ mol <sup>-1</sup> .									
Sm+++	gl	non-aq	25°C	100%	U		K1=<2	1989MGa (83893)	825
Medium: DMF, 0.10 M Et4NClO4									
Sm+++	ISE	non-aq	25°C	100%	C		K1=16.5	1986ALa (83894)	826
Medium: propylene carbonate, 0.1 M Et4NClO4									

Sm+++ gl alc/w 25°C 100% C I K1=7.00 1983ANb (83895) 827  
 The equilibration took 7-12 days. Medium: MeOH, 0.05 M Et4NC104  
 In propylene carbonate, 0.1 M Et4NC104, K1=14.9

\*\*\*\*\*  
 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
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Sm+++	gl	non-aq	25°C	100%	C		K1=5.18	1989BPa (84020)	828
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Medium: anhydrous propylene carbonate, 0.1 M Et4NC104

\*\*\*\*\*  
 C12H28N2O9P2 H4L (7242)  
 1,4,10-Trioxa-7,13-diazacyclopentadecane-7,13-diyl dimethylenediphosphonic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Sm+++	gl	R4N.X	25°C	0.10M	U		K1=14.01 K(Sm+HL)=10.63 K(Sm+H2L)=5.79	1996BJa (84164)	829
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Medium: 0.1 M Me4NC1

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Sm+++	gl	NaNO3	25°C	0.20M	C		K1=8.14	1991KKa (84352)	830
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Sm+++	gl	NaCl	20°C	0.10M	C		K1=10.1	1988SJB (84353)	831
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 C13H502F13S L (6997)  
 1-(2-Thienyl)-3-tridecafluorohexylpropane-1,3-dione; C6F13.CO.CH2.CO.C4H3S

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

Sm+++	gl	alc/w	22°C	80%	U		K1=5.62 B2=10.86 K3=4.57	1995MTa (84461)	832
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Medium: 0.1 M NaClO4 in 80% (v/v) EtOH/H2O.

\*\*\*\*\*  
 C13H8O3 H2L CAS 18931-22-1 (2913)  
 peri-Dihydroxynaphthindenone;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Sm+++	sp	alc/w	25°C	50%	U		K1=9.96	1982HMa (84507)	833
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\*\*\*\*\*  
 C13H9N2O4Cl HL CAS 36016-30-5 (182)  
 N-(4-Chlorophenyl)-3-nitrobenzohydroxamic acid; O2N.C6H4.CO.N(C6H4Cl).OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Sm+++	gl	diox/w	35°C	50%	A			K1=7.72 B2=13.95 K3=5.21	1977AKa (84606)	834

\*\*\*\*\*

C13H9N3OS L (6217)  
Acenaphthenequinone Monothiosemicarbazone; C12H6O:N.NH.CS.NH2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Sm+++	gl	diox/w	25°C	75%	U	TI		K1=8.92 B2=17.19	1986SSd (84625)	835

Medium: 0.1 M NaClO4. 30 C: K1=9.12, K2=8.48; 40 C: K1=8.91, K2=8.21; 50 C: K1=8.48, K2=7.62; I=0.01 M: K1= 9.80, K2=9.17; I=0.05: K1=9.27, K2=8.73

\*\*\*\*\*

C13H11NOS H2L (7306)  
2-(Salicylideneamino)thiophenol, Salicylaldehyde-2-mercaptoanil;  
HO.C6H4.CH:N.C6H4.SH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Sm+++	gl	alc/w	25°C	70%	U			K1=12.10 B2=23.10	1995IFa (85048)	836

Medium: 70% v/v EtOH/H2O, 0.10 M NaCl.

\*\*\*\*\*

C13H11NO2 HL CAS 304-88-1 (181)  
N-Phenylbenzohydroxamic acid; C6H5.CO.N(C6H5).OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Sm+++	dis	oth/un	23°C	0.01M	C				1997AAa (85176)	837

Method: extraction of 153Sm from 0.01 M borate buffer into benzene-ligand solution. K(Sm+3HL(org)=SmL3(org)+3H)=-15.36.

Sm+++	gl	diox/w	35°C	50%	A			K1=11.15 B2=20.80 K3=8.63	1977AKa (85177)	838
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Sm+++	gl	mixed	25°C	75%	U			K1=8.28 B2=14.63 K3=5.15	1969DSb (85178)	839
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Medium: 75% acetone, 0.1 M NaClO4

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C13H11NO4S H2L CAS 124452-52-4 (8496)  
2-[(Phenylimino)methy]phenol 4-sulfonic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Sm+++	gl	NaClO4	25°C	0.10M	U	T HM		K1=4.95 K(Sm(bpy)+L)=4.60 K(Sm(phen)+L)=4.50 K(Sm(his)+L)=3.80	1995SSd (85209)	840

Data for 35 and 45 C. DH and DS values reported.

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C13H11NS HL CAS 42152-36-3 (8401)

2-[(Phenylmethylene)amino]benzenethiol;

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Sm+++ gl alc/w 25°C 70% U K1=8.39 B2=16.52 1995IFa (85233) 841  
Medium: 70% v/v EtOH/H2O, 0.10 M NaCl. Also data for p-Cl, p-NMe2, p-OH,  
p-OCH3, p-CH3, p-NO2 substituted benzaldehyde Schiff bases.

\*\*\*\*\*

C13H11N2O3F3 HL (5563)  
3-(2-Acetylphenylhydrazone)-1,1,1-trifluoropentane-2,4-dione;  
CF3.CO.C(CO.CH3):N.HN.C6H4.COCH3

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Sm+++ gl diox/w 30°C 75% U K1=8.80 B2=16.12 1988ESb (85253) 842  
\*\*\*\*\*

C13H12N2O3S HL (6203)  
Salicylidenesulfanilamide, 4-(N-(2-Hydroxybenzylene))aminosulanilamide;  
H2NSO2C6H4N:CHC6H4OH

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Sm+++ gl oth/un 25°C 0.10M U K1=12.273 1987KSc (85365) 843  
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C13H12N4O L Diphenylcarbaz. CAS 538-62-5 (1195)  
Diphenylcarbazone; C6H5.NH.NH.CO.N:N.C6H5

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Sm+++ EMF alc/w 20°C 50% U K1=3.50 1971MAc (85418) 844  
Medium: 50% EtOH, 0.1 M NaCl04

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C13H12N4S L Dithizone CAS 60-10-6 (1801)  
Diphenylthiocarbazone; C6H5.NH.NH.CS.N:N.C6H5

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Sm+++ EMF alc/w 20°C 50% U K1=1.90 1971MAc (85473) 845  
Medium: 50% EtOH, 0.1 M NaCl04

\*\*\*\*\*

C13H14N2O3 HL (4940)  
3-(2-Acetylphenylhydrazone)pentane-2,4-dione; (CH3.CO)2C:N.NH.C6H4(CO.CH3)

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Sm+++ gl diox/w 30°C 75% U K1=10.85 B2=20.53 1988ESb (85616) 846  
\*\*\*\*\*

C13H15NO6 H3L (4999)  
2-Benzylinitrilotriethanoic acid;

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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Sm+++      oth oth/un 25°C 0.10M U      K1=11.6   B2=20.46  1962HKa (85743) 847
*****
C13H17N3O5      H2L      Tyr-Gly-Gly      CAS 21778-69-8 (863)
Tyrosyl-glycyl-glycine; H2N.CH(CH2.C6H4.OH).CO.NH.CH2.CO.NH.CH2.COOH
-----

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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Sm+++      gl   KNO3   25°C 0.10M U T H      1981SGf (86026) 848
                        K(Sm+HL)=3.60
Data for 35 and 45 C. DH(Sm+HL)=14.3 kJ mol-1, DS(Sm+HL)=118 J K-1 mol-1.
*****
C13H19NO3      H2L      (2031)
2-(1-(2-Hydroxyphenyl)-ethylimine)-3-methylbutanoic acid;
-----

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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Sm+++      gl   NaClO4 25°C 0.10M U TIH      K1=10.75   B2=19.75  1980SSc (86059) 849
*****
C13H20N2O8      H4L      CAS 123064-92-6 (7929)
trans-1,3-Cyclopentanedi-aminotetraethanoic acid;
-----

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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Sm+++      gl   KCl     25°C 1.0M U      K1=12.46      1989CMb (86127) 850
                        K(SmHL+H)=3.92
                        K(SmL+H)=4.60
*****
C13H22N2O8      H4L      CAS 1798-14-7 (921)
(Pentamethylenedinitrilo)tetraethanoic acid; ((HOOC.CH2)2N.CH2.CH2)2CH2
-----

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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Sm+++      gl   KNO3   25°C 0.10M C      K1=10.17      1982PPd (86205) 851
                        K(Sm+HL)=6.66
*****
C13H22N2O8      H4L      CAS 1198-14-7 (5004)
1,2-Diaminopentane-N,N,N',N'-tetraethanoic acid; (HOOCCH2)2NCH2CH(C3H7)N(CH2COOH)2
-----

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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Sm+++      vlt KNO3   20°C 0.10M U      K1=18.25      1974NLa (86235) 852
*****
C13H22N2O8      H4L      (7164)
2,4-Diaminopentane-N,N,N',N'-tetraethanoic acid;
(HOOCCH2)2NCH(CH3)CH2CH(CH3)N(CH2COOH)2
-----

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

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K(Sm(edta)+L)=8.36

B(Sm(edta)L)=21.20

\*\*\*\*\*

C14H9NO3 HL CAS 116-85-8 (1020)

1-Amino-4-hydroxyanthraquinone;

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

Sm+++ sp oth/un 30°C ? U K1=5.35 1972JAa (86798) 861

\*\*\*\*\*

C14H9N5Cl2 L CAS 7071-45-6 (8463)

1,5-Bis(4-chlorophenyl)-3-cyanoformazan;

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

Sm+++ gl diox/w 25°C 70% U K1=5.98 B2=11.91 1996DAb (86853) 862

Medium: 70% dioxane/H2O, 0.10 M NaClO4.

