

SC-Database

Software version = 5.81 Data version = 4.62
 Experiment list contains 1162 experiments for
 (no ligands specified)
 Metal : Gd+++
 (no references specified)
 (no experimental details specified)

 e- HL Electron (442)
 Electron;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	oth	none	25°C	0.0	U			1974JOb K(Gd+3e=Gd(s))=-115.1(-2.27V) K(Gd+e=Gd(II))=-61(-3.6V)	(511)	1

Method: Literature evaluated data

Gd+++	oth	none	25°C	0.0	U			1952LAb K(Gd+3e)=-121.5(-2400 mV)	(512)	2
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 AsO4--- H3L Arsenate CAS 7778-39-4 (1557)
 Arsenate;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	sol	none	25°C	0.0	C			1992FIa Kso(GdAsO4)=-21.67	(1147)	3

Equilibrium monitored by EDTA and iodine titrations.

 CN- HL Cyanide CAS 74-90-8 (230)
 Cyanide;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	dis	oth/un	25°C	0.50M	U			1971DGc K(Gd+HL)=1.9 K(Gd+HL=GdL+H)=-5.7 K(Gd+HL+H2O=Gd(OH)L+2H)=-13.9 K(Gd+HL+2H2O=Gd(OH)2L+3H)-22.9	(2689)	4

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	NaClO4	25°C	0.70M	C			K1=5.72 K(Gd+HCO3=GdHCO3)=1.31	2004LBb (3228)	5

Medium: 0.70 m NaClO4. Calculated for I=0, K1=7.39, B2=12.48,

$K(\text{Gd}+\text{HCO}_3=\text{GdHCO}_3)=2.36$, $K(\text{Gd}+\text{HL}=\text{GdL}+\text{H})=-2.94$, $K(\text{Gd}+2\text{HL}=\text{GdL}_2+2\text{H})=-8.18$

 Gd+++ dis NaClO4 25°C 0.70M C I K1=5.66 B2= 9.96 1998LBb (3229) 6
 Method: H2O/tributylphosphate distribution and ICP-mass spectrometry.
 Values calculated for I=0.0 M, K1=7.64, B2=13.04.

Gd+++ dis NaClO4 25°C 0.70M C 1995LBc (3230) 7
 B1eff=5.65
 B2eff=10.12
 Keff(Gd+HL)=1.66

By solvent extraction from 0.7 M NaClO4 into tributylphosphate using 88Y.
 $B1_{\text{eff}}=[\text{GdL}]/[\text{Gd}](\text{[L]}+\text{[NaL]})$. $K_{\text{eff}}=[\text{GdHL}]/[\text{Gd}](\text{[HL]}+\text{[NaHL]})$.

 Gd+++ dis NaClO4 25°C 0.70M C K1=5.68 B2=10.09 1993LBa (3231) 8
 $K(\text{Gd}+\text{HL})=1.83$

Gd+++ sol none 25°C 0.0 C 1986FMa (3232) 9
 $K_{\text{so}}(\text{Gd}_2(\text{CO}_3)_3)=-35.45$

Gd+++ sol none 25°C 0.0 C 1986HMa (3233) 10
 $K_{\text{so}}(\text{Gd}_2(\text{CO}_3)_3)=-35.45$

Method: spectrophotometry.

 Gd+++ dis oth/un 20°C 2.5M C 1979DBb (3234) 11
 B4=14.31

Media: 2.5 M (NH4)2NO3/hexane. Analysis by NAA. By competition with edta;
 $K1(\text{Gd}(\text{edta}))=17.26$ recalculated for I=2.5 from J.Am.Chem.Soc.,75 1953,4196

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Gd+++	cal	none	25°C	0.00	M	H		K1=3.59	1972SCd (3650)	12
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DH(K1)=4.4 kJ mol⁻¹, DS=83.3 J K⁻¹ mol⁻¹

Gd+++	con	oth/un	25°C	0.0	U			K1=3.74	1963DKb (3651)	13
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 Cl- HL Chloride CAS 7647-01-0 (50)
 Chloride;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Gd+++	dis	NaCl	25°C	1.0M	C			K1=-0.16	1997HTb (4924)	14
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Method: by solvent extraction from 1.0 M NaCl into CHCl3, 0.1 M
 1,1,1-trifluoro-4-(2-thienyl)-2,4-pentanedione.

Gd+++	cal	non-aq	25°C	100%	U	H		K1=2.80 K3=1.44 K4=1.11	B2=4.77 1991ITa (4925)	15
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Medium: DMF, 0.2 M Et4NClO4. DH(K1)=15.1 kJ mol⁻¹, DH(K2)=23.4, DH(K3)=20
 DH(K4)=46. DS(K1)=104, DS(K2)=116, DS(K3)=95 J K⁻¹ mol⁻¹

 Gd+++ dis NaClO4 20°C 3.00M U K1=0.56 B2=0.21 1982FKb (4926) 16

Gd+++ sol NaClO4 25°C ? U K1=0.33 1982MAa (4927) 17

Gd+++ cal non-aq 25°C 100% U K1=1.23 B2=2.94 1980VCa (4928) 18
 Medium: dimethylacetamide

Gd+++ sp NaClO4 25°C 3.0M U K1=-0.04 1971KBF (4929) 19
 Medium: LiClO4

Gd+++ ISE none 25°C 0.0 U 1963AKd (4930) 20
 Kso(Gd(OH)2.5Cl0.5)=-23.12

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

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

Gd+++ ix oth/un 25°C 0.02M C T H K1=3.71 B2= 6.07 2004LMa (6914) 21
 Medium: 0.025 M HNO3. Applying Pitzer parameters: at I=0, K1=9.77.
 Data for 5 to 45 C. DH(K1)=7.2 kJ mol⁻¹, DH(B2)=17.6.

Gd+++ ISE NaClO4 25°C 0.0 C I K1=4.24 2000Lba (6915) 22
 Method: Fluoride ISE. Values calc. from data for I=0.015-0.70 M NaClO4.
 At I=0.70 M, K1=3.313.

Gd+++ ix KNO3 25°C 0.02M C K1=3.69 B2= 6.08 1999SBc (6916) 23
 Medium: 0.025 M HNO3. Additional method: ICP-MS.
 Assumed K1(HF) = 3.03, derived from literature values.

Gd+++ dis NaClO4 25°C 0.68M U K1=3.20 B2=5.28 1993LBb (6917) 24

Gd+++ ISE none 25°C 0.0 C H K1=3.21 B2=6.56 1989MJa (6918) 25
 Kso=-17.3
 Also by conductivity and radiometry. DH(Kso)=50.8 kJ mol⁻¹; DS=-157.0.

Gd+++ ISE R4N.X 25°C 0.50M C K1=3.21 B2=6.56 1989MJb (6919) 26

Gd+++ cal NaClO4 25°C 1.00M C H 1988GBa (6920) 27
 DH(K1)=9.22 kJ mol⁻¹; DS(K1)= 94.4 J mol⁻¹ K⁻¹

Gd+++ ISE NaNO3 25°C 0.10M U H 1987SMd (6921) 28
 K(GdA+L)=1.73
 DH=2.00 kJ mol⁻¹, DS=40.7 J K⁻¹ mol⁻¹. H3A=HEDTA

Gd+++ ISE NaCl 25°C 1.00M C K1=3.083 1985BBb (6922) 29

Gd+++ gl KCl 25°C 1.00M U M 1981KTb (6923) 30
K(GdEDTA+F)=1.73
K(Gd(EDTA)F+F)=0.48

Gd+++ dis NaClO4 25°C 1.00M U T H K1=3.16 1975MHa (6924) 31
DH=-17.2 kJ mol⁻¹ and DS=2.5 J mol⁻¹ K⁻¹.

Gd+++ ISE NaClO4 25°C 0.50M U K1=3.38 B2=6.5 1969ALa (6925) 32

Gd+++ dis NaClO4 25°C 0.50M U K1=3.43 B2=6.71 1967LNa (6926) 33

Gd+++ nmr NaClO4 20°C 0.10M U K1=4.04 1967VSc (6927) 34

Gd+++ EMF NaClO4 25°C 1.0M U H K1=3.31 1967WCa (6928) 35
By calorimetry: DH(K1)=37.2 kJ mol⁻¹, DS=188.5 J K⁻¹ mol⁻¹

Gd+++ EMF NaClO4 25°C 0.50M U I K1=3.37 1953KUa (6929) 36
K(Gd+HF=GdF+H)=0.46

At I=0 corr: K1=4.26

I03- HL Iodate CAS 7782-68-5 (1257)
Iodate;

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

Gd+++ sol oth/un 25°C 0.0 U 1966FPb (8517) 37
Kso=-11.13

I04- HL Periodate CAS 13444-71-8 (6063)
Periodate;

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

Gd+++ sol oth/un 25°C dil U 1974LOa (8604) 38
Kso(Gd(H2IO6)(H2O)3)=-10.60

Mo04-- H2L Molybdate (443)
Molybdate;

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

Gd+++ sp oth/un 25°C ? U M 1997STa (8733) 39
K(Gd+H2L=GdL+2H)=-1.4

Ligand: nano-Molibdenomanganate, MnMo9032-----

Gd+++ con oth/un 25°C .001M U K1=4.40 1968DKc (8734) 40

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Gd+++	gl	oth/un	20°C	0.10M	U			1989SBb (8774)	41

B(GdHL)=8.13
B(Gd2L)=7.84

NH3		L		Ammonia				CAS 7664-41-7 (414)	
Ammonia									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Gd+++	gl	R4N.X	25°C	5.00M	U		K1=0.45	1985MMa (9159)	42
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NO3- Nitrate;		HL		Nitrate				CAS 7697-37-2 (288)	
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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Gd+++	cal	NaClO4	25°C	2.0M	C	IH	K1=-0.52	1998BMb (9688)	43
DH(K1)=0.4 kJ mol ⁻¹ . From Pitzer extrapolation to I=0.0, K1=0.28, DH(K1)=-0.8 kJ mol ⁻¹									

Gd+++	cal	NaNO3	25°C	2.0M	C	H	K1=-0.46	1998BMc (9689)	44
Method: By competition with xylitol.									

Gd+++	dis	none	25°C	0.0	U		K1=1.59	1992MSb (9690)	45
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Gd+++	dis	R4N.X	25°C	0.0	C		K1=1.59	1988MSg (9691)	46
Extraction into tributylphosphate from 0.1-2.74 M NH4NO3 medium.									

Gd+++	dis	NaClO4	25°C	1.00M	U	T	K1=1.20	1975MHa (9692)	47
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Gd+++	oth	oth/un	25°C	var	U		B2=0.66 K1<0.1	1971NIb (9693)	48
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Method: Raman spectra

Gd+++	oth	none	25°C	0.0	U		K1=1.2 Kout=0.6	1969GEc (9694)	49
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Method: ultrasonic absorption

Gd+++	dis	NaClO4	25°C	1.0M	U		K1=0.03	1969MKi (9695)	50
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OH- Hydroxide;		HL		Hydroxide			(57)		
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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Gd+++	gl	NaClO4	25°C	0.0	C	IH		2000KBa (11523)	51
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*K1=-7.83

In 0.7 M NaClO4, *K1=-8.14. DH(*K1)=53 kJ mol⁻¹.

Gd+++ gl NaCl 25°C 0.10M U I 1999FBa (11524) 52
*B(1,3)=-22.16

In 0.1 M Me4NCl, *B(1,3)=-22.76.

Gd+++ sol none 25°C 0.50M C TI 1991GLc (11525) 53
*K1=-7.87
*B2=-15.16

Also data at 70 C: *K1=-7.55, *B2=-13.04.

DH(*K1)=14 kJ mol⁻¹, DH(*B2)=92. In D2O: *K1=-8.17, *B2=-16.00.

Gd+++ con oth/un 25°C dil C 1988MCa (11526) 54
*K1=-4.70

Method: conductivity of 0.5 mM GdCl3 solution as function of pH.

Gd+++ sol NaClO4 23°C 1.0M C 1980KDC (11527) 55
*K1=-7.3
*B2=-14.6
*B3=-21.9
*B(3,4)=-19.0

*Kso=17.0 (fresh)

Gd+++ gl NaClO4 25°C 3.00M U 1974NBc (11528) 56
*K1=-9.2
*B(2,2)=-14.20
Kso(Gd(OH)3(s))=-24.53

Gd+++ gl NaClO4 25°C 3.00M U 1973AKa (11529) 57
*K1=-8.20

Medium: LiClO4

Gd+++ gl NaClO4 25°C 3.00M U 1973AKb (11530) 58
*K1=-8.34

Medium: D2O containing LiClO4. *K1: Gd+D2O=GdOD+D

Gd+++ EMF alc/w 20°C 25% U 1973SPe (11531) 59
*K1(GdA+H2O=GdAOH+H)=-7.05

Medium: ca.25 to 35% w/w MeOH or EtOH/H2O. H3A=NTA

Gd+++ EMF alc/w 25°C 25% U I 1972USa (11532) 60
*K1=-7.98

Medium: 25% v/v EtOH/H2O, 0.05 M NaClO4. *K1=-8.27(v=0), -7.50(v=50),
-7.94(v=0, I=0)

Gd+++ dis NaClO4 ? 0.10M U 1971GDb (11533) 61
*K1=-7.1

Medium: LiClO4

Gd+++ dis NaClO4 25°C 0.10M U 1969MGf (11534) 62
*K1=-8.45

*B2=-15.82

Medium: LiClO4 with tris-buffer

Gd+++ oth oth/un rt 10% U 1967PBb (11535) 63

Kso=-27.5
K(GdL3(s)=GdL3)=-4.9

Medium: 10% sea water.

Gd+++ gl NaClO4 25°C 0.30M U 1966FKa (11536) 64

*K1=-8.35

Gd+++ sol none 25°C 0.0 M 1963AKb (11537) 65

Kso=-26.89
K(GdL3(s)=GdL3)=-4

Gd+++ sol none 25°C 0.0 U 1963AKd (11538) 66

Kso(Gd(OH)3)=-26.88

Gd+++ EMF none 20°C 0.0 U 1962KBc (11539) 67

Kso(Gd(OH)3)=-26.95

Gd+++ gl oth/un 25°C var U 1951MFb (11540) 68

Kso(Gd(OH)3)=-22.74

Gd+++ gl oth/un 25°C var U 1944MKa (11541) 69

Kso(Gd(OH)3)=-21.7

Gd+++ sol oth/un 100°C var U 1932ENa (11542) 70

Kso=0.53 + y

Kso: K(Gd(OH)3(s)=Gd+3OH); y=Kso for Y+++

P04--- H3L Phosphate CAS 7664-38-2 (176)

Phosphate;

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

Gd+++ sol none 25°C 0.0 M 1997LBd (13200) 71

Kso(GdPO4)=-25.62

Calculated from data for 0.10 M HClO4 solution.

Gd+++ sol oth/un 25°C 0.0 C I 1993FKb (13201) 72

Kso(GdPO4)=-26.92

In synthetic seawater, Ks(GdPO4)=-24.26.

Gd+++ dis NaClO4 25°C 0.68M C I K1=9.30 1991BLb (13202) 73

K(Gd+HPO4)=4.11
K(Gd+2HPO4)=7.38
K(Gd+H2PO4)=1.71

Distribution of 153Gd between 0.68 m NaClO4 and TBP. Calculated for I=0, K1=12.19, K(Gd+HPO4)=5.91, K(Gd+2HPO4)=9.97, K(Gd+H2PO4)=2.74.

 Gd+++ sol none 25°C 0.0 C 1991FBa (13203) 74
 Kso(GdPO4)=-25.39

Gd+++ dis NaClO4 25°C 0.68M C 1989BBf (13204) 75
 K(Gd+HL)=3.89
 K(Gd+2HL)=6.94
 K(Gd+H2L)=1.70

Gd+++ gl NaClO4 20°C 0.10M U K1=3.58 1974PJa (13205) 76

Gd+++ sol NaClO4 25°C 0.50M U 1967TPb (13206) 77
 Kso=-22.26

 P207---- H4L Pyrophosphate CAS 2466-09-3 (198)
 Diphosphate; from (HO)2PO.O.PO(OH)2

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

Gd+++ gl KCl 25°C 0.50M U 1989APd (13593) 78
 K(Gd+H2L)=4.51

Gd+++ kin none 25°C 0.0 U B2=20.45 1967SSo (13594) 79

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

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

Gd+++ gl NaCl 25°C 0.15M C K1=8.37 B2=13.39 1999BCb (13861) 80
 K(Gd+HL)=5.10
 K(GdL+OH)=4.73

Gd+++ gl KNO3 25°C 0.10M U T H B2=8.9 1974KRa (13862) 81
 K(Gd+2HL)=6.6
 K(Gd+2HL)=7.0 and B2=9.2 (35 C), K(Gd+2HL)=6.5 and B2=8.6 (45 C)
 DH(Gd+2HL)=-11 kJ mol⁻¹; DH(B2)=-29

Gd+++ gl NaClO4 ? 0.10M U B2=16.92 1962RKa (13863) 82
 K(Gd+HL)=4.91
 K(Gd+2HL)=8.72

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

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

Gd+++ dis oth/un 25°C 1.0M C K1=0.40 1997HTb (15017) 83
 Method: by solvent extraction from 1.0 M NaSCN into CHCl3, 0.1 M
 1,1,1-trifluoro-4-(2-thienyl)-2,4-pentanedione.

Gd+++ sp NaClO4 ? 0.60M U T K1=0.21 1964KSe (15018) 84

S04-- H2L Sulfate CAS 7664-93-9 (15)
Sulfate;

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

Gd+++ sol oth/un 25°C 0.66M C K1=1.94 2004SBb (16216) 85
Method: solubility of BaSO4 in 0.117 m GdCl3 solution.
Calculated for I=0, K1=3.61.

Gd+++ cal none 25°C 0.0 U H 1974POa (16217) 86
DH(K1)=19.9 kJ mol-1

Gd+++ con oth/un 25°C 0.0 U K1=3.67 1973FPb (16218) 87

Gd+++ oth none 25°C 0.0 U K1=3.66 1973FPb (16219) 88
K1in=0.69
Method: ultrasonic absorption. In D2O: K1=3.66, K1is=0.83

Gd+++ kin none 25°C 0.0 U K1=3.65 1973RSb (16220) 89

Gd+++ cal oth/un 25°C 0.0 U H 1969FPa (16221) 90
DH(K1)=17.2 kJ mol-1

Gd+++ cal oth/un 25°C 0.0 U H K1=3.48 B2=5.21 1969IEa (16222) 91
DH(K1)=15.0 kJ mol-1, DH(K2)=6.37 J K-1 mol-1; DS(K1)=117.0, DS(K2)=53.9

Gd+++ ISE NaClO4 25°C 2.0M U H K1=1.33 B2=1.75 1967CCd (16223) 92
By calorimetry: DH(K1)=16.5 kJ mol-1, DS=80.7 J K-1 m-1; DH(K2)=7.11, DS=31.8

Gd+++ dis NaClO4 25°C 0.55M U K1=1.90 B2=2.99 1967LNa (16224) 93
I=0.5-0.6, By cation exchange: K1=1.90, B2=2.84

Gd+++ con oth/un 25°C 0.0 U K1=3.66 1954SJa (16225) 94

CHO3F3S HL CAS 1493-13-6 (6755)
Trifluoromethanesulfonic acid; CF3SO3H

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

Gd+++ sp non-aq 25°C 100% U K3=2.52 1993BCc (17463) 95

Medium: MeCN

CH4O L Methyl alcohol CAS 67-56-1 (597)
Methanol; CH3.OH

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

Gd+++ gl alc/w 25°C 100% M 1989TMa (17881) 96
K(Gd+H-1L)=8.9
K(Gd+2H-1L)=18.4
K(Gd+3H-1L)=23 approx

Medium: MeOH

C2H2O3 HL Glyoxylic acid CAS 298-12-4 (1142)
Glyoxylic acid; OHC.COOH

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

Gd+++ gl NaClO4 20°C 0.10M U K1=2.49 B2=4.53 1964PSd (18422) 97
K3=1.5

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

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

Gd+++ ix R4N.X 25°C 0.05M C K1=5.60 B2= 9.91 2001SBf (18909) 98
K(Gd+HL)=2.04

Medium: 0.05 M NH4NO3. At I=0, K1=6.53, B2=11.10.

Gd+++ gl KCl 25°C 1.0M U M 1988KTa (18910) 99
K(Gd(edta)+L)=3.10

Gd+++ gl KNO3 35°C 0.10M U M K1=6.56 1986RMb (18911) 100
B(GdL(cytidine))=9.94

Gd+++ ix oth/un 25°C 0.50M U K1=4.78 B2=8.68 1967LNa (18912) 101
By distribution: K1=4.76, B2=8.65

Gd+++ kin oth/un 25°C 0.0 U K1=7.01 1962YZa (18913) 102

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

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

Gd+++ gl NaClO4 25°C 0.10M U T H K1=6.50 B2=11.90 1983SSb (19254) 103
K3=4.18

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

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

Gd+++ gl none 25°C dil M T H K1=2.52 B2= 4.61 2000DCa (19973) 104
Self medium, 0.03-0.05 M. Data for 40-80 C. At 40 C, K1=2.65, B2=4.84.

DH(K1)=19.53 kJ mol⁻¹, DS(K1)=113.5 J K⁻¹ mol⁻¹; DH(B2)=30.57, DS=190.4

Gd+++ sp NaNO3 25°C 0.10M U K1=1.67 19850Ha (19974) 105

Gd+++ sp NaClO4 21°C 2.0M U K1=1.96 B2=3.11 1984BMa (19975) 106
B3=3.82
B4=3.79

Gd+++ gl alc/w 25°C 95% U H K1=4.98 B2=8.98 1967Gwa (19976) 107
B3=11.66
B4=12.83

Medium:95% MeOH, 0.5 M NaClO4. By calorimetry:DH(K1)=14.1 kJ mol⁻¹,DS=142.5
J K⁻¹ mol⁻¹; DH(K2)=7.1,DS=100.3; DH(K3)=6.6,DS=74.0; DH(K4)=-1.2,DS=16.7

Gd+++ cal NaClO4 25°C 2.0M C H 1964GRa (19977) 108
DH(K1)=7.816 kJ mol⁻¹, DS(K1)=61.9 J K⁻¹ mol⁻¹; DH(B2)=13.58, DS(B2)=106;
DH(B3)=14.82, DS(B3)=122.

Gd+++ gl NaClO4 20°C 0.10M U K1=2.16 B2=3.76 1962KPa (19978) 109

Gd+++ ix NaClO4 20°C 1.0M U K1=1.82 B2=3.13 1959SOa (19979) 110
B3=4.0

Gd+++ EMF NaClO4 20°C 2.0M U K1=1.84 B2=3.12 1958SOb (19980) 111
B3=3.72
B4=3.70

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

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

Gd+++ gl NaClO4 25°C 0.20M U K1=6.17 B2=12.07 1996PJa (20323) 112

Gd+++ gl NaClO4 20°C 0.10M U 1964PKa (20324) 113
K(Gd+HL)=2.01
K(GdHL+HL)=1.30

Gd+++ gl NaClO4 25°C 2.0M U 1962BCa (20325) 114
K(Gd+HL)=1.64
K(GdHL+HL)=0.8

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

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

Gd+++ gl NaClO4 25°C 0.20M U K1=6.18 B2=11.47 1996PJa (20544) 115

Gd+++ gl KNO3 32°C 0.10M U 1980PPF (20545) 116

$K(\text{Gd}+\text{HL}=\text{GdL}+\text{H})=-1.19$
 $*K(\text{GdL})=-6.34$
 $K(\text{Gd}+2\text{HL}=\text{GdL}_2+2\text{H})=-2.43$
 $*K(\text{GdL}_2)=-6.08$

 Gd+++ gl NaClO4 25°C 0.50M C T K1=2.52 B2=4.62 1977Cma (20546) 117
 B3=5.78
 B4=7.18

 Gd+++ cal NaClO4 25°C 2.0M C H 1964GRa (20547) 118
 DH(K1)=-2.569 kJ mol⁻¹, DS(K1)=39 J K⁻¹ mol⁻¹; DH(B2)=-7.255, DS(B2)=60.3;
 DH(B3)=-14.71, DS(B3)=60.7; DH(B4)=-17.9, DS(B4)=61.9.

 Gd+++ gl NaClO4 20°C 0.10M U K1=2.792 B2=4.86 1964PKb (20548) 119
 B3=6.00

 Gd+++ gl NaClO4 25°C 2.0M U K1=2.46 B2=4.33 1961CCa (20549) 120
 K3=1.56

 Gd+++ EMF NaClO4 20°C 3.0M U I K1=2.59 B2=4.60 1961SOa (20550) 121
 B3=6.1
 B4=6.8
 B5=6.8
 B6=6.6

Method:quinhydrone electrode. At I=0.2: K1=2.73,B2=4.79,B3=6.3,B4=7.1,B5=7.0

 Gd+++ EMF NaClO4 20°C 2.0M U I K1=2.48 B2=4.43 1959SOB (20551) 122
 B3=5.78
 B4=6.42
 B5=6.0

Method: quinhydrone electrode. Using ion exchange (I=1.0): K1=2.54, B2=4.48, B3=5.8

 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

 Gd+++ gl KNO3 25°C 0.0 M T H K1=5.89 2003MBa (21561) 123
 $K(\text{Gd}+\text{HL}=\text{GdL}+\text{H})=-3.75$

Extrapolated from data for I=0.07-0.32 M KNO3. DH(K1)=-131.0 kJ mol⁻¹,
 DS(K1)=-326.9 J K⁻¹ mol⁻¹; DH(Gd+HL)=-80.9, DS(Gd+HL)=-343.2.

