

SC-Database

Software version = 5.81 Data version = 4.62

Experiment list contains 514 experiments for  
(no ligands specified)

Metal : Tm+++

(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
Tm+++	oth	none	25°C	0.0	U				1974JOb (988)	1
								K(Tm+3e=Tm(s))=-117.7(-2.32V)		
								K(Tm+e=Tm(II))=-35(-2.1V)		

Method: literature evaluated data

Tm+++	oth	none	25°C	0.0	U				1969NBa (989)	2
								K(Tm+e=Tm(II))=-40.6(-2.4V)		

Method: Estimated data

Tm+++	sp	oth/un	25°C	0.00	U				1964BDb (990)	3
								K(Tm+e=Tm++) = -42, -2500 mV		

Tm+++	oth	none	25°C	0.0	U				1952LAb (991)	4
								K(Tm+3e)=-115.5(-2280 mV)		

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Tm+++	sol	none	25°C	0.0	C				1992FIa (1163)	5
								Kso(TmAsO4)=-23.08		

Equilibrium monitored by EDTA and iodine titrations.

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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
Tm+++	gl	NaClO4	25°C	0.70M	C			K1=5.96	2004LBb (3401)	6
								K(Tm+HCO3=TmHCO3)=1.47		

Medium: 0.70 m NaClO4. Calculated for I=0, K1=7.68, B2=13.27,  
K(Tm+HCO3=TmHCO3)=2.52, K(Tm+HL=TmL+H)=-2.65, K(Tm+2HL=TmL2+2H)=-7.39

Tm+++	dis	NaClO4	25°C	0.70M	C	I		K1=5.95 B2=10.75	1998LBb (3402)	7
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Method: H2O/tributylphosphate distribution and ICP-mass spectrometry.

Values calculated for I=0.0 M, K1=7.93, B2=13.83.

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 Tm+++ sol none 25°C 0.0 C 1986FMa (3403) 8  
 Kso(Tm2(CO3)3)=-31.58  
 -----

Tm+++ sol none 25°C 0.0 C 1986HMa (3404) 9  
 Kso(Tm2(CO3)3)=-31.58  
 -----

Method: spectrophotometry.

-----  
 Tm+++ dis oth/un 20°C 2.5M C 1979DBb (3405) 10  
 B4=15.71  
 -----

Media: 2.5 M (NH4)2NO3/hexane. Analysis by NAA. By competition with edta;  
 K1(Tm(edta))=19.24 recalculated for I=2.5 from J.Am.Chem.Soc.,75 1953,4196  
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C6N6Fe--- H3L Ferricyanide (2491)  
 Hexacyanoferrate (III); Fe(III)(CN)6---  
 -----

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Tm+++	cal	none	25°C	0.00	M	H	K1=3.67	1972SCd (3695)	11

DH(K1)=4.4 kJ mol<sup>-1</sup>, DS=84.9 J K<sup>-1</sup> mol<sup>-1</sup>  
 -----

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
Tm+++	cal	non-aq	25°C	100%	C	HM	K1=2.6 B(Tm(phen)Cl)=5.2 B(Tm(phen)Cl2)=6.9 B(Tm(phen)Cl3)=8.81	2002KNc (5900)	12

Medium: DMF, 0.20 M Et4NC104. DH(K1)=27 kJ mol<sup>-1</sup>, DH(Tm(phen)Cl)=4.0,  
 DH(Tm(phen)Cl2)=28, DH(Tm(phen)Cl3)=6.  
 -----

Tm+++ dis NaCl 25°C 1.0M C K1=-0.14 1997HTb (5901) 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.  
 -----

Tm+++ cal non-aq 25°C 100% U H K1=2.57 B2=5.33 1991ITa (5902) 14  
 K3=2.04  
 K4=1.55

Medium: DMF, 0.2 M Et4NC104. DH(K1)=27.4 kJ mol<sup>-1</sup>, DH(K2)=16.6, DH(K3)=21  
 DH(K4)=20. DS(K1)=141, DS(K2)=109, DS(K3)=108 J K<sup>-1</sup> mol<sup>-1</sup>  
 -----

Tm+++ sol NaClO4 25°C ? U K1=0.25 1982MAa (5903) 15  
 -----

Tm+++ cal non-aq 25°C 100% U K1=2.45 B2=4.82 1980VCa (5904) 16  
 Medium: diemthylacetamide  
 -----

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Tm+++	ix	oth/un	25°C	0.02M	C	T H		K1=3.77 B2= 6.09	2004LMa (7270)	17
Medium: 0.025 M HNO3. Applying Pitzer parameters: at I=0, K1=9.88. Data for 5 to 45 C. DH(K1)=10.6 kJ mol <sup>-1</sup> , DH(B2)=20.6.										
Tm+++		ISE NaClO4	25°C	0.0	C	I		K1=4.29	2000LBa (7271)	18
Method: Fluoride ISE. Values calc. from data for I=0.015-0.70 M NaClO4. At I=0.70 M, K1=3.361.										
Tm+++	ix	KNO3	25°C	0.02M	C			K1=3.75 B2= 6.35	1999SBc (7272)	19
Medium: 0.025 M HNO3. Additional method: ICP-MS. Assumed K1(HF) = 3.03, derived from literature values.										
Tm+++		ISE none	25°C	0.0	C	H		K1=3.25 B2=6.94 Kso=-16.1	1989MJa (7273)	20
Also by conductivity and radiometry. DH(Kso)=14.7 kJ mol <sup>-1</sup> ; DS=-294.										
Tm+++		ISE R4N.X	25°C	0.50M	C			K1=3.25 B2=6.94	1989MJb (7274)	21
Tm+++	cal	NaClO4	25°C	1.00M	C	H			1988GBa (7275)	22
DH(K1)=10.8 kJ mol <sup>-1</sup> ; DS(K1)= 104 J mol <sup>-1</sup> K-1										
Tm+++		ISE NaNO3	25°C	0.10M	U	H			1987SMd (7276)	23
K(TmA+L)=2.09 DH=-0.5kJ mol <sup>-1</sup> , DS=38.2 J K-1 mol <sup>-1</sup> . H3A=HEDTA										
Tm+++		ISE NaCl	25°C	1.00M	C			K1=3.155	1985BBb (7277)	24
Tm+++	gl	KCl	25°C	1.00M	U	M			1981KTb (7278)	25
K(TmEDTA+F)=1.65 K(Tm(EDTA)F+F)=0.60										
Tm+++	oth	NaClO4	25°C	0.10M	U			K1=3.58	1973MSg (7279)	26
method:electromigration or transference number										
Tm+++	EMF	NaClO4	25°C	1.0M	U	H		K1=3.56	1967WCa (7280)	27
By distribution: K1=3.57. By calorimetry: DH(K1)=36.2 kJ mol <sup>-1</sup> , DS=189.8 *****										
I03-		HL		Iodate				CAS 7782-68-5	(1257)	
Iodate;										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Tm+++	dis	NaClO4	25°C	0.10M	U			K1=1.33	1973CBd (8569)	28
Tm+++	sol	oth/un	25°C	0.0	U				1966FPb (8570)	29
Kso=-10.36										

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 IO4- HL Periodate CAS 13444-71-8 (6063)  
 Periodate;

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 Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
 -----  
 Tm+++ sol oth/un 25°C dil U 1974LOa (8616) 30  
 Kso(Tm(H2IO6)(H2O)3)=-9.37

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

-----  
 Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
 -----  
 Tm+++ gl oth/un 20°C 0.10M U 1989SBb (8783) 31  
 B(TmHL)=8.26  
 B(Tm2L)=7.29  
 B(TmH2L)=10.55

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

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 Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
 -----  
 Tm+++ cal NaClO4 25°C 2.0M C IH K1=-0.89 1998BMb (9968) 32  
 DH(K1)=7.1 kJ mol-1. From Pitzer extrapolation to I=0.0, K1=-0.11,  
 DH(K1)=5.6 kJ mol-1

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 Tm+++ dis NaClO4 25°C 1.0M U K1=-0.25 1965CSb (9969) 33  
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OH- HL Hydroxide (57)  
 Hydroxide;

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 Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
 -----  
 Tm+++ gl NaClO4 25°C 0.0 C IH 2000Kba (12342) 34  
 \*K1=-7.39  
 In 0.7 M NaClO4, \*K1=-7.70. DH(\*K1)=49 kJ mol-1.

-----  
 Tm+++ gl NaCl 25°C 0.10M U I 1999FBa (12343) 35  
 \*B(1,3)=-20.86  
 In 0.1 M Me4NCl, \*B(1,3)=-21.97.

-----  
 Tm+++ dis NaClO4 ? 0.10M U 1971GDb (12344) 36  
 \*K1=-4.4

Medium: LiClO4

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 Tm+++ gl NaClO4 25°C 0.30M U 1966FKa (12345) 37  
 \*K1=-7.95  
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Tm+++ gl oth/un 25°C var U 1944MKa (12346) 38  
Kso(Tm(OH)3)=-23.5

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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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Tm+++ sol none 25°C 0.0 M 1997LBd (13349) 39  
Kso(TmPO4)=-25.03

Calculated from data for 0.10 M HClO4 solution.

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Tm+++ sol oth/un 25°C 0.0 C I 1993FKb (13350) 40  
Kso(TmPO4)=-26.68

In synthetic seawater, Ks(TmPO4)=-24.08.

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Tm+++ sol none 25°C 0.0 C 1991FBa (13351) 41  
Kso(TmPO4)=-26.05

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

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Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
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Tm+++ gl KNO3 25°C 0.10M U T H B2=9.7 1974KRa (13915) 42  
K(Tm+2HL)=7.3

K(Tm+2HL)=7.5 and B2=9.8 (35 C), K(Tm+2HL)=7.1 and B2=9.4 (45 C)  
DH(Tm+2HL)=-19 kJ mol-1; DH(B2)=-28

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

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Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
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Tm+++ sp oth/un rt 1.00M U K1=-0.89 1970POa (14112) 43  
Medium: HReO4

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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  
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Tm+++ dis oth/un 25°C 1.0M C K1=0.42 1997HTb (15309) 44  
Method: by solvent extraction from 1.0 M NaSCN into CHCl3, 0.1 M  
1,1,1-trifluoro-4-(2-thienyl)-2,4-pentanedione.

-----  
Tm+++ cal non-aq 25°C 100% U H K1=1.7 B2=3.0 1992TIIa (15310) 45  
K3 = 0.4

Medium: DMF, 0.2 M R4NX. DH(K1)=9 kJ mol-1, DH(B2)=6, DH(B3)=40

Tm+++ dis oth/un 30°C 1.0M C T H K1=0.07 B2= 0.42 1980KMe (15311) 46  
 In 1.0 M NH4ClO4/NH4SCN. Extraction of 170Tm into hexane/ammonium dinonyl-  
 naphthalene sulfonate. Data for 15-45 C. DH(K1)=-1.5 kJ mol-1, DH(K2)=-4.9

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S04-- 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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Tm+++ sol oth/un 25°C 0.66M C K1=1.81 2004SBb (16610) 47  
 Method: solubility of BaS04 in 0.117 m TmCl3 solution.  
 Calculated for I=0, K1=3.48.

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 Tm+++ cal none 25°C 0.0 U H 1974POa (16611) 48  
 DH(K1)=20.0 kJ mol-1

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 Tm+++ cal oth/un 25°C 0.0 U H 1969FPa (16612) 49  
 DH(K1)=13.2 kJ mol-1

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 Tm+++ cal oth/un 25°C 0.0 U H K1=3.41 B2=5.21 1969IEa (16613) 50  
 DH(K1)=15.1 kJ mol-1, DH(K2)=3.6; DS(K1)=115.8 J K-1 mol-1, DS(K2)=44.7

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 Tm+++ ISE NaClO4 25°C 2.0M U H K1=1.15 B2=1.59 1967CCd (16614) 51  
 By calorimetry: DH(K1)=17.6 kJ mol-1, DS=81.1 J K-1 m-1; DH(K2)=4.2, DS=22.6

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CH03F3S HL CAS 1493-13-6 (6755)  
 Trifluoromethanesulfonic acid; CF3SO3H

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 Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
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Tm+++ sp non-aq 25°C 100% U K3=2.41 1993BCc (17470) 52

Medium: MeCN

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C2H02Cl3 HL Trichloroacetic CAS 76-03-9 (1205)  
 Trichloroethanoic acid; Cl3C.COOH

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 Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
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Tm+++ cal NaClO4 25°C 2.00M U K1=0.23 1980ECa (18336) 53

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C2H202Cl2 HL CAS 79-43-6 (1282)  
 Dichloroethanoic acid; Cl2CH.COOH

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 Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
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Tm+++ cal NaClO4 25°C 2.00M U K1=0.53 1980ECa (18402) 54

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C2H203 HL Glyoxylic acid CAS 298-12-4 (1142)  
 Glyoxylic acid; OHC.COOH

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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
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Tm+++     gl  NaClO4 20°C 0.10M U          K1=2.61  B2=4.61  1964PSd (18432) 55
                                         K3=1.7

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*****
C2H2O4          H2L  Oxalic acid      CAS 144-62-7 (24)
Ethanedioic acid; (COOH)2
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Tm+++     ix  R4N.X  25°C 0.05M C          K1=5.97  B2=10.46  2001SBf (19112) 56
                                         K(Tm+HL)=2.18
Medium: 0.05 M NH4NO3. At I=0, K1=6.89, B2=11.65.
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Tm+++     gl  KCl    25°C 1.0M U    M          1988KTa (19113) 57
                                         K(Tm(edta)+L)=3.50
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Tm+++     oth oth/un 25°C 0.10M U          K1=5.60  B2=9.52  1971STe (19114) 58
Method : electrical migration or transference number
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Tm+++     ix  oth/un 18°C 0.10M U          K1=3.40  B2=3.45  1967ABa (19115) 59
                                         B3=1.0
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*****
C2H3O2Cl        HL  Chloroacetic      CAS 79-11-8 (34)
Chloroethanoic acid; ClCH2.COOH
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
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Tm+++     cal NaClO4 25°C 2.00M U          K1=0.92          1980ECa (19388) 60
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*****
C2H4O2          HL  Acetic acid      CAS 64-19-7 (36)
Ethanoic acid; CH3.COOH
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
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Tm+++     gl  NaClO4 20°C 0.10M U          K1=2.02  B2=3.61  1962KPa (20207) 61
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*****
C2H4O2S        H2L  Thioglycolic      CAS 68-11-1 (596)
Mercaptoethanoic acid; HS.CH2.COOH
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
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Tm+++     gl  NaClO4 25°C 0.20M U          K1=5.71  B2=10.74  1998PJb (20377) 62
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Tm+++     gl  NaClO4 20°C 0.10M U          1964PKa (20378) 63
                                         K(Tm+HL)=1.98
                                         K(TmHL+HL)1.11
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*****
C2H4O3          HL  Glycolic acid     CAS 79-14-1 (33)
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2-Hydroxyethanoic acid; HO.CH2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Tm+++	gl	KN03	32°C	0.10M	U				1980PPf (20640)	64
								K(Tm+HL=TmL+H)=-0.38		
								*K(TmL)=-5.55		
								K(Tm+2HL=TmL2+2H)=-1.64		
								*K(TmL2)=-5.48		

