

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			K(Sm+e=Sm(II))=-25(-1.5V)	1974J0b (935)	1

Method:Estimated data

Sm+++	oth	none	25°C	0.0	U			K(Sm+3e)=-122.4(-2410 mV)	1952LAb (936)	2
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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			Kso(SmAsO4)=-22.73	1992FIa (1160)	3

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 K1in=-0.89	1973KPe (2309)	4

Medium: 50% w/w MeOH/H2O, 3 M LiClO4. K1=-0.16(0%); K1in=-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

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

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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---

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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

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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;

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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  
 -----

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: diemthylacetamide										
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
							K1in=-0.74			
Medium: 50% w/w MeOH/H2O, 3 M LiClO4. K1=-0.02(0%); K1=0.96, K1in=0.09(100%)										
Sm+++	sp	alc/w	25°C	50%	U I		K1=0.54		1971KBg (5708)	20
							K1in=-0.55			
Medium: 50% v/v EtOH/H2O, 3 M LiClO4. K1=0.97, K1in=0.09(90%)										
Sm+++	sp	none	25°C	0.0	U		K1=-2.03		1970KBe (5709)	21
							K1in=-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			
*****										
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 <sup>-1</sup> , 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 <sup>-1</sup> ; 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  
-----

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  
-----

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  
 -----

N3- HL Azide CAS 7782-79-8 (441)  
 Azide;  
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Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
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Sm+++ sp NaClO4 25°C 2.0M C K1=0.22 1978ABc (10257) 44  
 Medium pH 5.0. By ion exchange, K1=0.27.  
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Sm+++ sp NaClO4 25°C 2.0M U K1=4.22 1975EAb (10258) 45  
 -----

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 K1=-7.84 2000KBa (12124) 46  
 -----

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 \*K1=-9.05 1999CIa (12125) 47  
 -----

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 \*B(1,3)=-22.34 1999FBa (12126) 48  
 -----

In 0.1 M Me4NCl, \*B(1,3)=-22.78.  
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Sm+++ gl NaClO4 RT 1.0M C \*B4=-36.7 1983KDe (12127) 49  
 -----

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)	

-----  
Sm+++ gl oth/un 25°C var U 1951MFb (12140) 62  
Kso(Sm(OH)3)=-22.08  
-----

Sm+++ gl oth/un 25°C var U 1944MKa (12141) 63  
Kso(Sm(OH)3)=-21.2  
-----

Sm+++ sol oth/un 100°C var U 1932ENa (12142) 64  
Kso=0.90 + y  
-----

Kso:  $K(\text{Sm}(\text{OH})_3(\text{s})=\text{Sm}+3\text{OH})$ ;  $y=K_{\text{so}}$  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  
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Sm+++ sol none 25°C 0.0 M 1997LBd (13323) 65  
Kso(SmPO4)=-26.19  
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Calculated from data for 0.10 M HClO4 solution.

Sm+++ sol oth/un 25°C 0.0 C I 1993FKb (13324) 66  
Kso(SmPO4)=-27.64  
-----

In synthetic seawater,  $K_{\text{s}}(\text{SmPO}_4)=-24.36$ .

Sm+++ sol none 25°C 0.0 C 1991FBa (13325) 67  
Kso(SmPO4)=-25.99  
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P207---- H4L Pyrophosphate CAS 2466-09-3 (198)

Diphosphate; from  $(\text{HO})_2\text{PO}.0.\text{PO}(\text{OH})_2$   
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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)

Triphosphate; from  $(\text{HO})_2\text{PO}.0.\text{PO}(\text{OH}).0.\text{PO}(\text{OH})_2$   
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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 1974KRa (13900) 70  
K(Sm+2HL)=6.5  
-----

$K(\text{Sm}+2\text{HL})=6.9$  and  $B_2=8.9$  (35 C),  $K(\text{Sm}+2\text{HL})=6.4$  and  $B_2=8.4$  (45 C)

$\text{DH}(\text{Sm}+2\text{HL})=-11$  kJ mol<sup>-1</sup>;  $\text{DH}(B_2)=-28$   
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Sm+++ gl NaClO4 30°C 0.30M U K1=7.42 1963KUa (13901) 71  
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Sm+++ gl NaClO4 ? 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;

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 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 NaClO4 25°C 1.00M U I K1=0.13 B2=0.26 1993SMb (15254) 74

Sm+++ sp NaClO4 ? 0.60M U T K1=0.09 1964KSe (15255) 75

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

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 Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
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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 NaClO4 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 D2O: DH(K1)=15.7, DS=122.9

Sm+++ con oth/un 25°C 0.0 U K1=3.68 1973FPb (16540) 79

Sm+++ oth none 25°C 0.0 U K1=3.66 1973FPb (16541) 80  
 K1in=0.72

Method: ultrasonic absorption

Sm+++ con oth/un 25°C 0.0 U K1=3.68 1973FPb (16542) 81  
 Medium:D2O

Sm+++ oth none 25°C 0.0 U K1=3.68 1973FPb (16543) 82  
 K1is=0.73

Method: ultrasonic absorption. Medium:D2O

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

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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>

-----  
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

\*\*\*\*\*  
CH2O2 HL Formic acid CAS 64-18-6 (37)  
Methanoic acid; H.CO0H

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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.CO0H

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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

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

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.

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

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

C2H3N3S2 HL CAS 2349-67-9 (6245)  
2-Amino-5-mercapto-1,3,4-thiadiazole;

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
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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
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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
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Sm+++	EMF	NaClO4	20°C	2.0M	U			K1=2.01 B2=3.26 B3=3.85 B4=3.8	1958SOa (20167)	102
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Method: quinhydrone electrode

\*\*\*\*\*

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
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Sm+++	cal	NaClO4	25°C	2.0M	C	H			1964GRa (20366)	105
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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

-----  
Sm+++ gl NaClO4 25°C 2.0M U 1962BCa (20368) 107  
K(Sm+HL)=1.81  
K(SmHL+HL)=0.9

\*\*\*\*\*  
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 NaClO4 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 NaClO4 25°C 0.20M U K1=6.08 B2=11.71 1996PJa (20625) 109

-----  
Sm+++ gl NaClO4 25°C 0.20M U M K1=3.92 1986LSb (20626) 110  
K(Sm(EDTA)+L)=3.72

-----  
Sm+++ gl NaClO4 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 NaClO4 25°C 0.50M C T K1=2.54 B2=4.58 1977Cma (20629) 113  
B3=5.70  
B4=7.20

-----  
Sm+++ cal NaClO4 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 NaClO4 20°C 0.10M U K1=2.914 B2=5.01 1964PKb (20631) 115  
B3=6.57

-----  
Sm+++ EMF NaClO4 20°C 2.0M U K1=2.56 B2=4.53 1959SOb (20632) 116  
B3=5.9  
B4=6.4  
B5=6.0

Method: quinhydrone electrode

\*\*\*\*\*  
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(nta)+HL)=1.83, K(Sm(nta)+2HL+H2L)=5.55, K(Sm(nta)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 1990LSb (21706) 119  
K(Sm(phen)+L)=5.92  
-----

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 1987RRc (21708) 121  
K(Sm+HL)=3.82  
-----

Sm+++ gl NaClO4 25°C 0.20M U M K1=5.84 1986LSb (21709) 122  
K(Sm(EDTA)+L)=4.97  
-----

Sm+++ gl KNO3 35°C 0.10M U M 1986RMb (21710) 123  
K(Sm+HL)=3.82  
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 1977GMa (21712) 125  
K(SmA+L)=3.56  
K(SmA+HL)=3.00  
K(SmA+H2L)=3.08  
-----

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  
-----

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

\*\*\*\*\*  
 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>.  
 \*\*\*\*\*  
 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

\*\*\*\*\*  
 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.  
 \*\*\*\*\*  
 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.