\*\*\*\*\*

C14H11N3O HL CAS 24854-76-0 (1380)

2-(1H-Benzimidazol-2-yl-methylene-amino) phenol;

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

Sm+++ gl diox/w 25°C 50% U K1=7.45 B2=14.36 19820Ca (86997) 863

Medium: 50% dioxan, 0.1 M NaClO4

\*\*\*\*\*

C14H12N2O2Cl HL CAS 32939-57-4 (6242)

N-(4-Tolyl)-4'-chlorobenzohydroxamic acid; Cl.C6H4.CO.N(C6H4.CH3).OH

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

Sm+++ gl diox/w 25°C 50% U T H K1=9.73 B2=17.97 1983AGb (87076) 864

K3=7.38

35 C: K1=9.24 K2=7.75, K3=6.74

\*\*\*\*\*

C14H12N2O2F HL CAS 13664-15-8 (6241)

N-(4-Tolyl)-4'-fluorobenzohydroxamic acid; F.C6H4.CO.N(C6H4.CH3).OH

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

Sm+++ gl diox/w 25°C 50% U T H K1=10.00 B2=18.50 1983AGb (87085) 865

K3=7.50

35 C: K1=9.51 K2=8.01, K3=7.00

\*\*\*\*\*

C14H12N2O4 HL CAS 29556-26-1 (6244)

N-(4-Tolyl)-4'-nitrobenzohydroxamic acid; O2N.C6H4.CO.N(C6H4.CH3).OH

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

Sm+++ gl diox/w 25°C 50% U T H K1=9.41 B2=17.32 1983AGb (87246) 866

K3=6.90

35 C: K1=8.90, K2=7.40, K3=6.40

\*\*\*\*\*

C14H12N2O4 HL CAS 854-7-78-9 (183)

N-2-Tolyl-3-nitrobenzohydroxamic acid; O2N.C6H4.CO.N(C6H4.CH3).OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	diox/w	35°C	50%	A		K1=8.97 B2=16.42 K3=6.44	1977AKa (87254)	867

\*\*\*\*\*

C14H12N2O4 HL (179)

N-3-Tolyl-3-nitrobenzohydroxamic acid; O2N.C6H4.CO.N(C6H4.CH3).OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	diox/w	35°C	50%	A		K1=9.21 B2=16.92 K3=6.70	1977AKa (87266)	868

\*\*\*\*\*

C14H12N2O4 HL CAS 85407-74-5 (180)

N-4-Tolyl-2-nitrobenzohydroxamic acid; O2N.C6H4.CO.N(C6H4.CH3).OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	diox/w	35°C	50%	A		K1=9.46 B2=17.42 K3=6.95	1977AKa (87279)	869

\*\*\*\*\*

C14H12N2O4 HL (221)

N-4-Tolyl-3-nitrobenzohydroxamic acid; O2N.C6H4.CO.N(C6H4.CH3).OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	EMF	diox/w	35°C	50%	U		K1=9.46 B2=17.42 K3=6.95	1977AKa (87292)	870

\*\*\*\*\*

C14H13NO2 HL DPAHA CAS 4463-22-3 (880)

2,2'-Diphenylacetohydroxamic acid; (C6H5)2.CH.CO.NH.OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	alc/w	30°C	50%	U T H		K1=6.97	1981RSb (87408)	871

Medium: 50% v/v EtOH, 0.1 M KNO3. K1=8.08(I=0), 7.32(I=0.05)

\*\*\*\*\*

C14H13NO2 HL CAS 1503-92-0 (1817)

N-(4-Tolyl)benzohydroxamic acid; C6H5.CO.N(C6H4.CH3).OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	diox/w	25°C	50%	U T H		K1=10.20 B2=18.90 K3=7.70	1983AGb (87452)	872

35 C: K1=9.70, K2=8.22, K3=7.25

\*\*\*\*\*

C14H13NO4S H2L (3660)

2-Aminobenzenesulfonic acid 2-hydroxyacetophenone Schiff base;

HSO3.C6H4.N:C(CH3).C6H4.OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaClO4	25°C	0.10M	U T H		K1=5.48 B2= 9.87	1978GKb (87580)	873
Data for 25-35 C and I=0.01-0.10 M. At I=0.0 M, DH(K1)=51.0 kJ mol <sup>-1</sup> , DS(K1)=360 J K <sup>-1</sup> mol <sup>-1</sup> .									

\*\*\*\*\*

C14H14N2O2 HL (6168)

N-(2-Hydroxy-3-methoxybenzylidene)phenylhydrazine; C6H5.NH.N:CH.C6H3(OH)OCH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	diox/w	30°C	75%	U		K1=8.96	1988MKd (87659)	874

\*\*\*\*\*

C14H15N2O3Cl H2L (8285)

5,5'-Dimethylcyclohexane-2-(2'-hydroxy-4'-chlorophenyl)hydrazono-1,3-dione;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	mixed	30°C	0.10M	U T H		K1=11.78 B2=21.86	1988TRb (87725)	875
Medium: 0.1 M KNO3 in 75% v/v isopropanol/water									

\*\*\*\*\*

C14H16N2O2S HL CAS 189231-67-2 (8475)

2-Thiophenylhydrazodimedone;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	diox/w	25°C	75%	C T H		K1=13.40 B2=25.15	1997EIa (87874)	876
Medium: 75% v/v dioxane/H2O, 0.10 M KNO3. Data for 10-40 C. DH(K1)=-7.16 kJ mol <sup>-1</sup> , DS(K1)=-9.54 J K <sup>-1</sup> mol <sup>-1</sup> ; DH(K2)=-6.16, DS(K2)=-8.08.									

\*\*\*\*\*

C14H16N2O3 H2L (8284)

5,5'-Dimethylcyclohexane-2-(2'-hydroxyphenyl)hydrazono-1,3-dione;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	mixed	30°C	0.10M	U T H		K1=12.11 B2=22.48	1988TRb (87892)	877
Medium: 0.1 M KNO3 in 75% v/v isopropanol/water									

\*\*\*\*\*

C14H16N2O8 H4L CAS 40774-59-2 (1901)

1,2-Diaminobenzene-N,N,N',N'-tetraethanoic acid; C6H4(N(CH2.COOH)2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaClO4	25°C	1.00M	C H		K1=13.35	1992YNa (87967)	878

By calorimetry: DH(K1)=13.7 k Jmol<sup>-1</sup>, DS=301 J K<sup>-1</sup> mol<sup>-1</sup>

\*\*\*\*\*

C14H19NO7 HL (6775)  
16-Nitro-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  
-----  
Sm+++ gl R4N.X 25°C 0.10M C K1=3.23 1990CBe (88153) 879

\*\*\*\*\*

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  
-----  
Sm+++ dis non-aq 25°C 100% U B2=8.12 1990NIa (88374) 880  
B2=extraction eq.constant: M+3P+2(S)=ML2P3(S); solvent(S)=CH2Cl2, P=picrate

-----  
Sm+++ ISE R4N.X 25°C 0.10M C K1=2.37 1986XJa (88375) 881  
\*\*\*\*\*

C14H20O8S HL CAS 127461-53-4 (7818)  
2,3-Benzo-1,4,7,10,13-pentaoxacyclopentadeca-2-ene-4'-sulfonic acid;

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Sm+++ dis R4N.X 25°C 0.12M C K1=1.77 1998SUa (88397) 882  
Medium: 0.12 M Et4NBr.

Method:solvent extraction into cyclohexane/di(2-ethylhexyl)phosphoric acid  
\*\*\*\*\*

C14H22N2O8 H4L cis-1,2-CDTA CAS 92761-75-6 (2846)  
cis-1,2-Diaminocyclohexane-N,N,N',N'-tetraethanoic acid;

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Sm+++ gl KCl 25°C 1.0M U K1=4.72 1987CMe (88434) 883  
K(SmHL+H)=4.83  
K(SmL+H)=6.85

\*\*\*\*\*

C14H22N2O8 H4L cis-1,3-CDTA CAS 92681-23-7 (2847)  
cis-1,3-Diaminocyclohexane-N,N,N',N'-tetraethanoic acid;

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Sm+++ gl KCl 25°C 1.0M U K1=7.44 1987CMe (88448) 884  
K(SmHL+H)=5.21  
K(SmL+H)=7.71

\*\*\*\*\*

C14H22N2O8 H4L cis-1,4-CDTA CAS 92681-25-9 (2848)  
cis-1,4-Diaminocyclohexane-N,N,N',N'-tetraethanoic acid;

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





Sm+++ gl KCl 25°C 1.00M U K1=8.56 1984MFb (88868) 895  
 \*\*\*\*\*

C14H22N2O9 H2L CAS 93031-53-9 (5830)  
 1,4,7-Trioxa-10,13-diazacyclopentadecane-8,15-dione-10,13-diethanoic acid;

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

Sm+++ gl R4N.X 25°C 0.10M C K1=8.58 1988CCb (88886) 896  
 \*\*\*\*\*

C14H23N3O10 H5L DTPA CAS 67-43-6 (238)  
 Diethylenetriamine-pentaethanoic acid; H00C.CH2.N(CH2.CH2.N(CH2.COOH)2)2

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

Sm+++ cal KNO3 25°C 0.10M C T 1988MIa (89379) 897  
 DH(K1)=-32.9 kJ mol-1, DS=317.2 J mol-1 K-1. Also data for 283 and 313 K

Sm+++ cal NaClO4 25°C 0.10M C H 1987YJa (89380) 898  
 DH(K1)=-27.3 kJ mol-1, DS(K1)=336 J K-1 mol-1.

-----  
 Sm+++ gl NaClO4 25°C 0.10M M K1=20.99 1987ZGa (89381) 899  
 -----

Sm+++ gl NaClO4 25°C 0.10M M K1=21.51 1987ZGa (89382) 900  
 -----

Sm+++ cal NaClO4 25°C 0.50M U H 1977CGc (89383) 901  
 DH(K1)=-44.2 kJ mol-1

-----  
 Sm+++ gl NaClO4 25°C 0.50M U K1=20.72 1977GGb (89384) 902  
 -----

Sm+++ gl KNO3 30°C 0.10M U K1=22.80 1976GAa (89385) 903  
 -----

Sm+++ cal KNO3 27°C 0.10M U H 1968CLd (89386) 904  
 DH(K1)=-33.0 kJ mol-1, DS=316 J K-1 mol-1

-----  
 Sm+++ sp oth/un 19°C 0.10M U K1=22.36 1963GAd (89387) 905  
 K(Sm+HL)=13.35  
 B(Sm2L)=25.47

-----  
 Sm+++ EMF KNO3 25°C 0.10M U H K1=22.34 1962MTc (89388) 906  
 DH(K1)=-34.3 kJ mol-1, DS=313 J K-1 mol-1

-----  
 Sm+++ gl oth/un 25°C 0.10M U K1=22.84 1959HCa (89389) 907  
 \*\*\*\*\*

C14H24N2O8 H4L (5075)  
 1,2-Diaminoethane-N,N'-diethanoic-N,N'-di-2-butyric acid;

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

Sm+++ vlt KNO3 20°C 0.10M U K1=16.0 1969NDc (89518) 908  
 \*\*\*\*\*

C14H24N2O8 H4L (7165)  
 1,2-Diaminohexane-N,N,N',N'-tetraethanoic acid; (HOOCCH2)NCH2CH(C4H9)N(CH2COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	vlt	KNO3	20°C	0.10M	U		K1=18.24	1974NLa (89538)	909