 Gd+++ gl NaClO4 25°C 0.20M U K1=4.64 B2= 9.17 1996PJa (21562) 124

 Gd+++ gl NaCl 25°C 0.15M C 1992JTa (21563) 125
 B(GdH-1L)=-2.29
 B(GdH-2L)=-10.08
 B(GdH-3L)=-20.6
 B(GdHL)=11.94

Gd+++ gl KNO3 25°C 0.20M U M K1=6.11 1990LSb (21564) 126
K(Gd(phen)+L)=6.02

Gd+++ gl NaClO4 25°C 0.20M U K1=4.64 B2= 9.17 1987PPa (21565) 127

Gd+++ gl KNO3 35°C 0.10M U 1987RRc (21566) 128
K(Gd+HL)=3.72

Gd+++ gl KNO3 35°C 0.10M U M 1986RMb (21567) 129
K(Gd+HL)=3.72
K(Gd+HL+cytidine)=8.49

Gd+++ gl NaClO4 25°C 0.10M U 1981KBa (21568) 130
K(Gd+HL)=0.73

Gd+++ EMF KCl 25°C 1.0M U M 1977GMa (21569) 131
K(GdA+L)=3.70
K(GdA+HL)=3.00
K(GdA+H2L)=3.10

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

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

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

Gd+++ sp non-aq 25°C 100% U 1992MBb (22100) 132
K8=1.0
K9=0.5

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

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

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

Gd+++ gl NaClO4 22°C 0.10M U 1972Mcd (22146) 133
K(GdH-1L+H)=7.25

C2H6O6P2 H4L (5706)
Ethene-1,1-diphosphonic acid; H2C:C(P03H2)2

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

Gd+++ gl KCl 25°C 0.15M U I 1989AMa (22171) 134
K(Gd+H2L)=5.25

C2H8N2 L Ethylenediamine CAS 107-15-7 (23)

1,2-Diaminoethane; H2N.CH2.CH2.NH2

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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++      ISE non-aq 25°C 100% C  H   K1=2.05  B2=3.82  1992CBa (23162) 135
              B3=4.98
Medium: DMSO, 0.10 M Et4NC104. By calorimetry, DH(K1)=-14.0, DH(B2)=-31.3,
DH(B3)=-72.1 kJ mol-1.
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Gd+++      gl  KNO3   25°C 0.10M U TIH   K1=5.34  B2=10.19 1986NSa (23163) 136
              B(GdAL)=9.04
H2A=phthalic acid. DH(GdAL)=-46.6 kJ mol-1, DS=16.49J K-1 mol-1
*****
C2H8O7P2      H4L   HEDPA      CAS 2809-21-4 (436)
1-Hydroxyethane-1,1-diphosphonic acid; CH3.C(OH)(PO3H2)2
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++      sp  oth/un 25°C 0.70M U              1987APa (23375) 137
              K(Gd+H2L)=5.64
*****
C3H4O2      HL   Acrylic acid  CAS 79-10-7 (2044)
Propenoic acid; CH2:CH.COOH
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++      gl  oth/un 25°C  ?  U   M   K1=2.08      1998PAa (23987) 138
              K(GdL+acac)=5.72
              K(Gd(acac)L+acac)=4.33
Additional method: nmr. Medium not stated.
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Gd+++      gl  NaClO4 25°C 0.10M C  H   K1=1.88  B2=3.48  1996HBa (23988) 139
              B3=5.0
DH(K1)=12.7 kJ mol-1, DS=79 J K-1 mol-1
*****
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
-----
Gd+++      nmr NaClO4 25°C 2.00M U  H   K1=1.67      1980CCa (24052) 140
DH=-4.93 kJ mol-1. Alternative method: Calorimetry.
*****
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
-----
Gd+++      gl  NaClO4 25°C 0.10M M  M   K1=4.45      1987NCa (24460) 141
              K(Gd(nta)+L)=2.74
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Gd+++ gl NaClO4 25°C 0.10M U K1=4.81 B2=7.88 1972DCc (24461) 142

Gd+++ gl NaClO4 25°C 1.00M U K1=3.73 B2=6.24 1971DGa (24462) 143
B(GdHL)=6.49
B(GdHL2)=9.78

Gd+++ ix NaClO4 25°C 0.15M U 1968KKc (24463) 144
K(Gd+HL)=1.65
K(GdHL+HL)=1.2

Gd+++ gl KNO3 25°C 0.10M U K1=4.32 B2=6.97 1968PFa (24464) 145

Gd+++ gl oth/un 25°C ->0 U T H K1=4.61 1956GNb (24465) 146
K1=4.49(35 C). DH(K1)=-21 kJ mol⁻¹

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

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

Gd+++ gl KCl 25°C 0.20M U K1=3.83 1973LPb (24626) 147

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

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

Gd+++ gl diox/w 20°C 50% U K1=5.68 1971MAf (24643) 148
Medium: 50% dioxan, 0.1 M NaClO4

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

Gd+++ gl diox/w 20°C 50% U K1=6.70 B2=12.48 1971MAf (24805) 149
Medium: 50% dioxan, 0.1 M NaClO4

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

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

Gd+++ gl NaClO4 25°C 2.0M U K1=1.84 B2=3.17 1965CGa (25006) 150

Gd+++ gl NaClO4 20°C 0.10M U K1=2.09 B2=3.57 1964PKa (25007) 151

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	NaClO4	25°C	0.20M	U			K1=6.67 B2=12.76	1996PJa (25145)	152
Gd+++	gl	NaClO4	25°C	2.00M	U			K(Gd+HL)=1.75	1968CMA (25146)	153
Gd+++	gl	NaClO4	31°C	2.0M	U			K(Gd+HL)=1.62 K(GdHL+HL)=0.8	1963BCb (25147)	154

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	NaClO4	25°C	2.00M	U			K(Gd+HL)=1.71	1968CMA (25208)	155
Gd+++	gl	NaClO4	31°C	2.0M	U			K(Gd+HL)=2.03 K(GdHL+HL)=1.3	1963BCb (25209)	156

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	NaClO4	25°C	2.00M	U			K1=1.61	1969JcC (25265)	157

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	NaClO4	25°C	0.20M	U			K1=6.54 B2=12.47	1996PJa (25448)	158
Gd+++	gl	KNO3	30°C	0.10M	U			K(Gd+HL=GdL+H)=0.35 *K(GdL)=-4.71 K(Gd+2HL=GdL2+2H)=-0.72 *K(GdL2)=-4.12	1983MPc (25449)	159
Gd+++	gl	NaClO4	25°C	0.10M	U			K1=2.96 B2=5.09	1966GGb (25450)	160
Gd+++	gl	NaClO4	25°C	0.20M	U			K1=2.57 B2=4.72 K3=1.02 K4=0.47	1964DVa (25451)	161

Gd+++ gl NaClO4 20°C 0.10M U K1=2.892 B2=5.04 1964PKb (25452) 162
B3=6.24

Gd+++ gl NaClO4 25°C 2.0M U K1=2.53 B2=4.63 1961CCa (25453) 163
K3=1.28

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

Gd+++ gl NaClO4 20°C 0.10M U K1=2.06 B2=3.01 1964PKa (25598) 164

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

Gd+++ gl NaClO4 25°C 0.20M U K1=5.18 B2= 9.41 1996PJa (26179) 165

Gd+++ gl NaCl 25°C 0.15M C K1=4.3 1992JTa (26180) 166
B(GdH-1L)=-2.34

Gd+++ gl KNO3 25°C 0.20M U M K1=6.43 1990LSb (26181) 167
K(Gd(phen)+L)=6.32

Gd+++ gl KNO3 35°C 0.10M U K1=5.19 1990RSe (26182) 168

Gd+++ gl NaClO4 25°C 0.20M U K1=5.18 B2= 9.41 1987PPa (26183) 169

Gd+++ gl KNO3 15°C 0.10M U K1=4.6 1967EMb (26184) 170

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

Gd+++ gl NaClO4 20°C 0.0 U T H K1=7.950 B2=15.07 1980SDc (26782) 171
Extrapolated from data for I=0.10-1.0 M. Data for 35 and 45 C.
DH(K1)=-14.4 kJ mol⁻¹, DS(K1)=103 J K⁻¹ mol⁻¹; DH(K2)=-5.76, DS=117.

C3H7NO3 HL Serine CAS 56-45-1 (49)
2-Amino-3-hydroxypropanoic acid; H2N.CH(CH2.OH)COOH

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

Gd+++ gl NaClO4 25°C 0.20M U K1=4.66 B2= 8.79 1996PPa (27135) 172

Gd+++ gl NaClO4 25°C 0.20M U K1=4.66 B2= 8.79 1990Pjb (27136) 173

Gd+++ gl oth/un 25°C 0.10M U K1=3.59 1965PGe (27137) 174

 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

Gd+++ gl NaClO4 22°C 0.10M U 1972MCd (27676) 175
 K(GdH-1L+H)=7.15

 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

Gd+++ gl NaClO4 22°C 0.10M U 1972MCd (27733) 176
 K(GdH-1L+H)=7.10

 Gd+++ gl NaCl 25°C 0.10M U 1970PKe (27734) 177
 K(GdH-1L+H)=7.17

 C3H10N2 L Propanediamine CAS 109-76-2 (123)
 1,3-Diaminopropane; H2N.CH2.CH2.CH2.NH2

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

Gd+++ gl KNO3 27°C 0.10M M M 1979KSc (28303) 178
 K(GdL+phthalate)=6.47
 K(GdL+malonate)=5.68

 C3H11NO6P2 H4L (6772)
 (Dimethylamino)-N-methylenediphosphonic acid; (CH3)2N.CH(PO3H2)2

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

Gd+++ gl NaNO3 24°C 0.20M C K1=17.6 B2=20.7 1993BRa (28412) 179
 K(GdL+H)=12.9
 K(GdHL+H)=3.0
 K(GdL2+H)>13
 K(GdHL2+H)=10.5
 K(GdH2L2+H)=7.0, K(GdH3L2+H)=3.7, K(GdH4L2+H)=1.2

 C3H12NO9P3 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

Gd+++ gl KNO3 25°C 0.10M U K1=13.87 B2=25.46 2002KAa (28568) 180
 K(Gd+HL)=5.48
 K(Gd+2HL)=10.92

Gd+++ gl KNO3 25°C 0.10M C 1991SKb (28569) 181

K(GdL+H)=7.37
K(GdHL+H)=5.34

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

Gd+++ cal NaClO4 25°C 0.10M U H K1=2.87 B2=4.16 19760Ca (28650) 182
DH(K1)=8.4 kJ mol⁻¹, DS=83 J K⁻¹ mol⁻¹; DH(B2)=15.9, DS=133

Gd+++ gl NaClO4 25°C 0.10M C H K1=2.866 B2= 4.17 19760Cb (28651) 183
By calorimetry: DH(K1)=8.41 kJ mol⁻¹, DS(K1)=83.3 J K⁻¹ mol⁻¹;
DH(B2)=15.9, DS(B2)=133.

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

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

Gd+++ gl oth/un 25°C 0.10M U K1=2.060 1987TSb (28889) 184

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

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

Gd+++ gl oth/un 25°C 0.10M U T H K1=3.93 1987TSb (28913) 185
30 C:K=3.58; 35 C: 3.13. DH=-141 kJ mol⁻¹, DS=-397 J K⁻¹ mol⁻¹

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

Gd+++ gl oth/un 25°C ? U M K1=3.68 1998PAa (29078) 186

K(GdL+acac)=4.90
K(Gd(acac)L+acac)=4.06

Additional method: nmr. Medium not stated.

Gd+++ gl KNO3 25°C 0.10M U T HM K1=4.81 B2=8.08 1986NSa (29079) 187

B(GdAL)=8.34

H2A=phthalic acid. DH(GdAL)=-38.3 kJ mol⁻¹, DS=31.1J K⁻¹ mol⁻¹

Gd+++ gl NaClO4 25°C 0.10M U K1=3.79 1973CDc (29080) 188

Gd+++ gl NaClO4 25°C 1.00M U K1=2.97 B2=4.79 1973DMa (29081) 189

Gd+++ gl NaClO4 25°C 0.10M U K1=3.80 B2=5.91 1970RFa (29082) 190

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

Gd+++ gl NaClO4 25°C 0.10M C K1=2.59 1986LCa (29199) 191
B(GdHL)=6.14
K(Gd+HL)=2.06

Gd+++ gl KNO3 25°C 0.10M U T HM K1=3.05 1986NSa (29200) 192
B(GdAL)=6.22
H2A=phthalic acid. DH(GdAL)=-33.9 kJ mol⁻¹, DS=5.4 J K⁻¹ mol⁻¹

Gd+++ gl NaClO4 25°C 0.10M U K1=2.88 1973CDc (29201) 193

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

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

Gd+++ gl NaClO4 25°C 0.50M M K1=3.69 B2=7.37 1991MOa (29267) 194

Gd+++ gl oth/un 25°C ? U K1=5.5 B2=10.0 1956GNc (29268) 195

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

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

Gd+++ gl KCl 25°C 0.10M U K1=2.39 1995PAa (29698) 196

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

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

Gd+++ gl NaClO4 25°C 0.10M M M K1=3.42 1987NCa (29976) 197
K(Gd(nta)+L)=2.25

Gd+++ gl NaClO4 25°C 0.10M M H K1=3.42 1986CDb (29977) 198
DH=12.7 kJ mol⁻¹, DS=108 J K⁻¹ mol⁻¹

Gd+++ gl KNO3 25°C 0.10M U T HM K1=3.58 B2=6.58 1986NSa (29978) 199
B(GdAL)=7.08
H2A=phthalic acid. DH(GdAL)=-47.9 kJ mol⁻¹, DS=28.5 J K⁻¹ mol⁻¹

Gd+++ ix NaClO4 25°C 0.15M U 1968KKc (29979) 200
K(Gd+HL)=1.83

K(GdHL+HL)=1.3

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

Gd+++ gl KCl 25°C 0.20M U K1=4.21 B2=6.38 1975PLa (30126) 201

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

Gd+++ gl NaClO4 25°C 0.20M U K1=6.32 B2=11.86 1996PJa (30334) 202

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

Gd+++ gl NaClO4 25°C 0.20M U K1=6.33 B2=11.72 1996PJa (30632) 203

Gd+++ gl KNO3 30°C 0.10M U M 1984AIa (30633) 204
K(Gd(EDTA)+L)=2.325

Gd+++ gl NaClO4 25°C 0.10M C K1=4.75 B2=7.83 1980KBd (30634) 205
Stereoselectivity studied, data for DL-malic acid. With L-malic acid:
K1=4.74, K2=2.94

Gd+++ gl KNO3 20°C 0.10M U 1980SDa (30635) 206
B(GdHL)=7.81

Gd+++ gl KNO3 20°C 0.10M U K1=4.57 B2=7.49 1980Sdb (30636) 207
K(Gd+HL)=2.06

Gd+++ EMF NaClO4 25°C 2.00M U K1=3.92 B2=6.53 1969JPa (30637) 208

Gd+++ EMF KCl 25°C 0.20M U K1=4.28 1964DAb (30638) 209

C4H6O5 H2L Diglycolic acid CAS 110-99-6 (243)
Di(carboxy)methyl ether, 2,2'-Oxydiethanoic acid; HOOC.CH2.O.CH2.COOH

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

Gd+++ gl KNO3 25°C 0.10M M M K1=2.76 1989NDa (30876) 210
K(GdL+ida)=2.48
K(GdL+gly)=2.61
B(GdLA)=8.77
B(GdLB)=9.65

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	KCl	25°C	1.0M	U	M			1988KTa (32262)	225
K(Gd(edta)+L)=4.54										
Gd+++	gl	NaClO4	25°C	0.20M	U	M		K1=6.78 B2=12.31	1988VSc (32263)	226
K(Gd(HEDTA)+L)=5.68										
K(Gd(CDTA)+L)=4.65										
K(Gd(DTPA)+L)=4.19										
Gd+++	gl	NaClO4	25°C	0.20M	U	M		K1=6.78 B2=12.31	1987VSb (32264)	227
K(Gd(nta)+L)=5.76										
K(Gd(edta)+L)=4.44										
Gd+++	gl	KNO3	27°C	0.10M	M	M			1984KTb (32265)	228
K(GdA+L)=5.51										
K(GdB+L)=5.38										

H2A=Citraconic acid, H2B=Maleic acid

Gd+++	gl	KNO3	27°C	0.10M	U	M			1980KTb (32266)	229
K(GdA+L)=6.01										
K(GdB+L)=5.71										

H2A=phthalic acid, H2B=malonic acid

Gd+++	EMF	KCl	25°C	1.0M	U	M			1977GMa (32267)	230
K(GdA+L)=5.07										
K(GdA+H2L)=1.02										
K(GdA+H3L)=2.39										

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

Gd+++	cal	KNO3	20°C	0.10M	U	HM			1971GKb (32268)	231
K(GdA+L)=4.30										

DH(GdA+L)=-27.66 kJ mol⁻¹, DS=-12.1 J K⁻¹ mol⁻¹. DH(GdAL)=-34.89, DS=296.
 H4A=EDTA

Gd+++	gl	KNO3	25°C	0.10M	U	M		K1=6.68 B2=12.07	1962THa (32269)	232
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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
Gd+++	gl	diox/w	20°C	50%	U			K1=7.99 B2=14.97	1971MAf (32540)	233

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

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

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

Gd+++ gl NaClO4 30°C 0.10M U K1=3.85 B2=6.81 1984YLa (32700) 234

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

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

Gd+++ gl NaClO4 25°C 0.10M U 1981KBa (33027) 235
K(Gd+HL)=0.58

Gd+++ gl KCl 25°C 0.10M U K1=2.35 1973FMa (33028) 236

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

Gd+++ gl KCl 60°C 0.10M U K1=6.48 B2=10.88 1978NBa (33085) 237
B3=13.60

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

Gd+++ gl KNO3 30°C 0.10M U M 1984AIa (33106) 238
K(Gd(EDTA)+L)=3.195

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

Gd+++ gl NaClO4 25°C 2.00M U H K1=1.86 B2=3.20 1965CGa (33230) 239
By calorimetry: DH(K1)=14.4 kJ mol⁻¹, DS=84 J K⁻¹ mol⁻¹; DH(K2)=7.1, DS=49

Gd+++ gl NaClO4 25°C 0.50M U K1=1.87 B2=3.28 1964SPa (33231) 240

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

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

Gd+++ gl NaClO4 31°C 2.0M U K1=1.70 B2=2.60 1963BCb (33406) 241

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
Gd+++	gl	NaClO4	25°C	0.20M	U		K1=2.79 K3=1.5 K4=1.2	1964DVa (33475)	242
Gd+++	gl	NaClO4	20°C	0.10M	U		K1=3.076 B2=5.51 B3=7.19	1964PKb (33476)	243
Gd+++	gl	NaClO4	25°C	0.50M	U		K1=2.71 B2=4.97 B3=6.01	1964SPa (33477)	244
Gd+++	gl	NaClO4	25°C	2.0M	U		K1=2.82 B2=5.15 K3=1.62	1961CCa (33478)	245

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
Gd+++	gl	KNO3	25°C	0.10M	C		K1=3.03 B2=5.40 K3=1.68	1975PFb (33679)	246

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
Gd+++	EMF	KNO3	25°C	0.10M	U		K1=3.09 B2=5.50 K3=1.90	1976PKb (33699)	247
Gd+++	gl	NaClO4	25°C	0.50M	U		K1=2.69 B2=4.99 B3=6.41	1964SPa (33700)	248

C4H9NO3 HL Threonine CAS 72-19-5 (48)
 2-Amino-3-hydroxybutanoic acid; H2N.CH(CH(OH)).CH3)COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Gd+++	gl	KNO3	25°C	0.0	M T H		K1=5.21 K(Gd+HL=GdL+H)=-3.97	2003MBa (34303)	249
Extrapolated from data for I=0.07-0.32 M KNO3. DH(K1)=-119.0 kJ mol ⁻¹ , DS(K1)=-299.6 J K ⁻¹ mol ⁻¹ ; DH(Gd+HL)=-65.3, DS(Gd+HL)=-295.2.									
Gd+++	gl	NaClO4	25°C	0.20M	U		K1=4.64 B2= 9.04	1996PPa (34304)	250
Gd+++	gl	NaCl	25°C	0.15M	C		K1=4.40	1992JTa (34305)	251

B(GdH-1L)=3.14
B(GdH-2L)=-10.41
B(GdHL)=11.84

Gd+++ gl NaClO4 25°C 0.20M U K1=4.64 B2= 9.04 1990PJb (34306) 252

C4H11O4P HL (4276)
Diethylphosphoric acid; (C2H5O)2.PO.OH

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

Gd+++ kin oth/un 25°C U K1=1.75 1971MGb (35258) 253

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

Gd+++ EMF NaClO4 25°C 100% C H K1=5.69 B2=10.25 2000CDa (35782) 254
Medium: DMF, 0.10 M Et4N[CF3SO3]. Method: Ag/Ag+ electrode.
By calorimetry: DH(K1)=-46.8, DH(B2)=-111.4 kJ mol-1.

Gd+++ ISE non-aq 25°C 100% C H K1=3.08 B2=5.65 1993CCb (35783) 255
Medium: DMSO, 0.1 M Et4NClO4. Method: Ag+ ISE. By calorimetry, DH(K1)=-27.5
kJ mol-1, DS=-33; DH(B2)=-73.0, DS-137.

C4H14N2O6P2 H2L EDDPO CAS 1733-49-9 (2435)
1,2-Diaminoethane-N,N'-bis(methylenephosphonic) acid; (H2O3P.CH2.NH.CH2)2

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

Gd+++ gl KCl 25°C 0.10M U K(Gd+HL)=8.31 1965DKb (35882) 256

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

Gd+++ cal NaClO4 25°C 0.10M U H K1=2.98 B2=4.21 1978COa (35942) 257
DH(K1)=7.23 kJ mol-1, DS=81.5; DH(K2)=2.42, DS=31.4

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

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

Gd+++ cal NaClO4 25°C 1.0M C H 1990YKb (36054) 258
DH(K1)=-0.12 kJ mol-1, DS(K1)=47.5 J K-1 mol-1.

Gd+++ EMF NaClO4 25°C 1.0M C K1=2.50 B2= 4.58 1983KKb (36055) 259
B3=6.08

Method: Pt/quinhydrone electrode.

C5H4O2S HL 2-Thenoic acid CAS 527-72-0 (2312)

Thiophene-2-carboxylic acid; C4H3S.CO0H

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

Gd+++ gl NaClO4 25°C 0.10M U K1=1.92 B2=3.20 1969RFa (36257) 260

C5H4O3 HL 2-Furoic acid CAS 88-14-2 (2492)

Furan-2-carboxylic acid; C4H3O.CO0H

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

Gd+++ gl NaClO4 25°C 0.10M U K1=1.84 B2=3.03 1969RFa (36295) 261

C5H4O3 HL CAS 488-93-7 (1166)

Furan-3-carboxylic acid; C4H3O.CO0H

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

Gd+++ cal NaClO4 25°C 2.00M U H K1=1.64 1976YCa (36304) 262

DH=6.32 kJ mol⁻¹ and DS=52.14 J mol⁻¹ K⁻¹.

C5H5NO2 HL CAS 16867-04-2 (2316)

2,3-Dihydroxypyridine, 3-Hydroxypyridin-2(1H)-one; C5H3N(OH)2

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

Gd+++ gl diox/w 25°C 50% U K1=8.34 1970GDa (36789) 263

Medium: 50% dioxan, 0.1 M NaClO4

C5H5NO3 H2L CAS 99110-85-7 (2195)

1,4-Dihydroxy-2-pyridinone;

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

Gd+++ gl KCl 25°C 0.10M C 1992CMc (36845) 264

B(GdHL)=14.41

C5H5O3F3 HL (7056)

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

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

Gd+++ gl diox/w 25°C 50% M I K1=5.99 B2=11.09 1994SSa (37065) 265

K3=4.46

Medium: 50% dioxan, I=0 corr. At 35 C: K1=5.70, K2=4.97, K3=4.07

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

Gd+++ gl KCl 25°C 0.20M U K1=3.06 1989MFa (37422) 266
K(Gd+HL)=1.91

Gd+++ oth NaClO4 25°C 1.0M U K1=2.18 1972STd (37423) 267
B(GdHL)=6.49
B(GdH2L2)=12.76

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

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

Gd+++ gl diox/w 20°C 50% U K1=4.52 B2=8.10 1971MAF (37526) 268
Medium: 50% v/v dioxan, 0.1 M NaClO4

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

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

Gd+++ gl diox/w 20°C 50% U K1=5.60 B2=10.33 1971MAF (37703) 269

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

Gd+++ gl KCl 25°C 0.10M U K1=5.73 B2=10.16 1995PAa (37978) 270
K3=3.35

Gd+++ gl NaClO4 20°C 0.10M U M 1973TZa (37979) 271
K(Gd(EDTA)+L)=3.55

Gd+++ gl R4N.X 25°C 0.10M U M 1972FGa (37980) 272
K(Gd(EDTA)+L)=2.64

Gd+++ gl alc/w ? 50% U I K1=6.98 1971KOa (37981) 273
Medium: 5-80% MeOH, 0.005 GdCl3, 0.005 HL. K1(5%)=6.00, K1(80%)=8.23

Gd+++ gl NaClO4 25°C 2.0M U K1=5.42 B2=9.81 1964YCa (37982) 274

Gd+++ gl oth/un 30°C 0.10M U K1=5.90 B2=10.38 1960GFa (37983) 275
K3=3.41

 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

 Gd+++ gl KCl 25°C 0.20M U K1=4.49 1989ZPa (38242) 276
 In 70.4% v/v EtOH/H2O: K1 = 6.20

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

 Gd+++ gl NaClO4 25°C 0.10M U K1=3.33 B2=5.12 1970RFa (38261) 277

C5H8O4 H2L Glutaric acid CAS 110-94-1 (420)
 Pentanedioic acid; HOOC.CH2.CH2.CH2.COOH

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

 Gd+++ gl NaClO4 25°C 0.10M M M K1=3.19 1987NCa (38322) 278
 K(Gd(nta)+L)=2.23

Gd+++ gl NaClO4 25°C 0.10M M H K1=3.19 1986CDb (38323) 279
 DH=16.9 kJ mol⁻¹, DS=118 J K⁻¹ mol⁻¹

C5H8O7 H2L CAS 40120-71-6 (3022)
 2,3,4-Trihydroxypentanedioic acid, Trihydroxyglutaric acid; HOOC.(CH(OH))3.COOH

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

 Gd+++ gl KCl 24°C 0.20M U K1=3.64 1966DDa (38423) 280

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

 Gd+++ gl NaClO4 25°C 0.10M U T H K1=5.58 1984SGb (38616) 281
 35 C: K1=5.43; 45 C: 5,30. DH=-30.6 kJ mol⁻¹, DS=4.5 J K⁻¹ mol⁻¹

Gd+++ gl NaClO4 25°C 0.10M U B2=5.60 1981ZLa (38617) 282

 C5H9NO3 HL Hydroxyproline CAS 51-35-4 (416)
 4-Hydroxy-2-pyrrolidinecarboxylic acid; C4H7N(OH)(COOH)

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

 Gd+++ gl NaCl 37°C 0.15M U K1=3.92 1997GMa (38733) 283

 Gd+++ gl NaClO4 25°C 0.10M U B2=5.08 1981ZLa (38734) 284

 C5H9N04 H2L MIDA CAS 4408-64-4 (190)
 N-Methyliminodiethanoic acid; CH3.N(CH2.COOH)2

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

 Gd+++ gl KCl 25°C 0.10M U K1=6.68 B2=11.98 1980MGc (39255) 285
 B3=14.82
 B(Gd+20H+L)=16.56

C5H9N3O4S H2L CAS 16907-58-7 (2106)
 Thiosemicarbazone-diethanoic acid; H2N.CS.NH.N(CH2.COOH)2

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

 Gd+++ gl NaClO4 22°C 0.10M U K1=4.01 1983BTa (39566) 286

 C5H10N2O3 HL Glutamine CAS 56-85-9 (18)
 2-Aminopentanedioic acid 5-amide; H2N.CH(CH2.CH2.CO.NH2)COOH