Tm+++	gl	NaCl04	20°C	0.10M	U			K1=3.055 B2=5.33 B3=7.00	1964PKb (20641)	65
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 C2H5NO2 HL Glycine CAS 56-40-6 (85)  
 2-Aminoethanoic acid; H2N.CH2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Tm+++	EMF	KCl	25°C	1.0M	U	M			1977GMa (21737)	66
								K(TmA+L)=4.39		
								K(TmA+HL)=3.01		
								K(TmA+H2L)=3.03		

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

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 C2H6OS L DMSO CAS 67-68-5 (329)  
 Dimethylsulfoxide; (CH3)2.S0

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Tm+++	sp	non-aq	25°C	100%	U				1992MBb (22128)	67
								K8=0.7		
								K9=0.3		

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

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Tm+++	gl	NaCl04	22°C	0.10M	U				1972MCd (22159)	68
								K(TmH-1L+H)=6.80		

\*\*\*\*\*  
 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
Tm+++	ISE	non-aq	25°C	100%	C	H		K1=2.86 B2=5.36 B3=7.04	1992CBa (23242)	69

Medium: DMSO, 0.10 M Et4NClO4. By calorimetry, DH(K1)=-21.6, DH(B2)=-40.7, DH(B3)=-84.0 kJ mol-1.

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

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Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
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Tm+++ nmr NaClO4 25°C 2.00M U H K1=1.89 1980CCa (24075) 70  
DH=-4.64 kJ mol-1. Alternative method: Calorimetry.

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

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Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
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Tm+++ gl NaClO4 25°C 0.10M U K1=4.91 B2=7.95 1972DCc (24572) 71

Tm+++ gl NaClO4 25°C 1.00M U K1=3.85 B2=6.42 1971DGA (24573) 72  
B3=7.62  
B(TmHL)=6.26  
B(TmHL2)=9.98

-----  
Tm+++ gl KNO3 25°C 0.10M U K1=4.42 B2=7.01 1968PFa (24574) 73

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

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

Tm+++ gl KCl 25°C 0.20M U K1=3.67 1973LPb (24634) 74

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C3H5NO2 HL (4234)  
Isonitrosoacetone; CH3.CO.CH:N.OH, anti-Pyruvic aldehyde oxime

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Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
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Tm+++ gl diox/w 20°C 50% U K1=6.07 1971MAf (24651) 75

Medium: 50% dioxan, 0.1 M NaClO4

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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  
-----

Tm+++ gl diox/w 20°C 50% U K1=7.27 B2=13.42 1971MAF (24813) 76

Medium: 50% dioxan, 0.1 M NaClO4

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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
Tm+++	gl	NaClO4	25°C	2.0M	U		K1=1.61 B2=2.66	1965CGa (25062)	77
Tm+++	gl	NaClO4	20°C	0.10M	U		K1=1.91 B2=3.43	1964PKa (25063)	78
*****									
C3H6O2S		H2L		Thiolactic acid		CAS 79-42-5	(366)		
2-Mercaptopropanoic acid; CH3.CH(SH).COOH									
Tm+++	gl	NaClO4	25°C	0.20M	U		K1=6.44 B2=12.38	1998PJb (25175)	79
Tm+++	gl	NaClO4	25°C	2.00M	U		K(Tm+HL)=1.48	1968Cma (25176)	80
*****									
C3H6O2S		H2L				CAS 107-96-0	(437)		
3-Mercaptopropanoic acid; HS.CH2.CH2.COOH									
Tm+++	gl	NaClO4	25°C	2.00M	U		K(Tm+HL)=1.40	1968Cma (25231)	81
*****									
C3H6O3		HL				CAS 81598-26-7	(2521)		
3-Hydroxypropanoic acid; HO.CH2.CH2.COOH									
Tm+++	gl	NaClO4	25°C	2.00M	U		K1=1.45	1969JCc (25281)	82
*****									
C3H6O3		HL		L-Lactic acid		CAS 79-33-4	(82)		
L-2-Hydroxypropanoic acid; CH3.CH(OH).COOH									
Tm+++	gl	KNO3	30°C	0.10M	U		K(Tm+HL=TmL+H)=0.44 *K(TmL)=-4.55 K(Tm+2HL=TmL2+2H)=-0.64 *K(TmL2)=-3.86	1983MPc (25556)	83
Tm+++	gl	NaClO4	25°C	0.20M	U		K1=2.92 B2=5.26 K3=1.34 K4=0.65	1964DVa (25557)	84
Tm+++	gl	NaClO4	20°C	0.10M	U		K1=3.190 B2=5.71 B3=7.43	1964PKb (25558)	85
*****									

C3H6O3 HL Methoxyacetic CAS 625-45-6 (29)  
Methoxyethanoic acid; CH3.O.CH2.COOH

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Tm+++ gl NaClO4 20°C 0.10M U K1=2.08 B2=3.23 1964PKa (25609) 86  
\*\*\*\*\*

C3H7NO2 HL Alanine CAS 56-41-7 (86)  
2-Aminopropanoic acid; H2N.CH(CH3).COOH

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Tm+++ gl KNO3 25°C 0.10M U K1=4.7 1967EMb (26281) 87  
\*\*\*\*\*

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  
-----  
Tm+++ gl NaClO4 20°C 0.0 U T H K1=7.998 B2=15.90 1980SDc (26846) 88  
Extrapolated from data for I=0.10-1.0 M. Data for 35 and 45 C.  
DH(K1)=-22.8 kJ mol<sup>-1</sup>, DS=75 J K<sup>-1</sup> mol<sup>-1</sup>; DH(K2)=-34.4, DS(K2)=34.  
\*\*\*\*\*

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  
-----  
Tm+++ gl NaClO4 22°C 0.10M U 1972MCd (27687) 89  
K(TmH-1L+H)=6.85  
\*\*\*\*\*

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  
-----  
Tm+++ gl NaClO4 22°C 0.10M U 1972MCd (27755) 90  
K(TmH-1L+H)=6.75  
-----

Tm+++ gl NaCl 25°C 0.10M U 1970PKe (27756) 91  
K(TmH-1L+H)=6.50  
\*\*\*\*\*

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  
-----  
Tm+++ gl KNO3 25°C 0.10M C 1991SKb (28593) 92  
K(TmL+H)=7.01  
K(TmHL+H)=5.6

\*\*\*\*\*

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
Tm+++	cal	NaClO4	25°C	0.10M	U	H	K1=2.78 B2=4.21	19760Ca (28668)	93

DH(K1)=9.8 kJ mol<sup>-1</sup>, DS=86 J K<sup>-1</sup> mol<sup>-1</sup>; DH(B2)=16.8, DS=137

Tm+++	gl	NaClO4	25°C	0.10M	C	H	K1=2.779 B2= 4.22	19760Cb (28669)	94
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By calorimetry: DH(K1)=9.75 kJ mol<sup>-1</sup>, DS(K1)=85.8 J K<sup>-1</sup> mol<sup>-1</sup>;  
DH(B2)=16.8, DS(B2)=137.

\*\*\*\*\*

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
Tm+++	gl	NaClO4	25°C	0.10M	U		K1=3.62	1973CDc (29143)	95

Tm+++	gl	NaClO4	25°C	0.10M	U		K1=3.62 B2=5.64	1970RFa (29144)	96
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\*\*\*\*\*

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
Tm+++	gl	NaClO4	25°C	0.10M	C		K1=2.44 B(TmHL)=5.99 K(Tm+HL)=1.91	1986LCa (29223)	97

Tm+++	gl	NaClO4	25°C	0.10M	U		K1=2.81	1973CDc (29224)	98
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C4H5NO5 H2L (7375)  
Oxalohydroxamic acid; HOOC.CO.CH2.CO.NHOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Tm+++	gl	KNO3	25°C	0.1M	M		K1=11.71 B2=22.62 K3=10.25	1989LWa (29317)	99

\*\*\*\*\*

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
Tm+++	gl	KCl	25°C	0.20M	U		K1=4.38 B2=7.05	1975PLa (30140)	100

\*\*\*\*\*

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  
-----  
Tm+++ gl NaClO4 25°C 0.20M U K1=5.93 B2=11.58 1998Pjb (30369) 101  
\*\*\*\*\*  
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  
-----  
Tm+++ gl KNO3 30°C 0.10M U M 1984AIa (30742) 102  
K(Tm(EDTA)+L)=1.982  
-----

-----  
Tm+++ gl KNO3 20°C 0.10M U 1980SDa (30743) 103  
B(TmHL)=7.80  
-----

-----  
Tm+++ gl KNO3 20°C 0.10M U K1=4.75 B2=7.95 1980Sdb (30744) 104  
K(Tm+HL)=1.11  
-----

-----  
Tm+++ gl NaClO4 25°C 0.10M U K1=5.01 B2=8.50 1970RFa (30745) 105  
\*\*\*\*\*  
C4H6O5 H2L Diglycolic acid CAS 110-99-6 (243)  
Di(carboxy)methyl ether, 2,2'-Oxydiethanoic acid; HOOC.CH2.O.CH2.COOH  
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-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Tm+++ gl KCl 25°C 1.0M U M 1988KTa (30939) 106  
K(Tm(edta)+L)=1.30  
-----

-----  
Tm+++ cal NaClO4 25°C 1.0M C H 1963GRd (30940) 107  
DH(K1)=6.586 kJ mol<sup>-1</sup>, DS(K1)=128 J K<sup>-1</sup> mol<sup>-1</sup>; DH(B2)=4.874,  
DS(B2)=213; DH(B3)=-15.98, DS(B3)=200.  
-----

-----  
Tm+++ EMF NaClO4 20°C 1.00M U K1=5.49 B2=10.22 1963GTa (30941) 108  
B3=13.29  
-----

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  
-----  
Tm+++ ix NaClO4 25°C 0.10M U B2=6.35 198000a (31378) 109  
K(Tm+2HL)=4.10  
K(Tm+HL+L)=5.99  
-----

-----  
Tm+++ sp oth/un 25°C 0.0 U T H K1=5.31 1975YBa (31379) 110  
DH(K1)=11.7 kJ mol<sup>-1</sup>, DS=142.2 J K<sup>-1</sup> mol<sup>-1</sup>  
-----

-----  
Tm+++ gl alc/w 25°C 40% U I K1=5.09 1972SSj (31380) 111  
-----

Medium: 0-40% EtOH, 0.05 M. 40% EtOH, I=0: K1=6.51

\*\*\*\*\*

C4H7N04 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  
-----  
Tm+++ gl NaCl04 30°C 0.10M U K1=5.87 B2=10.80 1984YLa (31956) 112  
-----

Tm+++ gl KCl 25°C 0.10M U K1=6.10 B2=11.10 1968DRb (31957) 113  
\*\*\*\*\*

C4H7N04 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  
-----  
Tm+++ gl KCl 25°C 1.0M U M 1988KTa (32380) 114  
K(Tm(edta)+L)=3.03  
-----

Tm+++ EMF KCl 25°C 1.0M U M 1977GMa (32381) 115  
K(TmA+L)=5.12  
K(TmA+H2L)=0.98  
K(TmA+H3L)=2.21

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

-----  
Tm+++ cal KNO3 20°C 0.10M U HM 1971GKb (32382) 116  
K(TmA+L)=2.86

DH(TmA+L)=-27.20 kJ mol<sup>-1</sup>, DS=-38.1 J K<sup>-1</sup> mol<sup>-1</sup>. DH(SmAL)=-35.02, DS=305.  
H4A=EDTA

-----  
Tm+++ gl KNO3 25°C 0.10M U M K1=7.22 B2=12.90 1962THa (32383) 117  
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  
-----  
Tm+++ gl diox/w 20°C 50% U K1=8.63 B2=16.20 1971MAf (32552) 118  
Medium: 50% v/v dioxan, 0.1 M NaCl04  
\*\*\*\*\*

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  
-----  
Tm+++ gl NaCl04 30°C 0.10M U K1=4.22 B2=7.31 1984YLa (32735) 119  
\*\*\*\*\*

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
Tm+++	gl	KCl	60°C	0.10M	U			K1=6.41 B2=11.11 B3=10.95	1978NBa (33095)	120

\*\*\*\*\*  
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
Tm+++	gl	KNO3	30°C	0.10M	U	M		K(Tm(EDTA)+L)=2.143	1984AIa (33116)	121

\*\*\*\*\*  
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
Tm+++	gl	NaClO4	25°C	2.00M	U	H		K1=1.61 B2=2.67	1965CGa (33251)	122

By calorimetry: DH(K1)=22.6 kJ mol<sup>-1</sup>, DS=107 J K<sup>-1</sup> mol<sup>-1</sup>; DH(K2)=17.1, DS=78

Tm+++	gl	NaClO4	25°C	0.50M	U			K1=1.69 B2=2.28	1964SPa (33252)	123
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\*\*\*\*\*  
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
Tm+++	gl	NaClO4	25°C	0.20M	U			K1=3.10 K3=1.92 K4=1.62	1964DVa (33529)	124