\*\*\*\*\*

C14H24N2O8 H4L HMDTA CAS 1633-00-7 (920)  
 1,6-Diaminohexane-N,N,N',N'-tetraethanoic acid; ((HOOC.CH2)2N.CH2.CH2.CH2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	KCl	25°C	1.00M	U	M		1976BKa (89603)	910

K(SmEDTA+L)=3.8  
 K(SmEDTA+HL)=3.8  
 K(2SmEDTA+L)=7.8

Sm+++	gl	KCl	25°C	0.10M	U			1974KPd (89604)	911
-------	----	-----	------	-------	---	--	--	-----------------	-----

K(Sm+HL)=6.64

Sm+++	sp	oth/un	19°C	0.10M	U	M		1966GAb (89605)	912
-------	----	--------	------	-------	---	---	--	-----------------	-----

K(Sm+H3L)=1.52  
 K(2Sm+HL+H2L)=11.32  
 K(Sm2H3L2+HL)=4.61  
 K(Sm2H3L2+2A)=2.00

K(Sm2H3L2A3+HL)=4.06, K(Sm2H2L2A3+HL)=7.15, K(Sm2H3L2+3A)=2.78; HA=ethanoic acid

\*\*\*\*\*

C14H24N2O8 H4L CAS 1633-00-7 (5076)  
 4-Methyl-1,2-diaminopentane-N,N,N',N'-tetraethanoic acid;  
 (HOOCCH2)2NCH2CH(N(CH2COOH)2CH2CH(CH3)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	vlt	KNO3	20°C	0.10M	U		K1=18.20	1968NLb (89641)	913

\*\*\*\*\*

C14H24N2O8 H2L CAS 17619-53-3 (5833)  
 Diaminoethane-N,N'-Di(ethylaceto)-N,N'-diethanoic acid;  
 (-CH2.N(CH2.CO0H)CH2.CO0C2H5)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	R4N.X	25°C	0.10M	C		K1=10.36	1988CCb (89657)	914

\*\*\*\*\*

C14H24N2O8 H4L EDTP (2936)  
 Diaminoethane-N,N,N',N'-tetrapropanoic acid; (HOOC.CH2CH2)2N.CH2CH2.N(CH2CH2.CO0H)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaCl04	25°C	0.10M	U			1995HAa (89690)	915

K(Sm+HL)=4.79  
 K(Sm+H2L)=4.19  
 K(Sm+H3L)=3.11  
 B(SmHL)=14.22

B(SmH2L)=19.74, B(SmH3L)=22.83

\*\*\*\*\*

C14H24N2O9 H4L BPETA CAS 87720-52-3 (5077)  
 Bis-(3-di(carboxymethyl)aminopropyl)ether;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	KN03	25°C	0.10M	U		K1=11.87 K(Sm+HL)=7.20	1984TPa (89736)	916

\*\*\*\*\*

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaNO3	25°C	0.0	U		K1=16.75	1996KDb (89927)	917
Extrapolated from data for I=0.05-0.15 M NaNO3.									
Sm+++	gl	NaNO3	25°C	0.10M	U	I	K1=16.54	1996KDc (89928)	918
Data for 0.05 and 0.15 M NaNO3. At I=0, K1=16.74.									
Sm+++	gl	NaNO3	25°C	0.10M	M		K1=16.54	1996KDD (89929)	919
Data for 0.05-0.15 M NaNO3. At I=0, K1=16.74.									
Sm+++	gl	NaNO3	25°C	0.10M	M	I	K1=16.54	1995KDb (89930)	920
Data for 0.05 and 0.15 M NaNO3. At I=0, K1=16.74.									
Sm+++	gl	NaNO3	25°C	0.10M	M	I	K1=16.54	1995KDc (89931)	921
Data for 0.05 and 0.15 M NaNO3. At I=0, K1=16.74.									
Sm+++	gl	NaNO3	25°C	0.10M	M	I	K1=16.546	1995KDD (89932)	922
Data for 0.15 and 0.05 M NaNO3. At I=0, K1=16.745.									
Sm+++	gl	NaNO3	25°C	0.0	U	HM	K1=16.45 K(SmL+ala)=3.58 K(SmL+phe)=3.07	1991ADb (89933)	923
Extrapolated from data for 0.01-0.1 M NaNO3. Data for 35 and 45 C. At 35 C DH(SmL+ala)=-26.2 kJ mol <sup>-1</sup> , DS=-19.8; DH(SmL+phe)=-31.5, DS=-47.2.									
Sm+++	gl	KCl	25°C	1.0M	U	M	K2=1.52 K(SmL+ida)=1.5	1985KBb (89934)	924

Sm+++	EMF	KN03	20°C	0.10M	U		K1=16.88	1962MMc (89935)	925
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C14H24O9 H3L CAS 64020-01-5 (8224)  
 1,1,1-Tris[(2-carboxyethoxy)methyl]ethane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	R4N.X	25°C	0.10M	C		K1=3.82 K(SmL+H)=4.08	2001VSa (90053)	926
Medium: 0.10 M Me4NCl. Also data for N-ethyl-, N-CH2OH-, N-CH2O(CH2)2COOH-derivatives.									
*****									
C14H25N3O8		H4L	DEATA				CAS 97315-55-4	(5601)	
N,N-Bis(2-aminoethyl)ethylamine-N',N',N'',N''-tetraethanoic acid;									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	KNO3	25°C	0.10M	C		K1=17.79	1985TPa (90106)	927
*****									
C14H25N3O9		H4L					CAS 4454-15-3	(5078)	
((N-(2-Hydroxyethyl)-2,2'-iminodiethylene)dinitrilo)tetraethanoic acid;									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	vlt	KCl	?	0.10M	U		K1=13.45	1968VLa (90119)	928
*****									
C14H26N2O7		H2L					(1567)		
1,4,10-Trioxa-7,13-diazacyclopentadecane-N,N'-diethanoic acid;									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	R4N.X	25°C	0.10M	M		K1=11.72	1986COb (90205)	929
*****									
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
Sm+++	ISE	non-aq	25°C	100%	U	H	K1=9.8	1990MGa (90438)	930
In acetonitrile, 0.1 M Et4NClO4. DH=-50 kJ mol-1.									
Sm+++	ISE	non-aq	25°C	100%	C		K1=4.06	1989MGa (90439)	931
Medium: DMD, 0.10 M Et4NClO4									
Sm+++	ISE	non-aq	25°C	100%	C		K1=15.3	1986ALa (90440)	932
Medium: propylene carbonate, 0.1 M Et4NClO4									
Sm+++	gl	R4N.X	25°C	0.25M	C		K1=6.8	1981BBE (90441)	933
Medium: Me4NCl									
*****									
C14H28N2O6		HL					CAS 82353-42-2	(5850)	
1,4,10,13-Tetraoxa-7,16-diazacyclooctadecane-7-ethanoic acid;									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo

```

-----
Sm+++      gl  R4N.X  25°C 0.10M C          K1=7.51          1988CCc (90487) 934
*****
C14H28O7          L      21-Crown-7          CAS 33089-36-0 (2264)
1,4,7,10,13,16,19-Heptaoxacycloheneicosane;
-----

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```

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

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```

Sm+++      gl  non-aq 25°C 100% C          K1=7.46          1989BPa (90539) 935
Medium: anhydrous propylene carbonate, 0.1 M Et4NClO4
*****
C14H30O7          L          CAS 1072-40-8 (2499)
2,5,8,11,14,17,20-Heptaoheneicosane; CH3.0.(CH2.CH2.0)6.CH3
-----

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```

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

```

```

Sm+++      gl  non-aq 25°C 100% C          K1=6.84          1989BPa (90710) 936
Medium: anhydrous propylene carbonate, 0.1 M Et4NClO4
*****
C14H32N2O10P2      H4L          CAS 81963-60-2 (7240)
1,4,10,13-Tetraoxa-7,16-diazacyclooctadecane-7,16-diylldimethylenediphosphonic acid;
-----

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```

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

```

```

Sm+++      gl  R4N.X  25°C 0.10M U          K1=13.43          1996BJa (90772) 937
                                   K(Sm+HL)=11.08
                                   K(Sm+H2L)=5.92
Medium: 0.1 M Me4NCl
-----

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```

C14H37O12O12P4      H8L          (6910)
N'-Hexyl-diethylenetriamine-N,N,N",N"-tetra(methylenephosphonic acid);
-----

```

```

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

```

```

Sm+++      gl  NaClO4 25°C 0.10M M          K(Sm+HL)=6.99          1987ZGa (90934) 938
-----

```

```

Sm+++      gl  oth/un 25°C 0.10M U          K(Sm+HL)=6.99          1984ZGa (90935) 939
                                   K(Sm+H2L)=5.22
-----

```

```

C15H11NO4          HL          CAS 1776-18-7 (955)
3-Phenyl-1-(2'-hydroxy-5'-nitrophenyl)-2-propen-1-one;
-----

```

```

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

```

```

Sm+++      gl  alc/w  35°C 70% U          K1=6.33  B2=12.57  1982SLb (91082) 940
*****
C15H11N3O          HL      PAN          CAS 85-85-8 (572)
1-(2-Pyridylazo)-2-naphthol; C5H4N.N:N.C10H6.OH
-----

```

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	sp	alc/w	21°C	50%	U		K1=10.02	1988CMd (91238)	941
Sm+++	sp	alc/w	21°C	50%	U	I	K1=9.52	1981MCb (91239)	942
Medium: 50% MeOH, 0.1 M NaClO4. In 75% MeOH K1=10.92									
*****									
C15H11N3O2		L					CAS 74378-23-7	(2745)	
Phenanthrenequinone monosemicarbazone; C14H8(:O)(:N.NH.CO.NH2)									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	diox/w	25°C	75%	C	TIH	K1=6.83 B2=13.04	1989SVa (91310)	943
DH(K1)=-51.87 kJ mol-1									
*****									
C15H11O2Br		HL					CAS 1218-20-0	(954)	
3-Phenyl-1-(2'-hydroxy-5'-bromophenyl)-2-propen-1-one;									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	alc/w	35°C	70%	U		K1=7.06	1982SLb (91374)	944
*****									
C15H11O2Cl		HL					CAS 1218-24-2	(953)	
3-Phenyl-1-(2'-hydroxy-5'-chlorophenyl)-2-propen-1-one;									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	alc/w	35°C	70%	U		K1=6.86 B2=13.45	1982SLb (91398)	945
Sm+++	gl	alc/w	35°C	70%	U		K1=6.86 B2=13.45	1980SLb (91399)	946
*****									
C15H12OS		HL					(1261)		
mono-Thiodibenzoylmethane; C6H5.CO.CH2.CS.C6H5									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaClO4	30°C	0.05M	U		K1=8.48 B2=16.30	1979VMa (91502)	947
K3=7.00									
*****									
C15H12O2		HL					CAS 1214-47-7	(951)	
3-Phenyl-1-(2'-hydroxyphenyl)-2-propen-1-one, 2'-hydroxychalkone;									
C6H5.CH:CH.CO.C6H4.OH									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	alc/w	35°C	70%	U		K1=7.65 B2=15.03	1982SLb (91591)	948
Medium: 70% EtOH, 0.1 M KNO3									
Sm+++	gl	alc/w	35°C	70%	U		K1=7.65 B2=15.03	1980SLb (91592)	949

\*\*\*\*\*  
 C15H12O3                      H2L                      CAS 1469-94-9 (3445)  
 2-Hydroxydibenzoylmethane; HO.C6H4.CO.CH2.CO.C6H5  
 -----

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	diox/w	30°C	70%	U			1996SNa (91609)	950
							K(Sm+HL)=10.52 K(SmHL+HL)=9.25		

Medium: 70% v/v dioxane/H2O, 1.0 M NaClO4.