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

 Gd+++ gl NaCl 25°C 0.15M C 1992JTa (39817) 287
 B(GdH-2L)=-11.00
 B(GdH-3L)=-21.0

C5H10N2O3 HL Ala-Gly CAS 687-69-4 (55)
 Alanyl-glycine; H2N.CH(CH3).CO.NH.CH2.COOH

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

 Gd+++ gl KCl 25°C 0.10M U K1=2.40 1973FMa (39888) 288

 C5H10N2O3 HL Gly-DL-Ala CAS 926-77-2 (66)
 Glycyl-DL-alanine; H2N.CH2.CO.NH.CH(CH3).COOH

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

 Gd+++ gl KCl 25°C 0.10M U K1=2.40 1973FMa (39937) 289

 C5H10N2O4 HL Gly-Ser CAS 7361-43-5 (281)
 Glycyl-serine; H2N.CH2.CO.NH.CH(CH2.OH).COOH

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

 Gd+++ gl KCl 25°C 0.10M U K1=2.50 1973FMb (40102) 290

 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

Gd+++ gl KNO₃ 25°C 0.10M U K1=2.94 B2=5.28 1969PCa (40254) 291
K3=1.58

C5H10O3 HL CAS 617-31-2 (474)
2-Hydroxypentanoic acid; CH₃.CH₂.CH₂.CH(OH).COOH

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

Gd+++ gl NaClO₄ 25°C 1.0M U K1=2.45 1968GCa (40279) 292

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

Gd+++ gl NaClO₄ 25°C 0.10M U K1=2.37 B2=4.00 1970RDa (40297) 293
K3=1.23

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

Gd+++ gl KNO₃ 25°C 0.10M C K1=3.08 B2=5.44 1975PFb (40312) 294
K3=1.57

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

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

Gd+++ cal none 25°C 0.0 U H K1=0.76 1993MLa (40350) 295
DH(K1)=-15.1 kJ mol⁻¹, TDS=-10.8

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

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

Gd+++ gl NaClO₄ 25°C 0.20M U K1=5.10 B2= 9.90 1996PPa (40710) 296

Gd+++ gl NaCl 25°C 0.15M C 1992JTa (40711) 297
B(GdH-1L)=-2.97

Gd+++ gl KNO₃ 25°C 0.20M U M K1=6.03 1990LSb (40712) 298
K(Gd(phen)+L)=5.77

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-----
Gd+++      gl  NaClO4  25°C  0.20M  U          K1=5.10  B2= 9.90  1990PJb (40713) 299
-----
Gd+++      gl  KCl      25°C  0.10M  U T       K1=3.96          1974BFa (40714) 300
*****
C5H11NO2S          HL  Methionine      CAS 63-68-3 (42)
2-Amino-4-(methylthio)butanoic acid; H2N.CH(CH2.CH2.S.CH3)COOH
-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values          Reference ExptNo
-----
Gd+++      gl  NaClO4  25°C  0.20M  U          K1=4.93  B2= 9.31  1996PPa (41096) 301
-----
Gd+++      gl  NaClO4  25°C  0.20M  U          K1=4.93  B2= 9.31  1990PJb (41097) 302
*****
C5H11NO2S          H2L  D-Penicillamine CAS 52-67-5 (1323)
D-2-Amino-3-mercapto-3-methylbutanoic acid; (CH3)2C(SH)CH(NH2)COOH
-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values          Reference ExptNo
-----
Gd+++      gl  KCl      25°C  0.10M  U          B(GdHL)=13.46
*****
C5H12O5          L    Xylitol          CAS 87-99-0 (2139)
Xylitol; HO.CH2.HCOH.HOCH.HCOH.CH2.OH
-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values          Reference ExptNo
-----
Gd+++      cal NaClO4  25°C  2.0M  C  H       K1=0.76          1998BMc (41687) 304
*****
C6H5NO2          HL  Picolinic acid  CAS 98-98-6 (391)
2-Pyridine-carboxylic acid; C5H4N.COOH
-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values          Reference ExptNo
-----
Gd+++      gl  NaClO4  20°C  0.10M  U          K1=5.01          1987EGb (42541) 305
Soln. contains 0.5 M t-butanol
-----
Gd+++      gl  KNO3    25°C  0.20M  U  M       K1=4.64          1987LSc (42542) 306
K(Gd(nta)+L)=4.16, K(Gd(edta)+L)=4.06.
-----
Gd+++      gl  NaClO4  25°C  0.50M  U          K1=3.62  B2=6.91  1977GGb (42543) 307
B3=9.31
-----
Gd+++      gl  KNO3    25°C  0.10M  U          K1=3.98  B2=7.41  1968PIa (42544) 308
K3=2.83
K4=2.26
-----
Gd+++      gl  NaClO4  25°C  2.0M  U          K1=3.77  B2=6.84  1965YCa (42545) 309
-----
Gd+++      gl  KNO3    25°C  0.10M  U          K1=4.06  B2=7.34  1964THb (42546) 310

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B3=10.5

C6H5NO2 HL Nicotinic acid CAS 59-67-6 (419)
3-Pyridine-carboxylic acid; C5H4N.COOH

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

Gd+++ gl NaClO4 25°C 0.20M U K1=2.08 1973FDa (42672) 311

C6H5NO3 H2L CAS 874-24-8 (4356)
3-Hydroxypyridine-2-carboxylic acid; C5H3N.(OH)(COOH)

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

Gd+++ gl NaClO4 30°C 0.10M U 1969DNc (42751) 312

K(Gd+HL)=3.46
K(GdHL+HL)=3.24

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

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

Gd+++ gl R4N.X 25°C 0.10M C K1=1.64 1990CBe (42807) 313

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

Gd+++ gl NaClO4 25°C 2.0M U K1=2.93 B2=5.20 1965YCa (42834) 314

C6H5NO4 H2L 4-Nitrocatechol CAS 3316-09-4 (890)
1,2-Dihydroxy-4-nitrobenzene; O2N.C6H3(OH)2

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

Gd+++ gl KNO3 25°C 0.10M U K1=9.15 B2=15.67 1981BDa (42927) 315

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

Gd+++ sp KCl 25°C 0.10M M I K1=6.08 1989PEa (42953) 316

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

 Gd+++ sp KCl 25°C 0.10M U K1=5.27 1987PLa (43109) 317

 C6H5O4Cl HL Chlorokojic aci (3086)
 3-Chloro-5-hydroxy-2-hydroxymethyl-4-pyrone;

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

Gd+++ gl oth/un 30°C 0.10M U K1=5.98 B2=11.12 1972DSd (43132) 318

 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

Gd+++ sp KCl 25°C 0.10M U K1=5.37 1987PLa (43151) 319

 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

Gd+++ gl NaClO4 25°C 0.20M U K1=10.08 1996PJa (43762) 320

Gd+++ gl KNO3 25°C 0.10M U TIH K1=8.72 B2=14.42 1986NSa (43763) 321
 B(GdAL)=11.85
 H2A=phthalic acid. DH(GdAL)=-57.0 kJ mol⁻¹, DS=35.7 J K⁻¹ mol⁻¹

Gd+++ gl NaClO4 35°C 0.20M M K1=9.57 1982LTa (43764) 322

Gd+++ gl KNO3 25°C 0.05M M I K1=10.36 B2=19.62 1981BDc (43765) 323
 Also data for I=0.2 and 0.35 M. At I=0, K1=10.98, K2=9.73.

Gd+++ gl NaClO4 25°C 0.10M U T K1=10.67 B2=20.08 1979NDa (43766) 324
 At 45 C, K1=9.89, K2=9.03. Medium ionic strength not stated.

Gd+++ EMF NaCl 25°C 0.10M U K1=11.20 1969PKe (43767) 325

 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

Gd+++ gl NaClO4 25°C 0.20M U K1=10.05 1996PJa (43960) 326

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

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

Gd+++ gl NaClO4 30°C 0.10M U M K1=6.01 B2=11.21 1989NOB (44086) 327
 B(GdLA)=13.43
 K(GdA+L)=6.55
 K(GdB+L)=5.73
 K(GdC+L)=5.15

H2A=iminodiacetic acid, H2B=hydroxyethyliminodiethanoic acid, H3C=nitrilo-triethanoic acid

Gd+++ gl NaClO4 30°C 0.10M U K1=6.58 B2=11.91 1970DSc (44087) 328
 K3=3.95

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
Gd+++	gl	NaClO4	30°C	0.10M	U	M	K1=5.38 B2=10.34	1989NOB (44215)	329
							B(GdLA)=12.70		
							K(GdA+L)=5.74		
							K(GdB+L)=5.28		
							K(GdC+L)=4.77		

H2A=iminodiacetic acid, H2B=hydroxyethyliminodiethanoic acid, H3C=nitrilo-triethanoic acid

Gd+++ sp KCl 25°C 0.10M C I K1=6.004 1987PEa (44216) 330
 In 0.087 M KCl, K1=6.039.

Gd+++ gl oth/un 30°C 0.10M U K1=6.09 B2=11.21 1972DSd (44217) 331
 K3=4.05

Gd+++ gl NaClO4 25°C 2.0M U K1=5.49 B2=10.66 1964YCa (44218) 332

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Gd+++	gl	NaCl	20°C	0.10M	U		K1=4.56	1986SKb (44297)	333
							K(Gd+HL)=3.23		

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
Gd+++	gl	NaClO4	35°C	0.20M	M		K1=13.37	1982LTa (44449)	334

Gd+++ gl KNO3 25°C 0.10M U TIH K1=14.53 B2=28.04 1980BDd (44450) 335
 Data for I=0.05-0.2 M and for I=0.10 M (35 C). Also DH and DS values.

Gd+++ gl NaClO4 25°C 0.50M C K1=12.50 B2=21.14 1976LAb (44451) 336
B(GdHL2)=29.01

Gd+++ gl NaClO4 25°C 0.10M U K1=14.10 1970SSi (44452) 337
K(Gd+HL)=5.92

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

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

Gd+++ sp non-aq 25°C 100% U HM 1982KNa (44871) 338
K(GdA3+L)=2.40

Medium: CCl4. HA=dipivaloylmethane

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

Gd+++ gl KNO3 25°C 0.10M U TIH K1=6.26 B2=10.83 1986NSa (44929) 339
B(GdAL)=13.39

H2A=phthalic acid. DH(GdAL)=-64.2 kJ mol⁻¹, DS=40.5 J K⁻¹ mol⁻¹

Gd+++ gl mixed 25°C 50% U I K1=3.80 B2=6.66 1969BCa (44930) 340
Medium: 50% DMSO, 0.12 M NaClO4. In 0.12 M NaClO4, 50% dioxan: K1=5.04,
K2=4.33. Medium: 0.12 NaClO4, 50% EtOH: K1=4.48, K2=3.37

C6H7NO2 HL CAS 19365-01-6 (6771)
1-Methyl-3-hydroxy-2-pyridinone;

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

Gd+++ gl KCl 25°C 0.10M C K1=6.36 B2=11.64 1992CMc (45028) 341
B3=15.68

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

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

Gd+++ gl NaClO4 15°C 0.10M U K1=8.70 1980ZMa (45127) 342

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

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

Gd+++ gl diox/w 25°C 50% M I K1=6.01 B2=11.32 1994SSa (45186) 343
K3=4.69

Medium: 50% dioxan, I=0 corr. At 35 C: K1=5.64, K2=5.24, K3=4.34

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

Gd+++ gl KCl 25°C 0.20M U K1=3.72 1989ZPa (45468) 344
In 70.4% v/v EtOH/H2O: K1 = 5.91

C6H8O6 H3L Tricarballic CAS 99-14-9 (1620)
1,2,3-Propanetricarboxylic acid; HOOC.CH2.CH(COOH).CH2.COOH

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

Gd+++ gl NaCl 25°C 0.15M C K1=4.20 1991JTa (45565) 345
B(GdHL)=8.48
B(GdH-1L)=-4.47

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

Gd+++ gl NaClO4 25°C 2.00M U IH K(Gd+HL)=1.52 1988HSa (45641) 346

DH=3.7 kJ mol⁻¹, DS=41.5 J K⁻¹ mol⁻¹

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

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

Gd+++ gl NaClO4 25°C 0.10M U TIH K1=3.68 B2=6.87 1986AJc (45695) 347
DH(K1)=-6.3 kJ mol⁻¹, DS=49.7 J K⁻¹ mol⁻¹; DH(K2)=-4.4, DS=46.9

Gd+++ gl NaClO4 30°C 0.10M U IH K1=3.68 B2=6.87 1983ASa (45696) 348
DH(K1)=-6.2 kJ mol⁻¹, DH(K2)=-4.4

C6H8O7 H3L Citric acid CAS 77-92-9 (95)
2-Hydroxypropane-1,2,3-tricarboxylic acid; HOOCCH2.CH(OH)(COOH).CH2COOH

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

Gd+++ gl NaCl 25°C 0.15M C K1=6.86 B2=10.53 1991JTa (46117) 349
B(GdHL)=10.12
B(GdH-1L)=0.77
B(GdH-2L)=-7.08

Gd+++ gl KNO3 25°C 1.0M M 1986SZb (46118) 350

Gd+++ ISE KNO3 25°C 0.10M C K1=11.50 1980NSf (46832) 361
Competitive method using Cd ion-selective electrode.

Gd+++ gl diox/w 30°C 50% U M K(GdL+A)=5.34 1978SGf (46833) 362

HA=tropolone

Gd+++ gl NaClO4 25°C 0.50M U K1=11.11 1977GGb (46834) 363

Gd+++ EMF KCl 25°C 1.0M U M K(GdA+L)=6.09 1977GMa (46835) 364
K(GdA+H2L)=1.55
K(GdA+H3L)=2.11
K(GdA+H4L)=3.45

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

Gd+++ cal KNO3 20°C 0.10M U HM K(GdA+L)=4.86 1971GKb (46836) 365

H4A=EDTA. DH(GdA+L)=-33.14 kJ.mol⁻¹, DS=-19.7 J K⁻¹ mol⁻¹.
DH(GdLA)=-40.4 kJ mol⁻¹, DS=288 J K⁻¹ mol⁻¹

Gd+++ gl oth/un 20°C 0.20M U B(Gd1OH)=6.28 1970VMa (46837) 366

Gd+++ gl KCl 20°C 0.10M U K1=11.43 B2=20.78 1965ANb (46838) 367

Gd+++ vlt KNO3 20°C 0.10M U T K1=11.43 1964PCa (46839) 368

Gd+++ gl KNO3 25°C 0.10M U T H T K1=11.54 B2=20.80 1962MFb (46840) 369
15 C: K1=11.57, K2=9.46; 20 C: 11.54, 9.34; 30 C: 11.59, 9.23; 35 C: 11.57, 9.12
40 C: 11.60, 9.09. DH(K1)=4.3 kJ mol⁻¹, DS=235 J K⁻¹ m⁻¹; DH(K2)=-24.3, DS=95

Gd+++ vlt KNO3 20°C 0.10M U T K1=11.43 1958CGa (46841) 370

Gd+++ vlt KNO3 20°C 0.10M U B(Gd2L3)=36.89 1957NOa (46842) 371

C6H9N3O2 HL Histidine CAS 71-00-1 (1)
2-Amino-3-(4'-imidazolyl)propanoic acid; H2N.CH(CH2.C3H3N2)COOH

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

Gd+++ gl KNO3 35°C 0.10M U K(Gd+HL)=3.76 1987RRc (47561) 372

Gd+++ gl KNO3 35°C 0.10M U M K(Gd+HL)=3.76 1986RMb (47562) 373

K(Gd+HL+cytidine)=8.57

Gd+++ gl NaClO4 37°C 3.00M U T K1=4.94 B2=9.16 1971JWa (47563) 374
B(GdHL)=11.30

Gd+++ gl NaClO4 25°C 3.00M U T K1=4.39 B2=8.61 1970JWa (47564) 375
B(GdHL)=11.47

C6H10O2S HL (4370)
Ethyl thioacetoacetate; CH3.CS.CH2.CO.OCH2.CH3

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

Gd+++ gl mixed 30°C 75% U K1=7.08 B2=12.83 1970DRa (47963) 376
K3=5.46

Medium: 75% acetone, 0.1 M

C6H10O3 HL CAS 16841-19-3 (3649)
1-Hydroxycyclopentanecarboxylic acid; HO.C5H8.COOH

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

Gd+++ gl NaClO4 25°C 0.10M U K1=2.844 B2=5.06 1966PRb (47989) 377
K3=1.65
K4=1.49

C6H10O3 HL CAS 141-97-9 (3068)
Ethyl acetoacetate; CH3.CO.CH2.CO2.C2H5

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

Gd+++ gl mixed 30°C 75% U K1=6.30 B2=11.65 1969DRa (48013) 378

Medium: 75% acetone, 0.1 M NaClO4

C6H10O4 H2L Adipic acid CAS 124-04-9 (401)
1,6-Hexanedioic acid; HOOC.(CH2)4.COOH

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

Gd+++ gl NaClO4 25°C 0.10M M M K1=3.09 1987Nca (48072) 379
K(Gd(nta)+L)=2.34

Gd+++ gl NaClO4 25°C 0.10M M H K1=3.09 1986CDb (48073) 380
DH=16.5 kJ mol⁻¹, DS=114 J K⁻¹ mol⁻¹

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

Gd+++ oth NaClO4 25°C 0.10M U K1=4.84 1984AFa (48340) 381
Laser excitation spectroscopy, competition method.

Gd+++ gl NaClO4 25°C 1.00M C H K1=4.89 B2=7.87 1974GGa (48341) 382
B3=8.83
B(GdHL2)=10.21

C6H10O8 H2L Saccharic acid CAS 87-73-0 (1191)
D-2,3,4,5-Tetrahydroxy-1,6-hexanedioic acid, Glucaric acid; HOOC.(CHOH)4.COOH

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

Gd+++ gl NaClO4 25°C 0.10M U M K1=4.51 1997PPb (48475) 383
K(Gd(edta)+L)=4.01

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

Gd+++ gl alc/w 30°C 50% C K1=9.01 1994SOa (48734) 384
Medium: 50% v/v MeOH/H2O, 0.10 M NaClO4.

Gd+++ gl KNO3 20°C 1.00M U 1974CMd (48735) 385
K(GdL2(OH)+H)=10.72

Gd+++ oth NaNO3 20°C 0.10M U M K1=9.0 B2=16.95 1966JMc (48736) 386
Method: paper electrophoresis. Ternary complexes with HEDTA

Gd+++ vlt KCl 25°C 0.10M U B2=16.08 1965DTa (48737) 387

Gd+++ ISE KNO3 25°C 0.10M U K1=9.01 B2=17.05 1963TLa (48738) 388

C6H11N3O4 HL Gly-Gly-Gly CAS 556-33-2 (415)
Glycyl-glycyl-glycine; H2N.CH2.CO.NH.CH2.CO.NH.CH2.COOH

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

Gd+++ gl NaClO4 25°C 0.10M U 1981KBa (48976) 389
K(Gd+HL)=0.43

Gd+++ gl KCl 25°C 0.10M U K1=2.20 1973FMa (48977) 390

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

Gd+++ gl R4N.X 25°C 0.10M C K1=8.13 1988CCb (49241) 391

Gd+++ gl NaClO4 25°C 1.00M C H K1=8.25 B2=14.42 1974GGa (49242) 392
B(GdH2L)=17.60

Gd+++ gl KNO3 25°C 0.10M U K1=8.13 B2=14.21 1962THb (49243) 393

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

Gd+++ gl NaCl 20°C 0.10M U K1=3.16 1986GKb (49424) 394

C6H12O3 HL DiEtGlycolic CAS 3639-21-2 (421)

2-Ethyl-2-hydroxybutanoic acid; (C2H5)2.C(OH).COOH

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

Gd+++ EMF NaClO4 25°C 1.0M U K1=2.71 B2=4.65 1965TVa (49459) 395

K3=0.98

K4=0.86

Method: quinhydrone electrode

C6H12O3 HL CAS 92841-97-9 (3658)

2-Hydroxy-2,3-dimethylbutanoic acid; CH3.CH(CH3).C(OH)(CH3).COOH

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

Gd+++ EMF NaClO4 25°C 1.0M U K1=2.65 B2=4.70 1965TVa (49473) 396

K3=1.34

K4=0.94

Method: quinhydrone electrode

C6H12O4 HL CAS 1112-33-0 (1246)

2,3-Dihydroxy-2,3-dimethylbutanoic acid; (CH3)2.C(OH).C(OH)(CH3).COOH

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

Gd+++ gl KNO3 25°C 0.10M U K1=3.42 B2=5.96 1979PPa (49493) 397

K3=1.72

C6H12O7 HL Gluconic acid CAS 526-95-4 (904)

D-Gluconic acid, 2,3,4,5,6-Pentahydroxyhexanoic acid; HO.CH2(CHOH)4.COOH

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

Gd+++ EMF alc/w 25°C 80% U I K1=5.37 1966KRb (49719) 398

Medium: 80% MeOH. K1=4.64(50%)

Gd+++ gl KCl 25°C 0.20M U K1=2.56 B2=4.76 1963K0c (49720) 399

C6H13NO2 HL Isoleucine CAS 73-32-5 (424)

2-Amino-3-methylpentanoic acid; CH3.CH2.CH(CH3).CH(NH2).COOH

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

Gd+++ gl NaClO4 25°C 0.20M U K1=5.21 B2= 9.81 1987PPa (49903) 400

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

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

Gd+++ gl KNO3 25°C 0.20M U M K1=6.10 1990LSb (50075) 401
K(Gd(phen)+L)=5.87

Gd+++ gl NaClO4 25°C 0.20M U K1=5.21 B2= 9.52 1987PPa (50076) 402

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

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

Gd+++ gl NaClO4 22°C 0.10M M M K1=4.72 B2=9.37 1991DTa (50179) 403
B3=13.16
K(GdA+L)=8.08
H4A=trans-cyclohexane-1,2-diaminotetraethanoic acid. Definitions wrong?

Gd+++ gl KCl 20°C 0.20M U K1=3.90 B2=7.48 1990PLa (50180) 404

C6H13NO2 HL CAS 60-32-2 (1846)
6-Amino hexanoic acid; H2N.CH2.CH2.CH2.CH2.COOH

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

Gd+++ gl KCl 20°C 0.20M U K1=4.79 B2=9.04 1990PLa (50216) 405

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

Gd+++ gl KNO3 20°C 0.10M U K1=5.58 B2=10.43 1982RFa (50365) 406

Gd+++ gl KCl 30°C 0.10M U K1=5.84 B2=10.60 1973MSe (50366) 407

Gd+++ gl alc/w 20°C 50% U I K1=6.70 1970KRa (50367) 408
Medium: 0-80% MeOH, 0.03 M KCl. K1(0%)=5.59, K1(20%)=6.12, K1(80%)=7.73

Gd+++ oth NaNO3 20°C 0.10M U K1=7.7 B2=13.50 1966JMc (50368) 409
Method: paper electrophoresis

C6H13N3O3 HL Citrulline (579)

2-Amino-5-ureidovaleric acid; H2N.CO.NH.CH2.CH2.CH2.CH(NH2).COOH

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

Gd+++ g1 NaCl 37°C 0.15M U M K1=2.96 1997GMa (50577) 410
B(GdHL)=10.98
B(GdH2AL)=24.41

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

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

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

Gd+++ g1 KNO3 15°C 1.0M U T 1989SSg (50823) 411
K(Gd+HL)=3.02
K(GdHL+HL)=2.76

Also data for 30 C.

Gd+++ g1 NaCl04 20°C 0.10M U T H K1=7.42 B2=14.03 1983SDa (50824) 412
30 C: K1=7.12, K2=6.51, 40 C: K1=6.96, K2=6.34

C6H15N3O3 L (6613)
1,3,5-Triamino-1,3,5-trideoxy-cis-inositol,5-Amino-5-deoxy-streptamine;

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

Gd+++ g1 KCl 25°C 0.10M C 1998HGa (51452) 413
B(GdH-6L2)=-18.2

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

Gd+++ ISE non-aq 25°C 100% C H K1=4.40 B2=5.90 1993CCb (52198) 414
Medium: DMSO, 0.1 M Et4NClO4. Method: Ag+ ISE. By calorimetry, DH(K1)=-44.9
kJ mol⁻¹, DS=-66; DH(B2)=-72, DS=-129.

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

Gd+++ g1 NaCl 37°C 0.15M C K1=14.87 1995WJa (52337) 415
K(GdL+H)=6.99
K(GdHL+H)=5.88

Gd+++ g1 KNO3 25°C 0.10M C 1991SKb (52338) 416
K(GdL+H)=7.35

K(GdHL+H)=6.19

Gd+++ gl KCl 25°C 0.10M U K1=21.80 1967KDa (52339) 417
K(Gd+HL)=17.09
K(Gd+H2L)=13.12
K(Gd+H3L)=10.34
K(Gd+H4L)=8.04

K(Gd+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

Gd+++ gl NaNO3 25°C 0.10M U I M K1=5.83 1996KDC (52481) 418
*K(GdL)=-7.26
K(Gd(egta)+L)=5.12

Data for 0.05 and 0.15 M NaNO3. At I=0, K1=6.22, *K(GdL)=-7.45,
K(Gd(egta)+L)=5.49.

Gd+++ gl oth/un 24°C 0.20M U K1=5.27 1972PSd (52482) 419
Medium: LiCl

C7H5N04 H2L Dipicolinic aci CAS 449-83-2 (418)
2,6-Pyridinedicarboxylic acid; C5H3N.(COOH)2

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

Gd+++ cal NaClO4 25°C 0.50M C H 1963GRd (52776) 420
DH(K1)=-14.99 kJ mol⁻¹, DS(K1)=116 J K⁻¹ mol⁻¹; DH(B2)=-36.53,
DS(B2)=183; DH(B3)=-56.98, DS(B3)=224.

Gd+++ EMF oth/un 20°C 0.50M U K1=8.74 B2=16.06 1961GRa (52777) 421
K3=5.77

C7H5N04 HL CAS 121-92-6 (490)
3-Nitrobenzoic acid; O2N.C6H4.COOH

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

Gd+++ gl NaClO4 25°C 0.10M C H K1=1.68 1986CLc (52866) 422
DH=7.3 kJ mol⁻¹, DS=57 J K⁻¹ mol⁻¹

C7H5N04 HL CAS 62-23-7 (489)
4-Nitrobenzoic acid; O2N.C6H4.COOH

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

Gd+++ gl NaClO4 25°C 0.10M M H K1=1.73 1999YKa (52907) 423
By calorimetry: DH(K1)=7.60 kJ mol⁻¹, DS(K1)=58.6 J K⁻¹ mol⁻¹.

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

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

 Gd+++ gl NaClO4 25°C 0.10M C H K1=1.80 1986CLc (53235) 424
 DH=8.1 kJ mol⁻¹, DS=62 J K⁻¹ mol⁻¹

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

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

 Gd+++ gl NaClO4 25°C 0.10M C H K1=2.00 1986CLc (53255) 425
 DH=8.0 kJ mol⁻¹, DS=65 J K⁻¹ mol⁻¹

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

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

 Gd+++ gl NaClO4 25°C 0.10M C H T 1993ALa (53368) 426
 B(1,1,1)=12.38
 B(1,0,1)=7.40
 B(1,0,2)=12.35
 B(1,-1,1)=-0.54

B(p,q,r); pGd+qH+rL=(Gd)pHqLr. B(1,-2,1)=-9.22.