\*\*\*\*\*

C3H4O4 H2L Malonic acid CAS 141-82-2 (79)  
Propanedioic acid; CH2(COOH)2

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

\*\*\*\*\*

C3H4O6 H2L CAS 560-27-0 (4233)  
Dihydroxypropanedioic acid; HOOC.C(OH)2.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

\*\*\*\*\*

C3H5NO2 HL (4234)  
Isonitrosoacetone; CH3.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

\*\*\*\*\*

C3H6N2O2 L Methylglyoxime CAS 2140-03-6 (2981)  
Methylglyoxime; CH3.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

\*\*\*\*\*

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			K(Sm+HL)=2.06	1968Cma (25169)	147
Sm+++	gl	NaClO4	31°C	2.0M	U			K(Sm+HL)=1.83 K(SmHL+HL)=0.9	1963BCb (25170)	148

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			K(Sm+HL)=1.74	1968Cma (25225)	149
Sm+++	gl	NaClO4	31°C	2.0M	U			K(Sm+HL)=2.19 K(SmHL+HL)=1.3	1963BCb (25226)	150

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	KNO3	25°C	0.20M	U	M	K1=6.75	1990LSb (26260)	164	K(Sm(phen)+L)=6.32	
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	1986LSb (26262)	166	K(Sm(EDTA)+L)=5.37	
Sm+++	gl	NaClO4	25°C	0.20M	U	M	K1=6.68	1985LSe (26263)	167	K(Sm(edta)+L)=5.87.	
Sm+++	gl	NaClO4	25°C	0.20M	U	M	K1=6.88	1984LSd (26264)	168	K(Sm(edta)+L)=5.37	
Sm+++	sp	R4N.X	25°C	1.00M	U		K1=7.04	B2=11.70	1978SGa (26265)	169	B(Sm2L)=11.20 B(Sm2L2)=15.80
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			2002TKa (26477)	171	B(SmHL)=11.71 K(Sm+L=SmH-2(HL))=-1.83	
Sm+++	gl	NaClO4	25°C	0.20M	U	M	K1=6.40	1986LSb (26478)	172	K(Sm(EDTA)+L)=4.99	
Sm+++	gl	NaClO4	25°C	0.20M	U	M	K1=6.40	1984LSd (26479)	173	K(Sm(edta)+L)=4.99	
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		2003TKa (26833)	174	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.	
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 2002TKa (27173) 176

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

-----  
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 1995KDD (27175) 178

K(Sm(egta)+L)=3.67

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  
-----

\*\*\*\*\*  
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 1972MCD (27684) 180

K(SmH-1L+H)=7.55

\*\*\*\*\*  
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 1972MCD (27748) 181

K(SmH-1L+H)=7.25

-----  
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 2002KAa (28586) 183

K(Sm+HL)=5.74  
K(Sm+2HL)=11.09

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.

\*\*\*\*\*

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 1991M0a (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 NaClO4 25°C 0.20M U M K1=4.54 1985LSf (30038) 203  
K(Sm(edta)+L)=4.08

Sm+++ gl NaClO4 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 NaClO4 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 NaClO4 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 NaClO4 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 NaClO4 25°C 0.20M U K1=6.24 B2=12.00 1996PJa (30362) 210

Sm+++ gl NaClO4 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		2003SBa (30717)	213
							K(Sm+HL)=2.94			
Sm+++	gl	NaClO4	25°C	0.20M	U		K1=5.42	B2=10.00	1996PJa (30718)	214
Sm+++	gl	NaClO4	25°C	0.20M	U	M	K1=4.53		1986LSb (30719)	215
							K(Sm(EDTA)+L)=4.11			
Sm+++	gl	NaClO4	25°C	0.20M	U	M	K1=4.58		1985LSf (30720)	216
							K(Sm(edta)+L)=4.18			
Sm+++	gl	KNO3	30°C	0.10M	U	M			1984AIa (30721)	217
							K(Sm(EDTA)+L)=2.137			
Sm+++	gl	KNO3	20°C	0.10M	U				1980SDa (30722)	218
							B(SmHL)=7.62			
Sm+++	gl	KNO3	20°C	0.10M	U		K1=4.76	B2=7.82	1980SDB (30723)	219
							K(Sm+HL)=2.23			
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	1969JPa (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	2003TKa (30925)
								B3=13.53		223
Sm+++	gl	KCl	25°C	1.0M	U	M			1988KTa (30926)	224
							K(Sm(edta)+L)=2.55			
Sm+++	EMF	NaClO4	20°C	1.00M	U	T		K1=5.62	B2=10.01	1972G0a (30927)
								B3=13.03		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	1963GTa (30929)
								B3=12.79		227

Method: quinhydrone electrode

\*\*\*\*\*

C4H6O6                    H2L    L-Tartaric acid    CAS 87-69-4    (92)  
 L-Tartaric acid, L-2,3-Dihydroxybutanedioic acid; HOOC.CH(OH).CH(OH).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Sm+++	sp	oth/un	25°C	0.0	U T H			K1=5.21	1975YBa (31350)	228
DH(K1)=-11.3 kJ mol <sup>-1</sup> , DS=62.8 J K <sup>-1</sup> mol <sup>-1</sup>										
Sm+++	gl	alc/w	25°C	50%	U I			K1=5.65	1972SSj (31351)	229
Medium: 0-50% EtOH, 0.05 M. 50% EtOH, I=0: K1=7.33										
Sm+++		EMF	KNO3	20°C	0.10M	U		K1=3.5    B2=7.3	1969DMa (31352)	230
Sm+++		EMF	NaClO4	25°C	2.00M	U		K1=3.50    B2=5.54	1969JPa (31353)	231
Sm+++	gl	KCl	24°C	0.20M	U			K1=3.50	1966DDa (31354)	232

\*\*\*\*\*  
 C4H7NO3                    HL                                    CAS 543-24-8    (3586)  
 N-Acetylglycine; CH3.CO.NH.CH2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Sm+++		EMF	NaClO4	25°C	0.10M	U		K1=1.88	1971RCa (31508)	233

\*\*\*\*\*  
 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				2002TKa (31936)	234
B(SmH2L)=14.89 B(SmHL)=11.84 K(Sm+L=SmH-1(HL))=5.56 K(Sm+L=SmH-2(HL))=-1.80										
Sm+++	gl	NaClO4	25°C	0.20M	U			K1=5.89    B2=10.81	1996PJa (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	1986LSb (31940)	238
K(Sm(EDTA)+L)=5.37										
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
K1(30 C)=7.83; K1(50 C)=10.6; K2(50 C)=8.4										

\*\*\*\*\*

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 1964DVa (33515) 259  
K3=1.40  
K4=1.21  
-----  
Sm+++ EMF NaClO4 25°C 1.0M U K1=2.63 B2=4.76 1964EVa (33516) 260  
K3=1.33  
K4=1.15

Method: quinhydrone electrode

-----  
Sm+++ gl NaClO4 20°C 0.10M U K1=2.993 B2=5.39 1964PKb (33517) 261  
B3=6.77  
-----  
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 1961CCa (33519) 263  
K3=1.58

\*\*\*\*\*  
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 1975PFb (33685) 264  
K3=1.64  
\*\*\*\*\*

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 1976PKb (33711) 265  
K3=1.90  
-----  
Sm+++ gl NaClO4 25°C 0.50M U K1=2.86 B2=5.07 1964SPa (33712) 266  
B3=6.51  
\*\*\*\*\*

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

-----  
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  
-----

-----  
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  
-----

-----  
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  
-----

-----  
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 1965DKb (35893) 273  
\*\*\*\*\*  
C5H2O5 H2L Croconic acid CAS 488-86-8 (1643)  
4,5-Dihydroxycyclopent-4-ene-1,2,3-trione;  
-----

-----  
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  
-----



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 B2=10.71 1994SSa (37070) 282  
K3=4.25

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

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Sm+++ gl NaClO4 25°C 0.20M U M K1=5.34 1986LSb (37372) 283  
K(Sm(EDTA)+L)=4.49

-----  
Sm+++ gl NaClO4 25°C 0.20M U M K1=5.40 1985LSf (37373) 284  
K(Sm(edta)+L)=4.52

\*\*\*\*\*

C5H6O4 H2L Itaconic acid CAS 97-65-4 (398)

Methylenesuccinic acid; HOOC.CH2.C(:CH2).COOH

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Sm+++ gl KCl 25°C 0.20M U K1=3.10 1989MFa (37446) 285  
K(Sm+HL)=1.96