\*\*\*\*\*  
 C15H13NO2                      HL                      CAS 959-66-0 (245)  
 Benzoyl-acetanilide; C6H5.CO.CH2.CO.NH.C6H5  
 -----

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	alc/w	30°C	70%	M		K1=5.35	1978SAb (91635)	951

\*\*\*\*\*

C15H13NO2                      HL                      CAS 7369-44-0 (4066)  
 N-3-Diphenylpropenohydroxamic acid;  
 -----

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	dis	oth/un	RT	0.05M	C			1993ATa (91642)	952

Method: extraction from 0.05 M triethanolamine buffer into chloroform.

Analysis by spectrophotometry. K(Sm+3HL(org)=SmL3(org)+3H)=-17.99

\*\*\*\*\*

C15H14NOCl                      HL                      CAS 268214-29-5 (8398)  
 4-Chloro-3,5-dimethyl-2-[(phenylimino)methyl]phenol;  
 -----

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	diox/w	30°C	75%	M		K1=7.45	2000ANa (91695)	953

Medium: 75% v/v dioxan/H2O, 0.10 M NaClO4. Data for an extensive series of 4'-substituted phenylimino derivatives.

\*\*\*\*\*

C15H15NO2                      HL                      (1167)  
 N-(4-Tolyl)-4'-tolylhydroxamic acid; CH3.C6H4.CO.N(C6H4.CH3)OH  
 -----

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	diox/w	25°C	50%	U T H		K1=10.45 B2=19.41 K3=7.95	1983AGb (91847)	954

35 C: K1=9.96, K2=8.45, K3=7.46

\*\*\*\*\*

C15H15NO3                      HL                      (6240)  
 N-4-Tolyl-4'-methoxybenzohydroxamic acid; CH3O.C6H4.CO.N(C6H4.CH3).OH  
 -----

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

Sm+++ gl diox/w 25°C 50% U T H K1=10.75 B2=20.01 1983AGb (91869) 955  
K3=8.26

35 C: K1=10.10, K2=8.60, K3=7.63

\*\*\*\*\*

C15H18N2O3 HL CAS 116822-13-0 (6743)  
5,5-Dimethylcyclohexane-2-(2-hydroxy-4'-methylphenyl)-hydrazono-1,3-dione;

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

Sm+++ gl alc/w 20°C 75% U T H K1=10.50 B2=18.50 1993RAa (92036) 956  
Medium: 75% v/v MeOH/H2O; 0.10 M KNO3. Data also for 4-Cl and 4-Me analogues

-----  
Sm+++ gl mixed 30°C 0.10M U T H K1=12.28 B2=23.22 1988TRb (92037) 957  
Medium: 0.1 M KNO3 in 75% v/v isopropanol/water

\*\*\*\*\*

C15H20N2O6 H3L BEDTA CAS 65311-06-0 (2944)  
N-Benzylldiaminoethane-N,N',N'-triethanoic acid;

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

Sm+++ gl KNO3 25°C 0.10M C K1=12.19 1978MPb (92157) 958

\*\*\*\*\*

C15H23N3O2 L CAS 36763-33-4 (5176)  
N,N,N',N'-Tetraethyl-2,6-pyridinedicarboxamide;

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

Sm+++ sp non-aq 25°C 100% M K1=7.3 B2=14.40 1997RPb (92289) 959  
B3=22.0

Medium: acetonitrile.

\*\*\*\*\*

C15H25N3O10 H5L (5127)  
Diethylenetriamine-N,N,N'',N''-tetraethanoic acid-N'-propanoic acid;

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

Sm+++ EMF KCl ? 0.10M U K1=16.16 1966VL a (92382) 960

-----  
Sm+++ vlt oth/un ? ? U K1=18.4 1966VL a (92383) 961

\*\*\*\*\*

C15H25N3O10 H5L (6100)  
Diethylenetriamine-N,N,N',N''-tetraethanoic acid-N''-propanoic acid;

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

Sm+++ gl KNO3 25°C 0.10M C K1=19.58 1989SPa (92399) 962  
K(Sm+HL)=13.40

\*\*\*\*\*

C15H26N4O9 H4L (7685)  
Diethylenetriamine-N,N,N',N'',N''-pentaethanoic acid N'-methanamide;



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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Sm+++      gl  KCl      25°C 0.10M C      K1=19.48      2000SBb (92437) 963
*****
C15H26N4O9      H4L      CAS 137076-43-8 (5085)
Diethylenetriamine-N,N,N',N'',N''-pentaethanoic acid N-methylamide;
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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Sm+++      gl  KCl      25°C 0.10M C      K1=18.62      2000SBb (92452) 964
*****
C15H33NO6      L      CAS 70384-51-9 (838)
Tris(3,6-dioxaheptyl)amine; (CH3.CH2.O.CH2.CH2.O.CH2.)3N
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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Sm+++      ISE non-aq 25°C 100% C      K1=9.5      B2=17.6      1986ALa (92569) 965
Medium: propylene carbonate, 0.1 M Et4NClO4
*****
C16H9N2OBr3      HL      CAS 84317-74-8 (5169)
1-(2,4,6-Tribromophenylazo)-2-hydroxynaphthalene;
-----

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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Sm+++      kin oth/un 25°C 0.02M U      K1=4.87      1972GSe (92663) 966
*****
C16H11N5O4      H2L      (5153)
1,5-Bis(2-carboxyphenyl)-3-cyanoformazan;
-----

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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Sm+++      gl  diox/w 25°C 70% U I      K1=9.15      B2=17.93      1996DAb (92899) 967
Medium: 70% dioxane/H2O, 0.10 M NaClO4. In 50% EtOH/H2O, 0.10 M NaClO4,
K1=10.74, K2=8.99.
*****
C16H12N2O4S      H2L      CAS 13964-82-4 (3475)
1-(4-Sulfophenylazo)-2-hydroxynaphthalene;
-----

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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Sm+++      sp  oth/un 25°C dil U      B2=7.34      1969SPd (93004) 968
*****
C16H12N2O11S3      H5L      CAS 548-81-2 (5180)
2-(4'-Sulfophenylazo)chromotropic acid,
2-(4-sulfophenylazo)-1,8-dihydroxyaphthalene-3,6-diHSO3
-----

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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Sm+++      gl  oth/un 25°C 0.10M U      K1=7.39      B2=11.78      1985AAa (93100) 969

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Data also for 12 other 4-substituted phenyl analogues

\*\*\*\*\*

C16H12N3O4ClS H2L CAS 133131-00-7 (8468)

7-Amino-8-[(4-chlorophenyl)azo]-4-hydroxy-2-naphthalenesulfonic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaCl	25°C	0.10M	U		K1=10.52 B2=18.50 B3=25.23	1997IHa (93119)	970

Also data for the 4'-bromo-, 4'-fluoro-, 4'-nitro-, 4'-methoxy-, 4'-di-methylamino-, 4'-hydroxy-, 4'-carboxy-, 4'-AsO(OH)2-, 2'-hydroxy- analogue

\*\*\*\*\*

C16H12N5O3 L CAS 77251-11-7 (5928)

1-Phenyl-3-methyl-4(2'-nitrophenylhydrazo)-5-pyrazolone;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	diox/w	30°C	75%	M		K1=7.40	1987ESa (93135)	971

\*\*\*\*\*

C16H13N2O10AsS2 H5L Thorin I CAS 3688-92-4 (2609)

1-((2-Arsonophenyl)azo)-2-hydroxy-3,6-naphthalylldisulfonic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaCl04	30°C	0.10M	U		K(Sm+H2L=SmH2L)=5.51 K(SmHL+H)=7.44 K(SmL+H)=10.20	1976NDa (93208)	972

\*\*\*\*\*

C16H13N2O11AsS2 H6L Arsenazo I CAS 520-10-5 (277)

2-(2'-Arsonophenylazo)chromotropic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	sp	oth/un	20°C	0.10M	U		K(Sm+H2L)=8.39	1971SSd (93265)	973

\*\*\*\*\*

C16H14O2 HL CAS 1775-98-0 (952)

3-Phenyl-1-(2'-hydroxy-5'-methylphenyl)-2-propen-1-one;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	alc/w	35°C	70%	U		K1=7.90 B2=15.45	1982SLb (93534)	974

Medium: 70% EtOH, 0.1 M KNO3

\*\*\*\*\*

C16H14O3 H2L CAS 29976-82-7 (8522)

1-(2-Hydroxy-5-methylphenyl)-3-phenyl-1,3-propanedione;

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

Sm+++ gl diox/w 30°C 70% U 1996SNa (93541) 975

K(Sm+HL)10.35

K(SmHL+HL)=9.60

Medium: 70% v/v dioxane/H2O, 1.0 M NaClO4.

\*\*\*\*\*

C16H14O3 HL CAS 3327-24-0 (956)

3-(4''-Methoxyphenyl)-1-(2'-hydroxyphenyl)-2-propen-1-one;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Sm+++	gl	alc/w	35°C	70%	U			K1=7.50 B2=14.61	1982SLb (93576)	976

Sm+++	gl	alc/w	35°C	70%	U			K1=7.50 B2=14.61	1980SLb (93577)	977
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C16H14O4 HL BHMA (5929)

omega-Benzoyl-2-hydroxy-4-methoxy-3-methylacetophenone;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Sm+++	gl	alc/w	30°C	25%	M			K1=6.43 B2=12.44	1987DGb (93585)	978

Medium: 25% v/v EtOH/H2O

\*\*\*\*\*

C16H15N5 L CAS 7014-14-4 (8462)

1,5-Bis(4-methylphenyl)-3-cyanoformazan;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Sm+++	gl	diox/w	25°C	70%	U			K1=8.30 B2=16.10	1996DAb (93643)	979

Medium: 70% dioxane/H2O, 0.10 M NaClO4.