Tm+++	gl	NaClO4	20°C	0.10M	U			K1=3.515 B2=6.22 B3=8.39	1964PKb (33530)	125
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Tm+++	gl	NaClO4	25°C	0.50M	U			K1=3.13 B2=5.62 B3=7.84	1964SPa (33531)	126
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\*\*\*\*\*  
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
Tm+++	gl	KNO3	25°C	0.10M	C			K1=3.22 K3=1.83	1975PFb (33687)	127

\*\*\*\*\*  
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  
-----  
Tm+++ EMF KNO3 25°C 0.10M U K1=3.08 B2=5.60 1976PKb (33715) 128  
K3=2.04  
-----

Tm+++ gl NaClO4 25°C 0.50M U K1=2.85 B2=4.97 1964SPa (33716) 129  
B3=6.51  
-----

\*\*\*\*\*  
C4H11N L Butylamine CAS 109-73-9 (159)  
1-Aminobutane; CH3.CH2.CH2.CH2.NH2  
-----

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Tm+++ cal non-aq 25°C 100% U H K1=4.38 B2=7.82 1997CDa (34773) 130  
B3=10.17  
B4=11.67  
-----

Medium: MeCN. DH(K1)=-35.4 kJ mol<sup>-1</sup>, DS=35, DH(B2)=-70.4, DS=87;  
DH(B3)=-103, DS=151, DH(B4)=-135, DS=229  
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\*\*\*\*\*  
C4H11O4P HL (4276)  
Diethylphosphoric acid; (C2H5O)2.PO.OH  
-----

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Tm+++ oth oth/un 25°C U K1=2.18 1971MGb (35270) 131  
Estimated  
-----

\*\*\*\*\*  
C4H12N2O L CAS 2752-17-2 (312)  
Bis-(2-aminoethyl)ether; H2N.CH2.CH2.O.CH2.CH2.NH2  
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Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Tm+++ EMF non-aq 25°C 100% C H K1=2.68 B2= 4.64 2002Cdb (35509) 132  
Method: comp. reactn. using Ag electrode. Medium: DMSO, 0.10 M Et4NClO4.  
Calorimetry: DH(K1)=-12 kJ mol<sup>-1</sup>, DS=11 J K<sup>-1</sup> mol<sup>-1</sup>; DH(B2)=-30, DS=-11.  
-----

\*\*\*\*\*  
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  
-----  
Tm+++ EMF NaClO4 25°C 100% C H K1=6.57 B2=10.68 2000CDa (35819) 133  
Medium: DMF, 0.10 M Et4N[CF3SO3]. Method: Ag/Ag+ electrode.  
By calorimetry: DH(K1)=-49.1, DH(B2)=-96.9 kJ mol<sup>-1</sup>.  
-----

Tm+++ ISE non-aq 25°C 100% C H K1=3.97 B2=7.25 1993CCb (35820) 134  
Medium: DMSO, 0.1 M Et4NClO4. Method: Ag+ ISE. By calorimetry, DH(K1)=-34.8  
kJ mol<sup>-1</sup>, DS=-41; DH(B2)=-79.5, DS-128.  
-----

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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  
-----  
Tm+++ cal NaClO4 25°C 0.10M U H K1=2.91 B2=4.59 1978COa (35951) 135  
DH(K1)=11.0 kJ mol-1, DS=92.8; DH(K2)=7.02, DS=55.6  
-----

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

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Tm+++ cal NaClO4 25°C 2.00M U H K1=1.48 1976YCa (36312) 136  
DH=8.95 kJ mol-1 and DS=58.16 J mol-1 K-1.  
-----

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  
-----  
Tm+++ gl KCl 25°C 0.20M U K1=2.45 1989MFa (37453) 137  
K(Tm+HL)=1.57  
-----

C5H7NO3 HL (4313)  
Isonitrosoacetylacetone; HO.N:CH.CO.CH2.CO.CH3

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Tm+++ gl diox/w 20°C 50% U K1=5.38 B2=9.15 1971MAf (37534) 138  
Medium: 50% v/v dioxan, 0.1 M NaClO4  
-----

C5H8N2O3 H2L (4317)  
Methylacetylglyoxime; CH3.C(:N.OH).C(:N.OH).CO.CH3

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Tm+++ gl diox/w 20°C 50% U K1=6.28 B2=11.49 1971MAf (37711) 139  
-----

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  
-----  
Tm+++ dis NaClO4 25°C 1.0M C B2=10.43 1989ALa (38106) 140  
B3=13.82  
B4=15.66  
-----

Method: extraction of 170Tm from 1.0 M NaClO4 into benzene/HL.  
-----

Tm+++ gl NaClO4 20°C 0.10M U M 1973TZa (38107) 141  
K(Tm(EDTA)+L)=3.66

-----  
Tm+++ gl NaClO4 25°C 2.0M U K1=6.03 B2=10.75 1964YCa (38108) 142

-----  
Tm+++ gl oth/un 30°C 0.10M U K1=6.09 B2=10.85 1960GFa (38109) 143  
K3=3.48

\*\*\*\*\*  
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

-----  
Tm+++ gl KCl 25°C 0.20M U K1=4.51 1989ZPa (38252) 144  
In 70.4% v/v EtOH/H2O: K1 = 6.43

\*\*\*\*\*  
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

-----  
Tm+++ gl NaClO4 25°C 0.10M U K1=3.08 B2=5.14 1970RFa (38270) 145

\*\*\*\*\*  
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

-----  
Tm+++ gl NaClO4 25°C 0.10M U B2=6.08 1981ZLa (38649) 146

\*\*\*\*\*  
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

-----  
Tm+++ gl NaCl 37°C 0.15M U K1=3.47 1997GMa (38756) 147

-----  
Tm+++ gl NaClO4 25°C 0.10M U B2=5.55 1981ZLa (38757) 148

\*\*\*\*\*  
C5H9NO4 H2L MIDA CAS 4408-64-4 (190)  
N-Methyliminodiethanoic acid; CH3.N(CH2.COOH)2

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

-----  
Tm+++ gl KCl 25°C 0.10M U K1=7.35 B2=13.44 1980MGc (39288) 149  
B3=15.38

\*\*\*\*\*  
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	
Tm+++	gl	KNO3	25°C	0.10M	U			K1=3.37 K3=1.92	B2=6.13	1969PCa (40265)	150
*****											
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	
Tm+++	gl	NaClO4	25°C	0.10M	U			K1=2.31	B2=3.93	1970RDa (40305)	151
*****											
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	
Tm+++	gl	KNO3	25°C	0.10M	C			K1=3.15	B2=5.62	1975PFb (40320)	152
*****											
C6H5NO2		HL							CAS 98-98-6	(391)	
2-Pyridine-carboxylic acid; C5H4N.COOH											
-----											
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo	
Tm+++	gl	NaClO4	25°C	0.50M	U			K1=4.05	B2=7.52	1977GGb (42608)	153
*****											
Tm+++	gl	KNO3	25°C	0.10M	U			K1=4.33	B2=8.08	1968PIa (42609)	154
*****											
								K3=2.87			
								K4=2.04			
-----											
Tm+++	gl	NaClO4	25°C	2.0M	U			K1=4.31	B2=7.48	1965YCa (42610)	155
-----											
Tm+++	gl	KNO3	25°C	0.10M	U			K1=4.36	B2=7.98	1964THb (42611)	156
*****											
C6H5NO3		HHL							CAS 824-40-8	(878)	
Pyridine-2-carboxylic acid N-oxide (Picolinic acid N-oxide); C5H4N(O)COO											
-----											
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo	
Tm+++	gl	NaClO4	25°C	2.0M	U			K1=3.16	B2=5.85	1965YCa (42841)	157
*****											
C6H5NO4		H2L							CAS 3163-07-3	(2711)	
2,4-Dihydroxy-1-nitrobenzene; O2N.C6H3(OH)2											
-----											
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo	

Tm+++ sp KCl 25°C 0.10M M I K1=6.38 1989PEa (42961) 158  
 \*\*\*\*\*  
 C6H5O4Br L CAS 40838-32-2 (1084)  
 6-Bromo-5-hydroxy-2-(hydroxymethyl)-4H-pyran-4-one;

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

Tm+++ sp KCl 25°C 0.10M U K1=5.60 1987PLa (43117) 159  
 \*\*\*\*\*  
 C6H5O4I L (1085)  
 6-Iodo-5-hydroxy-2-hydroxymethyl-4H-pyran-4-one;

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

Tm+++ sp KCl 25°C 0.10M U K1=5.68 1987PLa (43159) 160  
 \*\*\*\*\*  
 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  
 -----

Tm+++ gl NaClO4 25°C 0.20M U K1=9.98 1998PJb (43853) 161  
 -----  
 Tm+++ EMF NaCl 25°C 0.10M U K1=11.56 1969PKe (43854) 162  
 \*\*\*\*\*  
 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  
 -----

Tm+++ gl NaClO4 25°C 0.20M U K1=11.08 1998PJb (43989) 163  
 \*\*\*\*\*  
 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  
 -----

Tm+++ sp KCl 25°C 0.10M C I K1=6.322 1987PEa (44246) 164  
 In 0.087 M KCl, K1=6.349.

-----  
 Tm+++ gl NaClO4 25°C 2.0M U K1=6.00 B2=11.55 1964YCa (44247) 165  
 \*\*\*\*\*  
 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  
 -----

Tm+++ gl NaClO4 25°C 0.50M C K1=12.96 B2=22.50 1976LAb (44503) 166  
 B(TmHL2)=30.06  
 -----

Tm+++ gl NaClO4 25°C 0.10M U K1=14.36 1970SSi (44504) 167  
K(Tm+HL)=5.67

\*\*\*\*\*  
C6H7NO HL 2-Aminophenol CAS 95-55-6 (2868)  
2-Amino-1-hydroxybenzene; HO.C6H4.NH2

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

Tm+++ gl mixed 25°C 50% U I K1=4.48 B2=8.50 1969BCa (44939) 168  
Medium: 50% DMSO, 0.12 M NaClO4. In 0.12 M NaClO4, 50% dioxan: K1=5.65,  
K2=4.34. Medium: 0.12 NaClO4, 50% EtOH: K1=5.01, K2=4.20

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

Tm+++ gl KCl 25°C 0.20M U K1=4.03 1989ZPa (45476) 169  
In 70.4% v/v EtOH/H2O: K1 = 6.16

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

Tm+++ gl NaClO4 25°C 2.00M U IH K(Tm+HL)=1.41 1988HSa (45663) 170

DH=6.8 kJ mol<sup>-1</sup>, DS=49.9 J K<sup>-1</sup> mol<sup>-1</sup>  
\*\*\*\*\*  
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  
-----

Tm+++ gl KNO3 25°C 1.0M M 1986SZb (46286) 171  
K(Tm+H3L=TmHL+2H)=-2.46  
K(Tm+H3L=TmL+3H)=-5.88  
K(Tm+H3L=TmH-1L+4H)=-11.13  
K(Tm+2H3L=TmH2L2+4H)=-6.35  
K(Tm+2H3L=TmL2+6H)=-13.70, K(Tm+2H3L=TmH-2L2+8H)=-28.1,  
K(Tm+2H3L=TmH-3L2+9H)=-27.5, K(Tm+2H3L=TmH-4L2+10H)=-35.4.

-----  
Tm+++ gl KNO3 25°C 0.10M U M 1975TDa (46287) 172  
B(Tm(IDA)L)=10.2

-----  
Tm+++ dis NaClO4 25°C 0.15M U 1973HHc (46288) 173  
K(Tm+HL+L)=11.43

-----  
Tm+++ gl alc/w 25°C 25% U I K1=8.84 1972BKd (46289) 174  
Medium: EtOH/H2O, 0.05 M (NaCl,NaClO4). 0%, K1=8.00; 50%, K1=9.99

-----  
 Tm+++ ix NaCl 25°C 0.10M U K1=7.51 B2=12.74 197200a (46290) 175  
 K(Tm+HL)=5.60  
 K(Tm+2HL)=9.01  
 -----

Tm+++ dis oth/un ? ? U 1972PGd (46291) 176  
 K(Tm+HL+L)=10.18  
 -----

Tm+++ oth oth/un 25°C 0.10M U K1=8.06 B2=11.36 1971STe (46292) 177  
 K(TmL+HL)=2.60

Constants obtained by survey of literature data

\*\*\*\*\*

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

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

Tm+++ ISE NaCl04 25°C 0.10M C I K1=11.98 1997LBb (47063) 178  
 Method: Cu ISE and competitive complexation by Cu. Data for 0.1-5.0 M.  
 At I=0.0 M, K1=13.83.  
 -----

Tm+++ ISE KNO3 25°C 0.10M C K1=12.20 1980NSf (47064) 179  
 Competitive method using Cd ion-selective electrode.  
 -----

Tm+++ gl KNO3 20°C 1.0M C K2=8.47 1978GHb (47065) 180  
 -----

Tm+++ gl NaCl04 25°C 0.50M U K1=11.95 1977GGb (47066) 181  
 -----

Tm+++ EMF KCl 25°C 1.0M U M 1977GMa (47067) 182  
 K(TmA+L)=5.73  
 K(TmA+H2L)=1.80  
 K(TmA+H3L)=2.25  
 K(TmA+H4L)=3.37

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

Tm+++ cal KNO3 20°C 0.10M U HM 1971GKb (47068) 183  
 K(TmA+L)=3.13  
 H4A=EDTA. DH(TmA+L)=-28.24 kJ mol<sup>-1</sup>, DS=-36.4 J K<sup>-1</sup> mol<sup>-1</sup>.  
 DH(TmLA)=-36.1 kJ mol<sup>-1</sup>, DS=307 J K<sup>-1</sup> mol<sup>-1</sup>  
 -----

Tm+++ gl oth/un 20°C 0.20M U 1970VMa (47069) 184  
 B(TmL(OH))=6.62  
 -----

Tm+++ gl KNO3 25°C 0.10M U T H T K1=12.22 B2=21.45 1962MFb (47070) 185  
 15 C: K1=12.21, K2=9.32; 20 C: 12.20, 9.25; 30 C: 12.28, 9.22; 35 C: 12.27, 9.17; 40 C: 12.30, 9.16. DH(K1)=8.0 kJ mol<sup>-1</sup>, DS=261; DH(K2)=-9.9, DS=144  
 -----