-----  
Sm+++ gl NaClO4 25°C 0.20M U M K1=4.47 1986LSb (37447) 286  
K(Sm(EDTA)+L)=4.32

-----  
Sm+++ gl NaClO4 25°C 0.20M U M K1=4.52 1985LSf (37448) 287  
K(Sm(edta)+L)=4.35

-----  
Sm+++ sol oth/un 25°C 1.0M U K1=3.78 1984Kpf (37449) 288  
in 1.0 M HCl

-----  
Sm+++ oth NaClO4 25°C 1.0M U K1=2.07 1972STd (37450) 289  
B(SmHL)=6.48  
B(SmH2L2)=12.72

\*\*\*\*\*

C5H7NO3 HL (4313)

Isonitrosoacetylacetone; HO.N:CH.CO.CH2.CO.CH3

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Sm+++ gl diox/w 20°C 50% U K1=4.48 B2=7.95 1971MAf (37532) 290

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 1977DPa (37542) 291  
B(SmH-1L)=-3.40  
B(Sm2H-3L3)=-8.60

\*\*\*\*\*  
C5H8N2O3 H2L (4317)  
Methylacetyl glyoxime; 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 1995PAa (38077) 293  
K3=3.47

-----  
Sm+++ gl diox/w 30°C 75% U K1=7.03 B2=12.77 1979MBc (38078) 294  
K3=4.26

-----  
Sm+++ gl NaClO4 20°C 0.10M U M 1973TZa (38079) 295  
K(Sm(EDTA)+L)=3.53

-----  
Sm+++ gl R4N.X 25°C 0.10M U M 1972FGa (38080) 296  
K(Sm(EDTA)+L)=2.42

-----  
Sm+++ gl alc/w ? 50% U I K1=6.89 1971K0a (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 1960GFa (38083) 299  
K3=2.90

-----  
Sm+++ gl oth/un 30°C 0.0 U K1=5.9 B2=10.4 1955IFa (38084) 300  
K3=3.2

\*\*\*\*\*  
C5H8O4 H2L CAS 601-75-2 (479)  
Ethylpropanedioic acid; HOOC.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 NaClO4 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 NaClO4 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 NaClO4 25°C 0.20M U M K1=4.26 1986LSb (38355) 304  
K(Sm(EDTA)+L)=3.51

-----  
Sm+++ gl NaClO4 25°C 0.20M U M K1=4.30 1985LSf (38356) 305  
K(Sm(edta)+L)=3.56

-----  
Sm+++ gl NaClO4 25°C 0.20M U M K1=4.20 1984LSd (38357) 306  
K(Sm(edta)+L)=3.51

-----  
Sm+++ sol oth/un 25°C 0.50M U K1=3.68 1970MKe (38358) 307  
\*\*\*\*\*

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 NaClO4 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 NaClO4 25°C 0.10M U B2=5.53 1981ZLa (38641) 310  
\*\*\*\*\*

C5H9NO3 HL Hydroxyproline CAS 51-35-4 (416)  
4-Hydroxy-2-pyrrolidinedicarboxylic 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	NaClO4	25°C	0.10M	U		B2=4.95	1981ZLa (38751)	312
*****									
C5H9N04		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
Sm+++	gl	KCl	30°C	0.10M	U T H		K1=4.087	1978AGb (39124)	313
Data for 40 C. DH and DS values reported.									
*****									
C5H9N04		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
Sm+++	gl	KCl	25°C	0.10M	U		K1=6.67 B2=11.90 B3=15.03 B(Sm+2OH+L)=16.52	1980MGc (39279)	314
Sm+++	gl	KNO3	25°C	0.10M	U		K1=7.05	1977TIa (39280)	315
*****									
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 K3=1.51	1969PCa (40262)	316
Sm+++	EMF	NaClO4	25°C	1.0M	U		K1=2.60 B2=4.74 K3=1.26 K4=1.14	1964EVa (40263)	317

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
Sm+++	gl	NaClO4	25°C	1.0M	U		K1=2.40	1968GCa (40286)	318
*****									
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

\*\*\*\*\*  
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.  
-----

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

C5H12O5 L Xylitol CAS 87-99-0 (2139)  
Xylitol; HO.CH2.HCOH.HOCH.HCOH.CH2.OH

-----  
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

\*\*\*\*\*

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
Sm+++	gl	R4N.X	25°C	0.10M	C			K1=1.48	1990CBe (42816)	341

\*\*\*\*\*

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
Sm+++	gl	NaNO3	25°C	0.0	U	M		K1=9.63	1996KDb (42941)	342

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
Sm+++	sp	KCl	25°C	0.10M	M	I		K1=6.22	1989PEa (42959)	344

\*\*\*\*\*

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
Sm+++	sp	KCl	25°C	0.10M	U			K1=5.27	1987PLa (43115)	345

\*\*\*\*\*

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
Sm+++	gl	oth/un	30°C	0.10M	U			K1=5.83 B2=10.91	1972DSd (43137)	346

\*\*\*\*\*

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

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

Sm+++ dis NaClO4 25°C 0.10M U K2=4.83 1960RYa (43421) 348  
K3=3.70

Extraction into hexane

-----  
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

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

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.

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

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

-----  
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.

-----  
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.

-----  
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.

-----  
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

-----  
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	1996PJa (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

\*\*\*\*\*  
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

-----  
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; HOOC.CH(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);

-----  
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(Sm+HL)=1.65

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

K(Sm+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

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 K(SmA+L)=5.85 1977GMa (47017) 399  
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 K(SmL+Citrate)=2.7 1974TDa (47018) 400

-----  
Sm+++ cal KNO3 20°C 0.10M U HM K(SmA+L)=5.00 1971GKb (47019) 401

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 B(SmL(OH))=6.17 1970VMa (47020) 402

-----  
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 K(Sm2L3)=36.7 1957NOa (47024) 406

-----  
Sm+++ vlt KNO3 20°C 0.10M U T K1=11.33 1956SGa (47025) 407

\*\*\*\*\*  
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.COOH

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.COOH

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

Sm+++ gl NaNO3 25°C 0.10M M M K1=5.92 1996KDd (49914) 435  
\*K(SmL)=-8.34  
\*K(Sm(OH)L)=-8.78  
K(Sm(egta)+L)=4.13

Data for 0.05-0.15 M NaNO3. At I=0, K1=6.09, K(Sm(egta)+L)=4.27.

-----  
Sm+++ gl NaClO4 25°C 0.20M U K1=5.35 B2= 9.72 1987PPa (49915) 436  
\*\*\*\*\*

C6H13NO2 HL Leucine CAS 61-90-5 (47)  
2-Amino-4-methylpentanoic acid; H2N.CH(CH2.CH(CH3)2).COOH

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

Sm+++ gl NaNO3 25°C 0.10M M M K1=5.89 1996KDd (50103) 437  
\*K(SmL)=-8.36  
\*K(Sm(OH)L)=-8.81  
K(Sm(egta)+L)=4.10

Data for 0.05-0.15 M NaNO3. At I=0, K1=6.12, K(Sm(egta)+L)=4.27.

-----  
Sm+++ gl KNO3 25°C 0.20M U M K1=5.78 1990LSb (50104) 438  
K(Sm(phen)+L)=5.60

-----  
Sm+++ gl NaClO4 25°C 0.20M U K1=5.39 B2= 9.38 1987PPa (50105) 439

-----  
Sm+++ gl NaClO4 25°C 0.20M U M K1=6.18 1986LSb (50106) 440  
K(Sm(EDTA)+L)=5.09

-----  
Sm+++ gl NaClO4 25°C 0.20M U M K1=6.18 1985LSe (50107) 441  
K(Sm(edta)+L)=5.09.

\*\*\*\*\*  
C6H13NO2 HL Norleucine CAS 616-06-8 (602)  
2-Amino-hexanoic acid (2-Aminocaproic acid) CH3.(CH2)3.CH(NH2).COOH

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

Sm+++ gl NaNO3 25°C 0.10M M M K1=5.82 1996KDd (50192) 442  
\*K(SmL)=-8.38  
\*K(Sm(OH)L)=-8.84  
K(Sm(egta)+L)=4.08

Data for 0.05-0.15 M NaNO3. At I=0, K1=6.04, K(Sm(egta)+L)=4.22.