\*\*\*\*\*

C16H18N2O3 HL (5564)

2-(2-Acetylphenylhydrazon)-5,5-dimethyl-1,3-cyclohexanedione;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Sm+++	gl	diox/w	30°C	75%	U			K1=10.73 B2=19.50	1988ESb (93786)	980

\*\*\*\*\*

C16H18N4 L CAS 172665-46-2 (7699)

N,N'-Dimethyl-1,10-phenanthroline-2,9-dimethanamine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Sm+++	gl	NaClO4	25°C	0.10M	U			K1=7.39 B(SmHL)=14.51	2001WZa (93847)	981

Also data for the N,N'-diethyl, isopropyl, butyl and isobutyl derivatives.

\*\*\*\*\*

C16H18N4O4 H2L CAS 161563-39-9 (8399)

1,3-Phenylenediamine bisazoacetylacetone;

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

-----  
 Sm+++ gl diox/w 25°C 50% U K1=10.83 B2=20.95 1997MAb (93863) 982  
 Medium: 50% v/v dioxan/H2O, 0.10 M NaClO4. For the 1,4-phenylenediamine  
 derivative, K1=12.30, K2=10.96.

\*\*\*\*\*

C16H18N4O4 H2L CAS 161563-40-2 (8400)  
 1,3-Phenylenediamine bisazobenzoylacetone;

-----  

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

 -----

Sm+++ gl diox/w 25°C 50% U K1=8.50 B2=16.16 1997MAb (93870) 983  
 Medium: 50% v/v dioxan/H2O, 0.10 M NaClO4. For the 1,4-phenylenediamine  
 derivative, K1=9.82, K2=9.16.

\*\*\*\*\*

C16H20N2O8 H4L CAS 6411-02-5 (1919)  
 1-Phenyl-ethylenediamine-N,N,N',N'-tetraethanoic acid (DL)

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

 -----

Sm+++ vlt KNO3 20°C 0.10M U K1=17.09 1969NDb (94049) 984

\*\*\*\*\*

C16H22O6 L (6733)  
 4'-Acetyl-2,3-benzo-1,4,7,10,13-pentaoxacyclopentadeca-2-ene;

-----  

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

 -----

Sm+++ dis non-aq 25°C 100% U 1993INa (94253) 985  
 $B(Sm+3P+2L)=7.77$

By solvent extraction into dichloromethane. B is the extraction constant  
 $Sm(aq)+picrate(aq)+L(org)=SmL2P3(org)$ .

\*\*\*\*\*

C16H23NO8 L CAS 53408-96-1 (1765)  
 2,3-(4'-Nitrobenzo)-1,4,7,10,13,16-hexaoxacyclooctadeca-2-ene;  
 4'-Nitrobenzo-18-crown-6

-----  

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

Sm+++ ISE R4N.X 25°C 0.10M C K1=2.81 1986XJa (94274) 986

\*\*\*\*\*

C16H23N5O4 L (6969)  
 12-(4-Nitrobenzyl)-1,4,7,10-tetraazacyclotridecane-11,13-dione;

-----  

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

 -----

Sm+++ gl NaClO4 30°C 0.10M M 1994LZa (94301) 987  
 $B(SmH-2L)=-11.04$

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C16H24O9S HL SB18C6 CAS 185099-14-3 (7819)  
 2,3-Benzo-1,4,10,13,16-hexaoxacyclooctadeca-2-ene-4'-sulfonic acid;

-----

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	dis	R4N.X	25°C	0.12M	C		K1=1.70	1998SUa (94482)	988
Medium: 0.12 M Et4NBr. Method:solvent extraction into cyclohexane/di(2-ethylhexyl)phosphoric acid *****									
C16H26N2O10		H2L					CAS 93031-54-0	(5831)	
1,4,7,10-Tetraoxa-13,16-diazacyclooctadecane-11,18-dione-13,16-diethanoic acid;									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	R4N.X	25°C	0.10M	C		K1=9.37	1988CCb (94576)	989
*****									
C16H27N5O8		H3L					(6621)		
1,4,7-Tris(carboxymethyl)-1,4,7,10,13-pentaazacyclopentadecan-9,14-dione;									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	sp	KCl	25°C	0.08M	U		K1=11.4	1994FCa (94676)	990
*****									
C16H27N5O8		H3L					(6915)		
4,10,13-Tris(carboxymethyl)-1,4,7,10,13-pentaazacyclopentadeca-8,15-dione;									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	sp	KCl	25°C	0.08M	U		K1=15.5	1994FCa (94690)	991
*****									
C16H28N2O8		H4L					(5167)		
1,2-Diaminoethane-N,N'-diethanoic-N,N'-di-2-(3-methyl)butanoic acid;									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	KNO3	20°C	0.10M	U		K1=12.87	1969NDc (94720)	992
*****									
C16H28N2O8		H4L					(5168)		
1,2-Diaminoethane-N,N'-diethanoic-N,N'-di-2-pentanoic acid;									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	vlt	KNO3	20°C	0.10M	U		K1=16.07	1969NDc (94746)	993
*****									
C16H28N2O8		H4L					(5138)		
1,2-Diaminooctane-N,N,N',N'-tetraethanoic acid;									
(HOOCCH2)2N.CH2.CH(C6H13)N(CH2COOH)2									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	vlt	KNO3	20°C	0.10M	U		K1=18.17	1979MBd (94772)	994
*****									
C16H28N4O8		H4L			DOTA		CAS 60239-18-1	(1017)	

1,4,7,10-Tetraazacyclododecane-1,4,7,10-tetraethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Sm+++	gl	NaCl	37°C	1.0M	C		K1=23.3	1994TBb (94926)	995
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Method: Competitive reaction with Eu3+ ion.

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C16H29N5O8                      H3L                      (6505)  
Diethylenetriaminepentaethanoic acid N,N'-bismethylamide;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Sm+++	gl	NaClO4	25°C	0.10M	C	H	K1=16.69	1993RCa (95001)	996
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DH(K1)=-25.1 kJ mol-1, DS(K1)=235 J K-1 mol-1

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C16H30N2O8                      H2L                      CAS 72912-01-7 (1568)  
1,4,10,13-Tetraoxa-7,16-diazacyclooctadecane-N,N'-diethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Sm+++	gl	R4N.X	25°C	0.10M	U		K1=12.12	1983CRb (95054)	997
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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
-------	-----	--------	------	------	-----	-------	-------------	-----------	--------

Sm+++	ISE	non-aq	25°C	100%	U		K1=11.6	1990MGa (95285)	998
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In acetonitrile, 0.1 M Et4NClO4.

Sm+++	ISE	non-aq	25°C	100%	C		K1=2.9	1989MGa (95286)	999
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Medium: DMF, 0.10 M Et4NClO4

Sm+++	gl	R4N.X	25°C	0.25M	C		K1=6.76	1981BBE (95287)	1000
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Medium: Me4NCl

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

Sm+++	cal	non-aq	25°C	100%	U	H	K1=3.01	1993LLa (95394)	1001
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Medium: MeCN. DH(K1)=-31.5 kJ mol-1.

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C16H41N3O12P4                      H8L                      (6911)  
N'-Octyl-diethylenetriamine-N,N,N'',N''-tetra(methylenephosphonic acid);

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

Sm+++	gl	NaClO4	25°C	0.10M	M			1987ZGa (95669)	1002
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K(Sm+HL)=6.98

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Sm+++ gl oth/un 25°C 0.10M U 1984ZGa (95670)1003

K(Sm+HL)=6.98

K(Sm+H2L)=5.21

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C17H12N03Cl HL (6197)

8-Formyl-7-hydroxy-4-methyl-2H-[1]-benzopyran-2-one-4-chloroanil;

Cl.C6H4.N:CH.C9H3O(OH)(CH3)(:O)

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

-----  
Sm+++ gl diox/w 30°C 70% U K1=5.28 B2=9.43 1987ECa (95694)1004

B3=12.63

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C17H12N2O5 HL (6198)

8-Formyl-7-hydroxy-4-methyl-2H-[1]-benzopyran-2-one-4-nitroanil;

NO2.C6H4.N:CH.C9H3O(OH)(CH3)(:O)

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

-----  
Sm+++ gl diox/w 30°C 70% U K1=5.16 B2=9.18 1987ECa (95711)1005

B3=12.32

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C17H13N03 HL CAS 98399-88-3 (6195)

8-Formyl-7-hydroxy-4-methyl-2H-[1]-benzopyran-2-one-anil;

C6H5.N:CH.C9H3O(CH3)(OH)(:O)

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

-----  
Sm+++ gl diox/w 30°C 70% U K1=5.76 B2=10.52 1987ECa (95741)1006

B3=14.35

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C17H13N4O3 HL (5927)

1-Phenyl-3-methyl-4-(2'-carboxyphenylhydrazo)-5-pyrazolone;

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

-----  
Sm+++ gl diox/w 30°C 75% M K1=15.85 B2=28.81 1987ESa (95772)1007

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C17H14N2O2 L CAS 4551-69-3 (698)

4-Benzoyl-3-methyl-1-phenyl-2-pyrazolin-5-one;

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

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Sm+++ gl NaNO3 20°C 0.10M U M 1981GCa (95899)1008

B(Sm+3L+3TBP)=25.30

B(Sm+3L+4TBPOxide)=31.8

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C17H15N4O2 L CAS 97671-53-9 (5926)

1-Phenyl-3-methyl-4-(2'-methoxyphenylhydrazo)-5-pyrazolone;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Sm+++	gl	diox/w	30°C	75%	M			K1=8.97 B2=17.18	1987ESa (96013)	1009
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C17H16O4		H2L						CAS 29976-84-9	(8523)	
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1-(2-Hydroxy-5-methylphenyl)-3-(4-methoxyphenyl)-1,3-propanedione;

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

Sm+++	gl	diox/w	30°C	70%	U				1996SNa (96128)	1010
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K(Sm+HL)=8.50

K(SmHL+HL)=7.30

Medium: 70% v/v dioxane/H2O, 1.0 M NaClO4.