Tm+++ vlt KNO3 20°C 0.10M U 1957NOa (47071) 186  
 B(Tm2L3)=38.28

\*\*\*\*\*

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
Tm+++	gl	NaClO4	25°C	0.10M	U			K1=3.110 K3=1.99 K4=1.30	1966PRb (47998)	187

\*\*\*\*\*

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
Tm+++	oth	NaClO4	25°C	0.10M	U			K1=4.69	1984AFa (48357)	188
Laser excitation spectroscopy, competition method.										
Tm+++	gl	NaClO4	25°C	1.00M	C	H		K1=4.64 B3=8.46 B(TmHL2)=9.51	1974GGa (48358)	189

\*\*\*\*\*

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
Tm+++	gl	KNO3	20°C	1.00M	U			K1=8.52 K(YbL2(OH)+H)=9.12	1974CMD (48801)	190
Tm+++	oth	NaNO3	20°C	0.10M	U	M		K1=9.1 B2=16.90	1966JMc (48802)	191
Method: paper electrophoresis. Ternary complexes with HEDTA										
Tm+++	gl	KCl	25°C	0.10M	U			K1=9.03 B2=16.34	1965DTa (48803)	192
Tm+++	ISE	KNO3	25°C	0.10M	U			K1=9.35 B2=17.23	1963TLa (48804)	193

\*\*\*\*\*

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
Tm+++	gl	R4N.X	25°C	0.10M	C			K1=8.75	1988CCb (49276)	194

\*\*\*\*\*

C6H12O2 HL CAS 142-62-1 (964)  
Hexanoic acid; CH3.(CH2)4.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Tm+++	gl	NaCl	20°C	0.10M	U			K1=2.37	1986GKb (49429)	195

\*\*\*\*\*

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
Tm+++	gl	KNO3	25°C	0.10M	U			K1=3.44 B2=5.75 K3=1.81	1979PPa (49501)	196

\*\*\*\*\*

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Tm+++	gl	KCl	20°C	0.20M	U			K1=4.18 B2=8.88	1990PLa (50196)	197

\*\*\*\*\*

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
Tm+++	gl	KNO3	20°C	0.10M	U			K1=5.35 B2=9.90	1982RFa (50414)	198
Tm+++	gl	KCl	30°C	0.10M	U			K1=5.52 B2=9.65	1973MSe (50415)	199

\*\*\*\*\*

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Tm+++	gl	NaCl	37°C	0.15M	U	M		K1=3.16 B(TmHL)=11.10 B(TmH2AL)=24.47	1997GMa (50589)	200

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

\*\*\*\*\*

C6H18N4 L Tren CAS 4097-89-6 (817)  
2,2',2''-Triaminotriethylamine; (H2N.CH2.CH2)3N

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Tm+++	ISE	non-aq	25°C	100%	C	H		K1=5.84 B2=7.27	1993CCb (52211)	201

Medium: DMSO, 0.1 M Et4NC104. Method: Ag+ ISE. By calorimetry, DH(K1)=-54.8 kJ mol<sup>-1</sup>, DS=-72; DH(B2)=-82.0, DS=-136.

\*\*\*\*\*

C6H20N2O12P4 H8L EDTPA CAS 1429-50-1 (434)  
Ethane-1,2-bis(iminobis(methylenephosphonic acid)); ((H2O3PCH2)2NCH2.)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Tm+++	gl	KNO3	25°C	0.10M	C				1991SKb (52367)	202

K(TmL+H)=7.29  
K(TmHL+H)=5.98

-----  
Tm+++ gl KCl 25°C 0.10M U K1=21.41 1967KDa (52368) 203  
K(Tm+HL)=16.17  
K(Tm+H2L)=12.88  
K(Tm+H3L)=10.28  
K(Tm+H4L)=8.04

K(Tm+H5L)=4

\*\*\*\*\*  
C7H4N2O7 H2L CAS 609-99-4 (400)  
3,5-Dinitrosalicylic acid; (O2N)2.C6H2(OH).COOH  
-----

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

-----  
Tm+++ gl oth/un 24°C 0.20M U K1=5.61 1972PSd (52503) 204  
Medium: LiCl

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

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

-----  
Tm+++ cal NaClO4 25°C 0.50M C H 1963GRd (52814) 205  
DH(K1)=-7.67 kJ mol<sup>-1</sup>, DS(K1)=143 J K<sup>-1</sup> mol<sup>-1</sup>; DH(B2)=-22.89,  
DS(B2)=239; DH(B3)=-53.85, DS(B3)=239.

-----  
Tm+++ EMF oth/un 20°C 0.50M U K1=8.83 B2=16.54 1961GRa (52815) 206  
K3=5.50

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

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

-----  
Tm+++ gl NaClO4 25°C 0.10M C H K1=1.60 1986CLc (52874) 207  
DH=9.3 kJ mol<sup>-1</sup>, DS=62 J K<sup>-1</sup> mol<sup>-1</sup>

\*\*\*\*\*  
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

-----  
Tm+++ gl NaClO4 25°C 0.10M C H K1=1.73 1986CLc (53243) 208  
DH=9.0 kJ mol<sup>-1</sup>, DS=63 J K<sup>-1</sup> mol<sup>-1</sup>

\*\*\*\*\*  
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

-----  
Tm+++ gl NaClO4 25°C 0.10M C H K1=1.85 1986CLc (53263) 209  
DH(K1)=11.0 kJ mol<sup>-1</sup>, DS=72 J K<sup>-1</sup> mol<sup>-1</sup>

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

Tm+++ gl NaClO4 25°C 0.10M C T 1993ALa (53377) 210  
B(1,1,1)=12.34  
B(1,0,1)=7.69  
B(1,0,2)=13.24  
B(1,-2,1)=-7.15

B(p,q,r); pTm+qH+rL=(Tm)pHqLr

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

Tm+++ gl KNO3 25°C 0.10M U K1=7.60 B2=13.99 1969CMB (53697) 211  
K3=5.40  
K4=3.80

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

Tm+++ cal NaClO4 25°C 0.10M U H K1=1.94 B2=3.63 1982CBc (53859) 212  
DH1= 9.9 kJ mol<sup>-1</sup>, DS1= 70 J K<sup>-1</sup> mol<sup>-1</sup>

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

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

Tm+++ gl NaClO4 25°C 0.1M C H 1996HYa (54317) 213  
By calorimetry: DH(K1)=3.34 kJ mol<sup>-1</sup>, DH(B2)=6.97 J K<sup>-1</sup> mol<sup>-1</sup>

-----  
Tm+++ gl NaClO4 25°C 0.10M C T 1989HMa (54318) 214  
K(Tm+HL)=1.75  
K(TmHL+HL)=1.92

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

Tm+++ gl NaCl04 25°C 0.10M C 1988LLa (54391) 215  
K(Tm+HL)=1.93  
\*\*\*\*\*  
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  
-----  
Tm+++ gl NaCl04 25°C 0.10M C 1988LLa (54435) 216  
K(Tm+HL)=2.08  
\*\*\*\*\*  
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  
-----  
Tm+++ gl NaCl04 25°C 0.20M U K1=10.58 1998PJb (54705) 217  
\*\*\*\*\*  
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  
-----  
Tm+++ gl NaCl04 20°C 1.0M U K1=7.28 B2=13.15 1972CBb (55060) 218  
-----  
Tm+++ sp NaCl04 20°C 0.10M U K1=8.34 B2=14.95 1968KTb (55061) 219  
K(Tm+HL)=2.27  
\*\*\*\*\*  
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  
-----  
Tm+++ gl NaCl04 25°C 0.50M C T K1=8.85 B2=14.70 1976LAc (55103) 220  
\*\*\*\*\*  
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  
-----  
Tm+++ gl NaCl04 25°C 0.10M C K1=2.22 B2=4.39 1989HMa (55267) 221  
\*\*\*\*\*  
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  
-----  
Tm+++ gl KCl 25°C 0.20M U K1=2.14 1977EBa (55395) 222  
\*\*\*\*\*  
C7H7NO3 H2L CAS 89-73-6 (204)

2-Hydroxybenzohydroxamic acid (salicylhydroxamic acid); HO.C6H4.CO.NHOH

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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Tm+++      gl  KNO3   25°C  0.1M M          K1=12.00 B2=23.05 1989LWa (55612) 223
                        K3=10.32
*****
```

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

```
-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Tm+++      gl  KCl     25°C  0.20M M T H     K1=8.85          1991BPb (55696) 224
                        K(Tm+OH+L)=16.06
```

DH(K1)=-115 kJ mol<sup>-1</sup>, DS(K1)=-216 J K<sup>-1</sup> mol<sup>-1</sup>. DH(Tm(OH)L)=-171,  
DS(Tm(OH)L)=-265. 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
-----
Tm+++      gl  mixed  25°C  50% U I          K1=4.74 B2=9.29 1969BCb (56080) 225
Medium: 50% DMSO, 0.12 M NaClO4. In 50% dioxan, 0.12 M NaClO4: K1=5.80,
K2=4.81; 50% EtOH, 0.12 M NaClO4: K1=5.36, K2=4.50
*****
```

```
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
-----
Tm+++      sp  KCl     25°C  0.10M M I          K1=6.70          1986PLb (56135) 226
*****
```

```
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
-----
Tm+++      sp  KCl     25°C  0.10M M I          K1=6.39          1986PLb (56154) 227
*****
```

```
C7H10O4          H2L          CAS 5802-62-3 (71)
Cyclopentane-1,1-dicarboxylic acid; C5H8.(COOH)2
-----
```

```
-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Tm+++      gl  KNO3   25°C  0.10M U          K1=4.25 B2=6.82 1971PJb (56737) 228
*****
```

```
C7H11NO4          H2L          CAS 499-82-1 (3163)
Piperidine-2,6-dicarboxylic acid; C5H9N(COOH)2
-----
```

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Tm+++	g1	KNO3	25°C	0.10M	U		K1=6.53 B2=12.30	1963THb (56814)	229
*****									
C7H11NO6			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
Tm+++	g1	KNO3	25°C	0.1M	U		K1=9.16	1982KKc (56853)	230
*****									
C7H11NO6			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
Tm+++	g1	KNO3	20°C	0.10M	U		K1=13.01 B2=22.70	1974RMg (56920)	231
*****									
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
Tm+++	g1	KNO3	25°C	0.10M	U		K1=4.70 B2=7.31	1968PFa (57373)	232
*****									
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
Tm+++	g1	KNO3	20°C	0.10M	U		K1=8.95 B2=16.77	1980RPa (57621)	233
*****									
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
Tm+++	g1	NaClO4	25°C	0.10M	C		K1=2.99 B2=4.88	1976SPa (57881)	234
*****									
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
Tm+++	g1	KNO3	20°C	0.10M	U		K1=5.07 B2=9.58	1982RFa (57944)	235
*****									
C8H5N5O6			H3L	Murexide			(453)		
Purpuric acid (Murexide is ammonium salt);									

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

-----  
Tm+++ sp KNO3 12°C 0.10M U 1965GEa (58542) 236  
K(Tm+H2L)=3.36

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

Tm+++ cal non-aq 25°C 100% C H 2004MIa (58689) 237  
Method: calorimetric titration. Medium: chloroform. DH(TmL3+A)=6.7 kJ  
mol-1, DS=77 J K-1 mol-1; DH(TmL3+2A)=-5.0, DS=77. HA is benzoic acid.  
-----

Tm+++ gl alc/w 22°C 80% U K1=6.35 B2=12.23 1995MTa (58690) 238  
K3=4.93

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  
-----

Tm+++ gl NaClO4 30°C 0.10M U K1=4.45 B2=7.80 1966KPb (59020) 239

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

Tm+++ cal NaClO4 25°C 0.10M U H K1=2.57 1982CBc (59062) 240  
DH= 17.15 kJ mol-1, DS= 107 J K-1 mol-1

\*\*\*\*\*  
C8H7NO2 HL CAS 532-54-7 (4363)  
Isonitrosoacetophenone, Phenylglyoxal 2-oxime;  
-----

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

Tm+++ gl diox/w 20°C 50% U K1=6.49 B2=12.10 1971MAf (59109) 241

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

\*\*\*\*\*  
C8H7NO3 HL (7376)  
benzoylhydroxamic acid; C6H5COCONHOH  
-----

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

Tm+++ gl KNO3 25°C 0.1M M K1=10.87 B2=20.99 1989LWa (59130) 242  
K3=9.19

\*\*\*\*\*  
C8H8N2O2 HL Phenylglyoxime (3222)  
Phenylglyoxime; C6H5.C(:N.OH).CH:N.OH

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Tm+++ gl diox/w 20°C 50% U K1=7.55 B2=14.07 1971MAf (59344) 243  
Medium: 50% dioxan, 0.1 M NaClO4

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

Tm+++ gl NaClO4 25°C 0.1M C H K1=1.73 1996HYa (59566) 244  
By calorimetry: DH(K1)=16.73 kJ mol-1  
-----

Tm+++ gl NaClO4 25°C 0.10M C H K1=1.73 1990HYa (59567) 245  
By calorimetry: DH(K1)=16.7 J K-1 mol-1  
-----

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

Tm+++ gl NaClO4 25°C 0.10M M H K1=1.83 1988CLb (59755) 246  
DH=10.7 kJ mol-1, DS=71 J K-1 mol-1  
-----

Tm+++ gl alc/w 25°C 42% U K1=2.5 1983PMa (59756) 247  
-----

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

Tm+++ gl NaClO4 25°C 0.10M C K1=3.20 B2=5.56 1989HMa (59881) 248  
-----

Tm+++ gl NaClO4 25°C 2.0M U T K1=2.71 1972DCb (59882) 249  
-----

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

Tm+++ gl NaClO4 25°C 0.10M M H K1=2.05 1988CLb (59921) 250  
DH=11.9 kJ mol-1, DS=79 J K-1 mol-1  
-----

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

Tm+++ gl NaClO4 25°C 0.10M M H K1=2.02 1988CLb (59965) 251  
-----

DH=14.5 kJ mol<sup>-1</sup>, DS=87 J K<sup>-1</sup> mol<sup>-1</sup>

\*\*\*\*\*

C8H8O4 HL CAS 520-45-6 (4478)  
3-Acetyl-2-hydroxy-6-methylpyran-4-one, Dehydroethanoic acid;

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Tm+++ gl diox/w 35°C 50% U K1=5.02 B2=8.89 1971MAa (60099) 252  
Medium: 50% dioxan, 0.1 M NaClO4

\*\*\*\*\*

C8H8O9 H4L (6951)  
Tetrahydrofuran-2,3,4,5-tetracarboxylic acid;

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Tm+++ cal NaClO4 25°C 0.10M C H 2000MNa (60137) 253  
DH(Tm+HL)=7.76 kJ mol<sup>-1</sup>, DS=185 J K<sup>-1</sup> mol<sup>-1</sup>. DH(Tm+H2L)=5.42, DS=137.