C7H6OS HL Thiotropolone CAS 1073-38-7 (8477)
 2-Mercapto-2,4,6-cycloheptatrien-1-one;

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

 Gd+++ gl diox/w 30°C 50% M I K1=5.11 B2= 9.78 1978SSi (53544) 427
 K3=3.58
 Medium: 50% v/v dioxane/H2O, 0.10 M NaClO4. Data for 0.005 and 0.2 M NaClO4.

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

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

 Gd+++ gl KNO3 25°C 0.10M U K1=7.04 B2=12.90 1969CMb (53674) 428
 K3=4.82
 K4=3.30

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

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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++     gl  alc/w  25°C 100% M          K1=8.4   B2=15.1  1989TMa (53833) 429
                                         B3=18.6

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Medium: MeOH

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Gd+++     cal NaClO4 25°C 0.10M U  H   K1=2.08  B2=3.70  1982CBc (53834) 430
DH1= 9.0 kJ mol-1, DS1= 70 J K-1 mol-1

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Gd+++     gl  alc/w  25°C 99% U          K1=6.51  B2=11.35 1974BPb (53835) 431
                                         K3=2.73

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

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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++     gl  NaClO4 25°C 0.1M C   H          1996HYa (54224) 432
By calorimetry: DH(K1)=1.93 kJ mol-1, DH(B2)=5.92 J K-1 mol-1

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Gd+++     gl  NaNO3  25°C 0.10M U  I M   K1=8.62          1996KDc (54225) 433
                                         *K(GdL)=-7.80
                                         K(Gd(egta)+L)=5.86

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Data for 0.05 and 0.15 M NaNO3. At I=0, K1=8.95, *K(GdL)=-7.90,
K(Gd(egta)+L)=6.13.

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-----
Gd+++     gl  NaClO4 25°C 0.10M C   T          1989HMa (54226) 434
                                         K(Gd+HL)=1.89
                                         K(GdHL+HL)=1.89

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-----
Gd+++     gl  alc/w  25°C 100% M          K(Gd+HL)=7.6
                                         K(Gd+2HL)=14.0
                                         K(Gd+3HL)=16.6

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Medium: MeOH

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-----
Gd+++     gl  KNO3   25°C 0.10M U  TIH T K1=9.98          1986NSa (54228) 436
                                         B(GdAL)=15.56
H2A=phthalic acid. DH(GdAL)=-48.9 kJ mol-1, DS=137.3 J K-1 mol-1

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Gd+++     ix  mixed  20°C 50% U          K(Gd+HL)=2.31
                                         K(Gd+2HL)=3.33
                                         K(Gd+2HL)=5.64

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

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-----
Gd+++     gl  alc/w  25°C 100% U          K1=6.16  B2=11.04 1973BPd (54230) 438
                                         K3=3.42

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Medium: 99.9% MeOH, 0.1 M NaCl

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

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

Gd+++ gl NaClO4 25°C 0.10M C H 1988LLa (54379) 439
K(Gd+HL)=2.10

DH=8.37 kJ mol-1, DS=68.2 J K-1 mol-1

Gd+++ gl alc/w 25°C 99% U K1=6.58 B2=11.83 1974BPb (54380) 440
K3=2.99

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

Gd+++ gl NaClO4 25°C 0.10M M H K1=1.85 1999YKa (54417) 441
By calorimetry: DH(K1)=10.14 kJ mol-1, DS(K1)=69.4 J K-1 mol-1.

Gd+++ gl NaClO4 25°C 0.10M C H 1988LLa (54418) 442
K(Gd+HL)=2.27

DH=8.49 kJ mol-1, DS=71.8 J K-1 mol-1

Gd+++ gl alc/w 25°C 99% U K1=6.78 B2=12.05 1974BPb (54419) 443
K3=3.25

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

Gd+++ gl NaClO4 25°C 0.20M U K1=10.68 1996PJa (54676) 444

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

Gd+++ gl KNO3 20°C 0.10M U T K1=7.78 1982DBa (55009) 445

Gd+++ gl NaClO4 20°C 1.0M U K1=6.93 B2=12.83 1972CBb (55010) 446

Gd+++ gl NaClO4 20°C 0.10M U K1=7.58 B2=13.65 1966TJb (55011) 447
K(GdL+H)=6.20

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
Gd+++	gl	NaClO4	25°C	0.50M	C	T	K1=8.59 B2=14.12	1976LAc (55096)	448

C7H7NOS HL (2034)									
N-Thioformyl-N-phenylhydroxylamine; H(C:S)N(C6H5)OH									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Gd+++	gl	diox/w	30°C	70%	U		K1=7.72 B2=13.52 K3=4.34	1981MBb (55152)	449

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
Gd+++	gl	NaClO4	25°C	0.10M	C		K1=2.36 B2=4.51	1989HMa (55226)	450

Gd+++	gl	NaClO4	25°C	0.10M	U	H	K1=4.34	1982KYc (55227)	451
By calorimetry, DH(K1)=5.40 kJ mol ⁻¹ , DS(K1)=101.38 J K ⁻¹ mol ⁻¹ .									

Gd+++	gl	non-aq	25°C	100%	U		K1=7.15 B2=12.99 K3=3.35 K4=2.65	1970BBh (55228)	452

Medium: MeOH, 0.1 M NaCl

 C7H7NO2 HL CAS 150-13-0 (1376)
 4-Aminobenzoic acid; H2N.C6H4.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Gd+++	gl	NaClO4	25°C	0.10M	M	H	K1=2.10	1999YKa (55380)	453
By calorimetry: DH(K1)=7.91 kJ mol ⁻¹ , DS(K1)=66.7 J K ⁻¹ mol ⁻¹ .									

Gd+++	gl	KCl	25°C	0.20M	U		K1=2.54	1977EBa (55381)	454

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Gd+++	gl	diox/w	35°C	50%	A		K1=10.00 B2=18.50 K3=7.49	1977AKa (55502)	455

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

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

Gd+++ gl mixed 25°C 75% U 1970SEa (55597) 456

K(Gd+HL)=7.35
K(GdHL+HL)=6.80
K(Gd(HL)2+HL)=4.60

Medium: 75% acetone, 0.1 M NaClO4

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

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

Gd+++ gl KCl 25°C 0.20M M T H K1=8.17 1991BPb (55688) 457

K(Gd+OH+L)=15.36

DH(K1)=-87 kJ mol⁻¹, DS(K1)=-134 J K⁻¹ mol⁻¹. DH(Gd(OH)L)=-241,
DS(Sm(OH)L)=-517. 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

Gd+++ gl mixed 25°C 50% U I K1=4.13 B2=7.95 1969BCb (56067) 458

Medium: 50% DMSO, 0.12 M LiClO4. In 50% dioxan, 0.12 M NaClO4: K1=5.28,
K2=4.13; 50% EtOH, 0.12 M NaClO4: K1=4.83, K2=3.73

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

Gd+++ sp KCl 25°C 0.10M M I K1=6.40 1986PLb (56127) 459

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

Gd+++ sp KCl 25°C 0.10M M I K1=6.05 1986PLb (56146) 460

C7H8O8P2 H4L (6892)
1,2-((Phenylenedioxy)methylene)diphosphonic acid); C6H4O2C(PO3H2)2

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

Gd+++ gl R4N.X 25°C 0.50M U K1=11.17 1985GMb (56168) 461

K(Gd+HL)=5.88

Medium: 0.5 M Me4NCl

C7H9NO2 HL CAS 30652-11-0 (2458)
3-Hydroxy-1,2-dimethylpyridin-4(1H)-one; (OH)(CH3)(O:)C5H2N.CH3

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

Gd+++ gl KCl 25°C 0.10M C K1=7.82 B2=3.47 1994MRa (56439) 462

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

Gd+++ gl KNO3 25°C 0.10M U K1=4.18 B2=6.67 1971Pjb (56733) 463

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

Gd+++ gl KNO3 25°C 0.10M U K1=6.09 B2=11.46 1963THb (56806) 464

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

Gd+++ gl KNO3 25°C 0.1M U K1=8.86 1982KKc (56844) 465

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

Gd+++ gl KNO3 20°C 0.10M U K1=12.24 B2=21.84 1974RMg (56910) 466

C7H12N2O3 HL Gly-Pro CAS 704-15-4 (257)
Glycyl-proline; H2N.CH2.CO.NC4H7.COOH

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

Gd+++ gl KNO3 25°C 0.15M M T H K1=3.74 1983SKb (57121) 467
Data for 35 and 45 C. At 35 C, DH(K1)=22 kJ mol⁻¹, DS(K1)=146 J K⁻¹ mol⁻¹.

Gd+++ gl KNO3 25°C 0.15M U T H K1=3.87 1979SKe (57122) 468
At 35 C, K1=3.95; at 45 C, K1=4.03. At 35 C, DH(K1)=14.5 kJ mol⁻¹,
DS(K1)=123 J K⁻¹ mol⁻¹

C7H12N2O3 HL Pro-Gly CAS 2578-97-6 (262)
Prolyl-glycine; C4H8N.CO.NH.CH2.COOH

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

Gd+++ gl KCl 25°C 0.10M U K1=3.00 1973FMa (57148) 469

C7H12O3 HL CAS 609-69-8 (3731)
2-Hydroxycyclohexanecarboxylic acid; HO.C6H10.COOH

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

Gd+++ gl NaClO4 25°C 1.0M U K1=2.29 B2=4.17 1967STd (57262) 470

C7H12O3 HL (4422)
3-Methyl ethylacetoacetate; CH3.CO.CH(CH3).CO.OCH2.CH3

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

Gd+++ gl mixed 30°C 75% U K1=8.08 1971DRb (57274) 471
Medium: 75% acetone, 0.1 M

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

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

Gd+++ gl KNO3 25°C 0.10M U K1=4.49 B2=7.05 1968PFa (57364) 472

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

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

Gd+++ gl NaCl 20°C 0.10M U K1=2.77 1977SSc (57399) 473

Gd+++ EMF NaClO4 25°C 1.0M U K1=2.64 B2=4.63 19670Ta (57400) 474
K3=1.44
K4=0.73

Method: quinhydrone electrode

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

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

Gd+++ gl KNO3 20°C 0.10M U K1=8.50 B2=16.20 1980RPa (57612) 475

C7H14N2O3S HL Gly-Met CAS 554-94-9 (726)
Glycyl-methionine; H2N.CH2.CO.NH.CH(CH2.CH2.S.CH3).COOH

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

Gd+++ gl KCl 25°C 0.10M U K1=2.50 1973FMa (57797) 476

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

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

Gd+++ EMF NaClO4 25°C 1.0M U K1=2.77 B2=5.13 1965TVa (57862) 477
K3=1.39
K4=1.14

Method: quinhydrone electrode

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

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

Gd+++ gl NaClO4 25°C 0.10M C K1=2.68 B2=4.38 1976SPa (57874) 478

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

Gd+++ gl KNO3 20°C 0.10M U K1=5.26 B2=9.80 1982RFa (57936) 479

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

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

Gd+++ sp NaNO3 25°C 0.10M U K1=3.90 19850Ha (58502) 480

Gd+++ sp non-aq 25°C 100% U K1=5.53 1983PSc (58503) 481
Medium: DMSO

Gd+++ sp NaClO4 30°C 0.10M C 1978BKd (58504) 482
K1eff=5.031
Medium pH 5.4 (acetate).

Gd+++ sp alc/w 12°C 50% U 1972BLa (58505) 483
K(Gd+H2L)=4.91
Medium: 50% EtOH, 0.1 M NaClO4

Gd+++ sp KNO3 12°C 0.10M U 1965GEa (58506) 484
K(Gd+H2L)=4.08

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

Gd+++ cal non-aq 25°C 100% C H 2004MIa (58624) 485
 Method: calorimetric titration. Medium: chloroform. DH(GdL3+A)=8.0 kJ
 mol-1, DS=84 J K-1 mol-1; DH(GdL3+2A)=6.9, DS=131. HA is benzoic acid.

 Gd+++ gl alc/w 22°C 80% U K1=6.44 B2=11.87 1995MTa (58625) 486
 K3=4.55
 Medium: 0.1 M NaClO4 in 80% (v/v) EtOH/H2O.

 Gd+++ gl mixed 25°C 50% U K1=5.80 1980SBc (58626) 487
 Medium: 50% MeCN

 Gd+++ dis non-aq 25°C 100% U M 1972KKd (58627) 488
 K(GdL3+bpy)=6.38
 K(GdL3+2bpy)=8.59
 K(GdL3+A)=4.54
 K(GdL3+2A)=6.59

A=4,4'-dipyridyl. Medium: benzene. K(GdL3+phen)=6.98, K(GdL3+2phen)=10.85

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
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Gd+++	gl	KNO3	25°C	0.10M	U			K1=3.82 B2=6.85	1986NSa (58971)	489
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Gd+++	gl	NaClO4	30°C	0.10M	U			K1=4.28 B2=7.58	1966KPb (58972)	490
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 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
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Gd+++	cal	NaClO4	25°C	0.10M	U	H		K1=2.73	1982CBc (59053)	491
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DH= 12.20 kJ mol-1, DS= 93 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
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Gd+++	gl	diox/w	20°C	50%	U			K1=6.05 B2=11.45	1971MAf (59101)	492
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Medium: 50% v/v dioxan, 0.1 M NaClO4

C8H7O2Cl HL CAS 1450-74-4 (6325)
 2-Hydroxy-5-chloro-acetophenone; Cl(HO)C6H3.CO.CH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Gd+++	gl	alc/w	25°C	20%	M	I		K1=6.24	1994KDa (59217)	493
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Medium: 20% v/v EtOH/H2O, 0.10 M NaNO3. Also data for 0.05 and 0.15 M

NaNO3. At I=0 (20% v/v), K1=6.52, *K(GdL)=-8.74, *K(Gd(OH)L)=-8.84.

C8H8N2O L CAS 4856-97-7 (3820)
2-(Hydroxymethyl)benzimidazole;

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

Gd+++ gl diox/w 30°C 50% U T H B2=16.55 1988NOa (59310) 494
40 C: B2=16.44; 50 C: B2=16.35. DH=-18.8 kJ mol⁻¹, DS=254 J K⁻¹ mol⁻¹

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

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

Gd+++ gl diox/w 20°C 50% U K1=7.01 B2=13.11 1971MAf (59336) 495
Medium: 50% dioxan, 0.1 M NaClO4

C8H8N4OS L (6097)
2-Acetylpyridinethiosemicarbazone; C5H4N.CO.CH:N.NH.CS.NH2

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

Gd+++ gl alc/w 25°C 75% C I K1=7.57 B2=14.58 1988GSa (59407) 496
In 75%(v/v) ethanol/water; 0.1M NaClO4. I=0.2 M: K1=7.51, K2=6.98;
I=0.05 M: K1=7.63, K2=7.10; I=0.02 M: K1=7.84, K2=7.26

C8H8O2 HL 2-Acetylphenol CAS 118-93-4 (1888)
2-Hydroxyacetophenone; HO.C6H4.CO.CH3

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

Gd+++ gl alc/w 25°C 20% M I K1=6.56 1994KDa (59464) 497
Medium: 20% v/v EtOH/H2O, 0.10 M NaNO3. Also data for 0.05 and 0.15 M
NaNO3. At I=0 (20% v/v), K1=6.81, *K(GdL)=-8.64, *K(Gd(OH)L)=-9.21.

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

Gd+++ gl NaClO4 25°C 0.1M C H K1=1.96 1996HYa (59546) 498
By calorimetry: DH(K1)=12.01 kJ mol⁻¹

Gd+++ gl NaClO4 25°C 0.10M C H K1=1.96 1990HYa (59547) 499
By calorimetry: DH(K1)=12.0 J K⁻¹ mol⁻¹

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	sp	alc/w	?	3%	U			K1=7.10	1967GDb (59597)	500
Medium: 3% EtOH, 0.2 M NaClO4										

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	alc/w	25°C	20%	M	I			1994KDa (59678)	501
K(Gd+HL)=6.39										
Medium: 20% v/v EtOH/H2O, 0.10 M NaNO3. Also data for 0.05 and 0.15 M NaNO3. At I=0 (20% v/v), K1=6.64, *K(GdHL)=-8.57, *K(Gd(OH)HL)=-8.98.										

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
Gd+++	gl	alc/w	25°C	100%	M			K1=8.2 B2=14.8 B3=17.6	1989TMa (59732)	502
Medium: MeOH										

Gd+++	gl	NaClO4	25°C	0.10M	M	H		K1=1.95	1988CLb (59733)	503
DH=8.42 kJ mol ⁻¹ , DS=66 J K ⁻¹ mol ⁻¹										

Gd+++	gl	alc/w	25°C	42%	U			K1=2.4	1983PMa (59734)	504
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Gd+++	gl	diox/w	30°C	76%	M			K1=5.79	1978PMa (59735)	505
Medium: 76% v/v dioxane/H2O, 0.10 M NaClO4.										

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	cal	alc/w	25°C	60%	U	H			1996YLa (59833)	506
K(GdL+Phen)=2.33										
Medium: 60% v/v MeOH/H2O. Phen: 1,10-phenanthroline.										
DH=-10.45 kJ mol ⁻¹ , DS=7.8 J K ⁻¹ mol ⁻¹ .										

Gd+++	gl	NaClO4	25°C	0.10M	C			K1=2.88 B2=5.01	1989HMa (59834)	507
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Gd+++	gl	NaClO4	?	2.0M	U	T		K1=2.42	1972DCb (59835)	508

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
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Gd+++ gl NaClO4 25°C 0.10M M H K1=2.07 1988CLb (59911) 509
DH=9.62 kJ mol-1, DS=72 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

Gd+++ gl NaClO4 25°C 0.10M M H K1=2.12 1988CLb (59952) 510
DH=10.3 kJ mol-1, DS=75 J K-1 mol-1

Gd+++ gl diox/w 30°C 76% M K1=6.03 1978PMa (59953) 511
Medium: 76% v/v dioxane/H2O, 0.10 M NaClO4.

C8H8O4 H3L CAS 480-66-0 (8525)
2,4,6-Trihydroxyacetophenone;

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

Gd+++ gl diox/w 25°C 50% M K1=3.69 1978AGc (60053) 512
Medium: 50% v/v dioxane/H2O, 0.10 M NaClO4.

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

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

Gd+++ gl diox/w 35°C 50% U K1=4.50 B2=8.23 1971MAa (60089) 513
Medium: 50% dioxan, 0.1 M NaClO4

C8H9NO2 HL CAS 5330-97-2 (6248)
Phenylacetohydroxamic acid; C6H5.CH2.CO.NH.OH

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

Gd+++ gl KNO3 30°C 0.10M C M K1=5.94 B2=11.56 1987RSc (60343) 514
K3=4.65
K(Gd(hedta)+L)=4.40
hedta is N-hydroxyethyldiaminoethane-N,N',N'-triethanoic acid.

Gd+++ gl KNO3 20°C 0.10M M T K1=5.98 B2=11.65 1986RSc (60344) 515
K3=4.71

Data for 20-50 C. At 30 C, K1=5.94, K2=5.62, K3=4.65.

C8H9NO4 H2L (4520)
Dehydroethanoic acid oxime;

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

Gd+++ gl diox/w 35°C 50% U 1971MAa (60495) 516
K(Gd+HL)=4.37
K(Gd+2HL)=7.86

Medium: 50% dioxan, 0.01 M NaClO4

C8H9N3O2 L CAS 7254-31-4 (1266)

Acylnicotinoyl hydrazide; C5H4N.CO.NH.NH.CO.CH3

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

Gd+++ gl NaClO4 25°C 0.10M U K1=13.80 B2=24.95 1980ZMa (60568) 517

C8H10N6O2S2 H2L (2746)

2,5-Dihydroxybenzoquinone bis-thiosemicarbazone;

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

Gd+++ gl diox/w 30°C 50% C TIH K1=5.23 B2=9.73 1989GDa (60814) 518
DH(K1)=-76.57 kJ mol⁻¹

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

Gd+++ gl alc/w 22°C 20% U K1=4.47 B2=7.97 1988ZTa (60848) 519
K3=3.08

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

Gd+++ gl KCl 30°C 0.10M C K1=5.91 B2=10.02 1996SZa (60868) 520
For the -5-en-2-exo isomer, K1=6.11, B2=10.82.

C8H11NO3 HL Vitamin B6 CAS 65-23-6 (254)

5-Hydroxy-6-methyl-3,4-pyridinedimethanol, Pyridoxine;

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

Gd+++ gl KCl 25°C 0.1M C 1999DNa (61119) 521
B(GdHL)=11.5

C8H11NO8 H4L CAS 7408-20-0 (2608)

Amino-di(butanedioic acid);HN(CH(COOH)CH2.COOH)2

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

Gd+++ gl KCl 25°C 0.10M U K1=11.20 B2=18.18 1979BEb (61208) 522

B(GdHL)=15.49

C8H1104P H2L (4536)
(alpha-Hydroxy-alpha-methylbenzyl)phosphonic acid;

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

Gd+++ gl NaCl 25°C 0.10M U 1973BSg (61309) 523
K(Gd+HL)=2.42

C8H12N2O3 H2L Barbitol CAS 57-44-3 (2744)
5,5-Diethylbarbituric acid, Veronal, Barbitone;

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

Gd+++ gl oth/un 25°C 0.10M U K1=2.161 1987TSb (61436) 524

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

Gd+++ gl KNO3 20°C 0.10M U K1=12.58 B2=17.16 1975DPa (61505) 525

Gd+++ vlt KNO3 25°C 0.10M U K1=10.78 1972GBd (61506) 526

C8H12O2 HL CAS 874-23-7 (3203)
2-Acetylcyclohexanone;

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

Gd+++ gl mixed 25°C 75% U K1=8.76 B2=17.61 1971DRa (61673) 527
K3=7.81

Medium: 75% acetone, 0.1 M NaClO4

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

Gd+++ gl NaClO4 25°C 0.10M M H K1=4.35 1986CDb (61709) 528
DH=16.2 kJ mol-1, DS=138 J K-1 mol-1

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

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

Gd+++ gl KNO3 20°C 0.10M U K1=9.53 B2=16.95 1974RMg (61763) 529

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	KNO3	20°C	0.10M	U			K1=11.25 B2=19.89	1974RMg (61787)	530

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	mixed	30°C	75%	U			K1=8.86	1971DRb (62078)	531

Medium: 75% acetone, 0.1 M

C8H16N2O3 HL Gly-Leu CAS 869-19-2 (255)
 Glycyl-leucine; H2N.CH2.CO.NH.CH(CH2.CH(CH3)2).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	KCl	25°C	0.10M	U			K1=2.30	1973FMa (62387)	532

C8H16N2O3 HL Leu-Gly CAS 686-50-0 (1248)
 Leucyl-glycine; H2N.CH(CH2.CH(CH3)2).CO.NH.CH2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	KCl	25°C	0.10M	U			K1=2.25	1973FMa (62432)	533

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	EMF	NaCl04	25°C	1.0M	U			K1=2.83 B2=5.03	1965TVa (62634)	534

Method: quinhydrone electrode

C8H19NO5 L Bis-tris CAS 6976-37-0 (2827)
 Bis-(2-hydroxyethyl)imino-tris(hydroxymethyl)methane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	NaCl	30°C	0.10M	C			K1=6.23 B2=10.93	2002Nwa (63060)	535

Constants expressed on the molality scale.

C8H22N2O6P2 H4L CAS 13516-59-1 (3850)
 2,2'-(Ethylenedi-imino)bis(propylphosphonic acid);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Gd+++ gl KCl 25°C 0.10M U K1=12.27 1965DKb (63339) 536
K(Gd+HL)=6.16

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

Gd+++ gl diox/w 35°C 75% U K1=7.00 B2=12.80 1971MAb (63564) 537
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

Gd+++ sp diox/w 20°C 50% U K1=2.62 B2=4.46 1977MBb (63608) 538

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

Gd+++ gl NaClO4 25°C 0.10M U K1=5.21 B2=9.85 1973MAa (63697) 539
K3=4.0

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

Gd+++ gl NaClO4 25°C 0.10M U I K1=5.55 B2=10.53 1987BCd (63802) 540
B3=14.96

Data also in 42% MeOH, 51.1% EtOH and 61.2% dioxan

Gd+++ gl NaClO4 35°C 0.20M M K1=6.08 1982LTa (63803) 541

Gd+++ gl oth/un 20°C 0.10M U K1=6.06 1977SKd (63804) 542

C9H6N3OC1S HL CAS 27004-41-7 (216)
2-(2'-Thiazolylazo)-4-chlorophenol; C3H2NS.N:N.C6H3(Cl).OH

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

Gd+++ gl KNO3 25°C 0.10M U K1=7.94 1974KSa (63924) 543

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
Gd+++	gl	NaClO4	25°C	0.10M	U	H	K1=5.05 K(Gd+HL)=2.94	1994CRa (63969)	544
DH(K1)=17.6 kJ mol ⁻¹ ; DS=156 J K ⁻¹ mol ⁻¹									

C9H7N		L					CAS 91-22-5	(1538)	
Quinoline;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Gd+++	gl	NaClO4	25°C	0.5M	M	H	K1=3.53	1991KBb (64061)	545
By calorimetry: DH(K1)=4.40 kJ mol ⁻¹ , DS(K1)=82.4 J K ⁻¹ mol ⁻¹ .									

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Gd+++	gl	KNO3	25°C	0.10M	U	TIH	K1=7.13 B2=13.23 B(GdAL)=15.58	1986NSa (64275)	546
H2A=phthalic acid. DH(GdAL)=-54.7 kJ mol ⁻¹ , DS=114.8 J K ⁻¹ mol ⁻¹									

Gd+++	sol	none	RT	0.0	U			1981FCa (64276)	547
Kso(GdL3)=-31.38									
Method: spectrophotometry.									