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C17H16O4		H2L						CAS 58134-82-0	(6193)	
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Benzoyl-2-hydroxy-4-methoxy-3-methylacetophenone;

C6H5.CO.CH2.CO.C6H2(OH)(OCH3)(CH3)

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

Sm+++	gl	alc/w	30°C	75%	U	M		B2=13.46	1991GDd (96162)	1011
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Medium: 75% v/v EtOH/H2O, 0.1 M NaClO4. K(Sm(Acetylacetone)+L)=11.60

Sm+++	gl	alc/w	30°C	75%	U	T	H	K1=7.40 B2=14.13	1987DGd (96163)	1012
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20 C:K1=7.46, K2=6.87; 40 C:K1=7.74, K2=6.89; 50 C:K1=8.05, K2=7.09

DH(K1)=-31 kJ mol<sup>-1</sup>, DS=42 J K<sup>-1</sup> mol<sup>-1</sup>

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C17H20N3O3F		HL						(7845)		
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1-Ethyl-6-fluoro-7-(4-methylpyperazine-1-yl)-4-oxo-1,4-dihydroquinoline-3-carboxylic acid;

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

Sm+++	gl	alc/w	22°C	0.1M	U			K1=6.21 B2=11.66	2000TBb (96290)	1013
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K3=4.20

Medium: 0.1 M NaClO4 in 70% v/v EtOH/H2O

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C17H23N4O4BrS		H2L						(1594)		
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2-(5-Bromo-2-pyridylazo)-5-(N-propyl-3-sulfopropylamino)phenol;

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

Sm+++	sp	NaNO3	25°C	0.10M	C			K1=8.58	19880Ha (96425)	1014
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K(Sm+HL)=2.80

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C17H27N04		L						CAS 71089-11-7	(7945)	
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13-Phenylmethyl-1,4,7,10-tetraoxa-13-azacyclopentadecane;



Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	cal	non-aq	25°C	100%	C	H		1993LLb (96538)	1015

K(SmNO<sub>3</sub>+L)=3.85

Medium: acetonitrile. DH(SmNO<sub>3</sub>+L)=-49.66 kJ mol<sup>-1</sup>.

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C17H29N3O10                      H4L                      CAS 89378-46-1 (5528)  
 (Bis(3-(bis(carboxymethyl)amino)propyl)methylammonio)ethanoate;

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

Sm+++	gl	KNO <sub>3</sub>	25°C	0.10M	U		K1=8.71 K(Sm+HL)=5.67	1984TPa (96577)	1016
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C18H15NO<sub>3</sub>                      HL                      (6196)  
 8-Formyl-7-hydroxy-4-methyl-2H-[1]-benzopyran-2-one 4-methylanil;  
 CH<sub>3</sub>.C<sub>6</sub>H<sub>4</sub>.N:CH.C<sub>9</sub>H<sub>3</sub>O(OH)(CH<sub>3</sub>)(O)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Sm+++	gl	diox/w	30°C	70%	U		K1=6.65    B2=12.36 B3=17.07	1987ECa (96998)	1017
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C18H16N<sub>2</sub>O<sub>3</sub>                      HL                      (5560)  
 2-(2-Acetylphenylhydrazon)-1-phenyl-but-1,3-dione;  
 C<sub>6</sub>H<sub>5</sub>.CO.C(CO.CH<sub>3</sub>):N.NH.C<sub>6</sub>H<sub>4</sub>.COCH<sub>3</sub>

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Sm+++	gl	diox/w	30°C	75%	U		K1=10.56    B2=19.76	1988ESb (97179)	1018
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C18H18N<sub>4</sub>                      L                      CAS 16858-01-8 (1528)  
 Tris(2-pyridylmethyl)amine; (C<sub>5</sub>H<sub>4</sub>NCH<sub>2</sub>)<sub>3</sub>N

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Sm+++	nmr	KCl	25°C	1.0M	C	H	K1=2.51	2004BRa (97272)	1019
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Method: 1H nmr measurements in D<sub>2</sub>O. DH(K1)=-12 kJ mol<sup>-1</sup>,  
 DS(K1)=6 J mol<sup>-1</sup>K<sup>-1</sup>

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C18H20N<sub>2</sub>O<sub>6</sub>                      H4L    EHPG                      CAS 10328-28-6 (429)  
 N,N'-Ethylene-bis-(2-(2'-hydroxyphenyl))glycine; (HOOCCH(C<sub>6</sub>H<sub>4</sub>OH)NHCH<sub>2</sub>)<sub>2</sub>

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Sm+++	EMF	KNO <sub>3</sub>	25°C	0.10M	C	T H	K1=18.62 K(SmL+H)=7.20	1985HWb (97440)	1020
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Method: Hg (and glass) electrode, using Hg(II) as competitive indicator  
 ion. Data for 10-35 C. DH(K1)=-61.7 kJ mol<sup>-1</sup>, DS(K1)=150 J K<sup>-1</sup> mol<sup>-1</sup>.

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C18H25N3O8                      H4L      BEATA                      CAS 87732-99-8 (5600)

N,N-Bis(2-aminoethyl)aniline-N',N'',N''',N'''-tetraethanoic acid;

-----  
Metal            Mtd Medium Temp Conc Cal Flags Lg K values            Reference ExptNo  
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Sm+++            gl    KNO3    25°C 0.10M C                      K1=15.66            1985TPa (97659)1021

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C18H26N6                      L                      (6628)

3,6,14,17,23,24-Hexaazatricyclo[17.3.1.1]tetracos-1(23),8,10,12(24),19,21-hexaene;

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

Sm+++            gl    KCl      25°C 0.10M M                      K1=9.0            1996MBb (97723)1022

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C18H28O5                      L                      CAS 15196-73-3 (2359)

2,3-(4'-Dimethylethylbenzo)-1,4,7,10,13-pentaoxacyclopentadeca-2-ene;

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

Sm+++            gl    non-aq 25°C 100% U                      K1=3.45            1982MDa (97812)1023

Medium: propylene carbonate

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C18H29NO4                      L                      CAS 207603-17-6 (9000)

7-(Phenylmethyl)-1,4,10,13-tetraoxa-7-azacyclohexadecane;

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

Sm+++            cal non-aq 25°C 100% C    H                      K1=2.46            1998LBc (97881)1024

Medium: acetonitrile. DH(K1)=-60.58 kJ mol<sup>-1</sup>, DS(K1)=-156.1 J K<sup>-1</sup> mol<sup>-1</sup>.

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C18H30N2O11                      H2L                      CAS 93049-99-1 (5832)

1,4,7,10,13-Pentaoxa-16,19-diazacycloeicosane-14,21-dione-16,19-diethanoic acid;

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

Sm+++            gl    R4N.X    25°C 0.10M C                      K1=9.71            1988CCb (97916)1025

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C18H30N4O12                      H6L      TTHA                      CAS 869-52-3 (694)

Triethylenetetraaminehexaethanoic acid;((HOOCH<sub>2</sub>)<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>N(CH<sub>2</sub>COOH)<sub>2</sub>)<sub>2</sub>

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

Sm+++            EMF KNO3    25°C 0.10M C T H                      K1=23.00            1987HCa (98085)1026

K(SmL+H)=4.50

K(SmHL+H)=2.73

Method: Hg electrode; competitive reaction with Hg(II).

Data for 15-35 C. At 25 C, DH(K1)=-126 kJ mol<sup>-1</sup>, DS(K1)=19.4 J K<sup>-1</sup> mol<sup>-1</sup>.

-----  
Sm+++            vlt R4N.X    30°C 0.01M C                      K1=19.54            1981GMh (98086)1027

Method: polarography, using Cd as indicator ion. Medium: 0.01 M Et4NBr.

Sm+++ vlt NaClO4 25°C 0.40M C K1=23.81 1978MNb (98087)1028  
 Medium: 0.40 M NaClO4, pH 4.80. Method: polarography, using Cd as  
 indicator ion.

Sm+++ gl KNO3 30°C 0.10M U K1=19.54 1976GAa (98088)1029

Sm+++ gl KNO3 25°C 0.10M U K1=15.7 1969LUa (98089)1030  
 K(SmL+H)=4.49  
 K(SmHL+H)=2.60  
 B(Sm2L)=20.8

Sm+++ gl KNO3 25°C 0.10M U K1=24.3 1968SCa (98090)1031  
 \*\*\*\*\*  
 C18H32N4O8 H4L TETA CAS 60239-22-7 (1019)  
 1,4,8,11-Tetraazacyclotetradecane-1,4,8,11-tetraethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Sm+++ gl NaNO3 25°C 0.20M C K1=14.47 1991KKa (98223)1032

Sm+++ EMF NaCl 80°C 1.00M C K1=14.97 1986LDb (98224)1033  
 K(SmL+H)=3.90

\*\*\*\*\*  
 C18H34N2O8 H2L CAS 68670-15-5 (5851)  
 1,4,10,13-Tetraoxa-7,16-diazacyclooctadecane-7,16-di-(3-propanoic acid);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Sm+++ gl R4N.X 25°C 0.10M C K1=7.44 1988CCc (98344)1034  
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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
-------	-----	--------	------	------	-----	-------	-------------	-----------	--------

Sm+++ ISE non-aq 25°C 100% U H K1=11.0 1990MGa (98727)1035  
 In acetonitrile, 0.1 M Et4NClO4. DH=-104.5 kJ mol<sup>-1</sup>.

Sm+++ ISE non-aq 25°C 100% C K1=2.7 1989MGa (98728)1036  
 Medium: DMF, 0.10 M Et4NClO4

Sm+++ ISE non-aq 25°C 100% C K1=17.3 1986ALa (98729)1037  
 Medium: propylene carbonate, 0.1 M Et4NClO4

Sm+++ ISE non-aq 25°C 100% U H K1=15.99 1984GBa (98730)1038  
 K = 16.39 at 0.9 mol L<sup>-1</sup>. DH=-96.3 kJ mol<sup>-1</sup>; DS=-17 J K<sup>-1</sup> mol<sup>-1</sup>  
 In propylene carbonate.