-----  
Sm+++ gl NaClO4 22°C 0.10M M M K1=5.06 B2=9.93 1991DTa (50193) 443  
B3=13.56  
K(SmA+L)=9.79

H4A=trans-cyclohexane-1,2-diaminotetraethanoic acid. Definitions wrong?

\*\*\*\*\*  
C6H13NO4 HL Bicine CAS 150-25-4 (2124)  
N,N-Bis(2-hydroxyethyl)glycine; (HO.CH2.CH2)2N.CH2.COOH

-----  
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  
-----



C7H5N04 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 1961GRa (52804) 462  
K3=5.35

\*\*\*\*\*

C7H5N04 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

\*\*\*\*\*

C7H5N04 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 1978SSi (53548) 468  
 K3=3.91

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 1969Cmb (53691) 469  
 K3=4.60

\*\*\*\*\*

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-1 DS1= 68 J K-1 mol-1

\*\*\*\*\*

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-1, DH(B2)=3.91 J K-1 mol-1

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

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 1989HMa (54294) 473  
 K(Sm+HL)=2.06  
 K(SmHL+HL)=1.76  
 -----

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 1996PJa (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; HOOC.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; HO3S.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 1977AKa (55515) 504  
K3=7.46

\*\*\*\*\*  
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 1995KDc (55680) 506  
K(Sm(egta)+L)=3.35

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 1991BPb (55694) 507  
K(Sm+OH+L)=15.24

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 1996KDb (56077) 508  
K(Sm(egta)+L)=5.87

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
*****									
C7H11N04			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
*****									
C7H11N06			H3L				(2926)		
2-Aminobutanoic-N-propane-1,3-dioic acid; HOOC.CH(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
*****									
C7H11N06			H3L	MNTA			(1026)		
Nitrilo(2-propanoic)-diethanoic acid; HOOC.CH(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

Sm+++ gl mixed 30°C 75% U K1=8.05 1971DRb (57278) 516  
Medium: 75% acetone, 0.1 M

\*\*\*\*\*

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

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

Sm+++ gl KNO3 25°C 0.10M U K1=4.33 B2=6.92 1968PFa (57371) 517

\*\*\*\*\*

C7H12O6 HL Quinic acid CAS 77-95-2 (2578)  
1,3,4,5-Tetrahydroxycyclohexane-1-carboxylic acid;

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

Sm+++ gl NaCl 20°C 0.10M U K1=2.84 1977SSc (57410) 518

Sm+++ EMF NaCl04 25°C 1.0M U K1=2.66 B2=4.65 19670Ta (57411) 519  
K3=1.43  
K4=0.72

Method: quinhydrone electrode

\*\*\*\*\*

C7H13NO6 H2L CAS 32013-58-4 (6079)  
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

Sm+++ gl KNO3 20°C 0.10M U K1=8.50 B2=16.02 1980RPa (57619) 520

\*\*\*\*\*

C7H14N2O3 HL Gly-Val CAS 7963-21-9 (973)  
Glycyl-valine; H2N.CH2.CO.NH.CH(CH(CH3)2).COOH

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

Sm+++ gl KNO3 30°C 0.15M U T H K1=3.91 1980SKe (57757) 521  
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.

\*\*\*\*\*

C7H14O3 HL CAS 63204-98-9 (3738)  
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

Sm+++ EMF NaCl04 25°C 1.0M U K1=2.71 B2=4.90 1965TVa (57866) 522  
K3=1.48  
K4=1.02

Method: quinhydrone electrode

\*\*\*\*\*

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

-----  
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

-----  
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);

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

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.

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

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

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Sm+++ gl NaNO3 25°C 0.10M M I M K1=4.64 1995KDb (59009) 528  
K(Sm(egta)+L)=4.25  
Data for 0.05 and 0.15 M NaNO3. At I=0, K1=4.96, K(Sm(egta)+L)=4.58.

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

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

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

C8H8N4OS 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  
-----

Sm+++ gl NaClO4 25°C 0.1M C H K1=2.13 1996HYa (59562) 538  
By calorimetry: DH(K1)=9.99 kJ mol-1

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

\*\*\*\*\*  
C8H8O2 HL CAS 583-80-2 (3191)  
beta-Methyltropolone;

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

Sm+++ sp alc/w ? 3% U K1=7.07 1967GDb (59604) 540  
Medium: 3% EtOH, 0.2 M NaClO4

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

Sm+++ gl alc/w 25°C 20% M I K(Sm+HL)=6.27 1994KDa (59683) 541

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  
-----

Sm+++ gl NaClO4 25°C 0.10M M H K1=2.10 1988CLb (59749) 542  
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

-----  
Sm+++ gl diox/w 30°C 76% M K1=6.48 1978PMa (59751) 544  
Medium: 76% v/v dioxane/H2O, 0.10 M NaClO4.

\*\*\*\*\*  
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

-----  
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>

\*\*\*\*\*  
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.

\*\*\*\*\*  
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.

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

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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=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
-----