-----  
Tm+++ gl NaClO4 25°C 0.10M C K1=10.37 B2=14.93 1995JNa (60138) 254  
B(TmH2L)=17.38  
B(TmHL)=14.78  
B(TmH-1L)=2.62  
B(TmH-2L)=-7.12

B(TmH2L2)=24.91, B(TmHL2)=20.00

\*\*\*\*\*

C8H9NO4 H2L (4520)  
Dehydroethanoic acid oxime;

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Tm+++ gl diox/w 35°C 50% U 1971MAa (60505) 255  
K(Tm+HL)=4.92  
K(Tm+2HL)=8.52

Medium: 50% dioxan, 0.1 M NaClO4

\*\*\*\*\*

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  
-----  
Tm+++ gl alc/w 22°C 20% U K1=4.77 B2=8.51 1988ZTa (60856) 256  
K3=3.37

\*\*\*\*\*

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  
-----  
Tm+++ gl KCl 30°C 0.10M C K1=5.71 B2=9.99 1996SZa (60877) 257  
For the -5-en-2-exo isomer, K1=6.07, B2=10.83.

\*\*\*\*\*  
 C8H11N08 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  
 -----  
 Tm+++ gl KCl 25°C 0.10M U K1=11.32 B2=18.05 1979BEb (61219) 258  
 B(TmHL)=15.77

\*\*\*\*\*  
 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  
 -----  
 Tm+++ gl KNO3 20°C 0.10M U K1=12.40 B2=18.28 1975DPa (61530) 259  
 -----  
 Tm+++ gl KNO3 25°C 0.10M U K1=11.32 1972GBd (61531) 260  
 By polarography K1=11.18

\*\*\*\*\*  
 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  
 -----  
 Tm+++ gl NaClO4 25°C 0.10M M H K1=4.33 1986CDb (61717) 261  
 DH=19.0 kJ mol-1, DS=147 J K-1 mol-1

\*\*\*\*\*  
 C8H13N06 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  
 -----  
 Tm+++ gl KNO3 20°C 0.10M U K1=10.42 B2=17.77 1974RMg (61772) 262

\*\*\*\*\*  
 C8H13N06 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  
 -----  
 Tm+++ gl KNO3 20°C 0.10M U K1=12.07 B2=20.81 1974RMg (61797) 263

\*\*\*\*\*  
 C8H19O4P HL CAS 107-66-4 (2130)  
 Dibutylphosphoric acid; (C4H9O)2P(O)OH

-----  
 Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
 -----  
 Tm+++ dis oth/un 26°C 0.10M C I 1992SNc (63194) 264  
 K(Tm+5HL(org))=TmL3(HL)2(org)+3H)=19.1. Method: extraction of 170Tm from  
 HNO3 solution into CFC-112. For extraction into benzene, K=6.2.

Tm+++ kin oth/un 25°C ? U K1=3.29 1971MGb (63195) 265  
\*\*\*\*\*

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  
-----

Tm+++ gl diox/w 35°C 75% U K1=7.60 B2=13.70 1971MAb (63572) 266  
K3=5.20

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  
-----

Tm+++ sp diox/w 20°C 50% U K1=2.88 B2=4.84 1977MBb (63615) 267  
\*\*\*\*\*

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  
-----

Tm+++ gl NaClO4 25°C 0.10M U K1=5.82 B2=10.55 1973MAa (63705) 268  
K3=3.9

\*\*\*\*\*

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  
-----

Tm+++ gl oth/un 20°C 0.10M U K1=6.50 1977SKd (63832) 269  
\*\*\*\*\*

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  
-----

Tm+++ gl NaClO4 25°C 0.10M U H K1=4.81 1994CRa (63978) 270  
K(Tm+HL)=2.88

DH(K1)=20.2 kJ mol<sup>-1</sup>; DS=160 J K<sup>-1</sup> mol<sup>-1</sup>

\*\*\*\*\*

C9H7NO HL Oxine CAS 148-24-3 (504)  
8-Hydroxyquinoline (8-quinolinol);

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

Tm+++ sol none RT 0.0 U 1981FCa (64363) 271  
Kso(TmL3)=-33.03

Method: spectrophotometry.

-----  
Tm+++ gl oth/un 20°C 0.10M U K1=7.55 1977SKd (64364) 272  
-----

Tm+++ gl diox/w 30°C 50% U K1=9.55 B2=18.13 1970Gmb (64365) 273  
Medium: 50% dioxan, 0.3 M NaClO4

\*\*\*\*\*  
C9H7NO2 HL CAS 1127-45-3 (4614)  
8-Hydroxyquinoline-N-oxide;  
-----

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

Tm+++ gl diox/w 30°C 50% U K1=7.40 1970Gmb (64412) 274  
Medium: 50% dioxan, 0.3 M NaClO4

\*\*\*\*\*  
C9H7NO4S H2L Sulfoxine CAS 84-88-8 (448)  
8-Hydroxyquinoline-5-sulfonic acid;  
-----

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

Tm+++ cal KNO3 20°C 0.10M U HM 1971Gkb (64583) 275  
K(TmA+L)=4.76

DH(TmA+L)=-25.24 kJ mol<sup>-1</sup>, DS=4.59 J K<sup>-1</sup> mol<sup>-1</sup>  
DH(TmAL): DH=-33.06, DS=347.4. H4A=EDTA  
\*\*\*\*\*  
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  
-----

Tm+++ sp NaNO3 25°C 0.10M C K1=8.34 19850Hb (64733) 276  
K(Tm+HL)=4.74  
K(TmL+H)=5.84

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

Tm+++ gl KCl 30°C 0.10M U K1=4.20 B2= 7.96 1996SZa (64983) 277

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

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

Tm+++ gl NaClO4 25°C 0.1M C H K1=1.91 B2= 3.45 1996HYa (65375) 278  
By calorimetry: DH(K1)=15.60 kJ mol<sup>-1</sup>, DH(B2)=14.24 J K<sup>-1</sup> mol<sup>-1</sup>

-----  
Tm+++ gl NaClO4 25°C 0.10M C H K1=1.91 B2=3.45 1990HYa (65376) 279  
By calorimetry: DH(K1)=15.6 J K<sup>-1</sup> mol<sup>-1</sup>, DH(K2)=-1.4

\*\*\*\*\*

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  
-----  
Tm+++ gl NaCl04 25°C 0.10M C K1=2.14 B2=3.86 1989HMa (65468) 280  
\*\*\*\*\*

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  
-----  
Tm+++ gl NaCl04 25°C 0.10M C K1=2.02 B2=3.78 1989HMa (65482) 281  
\*\*\*\*\*

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  
-----  
Tm+++ gl KCl 30°C 0.10M C K1=4.13 B2=6.68 1996SZa (65579) 282  
For the -2,5-dien-2-exo isomer, K1=4.20, B2=7.96.  
\*\*\*\*\*

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  
-----  
Tm+++ gl NaCl04 24°C 0.10M U K1=4.40 1986ZBa (65594) 283  
K(Tm+HL)=1.50  
\*\*\*\*\*

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  
-----  
Tm+++ gl KCl 30°C 0.10M U K1=5.15 B2= 8.14 1996SZa (65611) 284  
\*\*\*\*\*

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  
-----  
Tm+++ gl KCl 30°C 0.10M C K1=5.15 B2=8.14 1996SZa (65626) 285  
\*\*\*\*\*

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  
-----

Tm+++ gl NaCl 25°C 0.15M U H K1=3.88 1992ZNa (65981) 286  
By calorimetry: DH(K1)=3.41 kJ mol<sup>-1</sup>, DS(K1)=85.74 J K<sup>-1</sup> mol<sup>-1</sup>.

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

Tm+++ ISE KNO3 25°C 0.10M U K1=12.46 1983KBd (66748) 287  
Hg-electrode.

\*\*\*\*\*  
C9H13NO6 H3L (3881)  
2,6-Dicarboxypiperidyl-N-ethanoic acid;

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

Tm+++ gl KNO3 25°C 0.10M U K1=11.54 B2=20.17 1968TKe (66896) 288  
\*\*\*\*\*

C9H15NO6 H3L (7177)  
2-Aminopentanoic-N,N-diethanoic acid; C3H7C(COOH)N(CH2COOH)2

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

Tm+++ gl KNO3 20°C 0.10M U K1=11.93 B2=20.52 1974RMg (67416) 289  
\*\*\*\*\*

C9H16N2O6 H3L MEDTA CAS 40423-02-7 (5717)  
N-Methyldiaminoethane-N,N',N'-triethanoic acid; HOOC.CH2.N(CH3)CH2.CH2.N(CH2.COOH)2

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

Tm+++ cal NaClO4 25°C 0.50M M IH K1=13.74 1986RCa (67646) 290  
DH=-13.9 kJ mol<sup>-1</sup>, DS=216 J K<sup>-1</sup> mol<sup>-1</sup>

\*\*\*\*\*  
C9H16O4 H2L CAS 1636-27-7 (485)  
Dipropylpropanedioic acid (Di-n-propylmalonic acid);

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

Tm+++ gl KNO3 25°C 0.10M U K1=4.76 B2=7.39 1968PFa (67780) 291  
\*\*\*\*\*

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  
-----

Tm+++ gl alc/w 22°C 80% U K1=6.36 B2=11.88 1995MTa (68435) 292  
K3=5.56

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

\*\*\*\*\*

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  
-----

Tm+++ gl NaClO4 25°C 0.10M U H K1=4.58 1994CRa (68531) 293  
K(Tm+HL)=3.67

DH(K1)=25.4 kJ mol<sup>-1</sup>, DS=173 J K<sup>-1</sup> mol<sup>-1</sup>; DH(Tm+HL)=15.5, DS=122

\*\*\*\*\*

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  
-----

Tm+++ sp KCl 25°C 0.10M M I K1=4.38 1976PEa (68596) 294

\*\*\*\*\*

C10H7NO2 HL CAS 132-53-6 (2524)

2-Nitroso-1-naphthol;

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

Tm+++ gl KNO3 25°C 0.10M U K1=6.00 B2=11.42 1982LPc (68664) 295

\*\*\*\*\*

C10H7NO5S H2L CAS 14090-74-5 (2676)

1-Nitroso-2-hydroxynaphthalene-7-sulfonic acid;

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

Tm+++ gl KCl 25°C 0.10M M K1=4.26 1979LSb (68820) 296

\*\*\*\*\*

C10H7NO5S H2L (4766)

1-Nitroso-2-hydroxynaphthalene-6-sulfonic acid;

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

Tm+++ sp KCl 25°C 0.10M C K1=4.47 1973PMb (68856) 297

\*\*\*\*\*

C10H7NO5S H2L CAS 31005-79-9 (1814)

2-Nitroso-1-hydroxynaphthalene-8-sulfonic acid;

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

Tm+++ sp KCl 25°C 0.10M M K1=4.97 1978PPb (68953) 298

\*\*\*\*\*

C10H7NO8S2 H3L Nitroso-R acid CAS 525-05-3 (1811)

1-Nitroso-2-hydroxynaphthalene-3,6-disulfonic acid;

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

Tm+++ gl oth/un 25°C 0.10M U K1=5.32 B2=9.82 1990ATa (69032) 299

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

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Tm+++ gl diox/w 25°C 75% U K1=5.82 B2=11.46 1986MIa (69103) 300  
\*\*\*\*\*

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  
-----  
Tm+++ gl alc/w 22°C 80% U K1=7.41 B2=13.37 1995MTa (69164) 301  
K3=6.02

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

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

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Tm+++ gl diox/w 25°C 75% U K1=6.08 B2=11.89 1986MIa (69737) 302  
\*\*\*\*\*

C10H8O2 H2L CAS 92-44-4 (1658)  
2,3-Dihydroxynaphthalene;

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Tm+++ gl NaClO4 20°C 0.10M U M 1973PAc (69781) 303  
K(TmA+L)=7.95, H4A=EDTA

\*\*\*\*\*  
C10H8O5S H3L DHNSA (877)  
2,3-Dihydroxynaphthalene-6-sulfonic acid;

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Tm+++ gl NaClO4 25°C 0.50M C K1=10.37 B2=18.92 1976LAd (69866) 304  
B3=23.3  
B(TmHL2)=25.73

\*\*\*\*\*  
C10H10O6 H2L CAS 5411-14-3 (2394)  
1,2-Phenylenedioxodiethanoic acid; C6H4(O.CH2.COOH)2

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Tm+++ gl NaClO4 25°C 0.10M M K1=3.94 1977HCb (70862) 305  
\*\*\*\*\*

C10H12N2O4 H2L CAS 16598-05-3 (967)  
2-Pyridylmethyliminodiethanoic acid; C5H4N.CH2.N(CH2.COOH)2



-----  
 Tm+++ EMF KCl 25°C 0.10M U T 1974BKb (74255) 318  
 K(TmL+H)=0.8  
 -----

Tm+++ gl KCl 25°C 1.0M C K2=1.55 1974BKe (74256) 319  
 K(TmL+HL)=1.15  
 K(2TmL+L=Tm2L3)=4.28  
 -----

Tm+++ gl KNO3 25°C 0.10M U T M 1973TRb (74257) 320  
 K(TmL+HA)=5.10  
 K(TmL+A)=7.64  
 K(TmL+HA)(2 C)=5.30, K(35 C)=5.19, K(45 C)=4.95, K(TmL+A)(2 C)=7.80,  
 K(35 C)=7.71, K(45 C)=7.40, H5A=tripolyphosphoric acid  
 -----