Gd+++	gl	oth/un	20°C	0.10M	U		K1=7.16	1977SKd (64277)	548

Gd+++	gl	diox/w	30°C	50%	U		K1=9.03 B2=17.21	1970GMB (64278)	549
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
Gd+++	gl	diox/w	30°C	50%	U		K1=7.10	1970GMB (64405)	550
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
Gd+++	gl	NaClO4	35°C	0.20M	M		K1=6.60	1982LTa (64546)	551

Gd+++	cal	KNO3	20°C	0.10M	U	HM		1971GKb (64547)	552
K(GdA+L)=4.36									
DH(GdA+L)=-25.49 kJ mol ⁻¹ , DS=-3.76 J K ⁻¹ mol ⁻¹									

DH(GdAL): DH=-32.73, DS=303.9. H4A=EDTA

Gd+++ gl oth/un 25°C 0.0 U H K1=6.64 B2=12.37 1958F0b (64548) 553
K3=4.9

DH(K1)=-14.6 kJ mol⁻¹, DS=79 J K⁻¹ mol⁻¹; DH(K2)=-18.0, DS=50; DH(K3)=-19.7,
DS=29

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

Gd+++ sp NaNO3 25°C 0.10M C K1=8.10 19850Hb (64707) 554
K(Gd+HL)=4.71
K(GdL+H)=6.05

C9H8N2O4S2 HL CAS 219931-32-5 (8394)
3-Phenylsulfonamidorhodanine;

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

Gd+++ sp alc/w 30°C 20% C T H K1=7.28 B2=14.23 1998EGa (64830) 555
Medium: 20% v/v EtOH/H2O, 0.10 M KCl. Also data for 35 and 45 C.
DH and DS values reported

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

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

Gd+++ sp NaClO4 ? 0.20M U K1=7.91 1967GDc (64940) 556
B(GdHL)=10.56

Gd+++ gl NaClO4 25°C 0.20M U K1=8.02 B2=14.40 1966GDa (64941) 557
K3=3.82

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

Gd+++ gl KCl 30°C 0.10M U K1=4.34 1996SZa (64975) 558

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

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

Gd+++ gl diox/w 27°C 0.10M U K1=4.42 1982LMa (65160) 559

C9H1003 HL Atrolactic acid CAS 940-31-8 (3859)
2-Hydroxy-2-phenylpropanoic acid; CH3.C(OH)(C6H5).COOH

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

Gd+++ gl NaClO4 25°C 1.0M U K1=2.54 B2=4.61 1966TVa (65438) 560
K3=1.70
K4=1.33

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

Gd+++ gl NaClO4 25°C 0.10M C K1=2.14 B2=3.59 1989HMa (65460) 561

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

Gd+++ gl NaClO4 25°C 0.10M C K1=2.17 B2=4.12 1989HMa (65474) 562

C9H1004 HL CAS 1521-38-6 (8489)
2,3-Dimethoxybenzoic acid;

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

Gd+++ gl diox/w 25°C 76% M K1=5.23 1978PMa (65530) 563
Medium: 76% v/v dioxane/H2O, 0.10 M NaClO4.

C9H1004 HL CAS 91-52-1 (8490)
2,4-Dimethoxybenzoic acid;

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

Gd+++ gl diox/w 25°C 76% M K1=5.83 1978PMa (65537) 564
Medium: 76% v/v dioxane/H2O, 0.10 M NaClO4.

C9H1004 HL CAS 1466-76-8 (8491)
2,6-Dimethoxybenzoic acid;

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

Gd+++ gl diox/w 25°C 76% M K1=5.67 1978PMa (65544) 565
Medium: 76% v/v dioxane/H2O, 0.10 M NaClO4.

C9H1004 H2L (7232)
Bicyclo[2.2.1]hept-5-en-2-endo,3-cis-dicarboxylic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Gd+++	gl	KCl	30°C	0.10M	C		K1=4.17 B2=7.08	1996SZa (65571)	566

For the 2,5-dien-2-exoisomer, K1=4.34.

C9H1004		H2L					CAS 3853-88-1	(5687)	
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endo-cis-Bicyclo-[2,2,1]-5-hepten-2,3-dicarboxylic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Gd+++	gl	NaClO4	24°C	0.10M	U		K1=4.36 K(Gd+HL)=1.40	1986ZBa (65586)	567

C9H1005		H2L					CAS 54384-22-4	(8406)	
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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
Gd+++	gl	KCl	30°C	0.10M	U		K1=5.00 B2= 8.04	1996SZa (65603)	568

C9H1005		H2L					(7233)		
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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
Gd+++	gl	KCl	30°C	0.10M	C		K1=5.00 B2=8.04	1996SZa (65618)	569

C9H1008		H4L					CAS 3724-52-5	(1264)	
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cis-1,2,3,4-Cyclopentanetetracarboxylic acid; C5H6.(COOH)4

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Gd+++	gl	NaClO4	30°C	0.20M	U T		K1=10.20 K1=10.29 when T=40. K1=10.40 when T=50.	1979NSb (65644)	570

C9H11N02		HL					Phenylalanine CAS 63-91-2	(2)	
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2-Amino-3-phenylpropanoic acid; H2N.CH(CH2.C6H5)COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Gd+++	gl	NaCl	25°C	0.15M	U H		K1=3.47	1992ZNa (65940)	571

By calorimetry: DH(K1)=0.52 kJ mol⁻¹, DS(K1)=68.19 J K⁻¹ mol⁻¹.

Gd+++	gl	KNO3	35°C	0.10M	U		K1=4.98	1990RSe (65941)	572
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Gd+++	gl	KCl	25°C	0.10M	U		K1=4.25	1972BFe (65942)	573
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C9H11N03		H2L					Tyrosine CAS 60-18-4	(4)	
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2-Amino-3-(4-hydroxyphenyl)propanoic acid; HO.C6H4.CH2.CH(NH2).COOH

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

Gd+++ gl KNO3 25°C 0.10M U I 1976SAc (66222) 574
K(Gd+HL)=4.92
K(GdHL+HL)=4.43

Gd+++ gl KNO3 25°C 0.10M U T H 1976SAe (66223) 575
K(Gd+H2L)=4.63
K(GdH2L+H2L)=4.17

Gd+++ gl KCl 25°C 0.10M U 1972BFe (66224) 576
K(Gd+HL)=4.35
K(GdHL+HL)=4.2

C9H12N2O6 HL Uridine CAS 58-96-8 (828)
Uracil-1-beta-D-ribofuranoside;

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

Gd+++ gl KNO3 35°C 0.10M U M K1=4.68 1990RSc (66694) 577
K(GdA+L)=4.56
K(GdB+L)=4.43
K(GdC+L)=3.98

H2A=Iminodiethanoic acid, H3B=NTA, H4C=EDTA

Gd+++ gl KNO3 35°C 0.10M U M K1=4.26 1990RSe (66695) 578
K(GdL+Ala)=9.14
K(GdL+Phe)=8.90
K(GdL+Trp)=9.15

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

Gd+++ ISE KNO3 25°C 0.10M U K1=12.22 1983KBd (66735) 579
Hg-electrode.

C9H13NO2 L (7151)
1,2-Diethyl-3-hydroxy-4-pyridinone

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

Gd+++ gl KCl 25°C 0.10M C K1=8.09 B2=14.78 1994MRa (66796) 580
K3=4.98

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

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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++     gl  KNO3   25°C 0.10M U           K1=10.66 B2=18.62 1968TKe (66885) 581
*****
C9H13N2O9P          H3L   UMP-5           CAS 58-97-9 (2948)
Uridine-5'-monophosphoric acid;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++     gl  KNO3   35°C 0.10M U   M           1992RAd (66973) 582
                                     K(Gd+HL)=3.89
                                     K(GdHL+Gly)=4.00
                                     K(Gd+HL+His)=8.92
                                     K(Gd+HL+histamine)=8.12
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C9H13N3O5          L   Cytidine           CAS 65-46-3 (2152)
Cytidine, Cytosine-1-beta-D-ribofuranoside;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++     gl  KNO3   35°C 0.10M U   M   K1=3.13           1990RSc (67055) 583
                                     K(Gd+HA+L)=7.93
                                     B(GdLB)=15.08
                                     B(GdLC)=19.99

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H2A=Iminodiethanoic acid, H3B=NTA, H4C=EDTA

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Gd+++     gl  KNO3   35°C 0.10M U   M   K1=2.50           1990RSe (67056) 584
                                     K(GdL+Ala)=4.99
                                     K(GdL+Phe)=5.05
                                     K(GdL+Trp)=5.35
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Gd+++     gl  KNO3   35°C 0.10M U   M   K1=3.13           1986RMb (67057) 585
K(Gd+L+HGly)=8.41, K(Gd+L+HHis)=8.54, K(Gd+L+oxalate)=9.89
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C9H15NO6          H3L           (7177)
2-Aminopentanoic-N,N-diethanoic acid; C3H7C(COOH)N(CH2COOH)2
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++     gl  KNO3   20°C 0.10M U           K1=10.99 B2=19.46 1974RMg (67407) 586
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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
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++     cal NaClO4 25°C 0.50M M   IH   K1=12.63           1986RCa (67638) 587
DH=-11.3 kJ mol-1, DS=204 J K-1 mol-1
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C9H16N4O4 L CAS 157358-29-7 (7398)
N,N'-Bis(2-hydroxyiminopropionyl)propane-1,3-diamine;

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

Gd+++ gl NaCl 25°C 0.15M C 2004NJb (67724) 588
B(GdH-1L)=-0.84
B(GdH-2L)=-7.83
B(GdH-4L)=-22.88

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

Gd+++ gl KNO3 25°C 0.10M U K1=4.58 B2=7.30 1968PFa (67772) 589

C10H5O2F7S L (6996)
1-(2-Thienyl)-3-heptafluoropropylpropane-1,3-dione; C3F7.C(O)CH2C(O)C4H3S

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

Gd+++ gl alc/w 22°C 80% U K1=6.10 B2=11.80 1995MTa (68426) 590
K3=4.83

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

Gd+++ gl NaClO4 25°C 0.10M U H K1=4.78 1994CRa (68515) 591
K(Gd+HL)=3.80

DH(K1)=22.7 kJ mol⁻¹, DS=168 J K⁻¹ mol⁻¹; DH(Gd+HL)=9.0, DS=103

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

Gd+++ sp KCl 25°C 0.10M M I K1=4.44 1976PEa (68577) 592

Gd+++ sp oth/un ? ? U K1=2.96 1969MSb (68578) 593

C10H7NO2 HL CAS 132-53-6 (2524)
2-Nitroso-1-naphthol;

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

Gd+++ gl KNO3 25°C 0.10M U K1=5.75 B2=11.03 1982LPc (68646) 594

C10H7N02 HL Quinaldic acid CAS 93-10-7 (2209)
Quinoline-2-carboxylic acid;

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

Gd+++ gl NaClO4 30°C 0.10M U K1=2.58 B2=5.06 1969DNc (68710) 595

C10H7N02 HL CAS 86-59-9 (873)
Quinoline-8-carboxylic acid;

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

Gd+++ gl NaClO4 30°C 0.10M U K1=2.61 1969DNc (68761) 596

C10H7N05S H2L CAS 14090-74-5 (2676)
1-Nitroso-2-hydroxynaphalene-7-sulfonic acid;

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

Gd+++ gl KCl 25°C 0.10M M K1=4.43 B2=7.98 1979LSb (68812) 597

C10H7N05S H2L (4766)
1-Nitroso-2-hydroxynaphthalene-6-sulfonic acid;

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

Gd+++ sp KCl 25°C 0.10M C K1=4.57 1973PMb (68844) 598

Gd+++ sp oth/un ? ? U K1=2.25 1969MSa (68845) 599

C10H7N05S H2L CAS 3682-32-4 (1812)
2-Nitroso-1-hydroxynaphthalene-4-sulfonic acid;

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

Gd+++ gl KCl 25°C 0.10M U I K1=3.41 1967MAi (68884) 600
K1=4.50(I=0)

C10H7N05S H2L CAS 31005-79-9 (1814)
2-Nitroso-1-hydroxynaphthalene-8-sulfonic acid;

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

Gd+++ sp KCl 25°C 0.10M M K1=5.50 1978PPb (68945) 601

C10H7N08S2 H3L Nitroso-R acid CAS 525-05-3 (1811)
1-Nitroso-2-hydroxynaphthalene-3,6-disulfonic acid;

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

Gd+++ gl oth/un 25°C 0.10M U K1=4.62 B2=7.98 1990ATa (69011) 602

Gd+++ sp oth/un ? ? U K1=1.40 1969MSb (69012) 603

Gd+++ gl KCl 25°C 0.10M U K1=4.92 1968MAe (69013) 604

C10H7N08S2 H3L CAS 52664-45-6 (1627)
2-Nitroso-1-hydroxynaphthalene-4,6-disulfonic acid;

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

Gd+++ gl NaCl 25°C 0.10M U K1=3.702 B2=6.259 1974SAa (69051) 605

C10H7N08S2 H3L CAS 50332-99-3 (1628)
2-Nitroso-1-hydroxynaphthalene-4,7-disulfonic acid;

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

Gd+++ gl NaCl 25°C 0.10M U K1=3.831 B2=6.228 1974SAa (69061) 606

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

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

Gd+++ gl diox/w 25°C 75% U K1=5.03 B2=9.75 1986MIa (69096) 607

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

Gd+++ gl alc/w 22°C 80% U K1=6.45 B2=12.23 1995MTa (69149) 608
K3=5.18
Medium: 0.1 M NaClO4 in 80% (v/v) EtOH/H2O.

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

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

Gd+++ sp non-aq 25°C 100% C T K1=3.14 2005SYa (69577) 609
In ethylacetate; At 50 C K1=2.84

Gd+++ gl KNO3 25°C 0.10M U TIH K1=3.85 B2=6.80 1986NSa (69578) 610
B(GdAL)=11.33
H2A=phthalic acid. DH(GdAL)=-46.6 kJ mol-1, DS=16.5 J K-1 mol-1

Gd+++ gl NaNO3 25°C 0.50M U K1=0.8 1979HJa (69579) 611

Gd+++ cal non-aq 25°C 100% U M 1972KKc (69580) 612

K(GdA3+L)=3.71
K(GdA3+2L)=7.50

Medium : CHCl3. A=4,4,4-trifluoro-1-(2-thienyl)-1,3-butanedione

C10H8N4O3 HL CAS 43168-60-1 (6209)

5-Phenylazobarbituric acid;

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

Gd+++ gl diox/w 25°C 75% U K1=5.51 B2=10.51 1986MIa (69730) 613

C10H8O2 H2L CAS 92-44-4 (1658)

2,3-Dihydroxynaphthalene;

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

Gd+++ gl NaClO4 20°C 0.10M U M 1973PAc (69770) 614

K(GdA+L)=7.60, H4A=EDTA

C10H8O5S H3L DHNSA (877)

2,3-Dihydroxynaphthalene-6-sulfonic acid;

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

Gd+++ gl NaClO4 35°C 0.20M M K1=10.13 1982LTa (69847) 615

Gd+++ gl NaClO4 25°C 0.50M C K1=9.92 B2=17.49 1976LAd (69848) 616

B(GdHL)=14.2
B(GdHL2)=24.79

C10H8O8S2 H4L Chromotropic ac CAS 148-25-4 (1875)

1,8-Dihydroxynaphthalene-3,6-disulfonic acid;

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

Gd+++ gl KCl 25°C 0.10M M I 1974MLa (69952) 617

K(Gd+HL)=2.41

C10H9NO4S H2L CAS 29021-67-8 (3926)

2-Methyl-8-hydroxyquinoline-5-sulfonic acid;

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

Gd+++ gl NaClO4 30°C 0.10M U TI K1=5.39 B2=10.34 1988BCd (70197) 618

B3=14.25

in 42.5% MeOH-water: K1=6.36, B2=12.17, B3=16.68

51.8% EtOH-water: K1=6.77, B2=12.76, B3=17.34

C10H9N3OS HL CAS 60321-26-8 (4671)
2-(2-Thiazolylazo)methylphenol; C3H2NS.N:N.C6H3(CH3)OH

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

Gd+++ sp diox/w 25°C 10% U K1=9.61 B2=18.26 1973KSd (70360) 619
Medium: 10% dioxan, 0.1 M KNO3

C10H9N3O2S HL CAS 3012-52-0 (217)
2-(2'-Thiazolylazo)-4-methoxyphenol; CH3O.C6H3(OH).N:N.C3H2N2

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

Gd+++ sp KNO3 25°C 0.10M U K1=8.96 1974KSA (70399) 620

C10H10N4O2S HL Sulfadiazine CAS 68-35-9 (1885)
4-Amino-N-(2-pyrimidinyl)benzenesulfonamide; C4H3N2NHSO2C6H4NH2

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

Gd+++ gl alc/w 25°C 50% C M K1=4.53 1993EEa (70609) 621
K(Gd(NTA)+L)=8.76
Medium: 50% v/v EtOH/H2O, 0.10 M NaClO4.

Gd+++ gl NaNO3 25°C 0.10M U M 1988SSg (70610) 622
K(Gd(EDTA)+L)=2.70

C10H10O5 HL CAS 13522-48-0 (4722)
3-Mercapto-1-phenylbut-2-en-1-one; C6H5.CO.CH:CH.C(SH).CH3

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

Gd+++ gl mixed 30°C 75% U K1=3.92 B2=7.30 1969DNb (70635) 623
K3=3.02
Medium: 75% acetone, 0.1 M NaClO4

C10H10O2 HL Benzoylacetone CAS 93-91-4 (197)
1-Phenylbutane-1,3-dione; C6H5.CO.CH2.CO.CH3

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

Gd+++ gl alc/w 25°C 80% U K1=8.09 B2=14.30 1967DZa (70731) 624
K3=4.18
Medium: 80% MeOH, 0.1 M NaCl

Gd+++ gl alc/w 24°C 80% U K1=8.09 B2=14.30 1967DZb (70732) 625
K3 = 4.18
Medium: 80% v/v MeOH/H2O, 0.1 M NaCl

C10H10O6 H2L CAS 5411-14-3 (2394)

1,2-Phenylenedioxodiethanoic acid; C6H4(O.CH2.COOH)2

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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++      gl  NaClO4 25°C 0.10M M          K1=4.48  B2=7.07  1977HCb (70851) 626
*****
C10H11NOS          L                      (2831)
Acetothioacetanilide; CH3.CO.CH2.CS.NH.C6H5
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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++      gl  diox/w 25°C 50% U          K1=4.92  B2=9.12  1986NBa (70882) 627
*****
C10H11NO2          L                      CAS 102-01-2 (250)
Acetoacetanilide; CH3.CO.CH2.CO.NH.C6H5
-----
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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++      gl  diox/w 25°C 50% U          K1=5.57          1986NBa (70911) 628
*****
C10H11NO3          HL                     (1960)
N-Hydroxyacetoacetanilide; CH3.CO.CH2.CO.N(OH).C6H5
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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++      gl  diox/w 20°C 82% U          K1=6.79  B2=12.93  1979KSb (70939) 629
                        K3=5.92
*****
C10H11N5O          L                      CAS 105507-56-0 (8131)
N-Methylisatin-beta-amidinohydrazone;
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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++      gl  diox/w 30°C 50% C TIH    K1=5.05  B2= 9.20  1986SGc (71090) 630
Medium: 50% v/v dioxan/H2O, 0.10 M NaClO4. Data for 0.02-0.20 M NaClO4
and 30-50 C. DH(K1)=58.3 kJ mol-1, DS=289 J K-1 mol-1; DH(K2)=28.7, DS=174
*****
C10H11O2F7          HL                     CAS 17587-22-3 (1252)
1,1,1,2,2,3,3-Heptafluoro-7,7-dimethyl-4,6-octanedione;
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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++      dis R4N.X 25°C 0.10M U          B2=12.7      1970SBa (71109) 631
                        B3=18.7
                        B(GdL3(OH))=25.3
Medium: Et4NClO4
*****
C10H12N2O4          H2L                    CAS 16598-05-3 (967)
2-Pyridylmethyliminodiethanoic acid; C5H4N.CH2.N(CH2.COOH)2
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```

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	KNO3	25°C	0.10M	U			K1=8.76 B2=16.77	1964THa (71260)	632

C10H12N4O5		HL		Inosine				CAS 58-63-9	(2344)	
Hypoxanthine-9-beta-D-ribofuranoside;										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	KNO3	35°C	0.10M	U	M		K1=4.41 B(Gd(gly)L)=10.52 B(Gd(his)L)=10.96	1987RRc (71388)	633

C10H12N4O6		H2L		Xanthosine				CAS 5968-90-1	(1176)	
3,9-Dihydro-9-ribofuranosyl-1H-purine-2,6-dione;										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	KNO3	35°C	0.10M	U	M		K(Gd+HA+HL)=5.36 K(Gd+HB+HL)=4.72 K(Gd+HL)=3.62	1987RRc (71488)	634

HA=glycine, HB=histidine.

C10H12O2		HL						CAS 1946-74-3	(202)	
3-Isopropyltropolone;										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	diox/w	30°C	50%	U	M		K1=7.74 B2=14.49 K3=5.05 K(Gd(NTA)+L)=6.31	1980SGa (71583)	635

Gd+++	gl	alc/w	24°C	80%	U			K1=8.8 B2=16.13 K3=6.1 K4=4.6	1968DZb (71584)	636
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Medium: 80% MeOH, 0.1 M NaCl

Gd+++	sp	alc/w	?	3%	U			K1=7.15	1967GDb (71585)	637
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Medium: 3% EtOH, 0.2 M NaClO4

C10H12O4		HL						CAS 5936-18-9	(2743)	
2-Hydroxy-3,4-dimethoxyacetophenone; (HO)(CH3O)2C6H2.CO.CH3										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	diox/w	15°C	50%	C T H			K1=8.14 B2=15.52 K1(35, 40, 50 C) = 7.69, 7.68, 7.53 respectively. DH(K1)=-41.34 kJ mol ⁻¹	1987GBa (71652)	638

C10H12O5		HL						CAS 490-64-2	(8492)	

2,4,5-Trimethoxybenzoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	diox/w	25°C	76%	M			K1=5.81	1978PMa (71672)	639
Medium: 76% v/v dioxane/H2O, 0.10 M NaClO4.										

C10H12O5		HL						CAS 570-02-5	(8493)	
2,4,6-Trimethoxybenzoic acid;										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	diox/w	25°C	76%	M			K1=5.39	1978PMa (71679)	640
Medium: 76% v/v dioxane/H2O, 0.10 M NaClO4.										

C10H16N2O8		H4L			EDDS			CAS 52759-67-8	(1100)	
1,2-Diaminoethane-N,N'-di-1,4-butanedioic acid; (CH2.NH.CH(COOH)CH2.COOH)2										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	KCl	25°C	0.10M	U			K1=12.50 K(Gd+HL)=5.96	1980MMe (73136)	641
Gd+++	gl	KNO3	20°C	0.10M	U			K1=13.67	1975DPa (73137)	642
Gd+++	gl	NaClO4	30°C	0.10M	U			K(Gd+H2L=GdL+2H)=8.00	1974STb (73138)	643

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	vlt	KNO3	25°C	0.10M	U			K1=13.45	1971BGb (73139)	644

C10H16N2O8		H4L			EDTA			CAS 60-00-4	(120)	
1,2-Diaminoethane-N,N,N',N'-tetraethanoic acid, Sequestric acid;										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	sp	R4N.X	25°C	0.10M	C			K1=17.7	1994KCa (73805)	645
Medium: Me4NCl										
Gd+++	cal	NaClO4	25°C	0.10M	C	H			1987YJa (73806)	646
DH(K1)=-6.44 kJ mol ⁻¹ , DS(K1)=300 J K ⁻¹ mol ⁻¹ .										
Gd+++	gl	KCl	25°C	1.0M	U			K(GdL+H)=1.30	1984BKc (73807)	647
Gd+++	gl	NaClO4	20°C	0.02M	U	M		K(GdL+PO4)=3.33	1982MPd (73808)	648
Gd+++	vlt	KNO3	20°C	0.10M	U			K1=17.53	1978NLb (73809)	649
Gd+++	gl	NaClO4	25°C	0.50M	U			K1=16.28	1977GGb (73810)	650

Gd+++	gl	KCl	25°C	1.00M	U	K ₂ =3.43 K(GdL+HL)=2.38 K(2GdL+L)=6.54	1976BKa (73811)	651
Gd+++	gl	KCl	25°C	1.0M	U	K(GdL+H)=1.82	1976GMb (73812)	652
Gd+++	sp	KCl	25°C	0.10M	U	K ₂ =3.43 K(2GdL+L)=6.53 K(GdL+HL)=2.38	1975BKa (73813)	653
Gd+++	EMF	KCl	25°C	0.10M	U	T K(GdL+H)=1.53	1974BKb (73814)	654
Gd+++	gl	KCl	25°C	1.0M	C	K ₂ =3.43 K(GdL+HL)=2.38 K(2GdL+L=Gd ₂ L ₃)=6.53	1974BKe (73815)	655
Gd+++	gl	KNO ₃	25°C	0.10M	U T M	K(GdL+HA)=3.58 K(GdL+A)=5.31 (GdL+HA):K(2 C)=3.80, K(35 C)=3.61, K(45 C)=3.50, (GdL+A):K(2 C)=5.44 K(35 C)=5.29, K(45 C)=5.21, H ₅ A=tripolyphosphoric acid	1973TRb (73816)	656
Gd+++	gl	KNO ₃	25°C	0.10M	U T M	K(GdL+A)=4.3 K(2 C)=4.7, K(35 C)=4.6, K(45 C)=4.2, H ₄ A=adenosine triphosphate	1973TRb (73817)	657
Gd+++	cal	KNO ₃	20°C	0.10M	U	K(GdL(H ₂ O) _x =GdL(H ₂ O) _{x-1} +H ₂ O)=0.15	1971GKb (73818)	658
Gd+++	gl	NaClO ₄	25°C	0.10M	U M	K(GdL+A)=7.12, H ₄ A=tiron	1969AIb (73819)	659
Gd+++	dis oth/un		25°C	?	U	K ₁ =17.10 Method: paper electrophoresis. Medium: pH=1.86	1969PJa (73820)	660
Gd+++	ix	KCl	25°C	0.10M	U H	K ₁ =16.82 DH(K ₁)=1.8 kJ mol ⁻¹ , DS=328 J K ⁻¹ mol ⁻¹	1959BDb (73821)	661
Gd+++	cal	KNO ₃	20°C	0.10M	U H	DH(K ₁)=-4.6 kJ mol ⁻¹ , DS=316 J K ⁻¹ mol ⁻¹	1958SRa (73822)	662
Gd+++	gl	oth/un	20°C	0.01M	U	K ₁ =17.12 Polarography also used	1955WSa (73823)	663
Gd+++	gl	KCl	20°C	0.10M	U I T	K ₁ =17.10 By polarography, 0.1 M KNO ₃ , K ₁ =17.37	1954SGa (73824)	664

Gd+++ gl KCl 20°C 0.10M U I T K1=16.70 1953WSa (73825) 665
By polarography K1=17.0. In 0.1 M KNO3 K1=16.60

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

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

Gd+++ gl NaCl 25°C 0.15M C K1=6.34 B2= 9.98 1999BCb (74732) 666
K(Gd+HL)=4.28
K(Gd+H2L)=3.57

Gd+++ gl NaClO4 20°C 0.20M U T H K1=7.19 B2=11.04 1993VL a (74733) 667
K(Gd(nta)+L)=4.15
K(Gd(edta)+L)=4.00

Data for 30, 40 C. DH(K1)=17.2 kJ mol⁻¹, DS(K1)=197 J K⁻¹ mol⁻¹. DH(K2)=
24.9, DS(K2)=155; DH(Gd(nta)+L)=17.2, DS=138; DH(Gd(edta)+L)=16.3, DS=132.