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-----
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-hydroxyethyl diaminoethane-N,N',N'-triethanoic acid.
-----

```

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-----
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
-----

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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=13.75 B2=25.00  1980ZMa (60572) 560
*****
C8H10N6O2S2       H2L                      (2746)
2,5-Dihydroxybenzoquinone bis-thiosemicarbazone;
-----

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-----
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>

\*\*\*\*\*

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

\*\*\*\*\*

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  
-----

Sm+++ gl NaClO4 25°C 0.10M U K1=12.62 2002BBh (61319) 567  
B(SmHL)=20.11  
B(SmH2L)=24.42  
B(SmH-1L)=3.91  
B(SmH-2L)=-6.8

\*\*\*\*\*

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  
-----

Sm+++ gl oth/un 25°C 0.10M U K1=2.974 1987TSb (61442) 568

\*\*\*\*\*

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

Sm+++ vlt KNO3 25°C 0.10M U K1=10.97 1972GBd (61522) 570

\*\*\*\*\*

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 1971DRa (61677) 571  
K3=8.16

Medium: 75% acetone, 0.1 M NaClO4

\*\*\*\*\*

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

\*\*\*\*\*

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  
-----

Sm+++ gl NaClO4 25°C 0.10M M H K1=4.42 1986Cdb (61715) 573  
DH=15.3 kJ mol<sup>-1</sup>, DS=136 J K<sup>-1</sup> mol<sup>-1</sup>

\*\*\*\*\*

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

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

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

-----  
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);  
-----

-----  
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;  
-----

-----  
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);  
-----

-----  
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;  
-----

-----  
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  
-----

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

2-(2'-Thiazolylozo)-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   Hemimellitic ac CAS 569-51-7 (1621)
1,2,3-Benzenetricarboxylic acid; C6H3.(COOH)3
-----
```

```
-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Sm+++      gl  NaClO4 25°C 0.10M U   H    K1=5.08      1994CRa (63976) 588
                                K(Sm+HL)=2.75
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   Oxine          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          Kso(SmL3)=-30.80
1981FCa (64343) 590
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          K2K3=12.07
1960RYa (64346) 593
-----
```

```
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 1958FOb (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 1985OHb (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

\*\*\*\*\*

C9H1002 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 NaCl04 25°C 0.1M C H K1=2.19 B2= 3.75 1996HYa (65373) 603  
By calorimetry: DH(K1)=9.47 kJ mol<sup>-1</sup>, DH(B2)=18.16 J K<sup>-1</sup> mol<sup>-1</sup>  
-----

Sm+++ gl NaCl04 25°C 0.10M C H K1=2.19 B2=3.75 1990HYa (65374) 604  
By calorimetry: DH(K1)=9.5 J K<sup>-1</sup> mol<sup>-1</sup>, DH(K2)=8.7  
\*\*\*\*\*

C9H1003 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 NaCl04 25°C 1.0M U K1=2.57 B2=4.46 1966TVa (65444) 605  
K3=1.54  
K4=1.31  
-----

\*\*\*\*\*  
C9H1003 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 NaCl04 25°C 0.10M C K1=2.24 B2=3.64 1989HMa (65466) 606  
\*\*\*\*\*

C9H1003 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 NaCl04 25°C 0.10M C K1=2.24 B2=4.11 1989HMa (65480) 607  
\*\*\*\*\*

C9H1004 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 NaCl04.  
\*\*\*\*\*

C9H1004 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 NaCl04.  
\*\*\*\*\*

C9H1004 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.

\*\*\*\*\*

C9H1004 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.

\*\*\*\*\*

C9H1004 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

\*\*\*\*\*

C9H1005 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

\*\*\*\*\*

C9H1005 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

\*\*\*\*\*

C9H1008 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.

\*\*\*\*\*

C9H11N02 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



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  NaCl04 30°C 0.10M U          K1=2.64      1969DNc (68771) 636
*****
C10H7N05S          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
*****
C10H7N05S          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
*****
C10H7N05S          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)
*****
C10H7N05S          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
*****
C10H7N08S2          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
*****
C10H7N08S2          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;

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

Sm+++ gl NaCl 25°C 0.10M U K1=4.017 B2=6.271 1974SAa (69064) 644  
\*\*\*\*\*

C10H7N5O5 HL CAS 102964-51-2 (6212)  
5-(2'-Nitrophenylazo)barbituric acid;

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

Sm+++ gl diox/w 25°C 75% U K1=4.75 B2=9.29 1986MIa (69101) 645  
\*\*\*\*\*

C10H7O2F3 HL CAS 326-06-7 (196)  
3-Benzoyl-1,1,1-trifluoroacetone; CF3.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=6.72 B2=13.14 1995MTa (69162) 646  
K3=5.57

Medium: 0.1 M NaClO4 in 80% (v/v) EtOH/H2O.

\*\*\*\*\*

C10H8N2 L 2,2'-Bipyridyl CAS 366-18-7 (25)  
2,2'-Bipyridine; (C5H4N)2

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

Sm+++ sp non-aq 25°C 100% C T K1=2.72 2005SYa (69643) 647  
In ethylacetate; At 50 C K1=2.54

Sm+++ sp non-aq 25°C 100% C T K1=2.72 2005SYa (69644) 648  
In ethylacetate; At 50 C K1=2.54

Sm+++ gl NaNO3 25°C 0.50M U K1=0.9 1979HJa (69645) 649  
\*\*\*\*\*

C10H8N4O3 HL CAS 43168-60-1 (6209)  
5-Phenylazobarbituric acid;

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

Sm+++ gl diox/w 25°C 75% U K1=5.41 B2=10.29 1986MIa (69735) 650  
\*\*\*\*\*

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

\*\*\*\*\*

C10H805S 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

\*\*\*\*\*

C10H808S2 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

\*\*\*\*\*

C10H9N04S 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

\*\*\*\*\*

C10H9N30S 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

\*\*\*\*\*

C10H9N302S 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									

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

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  
\*\*\*\*\*

C10H11N02 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  
\*\*\*\*\*

C10H11N03 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

\*\*\*\*\*  
C10H11N50 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  
\*\*\*\*\*

C10H1102F7 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 1987RRc (71405) 673  
B(Sm(gly)L)=10.22  
B(Sm(his)L)=10.89

\*\*\*\*\*  
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 1987RRc (71500) 674  
K(Sm+HA+HL)=5.28  
K(Sm+HB+HL)=5.95  
K(Sm+HL)=4.52

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 1980SGa (71603) 675  
K3=5.62  
K(Sm(NTA)+L)=6.09  
-----  
Sm+++ gl alc/w 24°C 80% U K1=8.7 B2=15.99 1968DZb (71604) 676  
K3=6.0  
K4=4.6

Medium: 80% MeOH, 0.1 M NaCl

-----  
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-1

\*\*\*\*\*  
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;

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

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

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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=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;

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

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<sup>-1</sup>, DS(K1)=270 J K<sup>-1</sup> mol<sup>-1</sup>.

-----  
Sm+++ gl KCl 25°C 1.0M U K(SmL+H)=1.49 1984BKc (74145) 688

-----  
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		1982MPd (74149)	692
							K(SmL+PO4)=3.60		
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	1976BKa (74153)	696
							K(SmL+HL)=2.49		
							K(2SmL+L)=6.66		
Sm+++	gl	KCl	25°C	1.0M	U			1976GMb (74154)	697
							K(SmL+H)=2.03		
Sm+++	sp	KCl	25°C	0.10M	U		K2=3.65	1975BKa (74155)	698
							K(2SmL+L)=6.66		
							K(SmL+HL)=2.49		
Sm+++	EMF	KCl	25°C	0.10M	U	T		1974BKb (74156)	699
							K(SmL+H)=1.69		
Sm+++	gl	KCl	25°C	1.0M	C		K2=3.65	1974BKe (74157)	700
							K(SmL+HL)=2.49		
							K(2SmL+L=Sm2L3)=6.66		
Sm+++	gl	KNO3	20°C	0.10M	U	M		1974TDa (74158)	701
							K(SmL+Citrate)=2.8		
Sm+++	gl	KNO3	25°C	0.10M	U	T M		1973TRb (74159)	702
							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		
Sm+++	gl	KNO3	25°C	0.10M	U	T M		1973TRb (74160)	703
							K(SmL+A)=4.9		
							K(2 C)=4.8, K(35 C)=4.7, K(45 C)=4.6, H4A=adenosine triphosphate		
Sm+++	cal	KNO3	20°C	0.10M	U			1971GKb (74161)	704
							K(SmL(H2O)x=SmL(H2O)x-1+H2O)=-0.7		
Sm+++	gl	NaClO4	25°C	0.10M	U	M		1969AIb (74162)	705
							K(SmL+A)=6.69, H4A=tiron		

-----  
Sm+++ dis oth/un 25°C ? U K1=16.81 1969PJa (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 1959BDb (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 1993VLa (74816) 714  