Tm+++ gl KNO3 25°C 0.10M U T M 1973TRb (74258) 321  
 K(TmL+A)=6.5  
 K(2 C)=6.6, K(35 C)=6.4, K(45 C)=6.2, H4A=adenosine triphosphate  
 -----

Tm+++ dis oth/un 25°C ? U K1=18.04 1969PJa (74259) 322  
 Method: paper electrophoresis. Medium: pH=1.86  
 -----

Tm+++ ix KCl 25°C 0.10M U H K1=18.64 1959BDb (74260) 323  
 DH(K1)=6.6 kJ mol<sup>-1</sup>, DS=379 J K<sup>-1</sup> mol<sup>-1</sup>  
 -----

Tm+++ gl oth/un 20°C 0.01M U K1=19.49 1955WSa (74261) 324  
 -----

Tm+++ vlt KNO3 20°C 0.10M U T K1=19.32 1954SGa (74262) 325  
 -----

Tm+++ gl KCl 20°C 0.10M U I T K1=18.59 1953WSa (74263) 326  
 By polarography K1=18.62. In 0.1 M KNO3 K1=19.07  
 -----

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

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

Tm+++ gl R4N.X 25°C 0.10M C T K1=6.80 1991SMa (74834) 327  
 K(Tm+HL)=3.67  
 -----

IUPAC evaluation  
 -----

Tm+++ gl KCl 25°C 0.10M U K1=6.50 B2=10.56 1988SSd (74835) 328  
 K(Tm+HL)=4.09  
 -----

Tm+++ kin oth/un 25°C 0.05M C K1=7.42 1983Mcc (74836) 329  
 Method: inhibition of the hexokinase reaction, pH 8.0 (0.05 M TAPS).  
 -----

Tm+++ gl KNO3 35°C 0.10M U M 1972TRc (74837) 330  
 K(Tm(EDTA)+L)=6.8  
 -----

\*\*\*\*\*  
 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
Tm+++	gl	NaCl04	25°C	0.50M	U			K1=15.04	1977GGb (75520)	331
Tm+++	EMF	KCl	25°C	1.0M	U			K2=3.77 K(TmL+HL)=2.11 K(TmL+H2L)=0.16 K(TmL+H4L)=1.71	1977GMa (75521)	332

Method: Pt/H2 electrode.

Tm+++	EMF	KCl	25°C	1.0M	U	M		K(Tm(edta)+L)=2.50 K(Tm(edta)+HL)=1.95 K(Tm(edta)+H2L)=1.96 K(Tm(edta)+H3L)=1.74	1977GMa (75522)	333
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Method: Pt/H2 electrode.

Tm+++	gl	NaCl04	25°C	1.0M	U			K2=3.16 K(TmL+HL)=2.19 K(TmL+H2L)=1.09 K(TmL+H3L)=1.54	1973NMa (75523)	334
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Tm+++	ix	oth/un	?	?	U			K(TmL+HL)=2.65 K(TmL2H+H)=6.15	1968MDa (75524)	335
-------	----	--------	---	---	---	--	--	-----------------------------------	-----------------	-----

Tm+++	gl	KNO3	25°C	0.10M	U	M		K(TmL+A)=4.95 K(TmL+B)=4.26	1963TLb (75525)	336
-------	----	------	------	-------	---	---	--	--------------------------------	-----------------	-----

Id=iminodiacetic acid

Tm+++	EMF	oth/un	20°C	0.10M	U			K1=16.00	1962PMa (75526)	337
-------	-----	--------	------	-------	---	--	--	----------	-----------------	-----

Tm+++	gl	KNO3	15°C	0.10M	U	T H		K1=15.66 K1=15.64(20 C), 15.59(25 C), 15.62(30 C), 15.72(35 C), 15.69(40 C) DH(K1)=3.9 kJ mol <sup>-1</sup> (25 C), DS=312 J K <sup>-1</sup> mol <sup>-1</sup>	1961MFb (75527)	338
-------	----	------	------	-------	---	-----	--	--	-----------------	-----

Tm+++	gl	KNO3	25°C	0.10M	U			K1=15.38	1956SPa (75528)	339
-------	----	------	------	-------	---	--	--	----------	-----------------	-----

By polarography K1=15.5

\*\*\*\*\*  
C10H20N2O4 H2L (4753)

N,N'-Diethylethylenedinitrilo-N,N'-diethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Tm+++	gl	KNO3	25°C	0.10M	U			K1=7.1	1973PSb (75786)	340
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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

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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Tm+++     ISE non-aq 25°C 100% C          K1=3.63      1986BDa (76477) 341
Medium: propylene carbonate, 0.1 M Et4NClO4
*****
C11H8O3           L                      CAS 1133-72-8 (2614)
2-Aceto-1,3-indandione;
-----
```

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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Tm+++     gl mixed 22°C 60% U          K1=3.87 B2=7.36 K3=3.11 1979JMa (77047) 342
Medium: 60% acetone/H2O
*****
C11H8O4           HL                     CAS 7555-37-5 (4812)
3-Acetyl-4-hydroxycoumarin
-----
```

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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Tm+++     gl diox/w 35°C 50% U          K1=4.34 B2=7.42 1971MAa (77187) 343
Medium: 50% dioxan, 0.01 M NaClO4
*****
C11H8O6S          H3L                    CAS 66695-90-7 (1996)
1-Hydroxy-4-sulfo-2-naphthoic acid;
-----
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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Tm+++     gl NaClO4 25°C 0.10M C          K1=8.86 B2=15.52 K(Tm+HL)=1.88 1979LAb (77235) 344
*****
C11H8O9S2          H4L                    CAS 67097-84-1 (1995)
1-Hydroxy-4,7-disulfo-2-naphthoic acid;
-----
```

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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Tm+++     cal NaClO4 25°C 0.10M C  H          K1=9.01 B2=14.9 K(Tm+HL)=1.95 1986LLc (77288) 345
DH(Tm+HL)=8.1 kJ mol-1, DS=64 J K-1 mol-1
*****
C11H9NO4           H2L                    CAS 4321-82-7 (4829)
3-Acetyl-4-hydroxycoumarin oxime;
-----
```

```
-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Tm+++     gl diox/w 35°C 50% U          K(Tm+HL)=4.01 K(Tm+2HL)=6.88 1971MAa (77430) 346
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  
-----

Tm+++ sp NaNO3 25°C 0.10M C K1=10.57 19840Ha (77593) 347  
K(Tm+HL)=4.34  
\*K(TmHL)=-6.07

Medium pH 4.8-6.3.

-----  
Tm+++ sp KCl 20°C 0.10M U K(Tm+HL)=3.77 1971EKa (77594) 348  
-----

\*\*\*\*\*  
C11H10N4O3 HL CAS 92265-24-2 (6211)  
5-(2'-Methylphenylazo)barbituric acid;

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

Tm+++ gl diox/w 25°C 75% U K1=6.02 B2=11.45 1986MIa (77735) 349

\*\*\*\*\*

C11H10N4O4 HL CAS 92265-26-4 (6210)  
5-(2'-Methoxyphenylazo)barbituric acid;

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

Tm+++ gl diox/w 25°C 75% U K1=6.23 B2=12.25 1986MIa (77750) 350

\*\*\*\*\*

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  
-----

Tm+++ gl oth/un 30°C 0.10M U B2=21.85 1985EEb (78329) 351  
Medium: not stated. For 3'-sulfophenylhydrazo-, B2=22.11; for 2'-sulfo-  
phenylhydrazo-, B2=25.13; for 4'-methyl-2'-sulfophenylhydrazo-, B2=23.75.

\*\*\*\*\*

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  
-----

Tm+++ sp non-aq 20°C 100% C K1=7.0 B2=13.70 1997RPa (78539) 352  
B3=17.6

Medium: acetonitrile.

\*\*\*\*\*

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  
-----

-----  
Tm+++ gl KNO3 25°C 0.10M C K1=14.48 B2=26.48 1989YSa (78643) 353  
K(Tm+HL)=6.40  
-----

Tm+++ gl KNO3 20°C 0.10M U K1=14.53 B2=25.77 1983MSc (78644) 354  
\*\*\*\*\*  
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  
-----

Tm+++ gl KNO3 25°C 0.10M U K1=7.54 B2=12.81 1964THa (78894) 355  
\*\*\*\*\*  
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  
-----

Tm+++ vlt KNO3 20°C 0.10M U K1=15.69 1981NSc (79344) 356  
-----

Tm+++ EMF KNO3 25°C 0.10M U K1=16.47 1980KBc (79345) 357  
-----

Tm+++ vlt KNO3 20°C 0.10M U K1=20.05 1978NLb (79346) 358  
-----

Tm+++ vlt KNO3 20°C 0.10M U K1=20.08 1964ICb (79347) 359  
\*\*\*\*\*  
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  
-----

Tm+++ gl KNO3 25°C 0.10M U K1=11.12 1976GKd (79375) 360  
\*\*\*\*\*  
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  
-----

Tm+++ gl KNO3 25°C 0.10M M K1=15.31 1986PLc (79579) 361  
\*\*\*\*\*  
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  
-----

Tm+++ gl KNO3 25°C 0.10M U K1=12.34 1976GKd (79608) 362  
\*\*\*\*\*  
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
Tm+++	gl	KNO3	25°C	0.10M	U		K1=4.73 B2=7.34	1968PFa (79773)	363
*****									
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
Tm+++	gl	alc/w	22°C	80%	U		K1=6.28 B2=11.80 K3=5.36	1995MTa (80192)	364
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
Tm+++	sp	non-aq	25°C	100%	C	H	K1=2.06	2002KNc (80525)	365
Medium: N,N-dimethylformamide, 0.20 M Et4NClO4.									
By calorimetry: DH(K1)=-9.9 kJ mol-1.									
-----									
Tm+++	dis	non-aq	25°C	100%	C	HM		1998YHa (80526)	366
K(TmA3+L)=7.98									
Method: solvent extraction from 0.10 M NaClO4 into CHCl3. HA is									
1-(2-thienyl)-4,4,4-trifluoro-1,3-butanedione. DH(TmA3+L)=-11.9 kJ mol-1.									
*****									
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
Tm+++	sp	NaClO4	25°C	0.50M	U		K1=2.128	1987MSa (80976)	367
*****									
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
Tm+++	gl	alc/w	22°C	0.1M	U		K1=6.48 B2=12.15 K3=4.30	2000TBb (81083)	368
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
Tm+++	sp	NaClO4	25°C	0.50M	U		K1=2.276	1987MSa (81206)	369
*****									

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  
-----

Tm+++            gl    KNO3    25°C 0.10M C                    K1=6.03                    1988YSa (81821) 370  
\*\*\*\*\*

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  
-----

Tm+++            gl    R4N.X    25°C 0.10M C                    K1=6.53                    1988CCb (81845) 371  
\*\*\*\*\*

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  
-----

Tm+++            EMF   KNO3    25°C 0.10M U                    K1=14.22                    1985SGa (81881) 372

Tm+++            EMF   KNO3    25°C 0.10M U                    K1=15.63                    1980SGb (81882) 373  
\*\*\*\*\*

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  
-----

Tm+++            vlt   KNO3    20°C 0.10M U                    K1=20.52                    1968NLa (82036) 374  
\*\*\*\*\*

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  
-----

Tm+++            gl    KNO3    20°C 0.10M U                    K1=9.59    B2=15.54    1975DPa (82105) 375

Tm+++            gl    KNO3    25°C 0.10M U                    K1=9.26                    1973GBd (82106) 376  
\*\*\*\*\*

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  
-----

Tm+++            vlt   KNO3    20°C 0.10M U                    K1=18.91                    1976NKa (82147) 377  
\*\*\*\*\*

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
Tm+++	gl	NaClO4	25°C	0.10M	U	IH		K1=14.25 B(Tm+HL)=6.66	1988RNa (82181)	378
DH(K1)=3.74 kJ mol <sup>-1</sup> , DH(Tm+HL)=27.9, DS(K1)=285 J K <sup>-1</sup> mol <sup>-1</sup>										
*****										
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
Tm+++	gl	NaClO4	25°C	0.50M	M	H		K1=11.25 K(TmL+H)=6.05 K(TmHL+H)=4.85	1985CBa (82238)	379
DH(K1)=23.3 kJ mol <sup>-1</sup> , DS=293 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										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Tm+++	sp	NaClO4	20°C	0.10M	U			K1=20.44	1971ISa (82340)	380
Tm+++	vlt	oth/un	20°C	0.10M	U			K1=20.96	1966DMa (82341)	381
Tm+++	vlt	KNO3	20°C	0.10M	U			K1=20.96	1966NSb (82342)	382
*****										
C12H20N2O8		H4L						CAS 22968-57-6	(3992)	
meso-2,3-Diaminobutane-N,N,N',N'-tetraethanoic acid; (HOOC.CH2)2N.CH(CH3).CH(CH3).N(CH2.COOH)2										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Tm+++	sp	NaClO4	20°C	0.10M	U			K1=17.87	1971ISa (82424)	383
Tm+++	vlt	oth/un	20°C	0.10M	U			K1=17.87	1966DMa (82425)	384
*****										
C12H20N2O8S		H4L			TEDTA			CAS 923-74-0	(3394)	
2,2'-Thiobis(ethyliminodiethanoic acid); S(CH2.CH2.N(CH2.COOH)2)2										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Tm+++	gl	KNO3	25°C	0.10M	C			K1=14.41	1985TPa (82479)	385
*****										
C12H20N2O9		H4L			EEDTA			CAS 923-73-9	(2112)	
Oxa-bis(ethyleneimino)diethanoic acid; ((HOOC.CH2)2N.CH2.CH2)2O										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Tm+++ EMF KNO3 20°C 0.10M U K1=17.83 1962MMc (82572) 386  
\*\*\*\*\*

C12H20O8N2 H4L (6908)  
2-Methyl-1,2-diaminopropane-N,N,N'N'-tetraethanoic acid;  
(HOOC.CH2)2N.CH2.C(CH3)2.N(CH2.COOH)2

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

Tm+++ vlt KNO3 20°C 0.10M C K1=17.79 1978NLa (82683) 387  
\*\*\*\*\*

C12H21NO6 H3L (7209)  
1-Carboxy-1-aminoheptane-N,N-diethanoic acid; HOOC.CH(C6H13)N(CH2.COOH)2

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

Tm+++ gl alc/w 20°C 40% U K1=11.80 1985LBc (82707) 388  
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  
-----

Tm+++ gl R4N.X 25°C 0.10M C K1=13.19 1998CCb (83094) 389  
\*\*\*\*\*

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  
-----

Tm+++ gl alc/w 25°C 100% C K1=9.46 1983ANb (83912) 390  
The equilibration took 7-12 days. Medium: MeOH, 0.05 M Et4NClO4  
\*\*\*\*\*

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  
-----

Tm+++ gl non-aq 25°C 100% C K1=4.56 1989BPa (84026) 391  
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  
-----

Tm+++ gl R4N.X 25°C 0.10M U K1=13.80 1996BJa (84167) 392  
K(Tm+HL)=10.22  
K(Tm+H2L)=5.86

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
Tm+++	gl	NaNO3	25°C	0.20M	C			K1=8.95	1991KKa (84359)	393

Tm+++	gl	NaCl	20°C	0.10M	C			K1=10.4	1988SJB (84360)	394
-------	----	------	------	-------	---	--	--	---------	-----------------	-----

\*\*\*\*\*

C13H502F13S L (6997)  
 1-(2-Thienyl)-3-tridecafluorohexylpropane-1,3-dione; C6F13.CO.CH2.CO.C4H3S  
 -----

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Tm+++	gl	alc/w	22°C	80%	U			K1=5.72 K3=4.32	1995MTa (84463)	395

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

\*\*\*\*\*  
 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
Tm+++	dis	oth/un	23°C	0.01M	C				1997AAa (85182)	396

Method: extraction of 170Tm from 0.01 M borate buffer into benzene-ligand solution.  $K(Tm+3HL(org))=TmL3(org)+3H)=-13.54$ .

\*\*\*\*\*  
 C13H12N2O3S HL (6203)  
 Salicylidenesulfanilamide, 4-(N-(2-Hydroxybenzylene))aminosulanilamide;  
 H2NSO2C6H4N:CHC6H4OH  
 -----

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Tm+++	gl	oth/un	25°C	0.10M	U			K1=12.763	1987KSc (85367)	397

\*\*\*\*\*  
 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
Tm+++	EMF	alc/w	20°C	50%	U			K1=3.75	1971MAc (85420)	398

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
Tm+++	EMF	alc/w	20°C	50%	U			K1=2.25	1971MAc (85476)	399

Medium: 50% EtOH, 0.1 M NaClO4

\*\*\*\*\*

C13H20N2O8 H4L CAS 123064-92-6 (7929)  
trans-1,3-Cyclopentanediaminotetraethanoic acid;

---

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Tm+++	gl	KCl	25°C	1.0M	U			K1=14.43 K(TmHL+H)=3.06 K(TmL+H)=3.76	1989Cmb (86129)	400

\*\*\*\*\*

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
Tm+++	gl	KNO3	25°C	0.10M	C			K1=11.19 K(Tm+HL)=7.24	1982PPd (86210)	401

\*\*\*\*\*

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
Tm+++	vlt	KNO3	20°C	0.10M	U			K1=20.46	1974NLa (86238)	402

\*\*\*\*\*

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
Tm+++	vlt	KNO3	20°C	0.10M	U			K1=13.63	1981NSc (86266)	403

\*\*\*\*\*

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
Tm+++	vlt	KNO3	20°C	0.10M	U			K1=20.38	1968NLb (86293)	404

\*\*\*\*\*

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
Tm+++	gl	KNO3	25°C	0.10M	C			K1=14.97 K(Tm+HL)=9.29	1985PLa (86312)	405

\*\*\*\*\*

C14H8O4 H2L Alizarin CAS 72-48-0 (1058)

1,2-Dihydroxyanthraquinone;

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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Tm+++     gl  oth/un 25°C 0.10M U          K1=12.73      1981EIa (86652) 406
*****
C14H9N5Cl2          L          CAS 7071-45-6 (8463)
1,5-Bis(4-chlorophenyl)-3-cyanoformazan;
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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Tm+++     gl  diox/w 25°C 70% U          K1=6.39   B2=12.65  1996DAb (86854) 407
Medium: 70% dioxane/H2O, 0.10 M NaClO4.
*****
C14H11N5          L          CAS 7014-08-6 (8461)
1,5-Diphenyl-3-cyanoformazan;
-----
```