Gd+++ sp NaClO4 25°C 0.10M C K1=5.86 19910Ka (74734) 668
Method: competitive spectrophotometry using 5-Br-PAPS at pH 7.13 (HEPES).

Gd+++ gl KCl 25°C 0.10M U K1=6.52 B2=10.39 1988SSd (74735) 669
K(Gd+HL)=4.17

Gd+++ kin oth/un 25°C 0.05M C K1=7.06 1983Mcc (74736) 670
Method: inhibition of the hexokinase reaction, pH 8.0 (0.05 M TAPS).

Gd+++ gl KNO3 35°C 0.10M U M K(Gd(EDTA)+L)=4.6 1972TRc (74737) 671

C10H16O2 HL CAS 100563-25-5 (4706)
2-Butanoylcyclohexanone; CH3.CH2.CH2.CO.C6H9O

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

Gd+++ gl oth/un 30°C 0.10M U K1=9.42 B2=18.20 1972DSe (74921) 672
K3=8.45

C10H17N2O10P H5L CAS 69219-70-1 (7961)
Bis{[bis(carboxymethyl)amino]methyl}phosphinic acid;

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

Gd+++ gl NaCl 25°C 0.16M C K1=15.73 2001XRa (75022) 673
K(Gd+HL)=9.22
K(GdL+H)=2.76
B(GdHL)=18.48

C10H17N3O6S H3L Glutathione CAS 70-18-8 (333)
Glutamyl-cysteinyl-glycine;

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

Gd+++ gl NaClO4 25°C 0.10M U TIH K1=7.009 2003GSb (75120) 674
Values for 0.05-0.2 M NaClO4, 15-45 C and 10-30% MeOH/H2O, 20% EtOH/H2O,
20% DMF/H2O. At I=0, K1=8.130. DH(K1)=-36.4 kJ mol⁻¹, DS(K1)=-34.

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

Gd+++ gl NaClO4 25°C 0.50M U K1=14.80 1977GGb (75399) 675

Gd+++ EMF KCl 25°C 1.0M U K2=3.91 1977GMa (75400) 676
K(GdL+HL)=2.25
K(GdL+H4L)=1.99

Method: Pt/H2 electrode.

Gd+++ EMF KCl 25°C 1.0M U M 1977GMa (75401) 677

K(Gd(edta)+L)=3.40
K(Gd(edta)+HL)=2.06
K(Gd(edta)+H2L)=1.28

Method: Pt/H2 electrode.

Gd+++ gl NaClO4 20°C 0.10M U 1974PJa (75402) 678

K(GdL+A)=3.58
K(GdL+B)=3.70

HA=pentane-2,4-dione, B=1-phenylbutane-1,3-dione

Gd+++ gl NaClO4 25°C 1.0M U K2=3.21 1973NMa (75403) 679

K(GdL+HL)=2.37
K(GdL+H3L)=1.56

Gd+++ gl oth/un 20°C ? U 1971MNa (75404) 680

K(GdL+H3L)=0.85
K(GdL+H2L)=0.77
K(GdL+HL)=2.0
K(GdL+L)=3.32

Gd+++ gl KNO3 25°C 0.10M U M 1963TLb (75405) 681

K(GdL+A)=4.96
K(CdL+B)=4.57

H2A=iminodiethanoic acid, H2B=hydroxyethyleiminodiethanoic acid

Gd+++ EMF oth/un 20°C 0.10M U K1=15.44 1962PMa (75406) 682

Gd+++ gl KNO3 15°C 0.10M U T H K1=15.42 1961MFb (75407) 683

K1=15.31(20 C), 15.22(25 C), 15.16(30 C), 15.20(35 C), 15.11(40 C)
DH(K1)=-19.5 kJ mol⁻¹(25 C), DS=226 J K⁻¹ mol⁻¹

Gd+++ gl KNO3 25°C 0.10M U K1=15.10 1956SPa (75408) 684
By polarography K1=15.4

C10H19N3O4 H2L (8095)
1,4,7-Triazacyclononane-1,4-diethanoic acid;

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

Gd+++ gl KCl 25°C 1.0M U K1=11.08 2000LKc (75656) 685

C10H19N3O4 HL Leu-Gly-Gly CAS 1187-50-4 (1230)
Leucyl-glycyl-glycine; H2N.CH(CH2.CH(CH3)2).CO.NH.CH2.CO.NH.CH2.COOH

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

Gd+++ gl KNO3 25°C 0.10M U T H K1=3.36 1981SKg (75689) 686
Data for 35 and 45 C. DH(K1)=4.77 kJ mol⁻¹, DS(K1)=80.1 J K⁻¹ mol⁻¹.

Gd+++ gl KCl 25°C 0.10M U K1=1.95 1973FMa (75690) 687

C10H20N2O4 H2L (4753)
N,N'-Diethylethylenedinitrilo-N,N'-diethanoic acid;

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

Gd+++ gl KNO3 25°C 0.10M U K1=6.9 1973PSb (75782) 688

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

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

Gd+++ cal non-aq 25°C 100% U H K1=2.03 1993LLa (76003) 689
Medium: MeCN. DH(K1)=-33.7 kJ mol⁻¹.

Gd+++ dis non-aq 25°C 100% U B2=8.09 1990NIa (76004) 690

B2=extraction eq.constant: M+3P+2(S)=ML2P3(S); solvent(S)=CH2Cl2, P=picrate

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

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

Gd+++ ISE non-aq 25°C 100% C K1=4.49 1986BDa (76448) 691
Medium: propylene carbonate, 0.1 M Et4NC104

C10H26N4O6P2 H4L CAS 200951-96-8 (7643)
1,4,7,10-Tetraazacyclododecane-1,7-bis(methanephosphonic acid);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	KCl	25°C	0.10M	C			K1=18.2 *K(GdL)=-8.1 K(GdL+H)=7.0 B(GdHL2)=37.9	1998BRa (76804)	692

C11H8O3 L CAS 1133-72-8 (2614)
2-Aceto-1,3-indandione;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	diox/w	30°C	75%	U	T		K1=4.11 B2=8.06	1984APa (77032)	693
Gd+++	gl	mixed	22°C	60%	U			K1=3.84 B2=7.30 K3=3.08	1979JMa (77033)	694

Medium: 60% acetone/H2O

C11H8O3 H2L CAS 92-70-6 (1130)
2-Hydroxy-3-naphthoic acid (3-Hydroxy-2-naphthoic acid);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	diox/w	20°C	50%	U	T		K1=8.04 B2=16.34 B3=24.56 K3=8.22	1977SKf (77123)	695

C11H8O4 HL CAS 7555-37-5 (4812)
3-Acetyl-4-hydroxycoumarin

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	diox/w	35°C	50%	U			K1=3.73 B2=6.55	1971MAa (77177)	696

Medium: 50% dioxan, 0.01 M NaClO4

C11H8O4 HL CAS 6724-42-1 (6183)
8-Formyl-7-hydroxy-4-methyl-2H-1-benzopyran-2-one; CHO.C9H30(:O)(CH3)(OH)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	diox/w	30°C	50%	U	TI M		K1=5.17 B2=9.05 K3=2.71	1985ECa (77201)	697

20 C: K1=5.49, K2=4.15, K3=3.10; 40C: K1=4.87, K2=3.63, K3=2.35

C11H8O6S H3L CAS 66695-90-7 (1996)
1-Hydroxy-4-sulfo-2-naphthoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	NaClO4	25°C	0.10M	C			K1=8.46 B2=14.77	1979LAb (77227)	698

K(Gd+HL)=2.51

C11H8O6S H3L CAS 15509-36-1 (2658)

3-Hydroxy-7-sulfo-2-naphthoic acid;

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

Gd+++ gl NaClO4 25°C 0.10M C K1=7.73 1976MLb (77252) 699
K(Gd+HL)=2.62

C11H8O9S2 H4L CAS 67097-84-1 (1995)

1-Hydroxy-4,7-disulfo-2-naphthoic acid;

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

Gd+++ cal NaClO4 25°C 0.10M C H K1=8.67 B2=14.5 1986LLc (77280) 700
K(Gd+HL)=2.06

DH(Gd+HL)=7.0 kJ mol⁻¹, DS=63 J K⁻¹ mol⁻¹

C11H9NO2 H2L CAS 7470-09-9 (8481)

2-Hydroxy-1-naphthaldoxime;

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

Gd+++ gl diox/w 25°C 75% U K1=8.57 1978Mcd (77316) 701
Medium: 75% v/v dioxane/H2O, 0.10 M NaClO4.

C11H9NO4 H2L CAS 4321-82-7 (4829)

3-Acetyl-4-hydroxycoumarin oxime;

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

Gd+++ gl diox/w 35°C 50% U 1971MAa (77420) 702
K(Gd+HL)=3.52
K(Gd+2HL)=6.19

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

Gd+++ sp NaNO3 25°C 0.10M C K1=10.25 19840Ha (77546) 703
K(Gd+HL)=4.28
*K(GdHL)=-6.33

Medium pH 4.8-6.3.

Gd+++ sp KCl 20°C 0.10M U 1971EKa (77547) 704

K(Gd+HL)=3.52

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

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

Gd+++ gl diox/w 25°C 75% U K1=5.20 B2=9.88 1986MIa (77729) 705

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

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

Gd+++ gl diox/w 25°C 75% U K1=5.38 B2=10.37 1986MIa (77743) 706

C11H11N3O2S HL Sulfapyridine CAS 144-83-2 (8356)
4-Amino-N-2-pyridinyl-benzenesulfonamide;

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

Gd+++ gl alc/w 25°C 50% C M K1=10.88 B2=21.59 1993EEa (77930) 707
K(Gd(nta)+L)=5.64

Medium: 50% v/v EtOH/H2O, 0.10 M NaClO4.

C11H12N2O2 HL CAS 103314-23-4 (6182)
2-(N-2-Pyrrolidimino)benzoic acid; C4H7N:N.C6H4.COOH

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

Gd+++ gl NaClO4 25°C 0.10M U TIH B2=13.20 1986GSb (78017) 708
35 C: B2=13.80; 45 C:B2=13.90. DH(B2)=-63.5 kJ mol⁻¹, DS=58 J K⁻¹ mol⁻¹

C11H12N2O2 HL Tryptophan CAS 73-22-3 (3)
2-Amino-3-(3-indolyl)propanoic acid; H2N.CH(CH2.C8H6N)COOH

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

Gd+++ gl KNO3 35°C 0.10M U K1=5.25 1990RSe (78206) 709

Gd+++ gl KCl 25°C 0.10M U T H K1=4.8 1976BFc (78207) 710
For 55C K1= 4.18

Gd+++ gl KCl 25°C 0.10M U K1=5.0 B2=9.60 1972BFe (78208) 711

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

Gd+++ gl oth/un 30°C 0.10M U B2=22.08 1985EEb (78320) 712
Medium: not stated. For 3'-sulfophenylhydrazo-, B2=22.18; for 2'-sulfo-

phenylhydrazo-, B2=24.27; for 4'-methyl-2'-sulfophenylhydrazo-, B2=23.06.

C11H12N4O2S HL Sulfamerazine CAS 127-79-7 (8431)
4-Amino-N-(4-methyl-2-pyrimidinyl)benzenesulfonamide;

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

Gd+++ gl alc/w 25°C 50% C K1=6.05 B2=10.29 1993EEa (78356) 713
K(Gd(nta)+L)=7.40

Medium: 50% v/v EtOH/H2O, 0.10 M NaClO4.

C11H12O3 HL CAS 94-02-0 (3351)
Ethyl benzoylacetate; C6H5.CO.CH2.CO2.C2H5

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

Gd+++ gl mixed 25°C 75% U K1=8.27 B2=15.11 1971DRa (78400) 714

Medium: 75% acetone, 0.1 M NaClO4

C11H13NO3 H2L CAS 63467-38-9 (1961)
4-Methyl-N-hydroxyacetoacetanilide; CH3.CO.CH2.CO.N(OH).C6H4.CH3

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

Gd+++ gl diox/w 20°C 82% U K1=7.16 B2=13.27 1979KSb (78496) 715
K3=5.66

C11H13NO3 H2L CAS 67777-63-3 (8480)
N-[1-(2-Hydroxyphenyl)ethylidene]-beta-alanine;

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

Gd+++ gl NaClO4 25°C 0.10M U TI K1=9.46 B2=16.75 1978MSj (78525) 716
Also data for 30 and 35 C and 0.01 and 0.05 M NaClO4.

C11H13NO4S HL CAS 58943-48-9 (1411)
N-Acetylacetylidene-orthanilic acid; H03S.C6H4.N:C(CH3).CH2.CO.CH3

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

Gd+++ EMF NaClO4 25°C 0.10M U K1=18.80 1982MSc (78591) 717

C11H13NO5 H3L HBIDA CAS 7372-13-6 (1603)
N-(2-Hydroxybenzyl)iminodiethanoic acid; H0.C6H4.CH2.N(CH2.COOH)2

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

Gd+++ gl KNO3 25°C 0.10M C K1=13.55 B2=24.13 1989YSa (78626) 718
K(Gd+HL)=5.82
K(Gd+2HL)=12.23

Gd+++ gl KNO3 20°C 0.10M U K1=12.82 B2=23.36 1983MSc (78627) 719

C11H13NO6 H4L CAS 1911-59-2 (4852)
2,3-Dihydroxybenzyliminodiethanoic acid; (HO)2.C6H3.CH2.N(CH2.COOH)2

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

Gd+++ EMF oth/un ? ? U 1975DTa (78663) 720

K(Gd+HL)=14.4

C11H13NO6 H4L CAS 59036-09-8 (2111)
2,5-Dihydroxybenzyliminodiethanoic acid; (HO)2.C6H3.CH2.N(CH2.COOH)2

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

Gd+++ gl oth/un 25°C 0.0 U 1970TTb (78678) 721

K(Gd+HL)=14.4

C11H13NO6 H4L CAS 31477-66-7 (4853)
2,6-Dihydroxybenzyliminodiethanoic acid; (HO)2.C6H3.CH2.N(CH2.COOH)2

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

Gd+++ EMF oth/un ? ? U 1975DTa (78692) 722

K(Gd+HL)=12.4

C11H14N2O3 HL Gly-Phe CAS 3321-03-7 (829)
Glycyl-phenylalanine; H2N.CH2.CO.NH.CH(CH2.C6H5).COOH

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

Gd+++ gl KCl 25°C 0.10M U K1=2.40 1973FMa (78813) 723

C11H14N2O4 H2L Gly-Tyr CAS 658-79-5 (533)
Glycyl-tyrosine; H2N.CH2.CO.NH.CH(CH2.C6H4.OH).COOH

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

Gd+++ gl KCl 25°C 0.10M U 1973FMa (78858) 724

K(Gd+HL)=2.65

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

Gd+++ gl KNO3 25°C 0.10M U K1=6.71 B2=11.32 1964THa (78883) 725

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
Gd+++	vlt	KNO3	20°C	0.10M	U			K1=13.81	1981NSc (79285)	726
Gd+++	EMF	KNO3	25°C	0.10M	U			K1=15.93	1980KBc (79286)	727
Gd+++	vlt	KNO3	20°C	0.10M	U			K1=18.15	1978NLb (79287)	728
Gd+++	vlt	KNO3	20°C	0.10M	U			K1=18.21	1964ICb (79288)	729

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
Gd+++	gl	KNO3	25°C	0.10M	U			K1=9.96	1976GKd (79364)	730

C11H18N2O8 H4L CAS 4408-81-5 (923)
 1,3-Diaminopropane-N,N,N',N'-tetraethanoic acid; ((HOOC.CH2)2N.CH2.)2.CH2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	ix	KNO3	20°C	0.10M	U	H		K1=13.70	1971AWa (79445)	731

Polarography also used. DH=20.7 kJ mol⁻¹, DS=331 J K⁻¹ mol⁻¹

Gd+++	gl	KNO3	20°C	0.10M	U			K1=13.74	1964LAa (79446)	732
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Also K1=13.73. By polarography: K1=13.80

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
Gd+++	gl	KNO3	25°C	0.10M	M			K1=13.94	1986PLc (79557)	733

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
Gd+++	gl	KNO3	25°C	0.10M	U			K1=11.04	1976GKd (79595)	734

C11H18O2 HL CAS 40072-58-3 (4820)
 2-(3'-Methylbutanoyl)cyclohexanone (2-isovaleryl cyclohexanone);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	mixed	30°C	75%	U			K1=9.49 B2=18.42	1972DSd (79653)	735

K3=8.09

Medium: 75% acetone

C11H1802 HL CAS 5601-52-5 (4821)
2-Butanoyl-6-methylcyclohexanone (2-butyryl-6-methylcyclohexanone);

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

Gd+++ gl mixed 30°C 75% U K1=10.32 B2=20.26 1972DSd (79664) 736

Medium: 75% acetone

C11H1809 H3L CAS 64020-00-4 (8225)
1,1,1-Tris(carboxymethoxymethyl)ethane;

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

Gd+++ gl R4N.X 25°C 0.10M C K1=6.8 2001V5a (79674) 737

Medium: 0.10 M Me4NCl. Also data for N-ethyl-, N-phenyl-, N-NH2-,
N,N-dibenzyl- and N-CH2OCH2COOH- derivatives.

C11H2004 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

Gd+++ gl KNO3 25°C 0.10M U K1=4.54 B2=7.32 1968PFa (79768) 738

C11H2205 L 16-Crown-5 CAS 55477-28-8 (1592)
1,4,7,10,13-Pentaoxacyclohexadecane; cyclo(-(O.CH2.CH2)5.CH2.CH2-)

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

Gd+++ cal non-aq 25°C 100% U H K1=3.66 1993LLa (79853) 739

Medium: MeCN. DH(K1)=-22.8 kJ mol⁻¹.

C11H26N2O6 L Bistris-propane CAS 64431-96-5 (7920)
1,3-Bis[tris(hydroxymethyl)methylamino]propane;

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

Gd+++ gl NaClO4 25°C 0.10M C 2001GYb (79955) 740

K(2Gd+20H+2L)=23.44
K(2Gd+40H+2L)=34.90
K(2Gd+50H+2L)=33.39
K(2Gd+60H+2L)=42.73

C12H702F7 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

Gd+++ gl alc/w 22°C 80% U K1=6.19 B2=11.62 1995MTa (80183) 741
K3=4.62

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

Gd+++ sp non-aq 25°C 100% C H K1=1.3 2002KNc (80457) 742

Medium: N,N-dimethylformamide, 0.20 M Et4NClO4.

By calorimetry: DH(K1)=-10 kJ mol⁻¹.

Gd+++ dis non-aq 25°C 100% C HM 1998YHa (80458) 743

K(GdA3+L)=7.76

Method: solvent extraction from 0.10 M NaClO4 into CHCl3. HA is
1-(2-thienyl)-4,4,4-trifluoro-1,3-butanedione. DH(GdA3+L)=5.2 kJ mol⁻¹.

C12H10N6O4S H2L CAS 77327-19-6 (8343)

2-[4-Amino-3-(1,2,4-triazolylazo)]naphthol-4-sulphonic acid;

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

Gd+++ gl NaClO4 30°C 0.10M U T H B2=12.60 1982GMb (80782) 744

B3=18.10

Data for 40 and 50 C. Also DH and DS values.

C12H11N3OS HL (6787)

2-Hydroxy-1-naphthaldehyde thiosemicarbazone;

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

Gd+++ gl diox/w 20°C 75% U K1=6.55 B2=11.42 1992SSc (80889) 745

Medium: 75% v/v dioxan/H2O and other mixtures, 0.1 M NaClO4

C12H11N3O2 HL CAS 50536-09-5 (6323)

2-Hydroxy-1-naphthaldehyde-semicarbazone; HO.C10H6.CH:N.NH.CO.NH2

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

Gd+++ gl diox/w 20°C 75% U I K1=9.122 B2=16.541 1992SSc (80917) 746

Medium: 75% v/v dioxan/H2O; 0.1 M NaClO4

C12H11O4P HL CAS 838-85-7 (2133)

Diphenylphosphoric acid; (C6H5O)2P(O)OH

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

Gd+++ kin oth/un 25°C 0.02M U K1=2.38 1974GMc (80949) 747

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

Gd+++ sp NaClO4 25°C 0.50M U K1=2.077 1987MSa (80966) 748

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

Gd+++ gl alc/w 22°C 0.1M U K1=6.55 B2=12.19 2000TBb (81073) 749

K3=4.50

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

Gd+++ sp NaClO4 25°C 0.50M U K1=2.193 1987MSa (81196) 750

C12H14N4O2S L Sulfadimidine CAS 57-68-1 (6167)

2-(4-Aminobenzolsulfamido)-4,6-dimethylpyrimidine;

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

Gd+++ gl NaNO3 25°C 0.10M U M 1988SSg (81368) 751

K(Gd(EDTA)+L)=2.62

C12H15NO5 H3L (4930)

1-Hydroxy-4-methylphenyl-2-methyleneiminodiethanoic acid;

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

Gd+++ gl oth/un 25°C 0.0 U K1=14.28 1970TTb (81496) 752

C12H16O7S HL CAS 204931-01-1 (7817)

2,3-Benzo-1,4,7,10-tetraoxacyclododeca-2-ene-4'-sulfonic acid;

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

Gd+++ dis R4N.X 25°C 0.12M C K1=2.04 1998SUa (81697) 753

Medium: 0.12 M Et4NBr.

Method:solvent extraction into cyclohexane/di(2-ethylhexyl)phosphoric acid

C12H18N2O5S H2L CAS 80459-15-0 (1595)

2-Nitroso-5-(N-propyl-3-sulfopropylamino)phenol;


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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++      gl  KNO3   25°C 0.10M C      K1=5.70  B2=10.06  1988YSa (81812) 754
*****
C12H18N2O8      H2L                      CAS 93031-52-8 (5829)
1,4-Dioxa-7,10-diazacyclododecane-5,12-dione-7,10-diethanoic acid;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
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Gd+++      gl  R4N.X  25°C 0.10M C      K1=5.63                      1988CCb (81836) 755
*****
C12H18N2O8      H4L                      CAS 76079-31-7 (2587)
trans-1,2-Diaminocyclohexane-N,N'-di(propanedioic acid)
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
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Gd+++      EMF KNO3  25°C 0.10M U      K1=13.34                      1985SGa (81864) 756
-----
Gd+++      EMF KNO3  25°C 0.10M U      K1=15.65  B2=20.95  1980SGb (81865) 757
*****
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
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++      vlt KNO3  20°C 0.10M U      K1=18.56                      1968NLa (82025) 758
*****
C12H20N2O8      H4L                      CAS 40623-42-5 (1101)
1,2-Diaminoethane-N,N'-di(2-pentane-1,5-dioic acid); (CH2NHCH(COOH)CH2CH2COOH)2
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++      gl  KNO3   20°C 0.10M U      K1=8.61  B2=12.41  1975DPa (82071) 759
-----
Gd+++      gl  NaClO4 30°C 0.10M U                      1974STb (82072) 760
K(Gd+H2L=GdL+2H)=13.0
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Gd+++      gl  KNO3   25°C 0.10M U      K1=8.02                      1973GBd (82073) 761
*****
C12H20N2O8      H4L                      CAS 61368-60-3 (3389)
1,2-Diaminoethane-N,N'-diethanoic-N,N'-di-2-propanoic acid;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++      vlt KNO3  20°C 0.10M U      K1=16.96                      1976NKa (82133) 762
*****
C12H20N2O8      H4L                      CAS 40623-42-5 (3388)
1,2-Diaminoethane-N,N'-diethanoic-N,N'-dipropanoic acid;
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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	NaClO4	25°C	0.10M	U	IH		K1=13.21 B(Gd+HL)=6.23	1988RNa (82165)	763
DH(K1)=4.09 kJ mol ⁻¹ , DH(Gd+HL)=32.8, DS(K1)=267 J K ⁻¹ mol ⁻¹										
Gd+++	vlt	R4N.X	30°C	0.01M	C			K1=15.35	1981GMh (82166)	764
Method: polarography, using Cd as indicator ion. Medium: 0.01 M Et4NBr.										

C12H20N2O8		H4L						CAS 2458-58-4	(922)	
1,4-Diaminobutane-N,N,N',N'-tetraethanoic acid; (HOOC.CH2)2N.(CH2)4.N(CH2.COOH)2										
Gd+++	gl	NaClO4	25°C	0.50M	M	H		K1=9.94 K(GdL+H)=6.66 K(GdHL+H)=5.36	1985CBa (82219)	765
DH(K1)=24.3 kJ mol ⁻¹ , DS=272 J K ⁻¹ mol ⁻¹ (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										
Gd+++	sp	NaClO4	20°C	0.10M	U			K1=18.64	1971ISa (82302)	766
Gd+++	vlt	oth/un	20°C	0.10M	U			K1=18.84	1966DMa (82303)	767
Gd+++	vlt	KNO3	20°C	0.10M	U			K1=18.84	1966NSb (82304)	768

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										
Gd+++	sp	NaClO4	20°C	0.10M	U			K1=17.03	1971ISa (82397)	769
Gd+++	vlt	oth/un	20°C	0.10M	U			K1=16.51	1966DMa (82398)	770

C12H20N2O8S		H4L			TEDTA			CAS 923-74-0	(3394)	
2,2'-Thiobis(ethyliminodiethanoic acid); S(CH2.CH2.N(CH2.COOH)2)2										
Gd+++	gl	KNO3	25°C	0.10M	C			K1=14.76	1985TPa (82458)	771

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

Gd+++ EMF KNO3 20°C 0.10M U K1=18.13 1962MMc (82537) 772

C12H20N2O10 H4L CAS 10258-50-1 (3993)
(2,3-Dihydroxytetramethylenedinitrilo)tetraethanoic acid;

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

Gd+++ EMF KCl 25°C 0.10M U 1967SSa (82588) 773
K(Gd+H2L)=13.06
K(Gd+HL)=17.15

C12H20O8N2 H4L (6908)
2-Methyl-1,2-diaminopropane-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

Gd+++ vlt KNO3 20°C 0.10M C K1=17.09 1978NLa (82674) 774

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

Gd+++ gl alc/w 20°C 40% U K1=11.08 1985LBc (82697) 775
Medium: 40% v/v MeOH/H2O, 0.1 M KNO3

C12H21N3O6 H3L NOTA (5589)
1,4,7-Triazacyclononane-N,N',N''-triethanoic acid;

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

Gd+++ nmr KCl 25°C 0.10M U K1=13.7 1991BCa (82735) 776
K(Gd+HL=GdL+H)=2.30

Gd+++ sp NaCl 25°C 0.10M C 1990BSe (82736) 777
K(Gd+HL)=3.6

C12H23N3O6 H3L (7085)
2,5,8-Triazanonane-2,5,8-triethanoic acid;
CH3N(CH2COOH)CH2CH2N(CH2COOH)CH2CH2N(CH2COOH)CH3

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

Gd+++ gl KCl 25°C 0.10M C K1=13.12 1995PRa (83003) 778

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

Gd+++ gl R4N.X 25°C 0.10M C K1=13.06 1998CCb (83083) 779

Gd+++ gl KCl 25°C 0.10M C K1=19.4 1997HTa (83084) 780

C12H24O6 L 18-Crown-6 CAS 17455-13-9 (577)
1,4,7,10,13,16-Hexaoxacyclooctadecane;

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

Gd+++ dis R4N.X 25°C 0.12M C K1=<0.2 1998SUa (83363) 781
Medium: 0.12 M Et4NBr.
Method:solvent extraction into cyclohexane/di(2-ethylhexyl)phosphoric acid

Gd+++ dis non-aq 25°C 100% U 1993INa (83364) 782
B(GdPL)=6.55
B(GdPL2)=8.43

K is the equilibrium constant for extraction of the metal picrate (P) into CH2Cl2. For extraction from D2O, B=6.89 and 8.94.