Sm+++ gl alc/w 25°C 100% C I K1=9.70 1983ANb (98731)1039

The equilibration took 7-12 days. Medium: MeOH, 0.05 M Et4NC104  
In propylene carbonate, 0.1 M Et4NC104, K1=19.0

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Sm+++ gl R4N.X 25°C 0.25M C K1=5.94 1981BBe (98732)1040  
Medium: Me4NC1

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C18H40N2O10P2 H2L (7241)  
1,4,10,13-Tetraoxa-7,16-diazacyclooctadecane-7,16-diylldimethylenediphosphonic acid  
bis(Et-ester);

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

-----  
Sm+++ gl R4N.X 25°C 0.10M U K1=7.78 1996BJa (98898)1041  
Medium: 0.1 M Me4NC1

\*\*\*\*\*

C19H14O7S H4L Pyrocatechol Vi CAS 369596-29-2 (709)  
Pyrocatechol Violet,  
3-[3,4-Dihydroxyphenyl-3-hydroxy-4-oxo-2,5-cyclohexadien-1-ylidenemethyl-b.;

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

-----  
Sm+++ gl NaClO4 30°C 0.20M U M K1=9.29 1978MSk (99115)1042  
K(Sm(nta)+L)=6.98

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C19H16N4O L LAMI (5930)  
2-(2'-Lepidylazo)-N-methylisatin

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

-----  
Sm+++ gl diox/w 30°C 75% M I K1=9.72 B2=19.12 1987DGc (99168)1043  
Medium: 75% v/v dioxan/H2O, 0.15 M NaClO4

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C20H14N2O5S H3L EriochrBluBlk R CAS 2538-85-4 (3508)  
3-Hydroxy-4-(2-hydroxy-1-naphthylazo)naphthalene-1-sulfonic acid;

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

-----  
Sm+++ sp alc/w ? 98% U 1968RAa (99700)1044  
K(?)=5.2

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C20H14N2O11S3 H5L Chromotrope 8B CAS 5850-64-6 (2674)  
3-(4'-Sulfonaphthylazo)chromotropic acid;

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

-----  
Sm+++ sp NaClO4 25°C 0.10M C K1=5.96 1979PLb (99715)1045

\*\*\*\*\*

C20H14N2O11S3 H2L Hydroxynaphthol CAS 63451-35-4 (2835)  
Hydroxynaphthol blue, 1-(2-Hydroxy-4-sulfo-1-naphthylazo)-2-naphthol-3,

-----

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	sp	none	25°C	0.0	U			1978BRb (99735)	1046
							K <sub>leff</sub> =4.09		

K<sub>eff</sub> at pH 10

\*\*\*\*\*

C20H18N4O2 HL (5917)  
 Pyruvic monohydrazone-3-hydrazino-4-benzyl-6-phenylpyridazine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	diox/w	30°C	75%	U			1985RSb (99840)	1047
							K(Sm+HL)=5.30		
							K(Sm+2HL)=10.80		

\*\*\*\*\*

C20H24N2O6 H4L HBED CAS 3625-89-6 (2208)  
 N,N'-Di-(2-hydroxybenzyl)-diaminoethane-N,N'-diethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	KNO3	20°C	0.10M	U			1985SNb (100015)	1048
							K <sub>1</sub> =19.24		
							K(SmL+H)=5.51		
							K(SmHL+H)=4.98		

\*\*\*\*\*

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
Sm+++	cal	non-aq	25°C	100%	C	H	K <sub>1</sub> =3.84	1998LHa (100237)	1049
Medium: acetonitrile. DH(K <sub>1</sub> )=-3.01 kJ mol <sup>-1</sup> .									

Sm+++	gl	oth/un	25°C	0.0	U	H	K <sub>1</sub> =2.23	1991HJa (100238)	1050
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C20H24O12S2 H2L CAS 172985-47-6 (7820)  
 2,3:11,12-Dibenzo-1,4,7,10,13,16-hexaoxacyclooctadeca-2,11-diene-4',4''-disulfonic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	dis	R4N.X	25°C	0.12M	C		K <sub>1</sub> =1.77	1998SUa (100285)	1051
Medium: 0.12 M Et4NBr.									

Method:solvent extraction into cyclohexane/di(2-ethylhexyl)phosphoric acid

\*\*\*\*\*

C20H35N5O10 H5L (6545)  
 1,4,7,10,13-Pentaazacyclopentadecane-N,N',N'',N''',N''''-pentaethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaNO3	25°C	0.20M	C		K <sub>1</sub> =15.35	1991KKa (100545)	1052

C20H35N5O10 H3L (6623)  
1,4,7-Tris(carboxymethyl)-13,16-dioxo-1,4,7,10,19-pentaazacycloheptacosane-9,20-dione  
;

C20H43O4P	HL	CAS 7785-87-1	(2132)
Didecylphosphoric acid; (C10H21O)2P(O)OH			

C21H19N3O8S                      H4L              MeNaphtholOrange              (4151)  
N-(1'-Hydroxy-4'-(4''-sulfophenylazo)-2'-naphthylmethyl)-iminodiethanoic acid;

C22H14O9	H5L	CAS 4431-00-9	(3513)
Aurintricarboxylic acid;			

\*\*\*\*\*  
C22H17AsN4O14S3            H6L        Arsenazo   M            CAS 3563-69-7 (623)  
2-(2-Arsonophenylazo)-7-(3-sulfophenylazo)-1,8-dihydroxynaphthalene-3,6-disulfonic  
acid;

C22H18N4O14As2S2      H8L      Arsenazo III      CAS 1668-00-4      (1148)  
2,7-Bis(2'-arsonophenylazo)chromotropic acid;

K1eff=4.18  
B2eff=9.69  
B(2,2)eff=14.12

Method: spectral deconvolution. Medium: 0.1 M chloroacetate buffer, pH 3.5

Sm+++ sp oth/un 25°C var U I 1997HRb (101646)1059

K1(eff)=7.569

B(SmLC1)eff=7.791

B(SmL2Cl)eff=14.031

Conditional constants in chloride medium at pH 3.3. Also data in sulfate and perchlorate media. K(Sm+Cl)=1.822

Sm+++ sp oth/un 20°C ? U 1972SSi (101647)1060

K(Sm+H4L)=15.73

Sm+++ sp NaNO3 20°C 0.20M U 1963BUa (101648)1061

B(Sm2L2)=82.1

\*\*\*\*\*

C22H24N2O10 H4L CAS 132796-79-3 (8113)

1,2-Bis(2-aminophenoxy)ethane-N,N,N',N'-tetraethanoic acid;

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

Sm+++ EMF KNO3 25°C 0.10M C T H K1=10.92 1990HLA (101903)1062

K(SmL+H)=3.39

Method: Competitive reaction with Hg++, using Hg indicator electrode.

Data for 15-35 C. DH(K1)=-31.9 kJ mol<sup>-1</sup>, DS(K1)=102 J K<sup>-1</sup> mol<sup>-1</sup>.

\*\*\*\*\*

C22H26N4O10 H4L BAPTA (7230)

1,2-Bis(o-aminophenoxy)ethane-N,N,N',N'-tetraethanoic acid;

((HOOCCH2)2NCH(OC6H4NH2)2

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

Sm+++ gl R4N.X 25°C 0.10M C K1=10.87 1993YTa (101985)1063

\*\*\*\*\*

C22H28O13S2 H2L DSDB21C7 CAS 204931-02-2 (7821)

2,3:11,12-Dibenzo-1,4,7,10,13,16,19-heptaoxacycloheicosa-2,11-diene-4',4"-disulfo  
nic acid;

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

Sm+++ dis R4N.X 25°C 0.12M C K1=1.94 1998SUa (102081)1064

Medium: 0.12 M Et4NBr.

Method:solvent extraction into cyclohexane/di(2-ethylhexyl)phosphoric acid

\*\*\*\*\*

C22H29N3O12 H6L CAS 362606-74-4 (8226)

N,N'-[2-[[Bis(carboxymethyl)amino]methyl]-2-phenyl-1,3-propanediyl]bis[N-(carboxyme  
thyl)-glycine];

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

Sm+++ gl R4N.X 25°C 0.10M C K1=12.71 2001Vsa (102088)1065

K(SmL+H)=6.62

K(SmHL+H)=4.17

$$K(\text{SmH}_2\text{L}+2\text{H})=6.88$$

Medium: 0.10 M Me<sub>4</sub>NCl.

\*\*\*\*\*

C22H30N4 L CAS 250790-21-7 (7943)

N,N'-Bis(1,1-dimethylethyl)-1,10-phenanthroline-2,9-dimethanamine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaClO4	25°C	0.10M	U		K1=8.16 B(SmHL)=15.06	2001WZa (102118)	1066

Also data for the N,N'-diethyl, isopropyl, butyl and isobutyl derivatives.

\*\*\*\*\*

C22H37N5O14 H7L CAS 3234-59-1 (2425)

Tetraethylenepentamineheptaethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	vlt	R4N.X	30°C	0.01M	C		K1=20.50	1981GMh (102341)	1067

Method: polarography, using Cd as indicator ion. Medium: 0.01 M Et4NBr.

Sm+++	gl	KNO3	30°C	0.10M	U		K1=20.50	1976GAa (102342)	1068
Sm+++	gl	KNO3	25°C	0.10M	U		K1=20.50 K(Sm+HL)=14.43 B(SmH-1L)=5.29	1968MIc (102343)	1069

\*\*\*\*\*

C22H40N4O8 H4L CAS 138763-18-5 (8607)

5,7,12,14-Tetramethyl-1,4,8,11-tetraazacyclotetradecane-N,N',N'',N'''-tetraethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	KNO3	40°C	0.50M	U T		K1=18.18 K(SmL+H)=3.93	1995BIa (102360)	1070

Also data for 80 C.

\*\*\*\*\*

C23H16O9Cl2S H4L Chrome azurol S CAS 1667-99-8 (711)

Chromazurol S;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	sp	oth/un	25°C	?	U		K(?)=4.8	1967SAa (102572)	1071

\*\*\*\*\*

C23H18N2O3 HL (5561)

2-(2-Acetylphenylhydrazon)-1,3-diphenyl-prop-1,3-dione;

C6H5.CO.C(CO.C6H5):N.NH.C6H4.COCH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Sm+++ gl diox/w 30°C 75% U K1=10.90 B2=19.60 1988ESb (102601)1072  
\*\*\*\*\*

C23H18O9S H4L Eriochrome cyan CAS 3564-18-9 (433)  
4'-Hydroxy-3,3'-dimethyl-2''-sulfofuchsone-5,5'-dicarboxylic acid;

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

Sm+++ sp oth/un 25°C ? U B2=9.6 1968MDc (102636)1073  
\*\*\*\*\*

C23H24N4O2 L Trichachnine CAS 1251-85-0 (2606)  
4,4'-Diantiprylmethane,  
4,4'-phenylmethylen-bis-(1,2-dihydro-1,5-dimethyl-2-phenylpyrazol-3-one

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

Sm+++ sp diox/w 25°C 100% U K1=4.38 1995KMa (102678)1074  
\*\*\*\*\*

C24H16O16S8 H8L CAS 237770-97-7 (8854)  
25,26,27,28-Tetrahydroxy-2,8,14,20-tetrathiacalix[4]arene-5,11,17,23-tetrasulfonic  
acid;

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

Sm+++ cal oth/un 25°C 0.01M C H K1=3.37 2004LWa (102871)1075  
Medium: 0.01 M HCl. DH(K1)=7.2 kJ mol<sup>-1</sup>, DS(K1)=88.6 J K<sup>-1</sup> mol<sup>-1</sup>.  
\*\*\*\*\*

C24H32O14S2 H2L CAS 204931-03-3 (7822)  
2,3:11,12-Dibenzo-1,4,7,10,13,16,19,22-octaoxacyclotetracos-2,14-diene-4',4''-disul  
fonic acid;

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

Sm+++ dis R4N.X 25°C 0.12M C K1=2.07 1998SUa (103197)1076  
Medium: 0.12 M Et4NBr.