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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Tm+++     gl  diox/w 25°C 70% U          K1=7.33   B2=14.18  1996DAb (87003) 408
Medium: 70% dioxane/H2O, 0.10 M NaClO4.
*****
C14H12N2O3        H2L          CAS 4870-46-6 (3432)
2-Hydroxy-5-methyl-2'-carboxy-azobenzene; HO.C6H3(CH3).N:N.C6H4.COOH
-----
```

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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Tm+++     gl  diox/w 25°C 50% U I       K1=3.92   B2=7.78   1985ANa (87224) 409
*****
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
-----
Tm+++     gl  mixed 30°C 0.10M U T H     K1=12.68  B2=23.12  1988TRb (87727) 410
Medium: 0.1 M KNO3 in 75% v/v isopropanol/water
*****
C14H16N2O2S        HL          CAS 189231-67-2 (8475)
2-Thiophenylhydrazodimedone;
-----
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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Tm+++     gl  diox/w 25°C 75% C T H     K1=13.71  B2=25.81  1997EIa (87876) 411
Medium: 75% v/v dioxane/H2O, 0.10 M KNO3. Data for 10-40 C. DH(K1)=-8.48
kJ mol-1, DS(K1)=-13.50 J K-1 mol-1; DH(K2)=-7.38, DS(K2)=-11.63.
*****
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
-----
```

-----  
Tm+++ gl mixed 30°C 0.10M U T H K1=12.90 B2=23.65 1988TRb (87894) 412  
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  
-----

Tm+++ gl NaClO4 25°C 1.00M C H K1=15.87 1992YNa (87971) 413  
By calorimetry: DH(K1)=6.7 kJ mol<sup>-1</sup>, DS=326 J K<sup>-1</sup> mol<sup>-1</sup>

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

Tm+++ gl KCl 25°C 1.0M U K1=4.40 1987CMe (88436) 414  
K(TmHL+H)=5.13  
K(TmL+H)=6.93

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

Tm+++ gl KCl 25°C 1.0M U K1=8.30 1987CMe (88450) 415  
K(TmHL+H)=4.98  
K(TmL+H)=7.12

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

Tm+++ gl KCl 25°C 1.0M U K1=9.47 1987CMe (88464) 416  
K(TmHL+H)=5.42  
K(TmL+H)=5.75

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

Tm+++ gl KCl 25°C 1.0M U K1=20.98 1987CMe (88808) 417  
K(TmL+H)=1.22

-----  
Tm+++ gl KCl 25°C 1.00M U K1=20.98 1984MFa (88809) 418  
-----

Tm+++ gl NaClO4 25°C 0.50M U K1=19.58 1977GGb (88810) 419

-----  
Tm+++ EMF KNO3 25°C 0.10M U T H K1=20.46 1962MHa (88811) 420  
DH(K1)=-6.7 kJ mol<sup>-1</sup>, DS=368 J K<sup>-1</sup> mol<sup>-1</sup>. At 20 C: K(TmL+H)=2.20  
-----

Tm+++ vlt KNO3 20°C 0.10M U K1=20.96 1954SGa (88812) 421  
\*\*\*\*\*  
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  
-----

Tm+++ gl KCl 25°C 1.0M U K1=8.66 1987CMe (88843) 422  
K(TmHL+H)=4.44  
K(TmL+H)=7.12  
-----

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

Tm+++ gl KCl 25°C 1.0M U K1=9.69 1987CMe (88871) 423  
K(TmHL+H)=5.56  
K(TmL+H)=5.70  
-----

Tm+++ gl KCl 25°C 1.00M U K1=9.69 1984MFb (88872) 424  
\*\*\*\*\*  
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  
-----

Tm+++ gl R4N.X 25°C 0.10M C K1=7.98 1988CCb (88887) 425  
\*\*\*\*\*  
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  
-----

Tm+++ cal KNO3 25°C 0.10M C T 1988MIa (89418) 426  
DH(K1)=-26.52 kJ mol<sup>-1</sup>, DS=346.0 J mol<sup>-1</sup> K<sup>-1</sup>. Also data for 283 and 313 K  
-----

Tm+++ cal NaClO4 25°C 0.50M U H 1977CGc (89419) 427  
DH(K1)=-36.6 kJ mol<sup>-1</sup>  
-----

Tm+++ gl NaClO4 25°C 0.50M U K1=21.15 1977GGb (89420) 428  
-----

Tm+++ cal KNO3 27°C 0.10M U H 1968CLd (89421) 429  
DH(K1)=-27.6 kJ mol<sup>-1</sup>, DS=343 J K<sup>-1</sup> mol<sup>-1</sup>  
-----

Tm+++ EMF KNO3 25°C 0.10M U H K1=22.72 1962MTc (89422) 430  
-----

DH(K1)=-23.0 kJ mol<sup>-1</sup>, DS=358 J K<sup>-1</sup> mol<sup>-1</sup>

-----  
Tm+++ gl oth/un 25°C 0.10M U K1=22.97 1959HCa (89423) 431  
\*\*\*\*\*  
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  
-----  
Tm+++ vlt KNO3 20°C 0.10M U K1=18.45 1969NDc (89521) 432  
\*\*\*\*\*  
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  
-----  
Tm+++ vlt KNO3 20°C 0.10M U K1=20.40 1974NLa (89540) 433  
\*\*\*\*\*  
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  
-----  
Tm+++ gl KCl 25°C 1.00M U M 1976BKa (89610) 434  
K(TmEDTA+L)=2.4  
K(TmEDTA+HL)=2.2  
-----

Tm+++ gl KCl 25°C 0.10M U 1974KPd (89611) 435  
K(Tm+HL)=7.18  
\*\*\*\*\*  
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  
-----  
Tm+++ vlt KNO3 20°C 0.10M U K1=20.40 1968NLb (89644) 436  
\*\*\*\*\*  
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  
-----  
Tm+++ gl R4N.X 25°C 0.10M C K1=10.44 1988CCb (89658) 437  
\*\*\*\*\*  
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



Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Tm+++	gl	non-aq	25°C	100%	C		K1=6.25	1989BPa (90543)	445
Medium: anhydrous propylene carbonate, 0.1 M Et4NClO4									
*****									
C14H3007		L					CAS 1072-40-8	(2499)	
2,5,8,11,14,17,20-Heptaoxaheneicosane; CH3.O.(CH2.CH2.O)6.CH3									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Tm+++	gl	non-aq	25°C	100%	C		K1=5.34	1989BPa (90714)	446
Medium: anhydrous propylene carbonate, 0.1 M Et4NClO4									
*****									
C14H32N2O10P2		H4L					CAS 81963-60-2	(7240)	
1,4,10,13-Tetraoxa-7,16-diazacyclooctadecane-7,16-diylldimethylenediphosphonic acid;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Tm+++	gl	R4N.X	25°C	0.10M	U		K1=13.77 K(Tm+HL)=10.24 K(Tm+H2L)=6.11	1996BJa (90775)	447
Medium: 0.1 M Me4NCl									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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
Tm+++	gl	alc/w	20°C	75%	U T H		K1=12.15 B2=21.48	1993RAa (92040)	448
Medium: 75% v/v MeOH/H2O; 0.10 M KNO3									
*****									
Tm+++	gl	mixed	30°C	0.10M	U T H		K1=13.16 B2=24.74	1988TRb (92041)	449
Medium: 0.1 M KNO3 in 75% v/v isopropanol/water									
*****									
C15H20N2O6		H3L			BEDTA		CAS 65311-06-0	(2944)	
N-Benzylidiaminoethane-N,N',N'-triethanoic acid;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Tm+++	gl	KNO3	25°C	0.10M	C		K1=13.65	1978MPb (92159)	450
*****									
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
Tm+++	sp	non-aq	25°C	100%	M		K1=8.5 B2=16.00 B3=22.1	1997RPb (92291)	451
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  
-----

Tm+++ EMF KCl ? 0.10M U K1=16.71 1966VLa (92385) 452  
\*\*\*\*\*

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  
-----

Tm+++ gl KNO3 25°C 0.10M C K1=19.41 1989SPa (92401) 453  
K(Tm+HL)=13.11  
\*\*\*\*\*

C15H26N4O9 H4L (7685)  
Diethylenetriamine-N,N,N',N'',N''-pentaethanoic acid N'-methylamide;

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

Tm+++ gl KCl 25°C 0.10M C K1=20.4 2000SBb (92439) 454  
\*\*\*\*\*

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  
-----

Tm+++ gl KCl 25°C 0.10M C K1=19.1 2000SBb (92454) 455  
\*\*\*\*\*

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  
-----

Tm+++ kin oth/un 25°C 0.02M U K1=5.45 1972GSe (92667) 456  
\*\*\*\*\*

C16H11N3O10S2 H4L Chromotrope 2B CAS 548-80-1 (896)  
2-((4-Nitrophenyl)azo)chromotropic acid;

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

Tm+++ sp oth/un 25°C ? U K1eff=5.0 1967SAa (92870) 457  
\*\*\*\*\*

C16H11N5O4 H2L (5153)  
1,5-Bis(2-carboxyphenyl)-3-cyanoformazan;

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

Tm+++ gl diox/w 25°C 70% U I K1=11.06 B2=19.95 1996DAb (92901) 458

Medium: 70% dioxane/H2O, 0.10 M NaClO4. In 50% EtOH/H2O, 0.10 M NaClO4,  
 K1=11.86, K2=9.69.

\*\*\*\*\*

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  
 -----

Tm+++ gl NaClO4 30°C 0.10M U 1976NDa (93215) 459

K(Tm+H2L=TmH2L)=6.05

K(TmHL+H)=6.80

K(TmL+H)=8.80

K(TmL+OH)=3.10

\*\*\*\*\*

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  
 -----

Tm+++ sp oth/un 20°C 0.10M U 1971SSd (93271) 460

K(Tm+H2L)=8.33

\*\*\*\*\*

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  
 -----

Tm+++ gl diox/w 25°C 70% U K1=8.95 B2=16.80 1996DAb (93644) 461

Medium: 70% dioxane/H2O, 0.10 M NaClO4.