K(Sm(nta)+L)=4.19  
K(Sm(edta)+L)=4.04  
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 KNO3 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 B2=18.48 K3=8.44	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		K(Sm(edta)+L)=3.51 K(Sm(edta)+HL)=2.06 K(Sm(edta)+H2L)=1.82	1977GMa (75493)	723
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Method: Pt/H2 electrode.

Sm+++	gl	NaClO4	20°C	0.10M	U			K(SmL+A)=3.54 K(SmL+B)=3.64	1974PJa (75494)	724
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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+H2L)=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+++ gl 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 kJ mol<sup>-1</sup>(25 C), DS=228 J K<sup>-1</sup> mol<sup>-1</sup>  
-----

Sm+++ gl KNO3 25°C 0.10M U K1=15.17 1956SPa (75500) 730  
By polarography K1=15.3

\*\*\*\*\*  
C10H19N3O4 HL Leu-Gly-Gly CAS 1187-50-4 (1230)  
Leucyl-glycyl-glycine; H2N.CH(CH2.CH(CH3)2).CO.NH.CH2.CO.NH.CH2.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. DH(K1)=3.6 kJ mol<sup>-1</sup>, DS(K1)=78 J K<sup>-1</sup> mol<sup>-1</sup>.

\*\*\*\*\*  
C10H20N2O4 H2L CAS 58534-57-9 (2113)  
Hexamethylenediamine-N,N-diethanoic acid; H2N(CH2)6.N(CH2.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(Sm+HL)=7.07

\*\*\*\*\*  
C10H20O5 L 15-Crown-5 CAS 33100-27-5 (576)  
1,4,7,10,13-Pentaoxacyclopentadecane; cyclo(-(O.CH2.CH2)5-)  
-----

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

Sm+++ cal non-aq 25°C 100% U H K1=2.81 1993LLa (76126) 733  
Medium: MeCN. DH(K1)=-45.7 kJ mol<sup>-1</sup>.

-----  
Sm+++ dis non-aq 25°C 100% U B2=8.27 1990NIa (76127) 734  
B2=extraction eq.constant: M+3P+2(S)=ML2P3(S); solvent(S)=CH2Cl2, P=picrate

-----  
Sm+++ gl non-aq 25°C 100% C K1=7.34 B2=9.28 1989BPa (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 1986BDa (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 1975DJa (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 1984APa (77043) 740  
-----

Sm+++ gl mixed 22°C 60% U K1=4.06 B2=7.74 1979JMa (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 1975DJa (77065) 742  
-----

\*\*\*\*\*  
C11H8O3 HL CAS 483-35-6 (3347)  
2-Hydroxy-3-methyl-1,4-naphthoquinone;  
-----

-----  
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 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=5.31 1975DJa (77133) 745  
\*\*\*\*\*  
C11H8O4 HL CAS 7555-37-5 (4812)  
3-Acetyl-4-hydroxycoumarin  
-----

-----  
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; CHO.C9H30(:O)(CH3)(OH)  
-----

-----  
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;  
-----

-----  
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;  
-----

-----  
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 <sup>-1</sup> , DS=121 J K <sup>-1</sup> mol <sup>-1</sup>									
*****									
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 K3=4.34	1979MBc (78377)	760
*****									
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

\*\*\*\*\*

C11H13N03 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 NaCl04 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 NaCl04.

\*\*\*\*\*

C11H13N04 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.

\*\*\*\*\*

C11H13N04S 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 NaCl04 25°C 0.10M U K1=18.40 1982MSc (78596) 765

\*\*\*\*\*

C11H13N05 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

\*\*\*\*\*

C11H15N05 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; ((HOOCH2)2N.CH2.)2.CH2

-----  
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: KClO4. 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);

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Sm+++ gl mixed 30°C 75% U K1=9.63 B2=18.71 1972DSd (79657) 780  
K3=8.17

Medium: 75% acetone

\*\*\*\*\*

C11H18O2 HL CAS 5601-52-5 (4821)  
2-Butanoyl-6-methylcyclohexanone (2-butyryl-6-methylcyclohexanone);

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Sm+++ gl mixed 30°C 75% U K1=10.75 B2=21.01 1972DSd (79668) 781  
Medium: 75% acetone

\*\*\*\*\*

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; HOOC.C(C4H9)2.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 B2=12.09 1995MTa (80190) 785  
K3=5.46

Medium: 0.1 M NaClO4 in 80% (v/v) EtOH/H2O.

\*\*\*\*\*  
 C12H8N2 L Phenanthroline CAS 66-71-7 (144)  
 1,10-Phenanthroline;

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

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

\*\*\*\*\*  
 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

\*\*\*\*\*  
 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.COoH

-----  
 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

\*\*\*\*\*  
 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 1988RNa (82177) 804  
 B(Sm+HL)=6.16

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 1985CBa (82234) 806  
 K(SmL+H)=6.92  
 K(SmHL+H)=5.52

DH(K1)=27.2 kJ mol<sup>-1</sup>, DS=273 J K<sup>-1</sup> mol<sup>-1</sup> (by calorimetry)

\*\*\*\*\*  
 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

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-----
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
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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
-----

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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=14.76      1985TPa (82473) 812
*****
C12H20N2O9          H4L  EEDTA          CAS 923-73-9 (2112)
Oxa-bis(ethyleneimino)diethanoic acid; ((HOOC.CH2)2N.CH2.CH2)2O
-----

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-----
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
-----

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-----
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
-----

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-----
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-1.										

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	1989BPa (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-1.										

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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-1.										

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 Et4NClO4  
In propylene carbonate, 0.1 M Et4NClO4, 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  
-----

Sm+++ gl non-aq 25°C 100% C K1=5.18 1989BPa (84020) 828  
Medium: anhydrous propylene carbonate, 0.1 M Et4NClO4

\*\*\*\*\*  
C12H28N2O9P2 H4L (7242)  
1,4,10-Trioxa-7,13-diazacyclopentadecane-7,13-diylldimethylenediphosphonic acid;

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

Sm+++ gl R4N.X 25°C 0.10M U K1=14.01 1996BJa (84164) 829  
K(Sm+HL)=10.63  
K(Sm+H2L)=5.79

Medium: 0.1 M Me4NCl

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

Sm+++ gl NaNO3 25°C 0.20M C K1=8.14 1991KKa (84352) 830

Sm+++ gl NaCl 20°C 0.10M C K1=10.1 1988SJB (84353) 831

\*\*\*\*\*  
C13H50F13S 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 1995MTa (84461) 832  
K3=4.57

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  
-----

Sm+++ sp alc/w 25°C 50% U K1=9.96 1982HMa (84507) 833

\*\*\*\*\*  
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

\*\*\*\*\*

C13H11NO4S H2L CAS 124452-52-4 (8496)  
2-[(Phenylimino)methyl]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.

\*\*\*\*\*

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  
\*\*\*\*\*

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 NaClO4  
\*\*\*\*\*

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 NaClO4  
\*\*\*\*\*

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-Benzylnitriilotriethanoic acid;

-----  
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  
-----

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Sm+++ gl KNO3 25°C 0.10M U T H K(Sm+HL)=3.60 1981SGf (86026) 848  
Data for 35 and 45 C. DH(Sm+HL)=14.3 kJ mol<sup>-1</sup>, DS(Sm+HL)=118 J K<sup>-1</sup> mol<sup>-1</sup>.  
\*\*\*\*\*  
C13H19NO3 H2L (2031)  
2-(1-(2-Hydroxyphenyl)-ethylimine)-3-methylbutanoic acid;  
-----

-----  
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-Cyclopentanediaminotetraethanoic acid;  
-----

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Sm+++ gl KCl 25°C 1.0M U K1=12.46 K(SmHL+H)=3.92 K(SmL+H)=4.60 1989CMb (86127) 850  
\*\*\*\*\*  
C13H22N2O8 H4L CAS 1798-14-7 (921)  
(Pentamethylenedinitrilo)tetraethanoic acid; ((HOOC.CH2)2N.CH2.CH2)2CH2  
-----

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Sm+++ gl KNO3 25°C 0.10M C K1=10.17 K(Sm+HL)=6.66 1982PPd (86205) 851  
\*\*\*\*\*  
C13H22N2O8 H4L CAS 1198-14-7 (5004)  
1,2-Diaminopentane-N,N,N',N'-tetraethanoic acid; (HOOCCH2)2NCH2CH(C3H7)N(CH2COOH)2  
-----

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Sm+++ vlt KNO3 20°C 0.10M U K1=18.25 1974NLa (86235) 852  
\*\*\*\*\*  
C13H22N2O8 H4L (7164)  
2,4-Diaminopentane-N,N,N',N'-tetraethanoic acid;  
(HOOCCH2)2NCH(CH3)CH2CH(CH3)N(CH2COOH)2  
-----

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

-----  
 Sm+++ gl KNO3 20°C 0.10M U K1=11.82 1981NSc (86263) 853  
 \*\*\*\*\*  
 C13H22N2O8 H4L (5003)  
 3-Methyl-1,2-diaminobutane-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=18.12	1968NLb (86290)	854
*****										
		C13H22N2O9	H4L	DETAP				CAS 36829-96-6	(5602)	
Bis(2-aminoethyl)ether-N,N,N'-triethanoic acid-N'-(3-propanoic acid);										

-----