Gd+++ dis non-aq 25°C 100% U B2=8.43 1990NIa (83365) 783
B2=extraction eq.constant: M+3P+2(S)=ML2P3(S); solvent(S)=CH2Cl2, P=picrate

Gd+++ cal alc/w 25°C 100% U H K1=1.32 1977ILb (83366) 784
Medium: Methanol. DH=15.6 kJ mol⁻¹.

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

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

Gd+++ ISE non-aq 25°C 100% C K1=16.5 1986ALa (83841) 785
Medium: propylene carbonate, 0.1 M Et4NClO4

Gd+++ gl alc/w 25°C 100% C K1=7.67 1983ANb (83842) 786
The equilibration took 7-12 days. Medium: MeOH, 0.05 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

Gd+++ gl R4N.X 25°C 0.10M U K1=13.38 1996BJa (84156) 787
K(Gd+HL)=10.10
K(Gd+H2L)=5.66
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

 Gd+++ gl NaNO3 25°C 0.20M C K1=8.40 1991KKa (84329) 788

Gd+++ gl NaCl 20°C 0.10M C K1=9.8 1988SJB (84330) 789

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

 Gd+++ gl alc/w 22°C 80% U K1=5.40 B2=10.56 1995MTa (84454) 790
 K3=4.78

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

 C13H8O3 H2L CAS 18931-22-1 (2913)
 peri-Dihydroxynaphthindenone;

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

 Gd+++ sp alc/w 25°C 50% U K1=9.64 1982HMa (84503) 791

C13H9FO2S HL CAS 43191-66-8 (6154)
 1-(2'-Thienyl)-3"-fluoro-2"-hydroxyphenyl)-prop-1-one-2-ene;
 C4H3S.CH:CH.CO.C6H3(OH)F

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

 Gd+++ gl NaClO4 30°C 0.10M U K1=5.05 1989SHa (84514) 792

C13H9N2O4Cl HL CAS 36016-30-5 (182)
 N-(4-Chlorophenyl)-3-nitrobenzohydroxamic acid; O2N.C6H4.CO.N(C6H4Cl).OH

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

 Gd+++ gl diox/w 35°C 50% A K1=7.87 B2=14.19 1977AKa (84602) 793
 K3=5.29

 C13H11NOS H2L (7306)
 2-(Salicylideneamino)thiophenol, Salicylaldehyde-2-mercaptoanil;
 HO.C6H4.CH:N.C6H4.SH

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

 Gd+++ gl alc/w 25°C 70% U K1=12.72 B2=24.49 1995IFa (85043) 794
 Medium: 70% v/v EtOH/H2O, 0.10 M NaCl.

C13H11NO2 HL CAS 304-88-1 (181)
N-Phenylbenzohydroxamic acid; C6H5.CO.N(C6H5).OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	diox/w	35°C	50%	A			K1=11.43 B2=21.37 K3=8.91	1977AKa (85153)	795

Gd+++	gl	mixed	25°C	75%	U			K1=8.36 B2=14.68	1969DSb (85154)	796
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Medium: 75% acetone, 0.1 M NaClO4

C13H11NO4S H2L CAS 124452-52-4 (8496)
2-[(Phenylimino)methyl]phenol 4-sulfonic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	NaClO4	25°C	0.10M	U	T HM		K1=4.78 K(Gd(bpy)+L)=4.62 K(Gd(phen)+L)=4.58 K(Gd(his)+L)=3.53	1995SSd (85206)	797

Data for 35 and 45 C. DH and DS values reported.

C13H11NS HL CAS 42152-36-3 (8401)
2-[(Phenylmethylene)amino]benzenethiol;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	alc/w	25°C	70%	U			K1=7.86 B2=15.76	1995IFa (85228)	798

Medium: 70% v/v EtOH/H2O, 0.10 M NaCl. Also data for p-Cl, p-NMe2, p-OH, p-OCH3, p-CH3, p-NO2 substituted benzaldehyde Schiff bases.

C13H11N2O3F3 HL (5563)
3-(2-Acetylphenylhydrazone)-1,1,1-trifluoropentane-2,4-dione;
CF3.CO.C(CO.CH3):N.HN.C6H4.COCH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	diox/w	30°C	75%	U			K1=8.95 B2=16.25	1988ESb (85246)	799

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	oth/un	25°C	0.10M	U			K1=12.141	1987KSc (85359)	800

C13H12N4O L Diphenylcarbaz. CAS 538-62-5 (1195)
Diphenylcarbazone; C6H5.NH.NH.CO.N:N.C6H5

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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++     EMF alc/w 20°C 50% U      K1=3.45      1971MAc (85411) 801
Medium: 50% EtOH, 0.1 M NaClO4
*****
C13H12N4S          L      Dithizone          CAS 60-10-6 (1801)
Diphenylthiocarbazone; C6H5.NH.NH.CS.N:N.C6H5
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++     EMF alc/w 20°C 50% U      K1=1.80      1971MAc (85458) 802
Medium: 50% EtOH, 0.1 M NaClO4
*****
C13H14N2O3        HL          (4940)
3-(2-Acetylphenylhydrazone)pentane-2,4-dione;(CH3.CO)2C:N.NH.C6H4(CO.CH3)
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++     gl  diox/w 30°C 75% U      K1=11.05 B2=20.48 1988ESb (85609) 803
*****
C13H15N06        H3L          (4999)
2-Benzylnitriilotriethanoic acid;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++     oth oth/un 25°C 0.10M U      K2=8.97      1962HKa (85737) 804
*****
C13H19N03        H2L          (2031)
2-(1-(2-Hydroxyphenyl)-ethylimine)-3-methylbutanoic acid;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++     gl  NaClO4 25°C 0.10M U TIH  K1=11.10 B2=20.55 1980SSc (86054) 805
*****
C13H20N2O8        H4L          CAS 123064-92-6 (7929)
trans-1,3-Cyclopentanediaminotetraethanoic acid;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++     gl  KCl      25°C 1.0M U      K1=12.67      1989CMb (86120) 806
                    K(GdHL+H)=3.73
                    K(GdL+H)=4.29
*****
C13H22N2O8        H4L          CAS 1798-14-7 (921)
(Pentamethylenedinitrilo)tetraethanoic acid; ((HOOCH2)2N.CH2.CH2)2CH2
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
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Gd+++     gl  KNO3     25°C 0.10M C      K1=10.37      1982PPd (86195) 807
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K(Gd+HL)=6.79

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

Gd+++ vlt KNO3 20°C 0.10M U K1=18.53 1974NLa (86227) 808

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

Gd+++ gl KNO3 20°C 0.10M U K1=12.15 1981NSc (86254) 809

By polarography K1=12.28

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

Gd+++ vlt KNO3 20°C 0.10M U K1=18.44 1968NLb (86282) 810

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

Gd+++ gl KNO3 25°C 0.10M C K1=15.21 1985PLa (86303) 811

K(Gd+HL)=9.32

C13H23N3O6 H3L (6555)

1,4,7-Triazacyclodecane-N,N',N''-triethanoic acid;

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

Gd+++ nmr KCl 25°C 0.10M U K1=15.1 1991BCa (86389) 812

K(Gd+HL=GdL+H)=0.30

C13H26O5 L (6410)

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

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

Gd+++ cal non-aq 25°C 100% C H K1=3.62 1998LBc (86472) 813

Medium: acetonitrile. DH(K1)=-3.43 kJ mol⁻¹, DS(K1)=57.9 J K⁻¹ mol⁻¹.

C13H28N4O2 L CAS 17023-02-8 (7247)

3,3,9,9-Tetramethyl-4,8-diazaundecane-2,10-dione dioxime;
(HON:C(CH3)C(CH3)2NHCH2)2CH2

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

Gd+++ gl NaCl 25°C 0.15M C K1=15.53 2004NJa (86533) 814
B(GdH-1L)=7.64
B(GdH-2L)=0.27

C14H8O4 H2L Alizarin CAS 72-48-0 (1058)
1,2-Dihydroxyanthraquinone;

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

Gd+++ gl oth/un 25°C 0.10M U K1=12.14 1981EJa (86642) 815

C14H8O7S H3L DASA CAS 83-61-4 (950)
1,2-Dihydroxyanthraquinone-3-sulfonic acid, Alizarin Red S;

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

Gd+++ gl NaClO4 25°C 0.20M U M K1=10.18 1987VJa (86730) 816
K(Gd(cdta)+L)=6.03, K(Gd(dtpa)+L)=5.02.

Gd+++ sp oth/un 25°C ? U K(?)=8.6 1967SAa (86731) 817

C14H9N5Cl2 L CAS 7071-45-6 (8463)
1,5-Bis(4-chlorophenyl)-3-cyanoformazan;

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

Gd+++ gl diox/w 25°C 70% U K1=6.17 B2=12.20 1996DAb (86849) 818
Medium: 70% dioxane/H2O, 0.10 M NaClO4.

C14H10N2F HL CAS 87221-43-0 (6155)
1-(2'-Pyridyl)-3-(3-fluoro-2-hydroxyphenyl)-prop-1-one-2-ene;
C5H4N.CH:CH.CO.C6H3(OH)F

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

Gd+++ gl NaClO4 30°C 0.10M U K1=5.18 1989SHa (86884) 819

C14H11N3O HL CAS 24854-76-0 (1380)
2-(1H-Benzimidazol-2-yl-methylene-amino) phenol;

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

Gd+++ gl diox/w 25°C 50% U K1=7.43 B2=13.89 19820Ca (86994) 820

C14H11N5 L CAS 7014-08-6 (8461)
1,5-Diphenyl-3-cyanoformazan;

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

Gd+++ gl diox/w 25°C 70% U K1=7.06 B2=14.05 1996DAb (86999) 821
Medium: 70% dioxane/H2O, 0.10 M NaClO4.

C14H12NO2Br HL CAS 13664-21-6 (6243)
N-(4-Tolyl)-4'-bromobenzohydroxamic acid; Br.C6H4.CO.N(C6H4.CH3).OH

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

Gd+++ gl diox/w 25°C 50% U T H K1=9.85 B2=18.22 1983AGb (87046) 822
K3=7.36

35 C: K1=9.34, K2=7.86, K3=6.82

C14H12NO2Cl HL CAS 32939-57-4 (6242)
N-(4-Tolyl)-4'-chlorobenzohydroxamic acid; Cl.C6H4.CO.N(C6H4.CH3).OH

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

Gd+++ gl diox/w 25°C 50% U T H K1=9.88 B2=18.27 1983AGb (87072) 823
K3=7.38

35 C: K1=9.38 K2=7.90, K3=6.89

C14H12NO2F HL CAS 13664-15-8 (6241)
N-(4-Tolyl)-4'-fluorobenzohydroxamic acid; F.C6H4.CO.N(C6H4.CH3).OH

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

Gd+++ gl diox/w 25°C 50% U T H K1=10.15 B2=18.81 1983AGb (87081) 824
K3=7.65

35 C: K1=9.65 K2=8.15, K3=7.16

C14H12N2O3 H2L CAS 4870-46-6 (3432)
2-Hydroxy-5-methyl-2'-carboxy-azobenzene; HO.C6H3(CH3).N:N.C6H4.COOH

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

Gd+++ gl diox/w 25°C 50% U I K1=3.70 B2=7.10 1985ANa (87215) 825

C14H12N2O4 HL CAS 29556-26-1 (6244)
N-(4-Tolyl)-4'-nitrobenzohydroxamic acid; O2N.C6H4.CO.N(C6H4.CH3).OH

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

Gd+++ gl diox/w 25°C 50% U T H K1=9.55 B2=17.60 1983AGb (87242) 826
K3=7.04

35 C: K1=8.03, K2=7.54, K3=6.53

C14H12N2O4 HL CAS 854-7-78-9 (183)
N-2-Tolyl-3-nitrobenzohydroxamic acid; O2N.C6H4.CO.N(C6H4.CH3).OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Gd+++	gl	diox/w	35°C	50%	A		K1=9.10 B2=16.70 K3=6.60	1977AKa (87250)	827

C14H12N2O4 HL (179)
N-3-Tolyl-3-nitrobenzohydroxamic acid; O2N.C6H4.CO.N(C6H4.CH3).OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Gd+++	gl	diox/w	35°C	50%	A		K1=9.35 B2=17.20 K3=6.85	1977AKa (87261)	828

C14H12N2O4 HL CAS 85407-74-5 (180)
N-4-Tolyl-2-nitrobenzohydroxamic acid; O2N.C6H4.CO.N(C6H4.CH3).OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Gd+++	gl	diox/w	35°C	50%	A		K1=9.60 B2=17.70 K3=7.11	1977AKa (87274)	829

C14H12N2O4 HL (221)
N-4-Tolyl-3-nitrobenzohydroxamic acid; O2N.C6H4.CO.N(C6H4.CH3).OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Gd+++	EMF	diox/w	35°C	50%	U	T H	K1=9.60 B2=17.70 K3=7.11	1977AKa (87287)	830

C14H13NO2 HL DPAHA CAS 4463-22-3 (880)
2,2'-Diphenylacetohydroxamic acid; (C6H5)2.CH.CO.NH.OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Gd+++	gl	alc/w	30°C	50%	U	T H	K1=6.66 K1=7.77(I=0), 7.02(I=0.05)	1981RSb (87404)	831

C14H13NO2 HL CAS 1503-92-0 (1817)
N-(4-Tolyl)benzohydroxamic acid; C6H5.CO.N(C6H4.CH3).OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Gd+++	gl	diox/w	25°C	50%	U	T H	K1=10.35 B2=19.20 K3=7.84	1983AGb (87444)	832

35 C: K1=9.80, K2=8.56, K3=7.35

C14H13N04S H2L (3660)
2-Aminobenzenesulfonic acid 2-hydroxyacetophenone Schiff base;
HSO3.C6H4.N:C(CH3).C6H4.OH

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

Gd+++ gl NaClO4 25°C 0.10M U T H K1=5.76 B2=10.29 1978GKb (87575) 833
Data for 25-35 C and I=0.01-0.10 M. At I=0.0 M, DH(K1)=29.7 kJ mol⁻¹,
DS(K1)=297 J K⁻¹ mol⁻¹.

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

Gd+++ gl mixed 30°C 0.10M U T H K1=11.91 B2=22.26 1988TRb (87719) 834
Medium: 0.1 M KNO3 in 75% v/v isopropanol/water

C14H15O4P HL CAS 843-24-3 (2134)
Di(4-methylphenyl)phosphoric acid; (CH3C6H5O)2P(O)OH

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

Gd+++ kin oth/un 25°C 0.02M U K1=3.33 1974GMc (87792) 835

C14H16N2O2S HL CAS 189231-67-2 (8475)
2-Thiophenylhydrazodimedone;

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

Gd+++ gl diox/w 25°C 75% C T H K1=13.17 B2=24.70 1997EIa (87868) 836
Medium: 75% v/v dioxane/H2O, 0.10 M KNO3. Data for 10-40 C. DH(K1)=-6.27
kJ mol⁻¹, DS(K1)=-6.79 J K⁻¹ mol⁻¹; DH(K2)=-6.39, DS(K2)=-8.97.

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

Gd+++ gl mixed 30°C 0.10M U T H K1=12.12 B2=22.68 1988TRb (87886) 837
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

Gd+++ gl NaClO4 25°C 1.00M C H K1=13.84 1992YNa (87952) 838
By calorimetry: DH(K1)=14.6 kJ mol⁻¹, DS=315 J K⁻¹ mol⁻¹

C14H19N07 HL (6775)
16-Nitro-3,6,9,12-tetraoxabicyclo[12.3.1]octadeca-1(18),14,16-trien-18-ol;

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

Gd+++ gl R4N.X 25°C 0.10M C K1=3.18 1990CBe (88148) 839

C14H2005 L Benzo15-crown-5 CAS 14098-44-3 (608)
2,3-Benzo-1,4,7,10,13-pentaoxacyclopentadeca-2-ene;

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

Gd+++ dis non-aq 25°C 100% U B2=7.87 1990NIa (88269) 840
B2=extraction eq.constant: M+3P+2(S)=ML2P3(S); solvent(S)=CH2Cl2, P=picrate

Gd+++ ISE R4N.X 25°C 0.10M C K1=2.35 1986XJa (88270) 841

C14H2008S HL CAS 127461-53-4 (7818)
2,3-Benzo-1,4,7,10,13-pentaoxacyclopentadeca-2-ene-4'-sulfonic acid;

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

Gd+++ dis R4N.X 25°C 0.12M C K1=1.63 1998SUa (88393) 842
Medium: 0.12 M Et4NBr.

Method:solvent extraction into cyclohexane/di(2-ethylhexyl)phosphoric acid

C14H22N208 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

Gd+++ gl KCl 25°C 1.0M U K1=4.37 1987CMe (88430) 843
K(GdL+H)=7.00

C14H22N208 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

Gd+++ gl KCl 25°C 1.0M U K1=7.28 1987CMe (88442) 844
K(GdHL+H)=5.36
K(GdL+H)=7.91

C14H22N208 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

Gd+++ gl KCl 25°C 1.0M U K1=8.35 1987CMe (88456) 845
K(GdHL+H)=5.80

K(GdL+H)=6.57

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

Gd+++ gl KCl 25°C 1.0M U K1=18.97 1987CMe (88667) 846
K(GdL+H)=1.66

Gd+++ gl KCl 25°C 1.00M U K1=18.97 1984MFa (88668) 847

Gd+++ gl KNO3 27°C 0.10M U M 1981KSe (88669) 848
K(Gd+L+HA)=13.17
K(GdL+HA)=5.83

H2A=Citraconic acid

Gd+++ gl NaClO4 25°C 0.50M U K1=18.12 1977GGb (88670) 849

Gd+++ EMF KNO3 25°C 0.10M U T H K1=18.80 1962MHa (88671) 850
DH(K1)=24.3 kJ mol⁻¹, DS=439 J K⁻¹ mol⁻¹. At 20 C: K(GdL+H)=2.23

Gd+++ vlt KNO3 20°C 0.10M U K1=18.77 1954SGa (88672) 851

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

Gd+++ gl KCl 25°C 1.0M U K1=7.95 1987CMe (88836) 852
K(GdHL+H)=5.12
K(GdL+H)=7.48

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

Gd+++ gl KCl 25°C 1.0M U K1=8.56 1987CMe (88856) 853
K(GdHL+H)=5.95
K(GdL+H)=6.41

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

Gd+++ gl R4N.X 25°C 0.10M C K1=8.61 1988CCb (88880) 854

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
Gd+++	gl	NaClO ₄	25°C	0.10M	C			K ₁ =22.39	2001CCa (89256)	855
K ₁ from competitive titration using EDTA. In 0.10 M Me ₄ NCl, K ₁ =22.39.										
Gd+++	kin	KCl	25°C	1.0M	C			K(GdL+Eu)=1.3	2000SBc (89257)	856
Gd+++	kin	KCl	25°C	1.0M	C T			K(GdL+Cu)=1.1	2000SBc (89258)	857
At 37 C: K(GdL+Cu)=1.45.										
Gd+++	kin	KCl	25°C	1.0M	C T			K(GdL+Zn)=0.85	2000SBc (89259)	858
At 37 C: K(GdL+Zn)=1.1.										
Gd+++	gl	KCl	25°C	0.10M	C			K ₁ =22.52	1999SBd (89260)	859
Gd+++	sp	NaClO ₄	25°C	0.15M	U			K ₁ =21.04	1996GMa (89261)	860
Arsenazo III used as indicator. Also data for several DTPA-bis-anilides										
Gd+++	sp	R ₄ N.X	25°C	0.10M	C			K ₁ =22.2	1994KCa (89262)	861
Medium: Me ₄ NCl										
Gd+++	cal	KNO ₃	25°C	0.10M	C T				1988MIa (89263)	862
DH(K ₁)=-30.7 kJ mol ⁻¹ , DS=324.5 J mol ⁻¹ K ⁻¹ . Also data for 283 and 313 K										
Gd+++	cal	NaClO ₄	25°C	0.10M	C	H			1987YJa (89264)	863
DH(K ₁)=-27.0 kJ mol ⁻¹ , DS(K ₁)=339 J K ⁻¹ mol ⁻¹ .										
Gd+++	cal	NaClO ₄	25°C	0.50M	U	H			1977CGc (89265)	864
DH(K ₁)=-47.5 kJ mol ⁻¹										
Gd+++	gl	NaClO ₄	25°C	0.50M	U			K ₁ =20.73	1977GGb (89266)	865
Gd+++	sp	oth/un	20°C	dil	U			K ₁ =22.46	1969KAf (89267)	866
Gd+++	cal	KNO ₃	27°C	0.10M	U	H			1968CLd (89268)	867
DH(K ₁)=-32.6 kJ mol ⁻¹ , DS=321 J K ⁻¹ mol ⁻¹										
Gd+++	EMF	KNO ₃	25°C	0.10M	U	H		K ₁ =22.46	1962MTc (89269)	868
DH(K ₁)=-31.4 kJ mol ⁻¹ , DS=325 J K ⁻¹ mol ⁻¹										
Gd+++	gl	oth/un	25°C	0.10M	U			K ₁ =23.01	1959HCa (89270)	869

C ₁₄ H ₂₄ N ₂ O ₈ H ₄ L (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
Gd+++	vlt	KNO3	20°C	0.10M	U		K1=16.48	1969NDc (89509)	870

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
Gd+++	vlt	KNO3	20°C	0.10M	U		K1=18.47	1974NLa (89530)	871

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
Gd+++	gl	KCl	25°C	1.00M	U	M		1976BKa (89577)	872
							K(GdEDTA+L)=3.9		
							K(GdEDTA+HL)=3.7		
							K(2GdEDTA+L)=7.5		

Gd+++	gl	KCl	25°C	0.10M	U			1974Kpd (89578)	873
							K(Gd+HL)=6.61		

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
Gd+++	vlt	KNO3	20°C	0.10M	U		K1=18.48	1968NLb (89633)	874

C14H24N2O8		H2L					CAS 17619-53-3	(5833)	
Diaminoethane-N,N,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
Gd+++	gl	R4N.X	25°C	0.10M	C		K1=10.23	1988CCb (89651)	875

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
Gd+++	gl	NaClO4	25°C	0.10M	U			1995HAa (89683)	876
							K(Gd+HL)=4.67		
							K(Gd+H2L)=4.01		
							K(Gd+H3L)=2.97		
							B(GdHL)=14.10		

B(GdH2L)=19.56, B(GdH3L)=22.69

C14H24N2O9 H4L BPETA CAS 87720-52-3 (5077)

Bis-(3-di(carboxymethyl)aminopropyl)ether;

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

Gd+++ gl KNO3 25°C 0.10M U K1=11.74 1984TPa (89729) 877
K(Gd+HL)=7.30

C14H24N2O10 EGTA CAS 67-42-5 (349)

Ethyleneglycol-0,0'-bis(2-aminoethyl ether)-N,N,N',N'-tetraethanoic acid; H4L

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

Gd+++ gl NaNO3 25°C 0.10M U I K1=16.95 1996KDC (89867) 878
Data for 0.05 and 0.15 M NaNO3. At I=0, K1=17.10.

Gd+++ gl KCl 25°C 1.0M U M K2=1.56 1985KBb (89868) 879
K(GdL+ida)=1.5

Gd+++ EMF KNO3 20°C 0.10M U K1=16.94 1962MMc (89869) 880

C14H24O9 H3L CAS 64020-01-5 (8224)

1,1,1-Tris[(2-carboxyethoxy)methyl]ethane;

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

Gd+++ gl R4N.X 25°C 0.10M C K1=3.72 2001VSA (90051) 881
K(GdL+H)=4.20

Medium: 0.10 M Me4NCl. Also data for N-CH2OH-, N-CH2(CH2)2COOH-
derivatives.

C14H25N3O6 H3L (6556)

9-Methyl-1,4,7-triazacyclododecane-N,N',N''-triethanoic acid;

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

Gd+++ nmr KCl 25°C 0.10M U K1=14.7 1991BCa (90066) 882
K(Gd+HL=GdL+H)=-0.64

C14H25N3O7 H3L (5397)

1-Oxa-4,7,10-triazacyclododecane-4,7,10-triethanoic acid;

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

Gd+++ gl KCl 25°C 0.10M C K1=21.6 1993DSA (90085) 883
K(GdL+H)=1.45
K(Gd(OH)L+H)=10.35

C14H25N3O8 H4L DEATA CAS 97315-55-4 (5601)
N,N-Bis(2-aminoethyl)ethylamine-N',N',N'',N''-tetraethanoic acid;

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

Gd+++ gl KNO3 25°C 0.10M C K1=17.79 1985TPa (90100) 884

C14H25N3O9 H4L CAS 4454-15-3 (5078)
(N-(2-Hydroxyethyl)-2,2'-iminodiethylene)dinitrilo)tetraethanoic acid;

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

Gd+++ vlt KCl ? 0.10M U K1=13.45 1968VLa (90115) 885

C14H26N2O7 H2L (1567)
1,4,10-Trioxa-7,13-diazacyclopentadecane-N,N'-diethanoic acid;

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

Gd+++ gl R4N.X 25°C 0.10M M K1=11.66 1986COB (90191) 886

C14H26N4O6 H3L DOTRA (6701)
1,4,7,10-Tetraazacyclododecane-1,4,7-triethanoic acid;

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

Gd+++ gl R4N.X 25°C 0.10M C H K1=22.02 2000BCa (90248) 887
Medium: 0.10 M NMe4Cl. K1 corresponds to 3 weeks equilibration.
For complexes formed in minutes: K1=19.6, K(Gd+L+H)=22.5.