\*\*\*\*\*

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  
 -----

Tm+++ vlt KNO3 20°C 0.10M U K1=19.34 1969NDb (94054) 462

\*\*\*\*\*

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  
 -----

Tm+++ gl R4N.X 25°C 0.10M C K1=8.56 1988CCb (94578) 463

\*\*\*\*\*

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  
 -----

Tm+++ sp KCl 25°C 0.08M U K1=11.2 1994FCa (94678) 464

\*\*\*\*\*  
 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  
 -----  
 Tm+++ sp KCl 25°C 0.08M U K1=14.7 1994FCa (94692) 465  
 \*\*\*\*\*

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  
 -----  
 Tm+++ gl KNO3 20°C 0.10M U K1=15.20 1969NDc (94723) 466  
 By polarography: K1=15.31  
 \*\*\*\*\*

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  
 -----  
 Tm+++ vlt KNO3 20°C 0.10M U K1=18.45 1969NDc (94749) 467  
 \*\*\*\*\*

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  
 -----  
 Tm+++ vlt KNO3 20°C 0.10M U K1=20.39 1979MBd (94775) 468  
 \*\*\*\*\*

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  
 -----  
 Tm+++ gl NaCl 37°C 1.0M C K1=23.7 1994TBb (94935) 469  
 Method: Competitive reaction with Eu3+ ion.  
 \*\*\*\*\*

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  
 -----  
 Tm+++ gl R4N.X 25°C 0.10M U K1=11.10 1983CRb (95061) 470  
 \*\*\*\*\*

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

-----  
Tm+++ gl R4N.X 25°C 0.25M C K1=6.88 1981BBe (95304) 471  
Medium: Me4NCl

\*\*\*\*\*  
C16H35O4P HL CAS 298-07-7 (1625)  
Di-(2-ethylhexyl)-phosphoric acid; (C2H5C6H12O)2P(O)OH  
-----

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

Tm+++ dis oth/un 20°C 0.10M C 1992SNb (95516) 472  
Extraction of 170Tm from 0.10 M LiNO3/HNO3 medium into 90% CFC-112/benzene  
K(Tm+4HL(org))=TmL3(HL)(org)+3H)=5.58

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

Tm+++ gl NaNO3 20°C 0.10M U M 1981GCa (95904) 473  
B(Tm+3L+2TBP)=24.35  
B(Tm+3L+TBPOxide)=23.6  
B(Tm+3L+4TBPOxide)=34.7

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

Tm+++ gl alc/w 22°C 0.1M U K1=5.60 B2=10.08 2000TBb (96292) 474  
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  
-----

Tm+++ sp NaNO3 25°C 0.10M C K1=8.65 19880Ha (96427) 475  
K(Tm+HL)=2.76

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

Tm+++ gl KNO3 25°C 0.10M U K1=9.69 1984TPa (96579) 476  
K(Tm+HL)=6.34

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

Tm+++ EMF KNO3 25°C 0.10M C T H K1=21.39 1985HWb (97442) 477  
K(TmL+H)=6.96

Method: Hg (and glass) electrode, using Hg(II) as competitive indicator ion. Data for 10-35 C. DH(K1)=-83.4 kJ mol<sup>-1</sup>, DS(K1)=130 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  
-----

Tm+++ gl KNO3 25°C 0.10M C K1=14.79 1985TPa (97661) 478

\*\*\*\*\*

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  
-----

Tm+++ gl non-aq 25°C 100% U K1=2.81 1982MDa (97816) 479

Medium: propylene carbonate

\*\*\*\*\*

C18H30N2O11 H2L CAS 93049-99-1 (5832)

1,4,7,10,13-Pentaoxa-16,19-diazacycloeicosane-14,21-dione-16,19-diethanoic acid;

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

Tm+++ gl R4N.X 25°C 0.10M C K1=8.94 1988CCb (97918) 480

\*\*\*\*\*

C18H30N4O12 H6L TTHA CAS 869-52-3 (694)

Triethylenetetraaminehexaethanoic acid;((HOOC.CH2)2N.CH2.CH2.N(CH2.COOH).CH2)2

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

Tm+++ EMF KNO3 25°C 0.10M C T H K1=23.48 1987HCa (98100) 481

K(TmL+H)=5.04

K(TmHL+H)=2.57

Method: Hg electrode; competitive reaction with Hg(II).

Data for 15-35 C. At 25 C, DH(K1)=104 kJ mol<sup>-1</sup>, DS(K1)=799 J K<sup>-1</sup> mol<sup>-1</sup>.

\*\*\*\*\*

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  
-----

Tm+++ gl NaNO3 25°C 0.20M C K1=15.15 1991KKa (98232) 482

\*\*\*\*\*

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  
-----  
Tm+++ gl R4N.X 25°C 0.10M C K1=6.13 1988CCc (98347) 483  
\*\*\*\*\*  
C18H34N4O9 H3L DO3A-B (7301)  
10-[2,3-Dihydroxy-(1-hydroxymethyl)-propyl]-1,4,7,10-tetraazacyclododecane-1,4,7-triethanoic ac.;

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Tm+++ gl NaCl 25°C 0.10M C I K1=19.0 1996TKa (98385) 484  
In 0.1 M Me4NCl K=21.1  
\*\*\*\*\*  
C18H36N2O6 L Cryptand 2,2,2 CAS 23978-09-8 (514)  
1,10-Diaza-4,7,13,16,21,24-hexaoxabicyclo[8.8.8]hexacosane;

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Tm+++ gl alc/w 25°C 100% C K1=11.61 1983ANb (98762) 485  
The equilibration took 7-12 days. Medium: MeOH, 0.05 M Et4NClO4  
\*\*\*\*\*  
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  
-----  
Tm+++ gl R4N.X 25°C 0.10M U K1=6.47 1996BJa (98901) 486  
Medium: 0.1 M Me4NCl  
\*\*\*\*\*  
C20H14N2O11S3 H5L Chromotrope 8B CAS 5850-64-6 (2674)  
3-(4'-Sulfonaphthylazo)chromotropic acid;

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Tm+++ sp NaClO4 25°C 0.10M C K1=6.31 1979PLb (99718) 487  
\*\*\*\*\*  
C20H18N4O2 HL (5917)  
Pyruvic monohydrazone-3-hydrazino-4-benzyl-6-phenylpyridazine;

-----  
Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Tm+++ gl diox/w 30°C 75% U K(Tm+HL)=5.32  
K(Tm+2HL)=10.84  
\*\*\*\*\*  
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
Tm+++	gl	KNO3	20°C	0.10M	U		K1=20.31 K(TmL+H)=5.02 K(TmHL+H)=4.65	1985SNb (100017)	489

\*\*\*\*\*  
 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
Tm+++	gl	oth/un	25°C	0.0	U	H	K1=3.21	1991HJa (100255)	490

\*\*\*\*\*  
 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
Tm+++	gl	NaNO3	25°C	0.20M	C		K1=16.61	1991KKa (100548)	491

\*\*\*\*\*  
 C20H35N5O10 H3L (6623)  
 1,4,7-Tris(carboxymethyl)-13,16-dioxa-1,4,7,10,19-pentaazacycloheicosa-9,20-dione  
 ;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Tm+++	sp	KCl	25°C	0.08M	U		K1=17.1	1994FCa (100565)	492

\*\*\*\*\*  
 C21H17N5 L (7365)  
 2,6-Bis(1-methylbenzimidazol-2-yl)pyridine

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Tm+++	gl	non-aq	25°C	100%	C		K3=3.9	1997PBa (101094)	493

Medium: CH3CN; 0.1 M Et4NClO4  
 \*\*\*\*\*  
 C22H14O9 H5L CAS 4431-00-9 (3513)  
 Aurintricarboxylic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Tm+++	sp	oth/un	25°C	?	U		K(Tm+HL)=5.1(?)	1967SAa (101511)	494

\*\*\*\*\*  
 C22H17AsN4O14S3 H6L Arsenazo M CAS 3563-69-7 (623)  
 2-(2-Arsonophenylazo)-7-(3-sulfophenylazo)-1,8-dihydroxynaphthalene-3,6-disulfonic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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-----  
Tm+++ sp oth/un ? ? U K1=16.14 1971SSi (101555) 495  
\*\*\*\*\*  
C22H18N4O14As2S2 H8L Arsenazo III CAS 1668-00-4 (1148)  
2,7-Bis(2'-arsonophenylazo)chromotropic acid;  
-----

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

Tm+++ sp oth/un 20°C ? U 1972SSi (101653) 496  
K(Tm+H4L)=15.22  
\*\*\*\*\*

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  
-----

Tm+++ EMF KNO3 25°C 0.10M C T H K1=11.60 1990HLA (101905) 497  
K(TmL+H)=3.45

Method: Competitive reaction with Hg++, using Hg indicator electrode.  
Data for 15-35 C. DH(K1)=-42.0 kJ mol<sup>-1</sup>, DS(K1)=81.3 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;  
(HOOCH2)2NCH(OC6H4NH2)2  
-----

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

Tm+++ gl R4N.X 25°C 0.10M C K1=10.51 1993YTa (101988) 498  
\*\*\*\*\*

C22H37N5O14 H7L CAS 3234-59-1 (2425)  
Tetraethylenepentamineheptaethanoic acid;  
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Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----

Tm+++ gl KNO3 25°C 0.10M U K1=20.11 1968MIc (102346) 499  
K(Tm+HL)=13.98  
B(TmH-1L)=5.15  
\*\*\*\*\*

C23H18O9S H4L Eriochrome cyan CAS 3564-18-9 (433)  
4'-Hydroxy-3,3'-dimethyl-2''-sulfofuchsone-5,5'-dicarboxylic acid;  
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Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----

Tm+++ sp oth/un 25°C ? U B2=9.6 1968MDc (102638) 500  
\*\*\*\*\*

C23H24N4O2 L Trichachnine CAS 1251-85-0 (2606)  
4,4'-Diantipyrylmethane,  
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  
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Tm+++ sp diox/w 25°C 100% U K1=4.13 1995KMa (102680) 501  
\*\*\*\*\*

C24H42N6O12 H6L (6546)  
1,4,7,10,13,16-Hexaazacyclooctadecane-N,N',N'',N''',N''''-hexaethanoic acid;

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

Tm+++ gl NaNO3 25°C 0.20M C K1=24.09 1991KKa (103389) 502  
K(Tm+H2L)=16.82  
\*\*\*\*\*

C26H23N5O2 HL (5918)  
Hippuric monohydrazone-3-hydrazino-4-benzyl-6-phenylpyridazine;

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

Tm+++ gl diox/w 30°C 75% U K1=11.70 B2=22.28 1985RSb (103889) 503  
\*\*\*\*\*

C26H27N3O10 H4L (7231)  
2-((2-Amino-5-methylphenoxy)-methyl)-6-methoxy-8-aminoquinoline-N,N,N',N'-tetraethanoic acid;

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

Tm+++ gl R4N.X 25°C 0.10M C K1=14.35 1993YTa (103974) 504  
\*\*\*\*\*

C27H24N4O L BAHP (1023)  
Benzoylacetone-monohydrazone-3-hydrazino-4-benzyl-6-phenylpyridazine;

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

Tm+++ gl diox/w 30°C 75% U K1=8.82 1983RSa (104392) 505  
\*\*\*\*\*

C27H29N011 L Adriamycin CAS 25316-40-9 (2407)  
Doxorubicin;

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

Tm+++ sp oth/un 25°C 0.02M U T H K1=4.82 1985LSa (104464) 506  
Medium: 0.02M pH 7.6 buffer  
\*\*\*\*\*

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

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

Tm+++ gl non-aq 25°C 100% U K1=2.94 1980MDb (104853) 507  
Medium: Propylene carbonate.

Medium: propylene carbonate  
\*\*\*\*\*

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  
-----  
Tm+++ gl diox/w 30°C 75% U I K1=10.04 1983RRa (105411) 508  
In 75% MeOH: K1=7.79; 75% DMF: 6.63

\*\*\*\*\*  
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  
-----  
Tm+++ sp diox/w 25°C 100% C 1997KMa (105637) 509  
K(La(NO3)3+L)=4.07

\*\*\*\*\*  
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  
-----  
Tm+++ nmr KCl 25°C 1.0M C H K1=2.10 2004BRa (105976) 510  
Method: 1H nmr measurements in D2O. DH(K1)=29 kJ mol-1  
DS(K1)=138 J mol-1K-1

\*\*\*\*\*  
C36H60O3O L a-Cyclodextrin CAS 10016-20-3 (6946)  
alpha-Cyclodextrin, Cyclohexaamylose;

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Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Tm+++ gl NaCl 25°C 0.10M U I K1=2.65 1999FBa (106474) 511  
In 0.1 M Me4NCl, K1=3.0.

\*\*\*\*\*  
C37H44N2O13S H6L MeThymol Blue (428)  
3,3'-Bis(N,N-di(carboxymethyl)aminomethyl)thymolsulfonephthalein;

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Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Tm+++ gl NaClO4 30°C 0.10M U 1980NAb (106623) 512  
K(Tm+H3L)=4.65  
K(Tm+H2L)=7.59  
K(TmH2L+H)=4.20

Also data for TmHnL(OH) species

\*\*\*\*\*  
C47H46N6O4 L (7367)  
2,6-Bis(1-(3,5-dimethoxybenzyl)benzimidazol-2-yl)-4-(4-diethylamino)phenyl)pyridine  
;

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

-----  
Tm+++ gl non-aq 25°C 100% C K2=7.0 1997PBa (107321) 513  
K3=3.9

Medium: CH3CN; 0.1 M Et4NClO4

\*\*\*\*\*

C48H80O40 L g-Cyclodextrin CAS 17465-86-0 (7612)

Cyclooctaamylose;

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Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
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Tm+++ nmr oth/un 25°C C M 1999ZBa (107431) 514

K(Tm(DOTA)+L)=-0.48

K(2TM(DOTA)+L)=0.53

DOTA: 1,4,7,10-tetraazacyclododecane-1,4,7,10-tetraethanoic acid.

Method: 1H nmr. Medium: D2O

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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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