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Sm+++	gl	KNO3	25°C	0.10M	C			K1=15.29 K(Sm+HL)=9.59	1985PLa (86310)	855
*****										
		C13H26O5	L					(6410)		
15,15-Dimethyl-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%	C	H		K1=3.72	1998LBc (86487)	856
Medium: acetonitrile. DH(K1)=-7.36 kJ mol <sup>-1</sup> , DS(K1)=46.5 J K <sup>-1</sup> mol <sup>-1</sup> .										
*****										
		C14H8O4	H2L	Alizarin				CAS 72-48-0	(1058)	
1,2-Dihydroxyanthraquinone;										

-----

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Sm+++	gl	oth/un	25°C	0.10M	U			K1=11.98	1981EIa (86649)	857
*****										
		C14H8O7S	H3L	DASA				CAS 83-61-4	(950)	
1,2-Dihydroxyanthraquinone-3-sulfonic acid, Alizarin Red S;										

-----

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Sm+++	gl	NaClO4	25°C	0.20M	U	M		K1=10.24	1987Vsa (86754)	858
K(Sm(cdta)+L)=5.94, K(Sm(dtpa)+L)=5.28.										

-----

Sm+++	gl	NaClO4	25°C	0.10M	U	T	M		1985RMb (86755)	859
K(Sm(nta)+L)=5.02										
K(Sm(edta)+L)=5.42										
K(Sm(hedta)+L)=5.00										
K(Sm(cdta)+L)=6.41										

Also data for 35 C.  
 hedta is N-hydroxy-1,2-diaminoethane-N,N',N'-triethanoic acid.

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Sm+++	gl	NaClO4	25°C	0.20M	U	M		K1=10.21	1984LSe (86756)	860
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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

\*\*\*\*\*

C14H12NO2Cl 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

\*\*\*\*\*

C14H12NO2F 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 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 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 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 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 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 1.0M U K1=8.02 1987CMe (88462) 885  
 K(SmHL+H)=6.06  
 K(SmL+H)=7.07

\*\*\*\*\*

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

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

Sm+++ gl KCl 25°C 1.0M U K1=18.50 1987CMe (88771) 886  
 K(SmL+H)=1.78

-----  
 Sm+++ gl KCl 25°C 1.00M U K1=18.50 1984MFa (88772) 887  
 -----

Sm+++ gl NaClO4 30°C 0.10M U I M 1982MMd (88773) 888  
 K(SmL+A)=6.36  
 K(SmL+B)=3.68  
 K(SmL+C)=3.28

Data for 0.00-0.25 M NaClO4 and 25-75% dioxane/H2O. H3A is alizarin red S,  
 H2B is 8-hydroxyquinoline-5-sulfonic acid, H2C is iminodiethanoic acid.

-----  
 Sm+++ gl NaClO4 25°C 0.50M U K1=17.91 1977GGb (88774) 889  
 -----

Sm+++ sp none 25°C 0.0 C K1=15.83 1977HAa (88775) 890  
 Medium not reported.

-----  
 Sm+++ EMF KNO3 25°C 0.10M U H K1=18.63 1962MHa (88776) 891  
 DH(K1)=20.9 kJ mol-1, DS=427 J K-1 mol-1. At 20 C: K(SmL+H)=2.18  
 -----

Sm+++ vlt KNO3 20°C 0.10M U K1=18.38 1954SGa (88777) 892  
 \*\*\*\*\*

C14H22N2O8 H4L trans-1,3-CDTA CAS 92681-24-8 (2849)  
 trans-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=8.05 1987CMe (88841) 893  
 K(SmHL+H)=5.35  
 K(SmL+H)=7.50

\*\*\*\*\*

C14H22N2O8 H4L trans-1,4-CDTA CAS 92681-26-0 (2843)  
 trans-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 1.0M U K1=8.56 1987CMe (88867) 894  
 K(SmHL+H)=6.02  
 K(SmL+H)=6.45  
 -----

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; HOOC.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<sup>-1</sup>, DS=317.2 J mol<sup>-1</sup> K<sup>-1</sup>. 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<sup>-1</sup>, DS(K1)=336 J K<sup>-1</sup> mol<sup>-1</sup>.

-----  
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<sup>-1</sup>

-----  
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<sup>-1</sup>, DS=316 J K<sup>-1</sup> mol<sup>-1</sup>

-----  
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<sup>-1</sup>, DS=313 J K<sup>-1</sup> mol<sup>-1</sup>

-----  
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.COOH)CH2.COOC2H5)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.COOH)2

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

Sm+++ gl NaClO4 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	KNO3	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	KNO3	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;

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

Sm+++ gl R4N.X 25°C 0.10M C K1=3.82 2001V Sa (90053) 926  
K(SmL+H)=4.08

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;

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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=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 1968V La (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;  
 -----

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

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.O.(CH2.CH2.O)6.CH3  
 -----

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-diyl dimethylenediphosphonic acid;  
 -----

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  
 \*\*\*\*\*  
 C14H37O12N2P4 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

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-----
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)
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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;
-----

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-----
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;
-----

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-----
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
-----

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-----
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
-----

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-----
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
-----

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\*\*\*\*\*

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.  $K(\text{Sm}+3\text{HL}(\text{org})=\text{SmL}_3(\text{org})+3\text{H})=-17.99$

\*\*\*\*\*

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 1983AGb (91847) 954  
K3=7.95

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-Benzyl diaminoethane-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 1966VLa (92382) 960

Sm+++ vlt oth/un ? ? U K1=18.4 1966VLa (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'-methyamide;

-----  
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;  
-----

-----  
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  
-----

-----  
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;  
-----

-----  
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;  
-----

-----  
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;  
-----

-----  
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  
-----

-----  
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  
-----

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 1997IHa (93119) 970  
B3=25.23

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-naphthalylidysulfonic acid;

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Sm+++ gl NaCl04 30°C 0.10M U 1976NDa (93208) 972  
K(Sm+H2L=SmH2L)=5.51  
K(SmHL+H)=7.44  
K(SmL+H)=10.20  
\*\*\*\*\*

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 1971SSd (93265) 973  
K(Sm+H2L)=8.39  
\*\*\*\*\*

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.

\*\*\*\*\*

C16H1403 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  
 \*\*\*\*\*

C16H1404 HL BHMMA (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-Acetylphenylhydrazone)-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)

-----  
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  
-----

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

\*\*\*\*\*

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  
 -----

Sm+++ gl NaCl 37°C 1.0M C K1=23.3 1994TBb (94926) 995  
 Method: Competitive reaction with Eu3+ ion.

\*\*\*\*\*

C16H29N5O8 H3L (6505)  
 Diethylenetriaminepentaethanoic acid N,N'-bismethylamide;

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

Sm+++ gl NaClO4 25°C 0.10M C H K1=16.69 1993RCa (95001) 996  
 DH(K1)=-25.1 kJ mol-1, DS(K1)=235 J K-1 mol-1

\*\*\*\*\*

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  
 -----

Sm+++ gl R4N.X 25°C 0.10M U K1=12.12 1983CRb (95054) 997

\*\*\*\*\*

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  
 In acetonitrile, 0.1 M Et4NClO4.

-----  
 Sm+++ ISE non-aq 25°C 100% C K1=2.9 1989MGa (95286) 999  
 Medium: DMF, 0.10 M Et4NClO4

-----  
 Sm+++ gl R4N.X 25°C 0.25M C K1=6.76 1981BBe (95287)1000  
 Medium: Me4NCl

\*\*\*\*\*

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  
 Medium: MeCN. DH(K1)=-31.5 kJ mol-1.

\*\*\*\*\*

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

K(Sm+HL)=6.98

-----  
Sm+++ gl oth/un 25°C 0.10M U 1984ZGa (95670)1003

K(Sm+HL)=6.98

K(Sm+H2L)=5.21

\*\*\*\*\*

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

\*\*\*\*\*

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

\*\*\*\*\*

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

\*\*\*\*\*

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

\*\*\*\*\*

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

-----  
Sm+++ gl NaNO3 20°C 0.10M U M 1981GCa (95899)1008

B(Sm+3L+3TBP)=25.30

B(Sm+3L+4TBPOxide)=31.8

\*\*\*\*\*

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  
-----  
Sm+++ gl diox/w 30°C 75% M K1=8.97 B2=17.18 1987ESa (96013)1009  
\*\*\*\*\*  
C17H16O4 H2L CAS 29976-84-9 (8523)  
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  
K(Sm+HL)=8.50  
K(SmHL+HL)=7.30