Method:solvent extraction into cyclohexane/di(2-ethylhexyl)phosphoric acid  
\*\*\*\*\*

C24H42N6O12 H6L (6546)  
1,4,7,10,13,16-Hexaazacyclooctadecane-N,N',N'',N''',N''',N''''-hexaethanoic acid;

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

Sm+++ gl NaNO3 25°C 0.20M C K1=21.24 1991KKa (103385)1077  
K(Sm+H2L)=16.41  
\*\*\*\*\*

C25H32N2O7 H2L (7374)  
1,15-Diaza-3,4:12,13-dibenzo-5,8,11-trioxacyclooctadecane-N,N'-diethanoic acid;

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

Sm+++ gl KNO3 25°C 0.5M C K1=5.46 1993YNa (103735)1078

\*\*\*\*\*

C26H23N5O2 HL (5918)  
Hippuric monohydrazone-3-hydrazino-4-benzyl-6-phenylpyridazine;

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Sm+++ gl diox/w 30°C 75% U K1=11.72 B2=22.41 1985RSb (103887)1079  
\*\*\*\*\*

C26H27N3O10 H4L (7231)  
2-((2-Amino-5-methylphenoxy)-methyl)-6-methoxy-8-aminoquinoline-N,N,N',N'-tetraetha  
noic acid;

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Sm+++ gl R4N.X 25°C 0.10M C K1=13.28 1993YTa (103971)1080  
\*\*\*\*\*

C26H34N6O8 H4L CAS 132709-65-0 (8941)  
3,6,14,17,23,24-Hexaazatricyclotetracos-1,8,10,12,19,21-hexaene-3,6,14,17-tetraace  
tic acid;

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Sm+++ gl KCl 25°C 0.10M M K1=ca. 22 1996MBb (104100)1081  
\*\*\*\*\*

C27H24N4O L BAHF (1023)  
Benzoylacetone-monohydrazone-3-hydrazino-4-benzyl-6-phenylpyridazine;

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Sm+++ gl diox/w 30°C 75% U K1=8.10 1983RSa (104390)1082  
\*\*\*\*\*

C28H24O16S4 H8L CAS 206559-10-6 (7767)  
25,26,27,28-Tetrahydroxycalix[4]arene-5,11,17,23-tetrasulfonic acid;

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Sm+++ cal oth/un 25°C 0.10M C H 2001BIa (104702)1083  
K(Sm+H4L)=3.82

Medium: 0.10 m Na4H4L, pH=2. DH(Sm+H4L)=10.4 kJ mol<sup>-1</sup>.

\*\*\*\*\*

C28H36N2O14S2 L CAS 84162-07-2 (7948)  
15,15'-Dithiobis[2,3,5,6,8,9,11,12-octahydro-16-nitro-1,4,7,10,13-benzopentaoxacycl  
opentadecin]

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Sm+++ sp non-aq 25°C 100% C T H 1997LQa (104793)1084  
K(SmNO3+L)=2.98

Medium: acetonitrile. Data for 20-35 C. DH(SmNO3+L)=7.73 kJ mol<sup>-1</sup>.

\*\*\*\*\*

C28H40N4O4                      H2L                      CAS 138110-63-1 (8608)  
7,14-Dimethyl-5,12-diphenyl-1,4,8,11-tetraazacyclotetradecane-1,8-diethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Sm+++	gl	KCl	40°C	0.50M	M			K1=9.38	1997BZa (104828)	1085

\*\*\*\*\*

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
Sm+++	gl	non-aq	25°C	100%	U			K1=4.00	1980MDb (104850)	1086

Medium: Propylene carbonate.

Medium: propylene carbonate. K1=7.60 with Sm++

\*\*\*\*\*

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
Sm+++	ISE	non-aq	25°C	100%	U			K1=3.75	1982MDa (104909)	1087

Medium: propylene carbonate

\*\*\*\*\*

C28H52N4O10                      H5L                      CAS 137203-80-6 (8096)  
1-N-Dodecyltriethylenetetramine-N,N',N'', N''',N''''-pentaethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Sm+++	gl	alc/w	25°C	50%	C			K1=17.5 K(SmL+H)=4.4	2001SYb (104990)	1088

Medium: 50% EtOH/H2O, 0.10 M KNO3.

\*\*\*\*\*

C31H24N4O                      HL                      CAS 88700-85-0 (1409)  
1,2-Diphenyl-1,2-ethanedione-3-(4-benzyl-6-phenyl)-pyridazinyl hydrazone;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Sm+++	gl	diox/w	30°C	75%	U	I		K1=9.05	1983RRa (105409)	1089

In 75% MeOH: K1=7.65; 75% DMF: 6.08

\*\*\*\*\*

C31H32N2O13S                      H6L                      Xylenol orange                      CAS 63721-85-5 (432)  
5,5'-Bis-N,N-bis(carboxymethyl)aminomethyl-4'-hydroxy-3,3'-dimethylfuchsone-2''-sulfonic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Sm+++	sp	NaNO3	20°C	0.20M	U			B(Sm2L2)=47.0	1963BBb (105493)	1090

\*\*\*\*\*

C32H28N8O10S2            H4L    Diantiprylazo    CAS 14918-39-9    (5368)  
2,7-Bis(antipyrinylphenylazo)chromotropic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	sp	KNO3	?	0.20M	U		K(?)=78.9	1968BBa (105572)	1091

\*\*\*\*\*  
C32H34N4O2                            L                            CAS 163892-66-8    (7329)  
1-Phenyl-1,1-di(2,3-dimethyl-1-phenyl-3-pyrazolyl-5-one)butane;C6H5C(C3H7)((C2N2(O)  
(CH3)2(C6H5))2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	sp	diox/w	25°C	100%	C		K(La(NO3)3+L)=4.13	1997KMa (105636)	1092

\*\*\*\*\*  
C33H36N4O6                            L            Bilirubin                            CAS 635-65-4    (2623)  
Bilirubin

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	sp	non-aq		50%	U		K1=5.52 K(SmL+Sm)=4.68	1972KPb (105898)	1093

Medium: 1:1 v/v CHCl3:EtOH

\*\*\*\*\*  
C33H45N7O3                            L                            CAS 345349-93-1    (9178)  
Tris[6-((2-N,N-diethylcarbamoyl)pyridyl)methyl]amine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	nmr	KCl	25°C	1.0M	C	H	K1=2.29	2004BRa (105974)	1094

Method: 1H nmr measurements in D2O. DH(K1)=18 kJ mol-1  
DS(K1)=104 J mol-1K-1

\*\*\*\*\*  
C36H32O24S4                            H8L                            CAS 171798-10-0    (9139)  
25,26,27,28-Tetrakis(hydroxycarbonylmethoxy)calix[4]arene-5,11,17,23-tetrasulfonic  
acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	cal	oth/un	25°C	0.01M	C	H	K1=4.08	2004LWa (106231)	1095

Medium: 0.01 M HCl. DH(K1)=3.9 kJ mol-1, DS(K1)=91.3 J K-1 mol-1.

\*\*\*\*\*  
C36H54O12                            L                            (6732)  
1,8-Dioxooctamethylenebis(4'-2,3-benzo-1,4,7,10,13-pentaoxacyclopentadecane);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	dis	non-aq	25°C	100%	U			1993INa (106426)	1096

$$B(\text{Sm}+3\text{P}+2\text{L})=8.91$$

By solvent extraction into dichloromethane. B is the extraction constant  
 $\text{Sm}(\text{aq})+\text{picrate}(\text{aq})+\text{L}(\text{org})=\text{SmL2P3}(\text{org})$ .

\*\*\*\*\*

C36H60O30 L a-Cyclodextrin CAS 10016-20-3 (6946)  
 alpha-Cyclodextrin, Cyclohexaamylose;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaCl	25°C	0.10M	U	I	K1=2.7	1999FBa (106472)	1097

In 0.1 M Me4NCl, K1=3.18.

\*\*\*\*\*

C37H33N5O4 L (7366)  
 2,6-Bis(1-(3,5-dimethoxybenzyl)benzimidazol-2-yl)pyridine

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	non-aq	25°C	100%	C		K2=5.5 K3=3.6	1997PBa (106553)	1098

Medium: CH3CN; 0.1 M Et4NClO4

\*\*\*\*\*

C37H44N2O13S H6L MeThymol Blue (428)  
 3,3'-Bis(N,N-di(carboxymethyl)aminomethyl)thymolsulfonephthalein;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	NaClO4	30°C	0.10M	U		K(Sm+H3L)=4.20 K(Sm+H2L)=6.47 K(SmH2L+H)=4.97	1980NAb (106618)	1099

Also data for SmHnL(OH) species

\*\*\*\*\*

C45H66N10O6 L CAS 362613-35-2 (7912)  
 Tris[3-(6-diethylcarbamoylpyridine-2-carboxamide)propyl]amine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	sp	non-aq	25°C	100%	C	I	K1=6.6 K(Sm+HL)=6.3	2001RDa (107233)	1100

Medium: CH3CN. In 95% v/v CH3CN/H2O, K1=5.1, K(Sm+HL)=5.4.

\*\*\*\*\*

C47H46N6O4 L (7367)  
 2,6-Bis(1-(3,5-dimethoxybenzyl)benzimidazol-2-yl)-4-(4-diethylamino)phenylpyridine  
 ;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	gl	non-aq	25°C	100%	C		K3=6.0	1997PBa (107319)	1101

Medium: CH3CN; 0.1 M Et4NClO4

\*\*\*\*\*

C62H94N2O4S2 L (8109)  
5,11,17,23-Tetrakis(1,1-dimethylethyl)-25-27-bis[2-methylthio]ethoxy]...calix(4)arene;  
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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	cal	non-aq	25°C	100%	U	H	K1=4.14	2001NJ	a (107708)1102

Method: microcalorimetry. Medium: MeCN.. DH(K1)=-164 kJ mol<sup>-1</sup>  
\*\*\*\*\*

C76H116N4O8 L (8156)  
p-tert-Butylcalix(4)arene tetradiisopropylethanoamide;  
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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Sm+++	cal	non-aq	25°C	100%	U	H	K1=5.09	2001NJ	a (107885)1103

Method: microcalorimetry. Medium: MeCN.. DH(K1)=-86.4 kJ mol<sup>-1</sup>

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#### EXPLANATORY NOTES

DATA Flags are :-

T Data at other TEMPERATURES  
 I Data with various BACKGROUNDS  
 H Data for THERMOCHEMICAL quantities  
 M Data for TERNARY Complexes

EVALUATION Flags are :-

T or IUP=T signifies EVALUATION RATING = Tentative by IUPAC

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