Medium: 70% v/v dioxane/H2O, 1.0 M NaClO4.

\*\*\*\*\*  
C17H16O4 H2L CAS 58134-82-0 (6193)  
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  
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  
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>

\*\*\*\*\*  
C17H20N3O3F HL (7845)  
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  
K3=4.20

Medium: 0.1 M NaClO4 in 70% v/v EtOH/H2O

\*\*\*\*\*  
C17H23N4O4BrS H2L (1594)  
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  
K(Sm+HL)=2.80

\*\*\*\*\*  
C17H27N04 L CAS 71089-11-7 (7945)  
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(SmNO3+L)=3.85										
Medium: acetonitrile. DH(SmNO3+L)=-49.66 kJ mol <sup>-1</sup> .										
*****										
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	KNO3	25°C	0.10M	U			K1=8.71 K(Sm+HL)=5.67	1984TPa (96577)	1016
*****										
C18H15NO3		HL						(6196)		
8-Formyl-7-hydroxy-4-methyl-2H-[1]-benzopyran-2-one 4-methylanil; CH3.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=6.65 B2=12.36 B3=17.07	1987ECa (96998)	1017
*****										
C18H16N2O3		HL						(5560)		
2-(2-Acetylphenylhydrazone)-1-phenyl-but-1,3-dione; C6H5.CO.C(CO.CH3):N.NH.C6H4.COCH3										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Sm+++	gl	diox/w	30°C	75%	U			K1=10.56 B2=19.76	1988ESb (97179)	1018
*****										
C18H18N4		L						CAS 16858-01-8	(1528)	
Tris(2-pyridylmethyl)amine; (C5H4NCH2)3N										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Sm+++	nmr	KCl	25°C	1.0M	C	H		K1=2.51	2004BRa (97272)	1019
Method: 1H nmr measurements in D2O. DH(K1)=-12 kJ mol <sup>-1</sup> , DS(K1)=6 J mol <sup>-1</sup> K <sup>-1</sup>										
*****										
C18H20N2O6		H4L			EHPG			CAS 10328-28-6	(429)	
N,N'-Ethylene-bis-(2-(2'-hydroxyphenyl))glycine; (HOOCCH(C6H4OH)NHCH2.)2										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Sm+++	EMF	KNO3	25°C	0.10M	C	T H		K1=18.62 K(SmL+H)=7.20	1985HWb (97440)	1020
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> .										
*****										

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  
-----

Sm+++ gl KNO3 25°C 0.10M C K1=15.66 1985TPa (97659)1021  
\*\*\*\*\*

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  
\*\*\*\*\*

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  
\*\*\*\*\*

C18H29N04 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>.  
\*\*\*\*\*

C18H30N2O11 H2L CAS 93049-99-1 (5832)  
1,4,7,10,13-Pentaoxa-16,19-diazacycloeicosane-14,21-dione-16,19-diethanoic 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 C K1=9.71 1988CCb (97916)1025  
\*\*\*\*\*

C18H30N4O12 H6L TTHA CAS 869-52-3 (694)  
Triethylenetetraaminehexaethanoic acid;((HOOC.CH2)2N.CH2.CH2.N(CH2.COOH).CH2)2

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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
Sm+++	gl	NaNO3	25°C	0.20M	C			K1=14.47	1991KKa (98223)	1032

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Sm+++	EMF	NaCl	80°C	1.00M	C			K1=14.97 K(SmL+H)=3.90	1986LDb (98224)	1033
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 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
Sm+++	gl	R4N.X	25°C	0.10M	C			K1=7.44	1988CCc (98344)	1034

\*\*\*\*\*

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>.  
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Sm+++	ISE	non-aq	25°C	100%	C			K1=2.7	1989MGa (98728)	1036
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Medium: DMF, 0.10 M Et4NClO4  
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Sm+++	ISE	non-aq	25°C	100%	U	H		K1=17.3	1986ALa (98729)	1037
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Medium: propylene carbonate, 0.1 M Et4NClO4  
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Sm+++	ISE	non-aq	25°C	100%	U	H		K1=15.99	1984GBa (98730)	1038
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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.  
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Sm+++	gl	alc/w	25°C	100%	C	I		K1=9.70	1983ANb (98731)	1039
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The equilibration took 7-12 days. Medium: MeOH, 0.05 M Et4NC1O4  
In propylene carbonate, 0.1 M Et4NC1O4, K1=19.0

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Sm+++ gl R4N.X 25°C 0.25M C K1=5.94 1981BBe (98732)1040  
Medium: Me4NC1

\*\*\*\*\*  
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

\*\*\*\*\*  
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

\*\*\*\*\*  
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

\*\*\*\*\*  
C20H14N2O11S3 H5L Chromotrope 8B CAS 5850-64-6 (2674)  
3-(4'-Sulfonaphthylazo)chromotropic acid;

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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			K1eff=4.09	1978BRb (99735)	1046

Keff 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			K(Sm+HL)=5.30 K(Sm+2HL)=10.80	1985RSb (99840)	1047

\*\*\*\*\*  
 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			K1=19.24 K(SmL+H)=5.51 K(SmHL+H)=4.98	1985SNb (100015)	1048

\*\*\*\*\*  
 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		K1=3.84	1998LHa (100237)	1049

Medium: acetonitrile. DH(K1)=-3.01 kJ mol<sup>-1</sup>.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Sm+++	gl	oth/un	25°C	0.0	U	H		K1=2.23	1991HJa (100238)	1050

\*\*\*\*\*  
 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			K1=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			K1=15.35	1991KKa (100545)	1052



Sm+++ sp oth/un 25°C var U I 1997HRb (101646)1059

K1(eff)=7.569  
B(SmLCl)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-heptaoxacycloheneicosa-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	NaClO <sub>4</sub>	25°C	0.10M	U		K <sub>1</sub> =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		K <sub>1</sub> =20.50	1981GMh (102341)	1067

Method: polarography, using Cd as indicator ion. Medium: 0.01 M Et<sub>4</sub>NBr.

Sm+++	gl	KNO <sub>3</sub>	30°C	0.10M	U		K <sub>1</sub> =20.50	1976GAa (102342)	1068
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Sm+++	gl	KNO <sub>3</sub>	25°C	0.10M	U		K <sub>1</sub> =20.50 K(Sm+HL)=14.43 B(SmH-1L)=5.29	1968MIc (102343)	1069
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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	KNO <sub>3</sub>	40°C	0.50M	U T		K <sub>1</sub> =18.18 K(SmL+H)=3.93	1995BIa (102360)	1070

Also data for 80 C.

\*\*\*\*\*

C23H16O9Cl<sub>2</sub>S H4L Chrome azuro<sub>1</sub> S CAS 1667-99-8 (711)

Chromazuro<sub>1</sub> 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-Acetylphenylhydrazone)-1,3-diphenyl-prop-1,3-dione;

C<sub>6</sub>H<sub>5</sub>.CO.C(CO.C<sub>6</sub>H<sub>5</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=10.90 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'-phenylmethylene-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-octaoxacyclotetracosane-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-Hexaazatricyclohexatetracos-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 BAHP (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 2001SYb (104990)1088

K(SmL+H)=4.4

Medium: 50% EtOH/H2O, 0.10 M KNO3.

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C31H24N4O HL CAS 88700-85-0 (1409)

1,2-Diphenyl-1,2-ethanedione-3-(4-benzyl-6-phenyl)-pyridazinyl hydrazone;

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

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Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
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Sm+++ sp NaNO3 20°C 0.20M U 1963BBb (105493)1090

B(Sm2L2)=47.0

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C32H28N8O10S2 H4L Diantipyrylazo CAS 14918-39-9 (5368)  
2,7-Bis(antipyrynylphenylazo)chromotropic acid;

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Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Sm+++ sp KNO3 ? 0.20M U 1968BBa (105572)1091  
K(?)=78.9

\*\*\*\*\*  
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

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Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Sm+++ sp diox/w 25°C 100% C 1997KMa (105636)1092  
K(La(NO3)3+L)=4.13

\*\*\*\*\*  
C33H36N4O6 L Bilirubin CAS 635-65-4 (2623)  
Bilirubin

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Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Sm+++ sp non-aq 50% U K1=5.52 1972KPb (105898)1093  
K(SmL+Sm)=4.68

Medium: 1:1 v/v CHCl3:EtOH

\*\*\*\*\*  
C33H45N7O3 L CAS 345349-93-1 (9178)  
Tris[6-((2-N,N-diethylcarbamoyl)pyridyl)methyl]amine;

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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;

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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);

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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

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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;

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Sm+++ cal non-aq 25°C 100% U H K1=4.14 2001NJa (107708)1102  
Method: microcalorimetry. Medium: MeCN.. DH(K1)=-164 kJ mol-1

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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 2001NJa (107885)1103  
Method: microcalorimetry. Medium: MeCN.. DH(K1)=-86.4 kJ mol-1

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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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