Gd+++ gl R4N.X 25°C 0.10M C K1=22.02 1996BCd (90249) 888
Medium: Me4NCl

Gd+++ sp R4N.X 25°C 0.10M C K1=21.0 1994KCa (90250) 889
Medium: Me4NCl

Gd+++ sp NaCl 25°C 1.00M C K(GdL+H)=2.06 1993KCa (90251) 890

C14H28N2O4 L Cryptand 2,1,1 CAS 31250-06-3 (836)
1,10-Diaza-4,7,13,18-tetraoxabicyclo[8,5,5]eicosane (2,1,1);

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

Gd+++ ISE non-aq 25°C 100% C K1=15.4 1986ALa (90367) 891
Medium: propylene carbonate, 0.1 M Et4NClO4

Gd+++ sp non-aq 25°C 100% U K1=3.87 1983PSc (90368) 892
Medium: DMSO

C14H28N2O6 HL CAS 82353-42-2 (5850)
1,4,10,13-Tetraoxa-7,16-diazacyclooctadecane-7-ethanoic acid;

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

Gd+++ gl R4N.X 25°C 0.10M C K1=7.29 1988CCc (90480) 893

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

Gd+++ gl R4N.X 25°C 0.10M U K1=12.71 1996BJa (90764) 894
K(Gd+HL)=10.73
K(Gd+H2L)=5.85

Medium: 0.1 M Me4NCl

C14H34N4O6P2 H4L CAS 200952-02-9 (7644)
1,4,7,10-Tetraazacyclododecane-1,7-bis(methanephosphonic acid monoethyl ester);

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

Gd+++ gl KCl 25°C 0.10M C K1=9.81 1998BRa (90843) 895

C15H11N04 HL CAS 1776-18-7 (955)
3-Phenyl-1-(2'-hydroxy-5'-nitrophenyl)-2-propen-1-one;

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

Gd+++ gl alc/w 35°C 70% U K1=6.46 B2=12.86 1982SLb (91077) 896

C15H11N3O HL PAN CAS 85-85-8 (572)
1-(2-Pyridylazo)-2-naphthol; C5H4N.N:N.C10H6.OH

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

Gd+++ sp alc/w 21°C 50% U K1=9.29 1988CMd (91217) 897

Gd+++ sp alc/w 21°C 50% U I K1=8.80 1981MCb (91218) 898
Medium: 50% MeOH, 0.1 M NaClO4. In 75% MeOH K1=10.23

C15H11O2Br HL CAS 1218-20-0 (954)
3-Phenyl-1-(2'-hydroxy-5'-bromophenyl)-2-propen-1-one;

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

Gd+++ gl alc/w 35°C 70% U K1=7.10 1982SLb (91370) 899

C15H11O2Cl HL CAS 1218-24-2 (953)
3-Phenyl-1-(2'-hydroxy-5'-chlorophenyl)-2-propen-1-one;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	alc/w	35°C	70%	U			K1=7.00 B2=13.59	1982SLb (91389)	900

Gd+++	gl	alc/w	35°C	70%	U			K1=7.00 B2=13.59	1980SLb (91390)	901

C15H12OS			HL					(1261)		
mono-Thiodibenzoylmethane; C6H5.CO.CH2.CS.C6H5										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	NaClO4	30°C	0.05M	U			K1=8.64 B2=16.58 K3=7.36	1979VMa (91492)	902

C15H12O2			HL			Diphenylacac		CAS 120-46-7 (362)		
1,3-Diphenylpropane-1,3-dione, Dibenzoylmethane; C6H5.CO.CH2.CO.C6H5										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	mixed	15°C	50%	U	T H		K1=8.46	1982BSb (91549)	903
Medium: 50%CH3CN in H2O										

C15H12O2			HL					CAS 1214-47-7 (951)		
3-Phenyl-1-(2'-hydroxyphenyl)-2-propen-1-one, 2'-hydroxychalkone; C6H5.CH:CH.CO.C6H4.OH										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	alc/w	35°C	70%	U			K1=7.68 B2=15.10	1982SLb (91583)	904
Medium: 70% EtOH, 0.1 M KNO3										

Gd+++	gl	alc/w	35°C	70%	U			K1=7.68 B2=15.10	1980SLb (91584)	905

C15H13NO2			HL					CAS 959-66-0 (245)		
Benzoyl-acetanilide; C6H5.CO.CH2.CO.NH.C6H5										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	alc/w	30°C	70%	M			K1=5.29	1978SAb (91632)	906

C15H13NO2			HL					CAS 7369-44-0 (4066)		
N-3-Diphenylpropenohydroxamic acid;										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	dis	oth/un	RT	0.05M	C				1993ATa (91637)	907
Method: extraction from 0.05 M triethanolamine buffer into chloroform.										
Analysis by spectrophotometry. K(Gd+3HL(org)=GdL3(org)+3H)=-17.98										

C15H13N3O HL CAS 104992-04-3 (6852)
2-((1H-Benzimidazo-2-yl-methyl)-iminomethyl)phenol;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	alc/w	30°C	60%	U	M		K1=6.13 B2=11.19 K(GdA+L)=4.93 K(GdB+L)=4.63 K(GdC+L)=4.29	1990DOb (91664)	908

H2A=iminodiethanoic acid, H3B=hydroxyethyliminodiethanoic acid, H3C=NTA.
Data also for 3-chloro and 3-methoxysalicylidene analogues

C15H14NOCl HL CAS 268214-29-5 (8398)
4-Chloro-3,5-dimethyl-2-[(phenylimino)methyl]phenol;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	diox/w	30°C	75%	M			K1=7.00	2000ANa (91691)	909

Medium: 75% v/v dioxan/H2O, 0.10 M NaClO4. Data for an extensive series of 4'-substituted phenylimino derivatives.

C15H14O3S H2L (6191)
1-(2-Hydroxy-3,5-dimethylphenyl)-3-(2-thiophene)-propan-1,3-dione;
C4H3S.CO.CH2.CO.C6H2(OH)(CH3)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	diox/w	30°C	50%	U			K(Gd+HL)=8.00 K(GdHL+HL)=5.75	1987DDc (91784)	910

C15H14O3S H2L CAS 57051-65-7 (6190)
1-(2-Hydroxy-4,5-dimethylphenyl)-3-(2-thiophene)-propan-1,3-dione;
C4H3S.CO.CH2.CO.C6H2(OH)(CH3)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	diox/w	30°C	50%	U			K(Gd+HL)=7.67 K(GdHL+HL)=6.58	1987DDc (91790)	911

C15H14O4 H2L CAS 60403-51-2 (2361)
1-(2-Furyl)-3-(2-hydroxy-3,4-dimethylphenyl)-propan-1,3-dione;
C4H3O.CO.CH2.CO.C6H2(OH)(CH3)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	diox/w	30°C	50%	U			K(Gd+HL)=7.56 K(GdHL+HL)=7.22	1987DDc (91796)	912

C15H14O4 H2L CAS 60403-52-3 (6186)
1-(2-Furyl)-3-(2-hydroxy-3,5-dimethylphenyl)-propan-1,3-dione;
C4H3O.CO.CH2.CH2.C6H2(OH)(CH3)2

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

Gd+++ gl diox/w 30°C 50% U 1987DDc (91802) 913
K(Gd+HL)=6.84

C15H14O4 H2L CAS 60403-54-5 (6187)
1-(2-Furyl)-3-(2-hydroxy-3,6-dimethylphenyl)-propan-1,3-dione;
C4H3O.CO.CH2.CH2.C6H2(OH)(CH3)2

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

Gd+++ gl diox/w 30°C 50% U 1987DDc (91808) 914
K(Gd+HL)=7.67
K(GdHL+HL)=6.58

C15H15NO2 HL (1167)
N-(4-Tolyl)-4'-tolylhydroxamic acid; CH3.C6H4.CO.N(C6H4.CH3)OH

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

Gd+++ gl diox/w 25°C 50% U T H K1=10.60 B2=19.71 1983AGb (91842) 915
K3=8.10

35 C: K1=10.09, K2=8.61, K3=7.61

C15H15NO3 HL (6240)
N-4-Tolyl-4'-methoxybenzohydroxamic acid; CH3O.C6H4.CO.N(C6H4.CH3).OH

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

Gd+++ gl diox/w 25°C 50% U T H K1=10.75 B2=20.01 1983AGb (91864) 916
K3=8.26

35 C: K1=10.26, K2=8.75, K3=7.77

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

Gd+++ gl alc/w 20°C 75% U T H K1=10.91 B2=18.78 1993RAa (92023) 917
Medium: 75% v/v MeOH/H2O; 0.10 M KNO3

Gd+++ gl mixed 30°C 0.10M U T H K1=12.30 B2=23.29 1988TRb (92024) 918
Medium: 0.1 M KNO3 in 75% v/v isopropanol/water

C15H20N2O6 H3L BEDTA CAS 65311-06-0 (2944)

N-Benzyl diaminoethane-N,N',N'-triethanoic acid;

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

Gd+++ gl KNO3 25°C 0.10M C K1=12.40 1978MPb (92151) 919

C15H20N2O7 H4L HBET (6954)
N-(Hydroxobenzyl) diaminoethane-N,N',N'-triethanoic acid;
HO.C6H4.CH2.N(CH2COOH)CH2CH2.N(CH2COOH)2

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

Gd+++ gl KCl 25°C 0.10M C K1=17.54 1995MMa (92169) 920
B(GdHL)=23.55
B(GdH2L)=26.38

C15H22N4O4 H2L (7082)
3,6,9,15-Tetraazabicyclo[9.3.1]pentadeca-1(15),11,13-triene-3,9-diethanoic acid;

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

Gd+++ gl KCl 25°C 0.10M C K1=16.6 1995KHa (92246) 921

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

Gd+++ sp non-aq 25°C 100% M K1=7.9 B2=14.70 1997RPb (92283) 922
B3=22.6

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

Gd+++ EMF KCl ? 0.10M U K1=16.71 1966VLa (92371) 923

Gd+++ vlt oth/un ? ? U K1=18.4 1966VLa (92372) 924

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

Gd+++ gl KNO3 25°C 0.10M C K1=19.74 1989SPa (92393) 925
K(Gd+HL)=13.38

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

Gd+++ gl KCl 25°C 0.10M C K1=19.9 2000SBb (92431) 926

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

Gd+++ gl KCl 25°C 0.10M C K1=19.4 2000SBb (92446) 927

C15H27N3O6 H3L (6557)
9,9-Dimethyl-1,4,7-triazacyclodecane-N,N',N''-triethanoic acid;

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

Gd+++ nmr KCl 25°C 0.10M U K1=10.4 1991BCa (92467) 928
K(Gd+HL=GdL+H)=-3.47

C15H27N3O9 H4L CAS 319016-32-5 (7716)
N'-(2-Hydroxypropyl)-diethylenetriamine-N,N,N'',N''-tetraethanoic acid;

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

Gd+++ gl R4N.X 25°C 0.10M M K1=18.48 2000Cwa (92484) 929
Medium: 0.1 M NMe4NO3.

C15H30N4O6 H3L (6472)
Tris(4-Carboxy-3-methyl-3-azabutyl)amine; N(CH2.CH2.N(CH3).CH2.COOH)3

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

Gd+++ gl KCl 25°C 0.10M C K1=9.98 1992GBa (92538) 930

C15H33N06 L CAS 70384-51-9 (838)
Tris(3,6-dioxaheptyl)amine; (CH3.CH2.O.CH2.CH2.O.CH2.)3N

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

Gd+++ ISE non-aq 25°C 100% C K1=9.1 B2=16.7 1986ALa (92566) 931
Medium: propylene carbonate, 0.1 M Et4NClO4

C15H36N3O9P3 H3L (6749)
1,4,7-Triazacyclononane-N,N',N''-tris(methylenephosphonate monoethylester)

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

Gd+++ gl R4N.X 25°C 0.10M C K1=10.3 1992LRa (92612) 932

 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

Gd+++ kin oth/un 25°C 0.02M U K1=5.03 1972GSe (92653) 933

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

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

Gd+++ gl diox/w 25°C 70% U I K1=12.13 B2=21.26 1996DAb (92895) 934
 Medium: 70% dioxane/H2O, 0.10 M NaClO4. In 50% EtOH/H2O, 0.10 M NaClO4,
 K1=11.15, K2=8.94.

C16H12N2O11S3 H5L CAS 548-81-2 (5180)
 2-(4'-Sulfophenylazo)chromotropic acid,
 2-(4-sulfophenylazo)-1,8-dihydroxyaphthalene-3,6-diHSO3

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

Gd+++ gl oth/un 25°C 0.10M U K1=7.59 B2=12.17 1985AAa (93094) 935
 Data also for 12 other 4-substituted phenyl analogues

C16H12N3O4ClS H2L CAS 133131-00-7 (8468)
 7-Amino-8-[(4-chlorophenyl)azo]-4-hydroxy-2-naphthalenesulfonic acid;

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

Gd+++ gl NaCl 25°C 0.10M U K1=10.77 B2=20.31 1997IHa (93114) 936
 B3=27.72

Also data for the 4'-bromo-, 4'-fluoro-, 4'-nitro-, 4'-methoxy-, 4'-di-
 methylamino-, 4'-hydroxy-, 4'-carboxy-, 4'-AsO(OH)2-, 2'-hydroxy- analogue

C16H12N5O3 L CAS 77251-11-7 (5928)
 1-Phenyl-3-methyl-4(2'-nitrophenylhydrazo)-5-pyrazolone;

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

Gd+++ gl diox/w 30°C 75% M K1=7.38 1987ESa (93129) 937

C16H13N2O10AsS2 H5L Thorin I CAS 3688-92-4 (2609)
 1-((2-Arsonophenyl)azo)-2-hydroxy-3,6-naphthalylldisulfonic acid;

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

Gd+++ gl NaClO4 30°C 0.10M U 1976NDa (93193) 938
 K(Gd+H2L=GdH2L)=5.59

K(GdHL+H)=7.30

K(GdL+H)=9.74

K(GdL+OH)=2.70

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

Gd+++ sp oth/un 20°C 0.10M U 1971SSd (93255) 939
K(Gd+H2L)=8.34

Gd+++ sp oth/un ? 0.0 U 1970KLe (93256) 940
K(Gd+H2L)=8.15

C16H13O5Cl H3L (261)
3',4',7-Trihydroxy-3-methoxyflavylium chloride; (HO)2C6H3.C9H4O(OH)(OCH3)Cl

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

Gd+++ sp none 25°C 0.00 U 1997EFa (93398) 941
K(Ga+H2L=GaL+2H)=-3.56

C16H14N2O5 H2L (7017)
4-Hydroxy-1-carboxy-7-dimethylaminophenoxaz-3-one methyl ester;

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

Gd+++ sp alc/w 25°C 10% U I 1979KRb (93439) 942
B3=19.59

Medium: 10% w/w EtOH/H2O, 0.1 M NaClO4. In 30%: B3=19.98

C16H14O2 HL CAS 1775-98-0 (952)
3-Phenyl-1-(2'-hydroxy-5'-methylphenyl)-2-propen-1-one;

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

Gd+++ gl alc/w 35°C 70% U K1=7.93 B2=15.54 1982SLb (93530) 943
Medium: 70% EtOH, 0.1 M KNO3

C16H14O3 HL CAS 3327-24-0 (956)
3-(4''-Methoxyphenyl)-1-(2'-hydroxyphenyl)-2-propen-1-one;

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

Gd+++ gl alc/w 35°C 70% U K1=7.52 B2=14.78 1982SLb (93567) 944

Gd+++ gl alc/w 35°C 70% U K1=7.52 B2=14.78 1980SLb (93568) 945

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
-----
Gd+++      gl  diox/w 25°C 70% U      K1=7.82  B2=15.43  1996DAb (93639) 946
Medium: 70% dioxane/H2O, 0.10 M NaClO4.
```

```
*****
C16H15N5O7S2      H2L      Cefixime      CAS 79350-37-1 (8532)
5-Thia-1-azabicyclo[4,2,0]oct-2-ene-2-carboxylic acid;
```

```
-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++      con non-aq 25°C 100% C      K1=5.06  B2= 7.18  2003GNa (93651) 947
Medium: DMSO.
```

```
*****
C16H18N2O3      HL      (5564)
2-(2-Acetylphenylhydrazone)-5,5-dimethyl-1,3-cyclohexanedione;
```

```
-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++      gl  diox/w 30°C 75% U      K1=11.32 B2=20.20  1988ESb (93778) 948
*****
```

```
C16H18N4      L      CAS 172665-46-2 (7699)
N,N'-Dimethyl-1,10-phenanthroline-2,9-dimethanamine;
```

```
-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++      gl  NaClO4 25°C 0.10M U      K1=7.60      2001WZa (93842) 949
B(GdHL)=14.62
```

```
Also data for the N,N'-diethyl, isopropyl, butyl and isobutyl derivatives.
*****
C16H18N4O4      H2L      CAS 161563-39-9 (8399)
1,3-Phenylenediamine bisazoacetylacetone;
```

```
-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++      gl  diox/w 25°C 50% U      K1=10.15 B2=19.51  1997MAb (93859) 950
Medium: 50% v/v dioxan/H2O, 0.10 M NaClO4. For the 1,4-phenylenediamine
derivative, K1=10.95, K2=10.30.
```

```
*****
C16H18N4O4      H2L      CAS 161563-40-2 (8400)
1,3-Phenylenediamine bisazobenzoylacetone;
```

```
-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++      gl  diox/w 25°C 50% U      K1=7.96  B2=14.96  1997MAb (93866) 951
Medium: 50% v/v dioxan/H2O, 0.10 M NaClO4. For the 1,4-phenylenediamine
derivative, K1=9.25, K2=8.36.
```

```
*****
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
-----
Gd+++      vlt KNO3  20°C 0.10M U          K1=17.40      1969NDb (94038) 952
*****
C16H22O6          L                      (6733)
4'-Acetyl-2,3-benzo-1,4,7,10,13-pentaoxacyclopentadeca-2-ene;
-----
```

```
-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++      dis non-aq 25°C 100% U          B(Gd+3P+2L)=7.51      1993INa (94249) 953
-----
```

By solvent extraction into dichloromethane. B is the extraction constant
 $Gd(aq)+picrate(aq)+L(org)=GdL2P3(org)$.

```
*****
C16H23NO8          HL                      (6776)
19-Nitro-3,6,9,12,15-pentaoxabicyclo[15.13.1]heneicosa-1(21),17,19-trien-21-ol;
-----
```

```
-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++      gl  R4N.X  25°C 0.10M C          K1=3.03      1990CBe (94259) 954
*****
C16H23NO8          L                      CAS 53408-96-1 (1765)
2,3-(4'-Nitrobenzo)-1,4,7,10,13,16-hexaoxacyclooctadeca-2-ene;
4'-Nitrobenzo-18-crown-6
-----
```

```
-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++      ISE R4N.X  25°C 0.10M C          K1=2.98      1986XJa (94266) 955
*****
C16H24O9S          HL      SB18C6          CAS 185099-14-3 (7819)
2,3-Benzo-1,4,10,13,16-hexaoxacyclooctadeca-2-ene-4'-sulfonic acid;
-----
```

```
-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++      dis R4N.X  25°C 0.12M C          K1=1.39      1998SUa (94478) 956
Medium: 0.12 M Et4NBr.
-----
```

Method:solvent extraction into cyclohexane/di(2-ethylhexyl)phosphoric acid

```
*****
C16H26N2O10        H2L                      CAS 93031-54-0 (5831)
1,4,7,10-Tetraoxa-13,16-diazacyclooctadecane-11,18-dione-13,16-diethanoic acid;
-----
```

```
-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++      gl  R4N.X  25°C 0.10M C          K1=9.59      1988CCb (94569) 957
*****
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
Gd+++	sp	KCl	25°C	0.08M	U			K1=11.4	1994FCa (94668)	958
Gd+++	gl	KCl	25°C	0.10M	C			K1=11.15 K(GdL+H)=2.87	1992CKa (94669)	959

Data also for some related ligands

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
Gd+++	sp	KCl	25°C	0.08M	U			K1=15.3	1994FCa (94684)	960

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
Gd+++	gl	KNO3	20°C	0.10M	U			K1=13.39	1969NDc (94711)	961

By polarography: K1=13.47

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
Gd+++	vlt	KNO3	20°C	0.10M	U			K1=16.60	1969NDc (94737)	962

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
Gd+++	vlt	KNO3	20°C	0.10M	U			K1=18.43	1979MBd (94763)	963

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
Gd+++	gl	R4N.X	25°C	0.10M	C	H		K1=24.67	2000BCa (94896)	964

Medium: 0.10 M NMe4Cl. K1 corresponds to 3 weeks equilibration.
For complexes formed in minutes: K1=21.2, K(Gd+L+H)=24.5.

Gd+++	gl	R4N.X	25°C	0.10M	C			K1=24.67	1996BCd (94897)	965
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Medium: Me4NCl

Gd+++ gl NaCl 25°C 1.00M C 1994TBa (94898) 966
 K(GdL+H)=1.1
 K(GdHL+H)=-0.9

 Gd+++ gl NaCl 37°C 1.0M C K1=23.6 1994TBb (94899) 967
 Method: Competitive reaction with Eu3+ ion.

 Gd+++ sp NaCl 25°C 1.00M C 1993KCa (94900) 968
 K(GdL+H)=2.8

 Gd+++ gl R4N.X 25°C 0.10M C K1=27.0 1992AAb (94901) 969

 Gd+++ kin NaCl 25°C 1.00M U K1=22.1 1992WJa (94902) 970

 Gd+++ EMF KCl 25°C 0.10M C K1=24.0 1991CMb (94903) 971
 K(GdL+H)=2.3

 C16H29N3O8 H3L (6699)
 1,7-Dioxa-4,10,13-triazacyclopentadecane-N,N',N''-triethanoic acid;

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

 Gd+++ sp KCl 25°C 0.10M U K1=17.26 1997WHa (94974) 972
 Method: luminescence spectroscopy

 Gd+++ gl KCl 25°C 0.10M C K1=17.23 1993DSa (94975) 973
 K(GdL+H)=2.32
 K(Gd(OH)L+H)=10.79

 C16H29N3O9 H4L TTDA-HP (7932)
 N'-(2-Hydroxypropyl)di(carboxymethyl)triazadodecanedioic acid;

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

 Gd+++ gl R4N.X 25°C 0.10M M K1=17.33 2001Cwa (94982) 974
 Medium: 0.10 M Me4NNO3. Method: by competition with EDTA

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

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

 Gd+++ gl NaClO4 25°C 0.10M C H 1993RCa (94997) 975
 DH(K1)=-25.3 kJ mol-1, DS(K1)=238 J K-1 mol-1

 Gd+++ gl NaCl 25°C 0.10M U K1=16.85 1990CQa (94998) 976

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
Gd+++	gl	R4N.X	25°C	0.10M	U		K1=11.93	1983CRb (95041)	977

C16H30N4O6			H2L				(6295)		
1,2-Diaminoethane-N,N'-bis(2-propylethanoamide)-N,N'-diethanoic acid;(Me2CHNHCOCH2N(CH2COOH)CH2)2									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Gd+++	gl	KCl	25°C	0.10M	U		K1=12.79 B2=18.96	1999WWa (95069)	978

C16H30N4O7			H3L				(6917)		
10-(2-Hydroxyethyl)-1,4,7,10-tetraazacyclododecane-1,4,7-triethanoic acid;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Gd+++	sp	R4N.X	25°C	0.10M	C		K1=22.3 K(Gd+HL)=2.04	1994KJa (95075)	979
Medium: Me4NC1									

C16H30N4O12P2			H6L				CAS 330623-46-6 (8581)		
1,5,8,12-Tetraaza-3,10-dihydroxy-3,10-dioxide-3,10-diphosphacyclotetradecane-1,5,8,12-tetraOAc;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Gd+++	gl	NaCl	25°C	0.16M	C		K1=12.74 K(Gd+HL)=10.62 K(Gd+H2L)=7.11	2002SSa (95086)	980

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
Gd+++	sp	non-aq	25°C	100%	U		K1=3.26	1983PSc (95208)	981
Medium: DMSO									

C16H32N4O6			H2L				(7344)		
4,10-Bis(2-hydroxyethyl)-1,4,7,10-Tetraazacyclododecane-1,7-bis(ethanoic acid);									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Gd+++	gl	KCl	25°C	0.10M	C		K1=21.1	1997HTa (95327)	982

C16H32N8O4			L				CAS 157599-02-5 (8676)		
1,4,7,10-Tetraazacyclododecane-1,4,7,10-tetraacetamide;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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 Gd+++ gl NaNO3 25°C 0.10M C K1=10.05 1995MHa (95375) 983

 C16H32O7 L (6411)
 15-(2,5-Dioxaheptyl)-15-methyl-1,4,7,10,13-pentaoxacyclohexadecane;

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

Gd+++ cal non-aq 25°C 100% U H K1=3.10 1993LLa (95383) 984
 Medium: MeCN. DH(K1)=-31.9 kJ mol⁻¹.

 C16H38N4O6P2 H2L CAS 583879-34-9 (9251)
 4,10-Dimethyl-1,4,7,10-tetraazacyclododecane-1,7-bis(methanephosphonic acid
 monoethyl ester);

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

Gd+++ gl R4N.X 25°C 0.10M C K1=9.75 2003BGa (95594) 985
 Medium: 0.10 M Me4NCl.

 C17H12N3O3Cl HL (6197)
 8-Formyl-7-hydroxy-4-methyl-2H-[1]-benzopyran-2-one-4-chloroanil;
 Cl.C6H4.N:CH.C9H3O(OH)(CH3)(:O)

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

Gd+++ gl diox/w 30°C 70% U K1=5.22 B2=9.18 1987ECa (95690) 986
 B3=11.93

 C17H12N2O5 HL (6198)
 8-Formyl-7-hydroxy-4-methyl-2H-[1]-benzopyran-2-one-4-nitroanil;
 NO2.C6H4.N:CH.C9H3O(OH)(CH3)(:O)

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

Gd+++ gl diox/w 30°C 70% U K1=5.05 B2=8.82 1987ECa (95707) 987
 B3=11.47

 C17H12O4 H2L CAS 60430-57-8 (6189)
 1-(2-Furyl)-3-(2-naphthol)-propan-1,3-dione; C4H3O.CO.CH2.CO.C10H6.OH

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

Gd+++ gl diox/w 30°C 50% U 1987DDc (95732) 988
 K(Gd+HL)=8.00
 K(GdHL+HL)=6.45

 C17H13NO3 HL CAS 98399-88-3 (6195)
 8-Formyl-7-hydroxy-4-methyl-2H-[1]-benzopyran-2-one-anil;
 C6H5.N:CH.C9H3O(CH3)(OH)(:O)

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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++     gl  diox/w 30°C 70% U          K1=5.75  B2=10.31 1987ECa (95738) 989
                               B3=13.64

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*****
C17H13N4O3          HL                      (5927)
1-Phenyl-3-methyl-4-(2'-carboxyphenylhydrazo)-5-pyrazolone;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++     gl  diox/w 30°C 75% M          K1=15.86 B2=28.79 1987ESa (95766) 990
*****
C17H14N2O2          L                      CAS 4551-69-3 (698)
4-Benzoyl-3-methyl-1-phenyl-2-pyrazolin-5-one;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++     gl  NaNO3 20°C 0.10M U    M                      1981GCa (95883) 991
                               B(Gd+3L+3TBP)=25.65
                               B(Gd+3L=4TBPoxide)=32.8
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Gd+++     dis non-aq 25°C 100% U    M                      1973TEc (95884) 992
                               K(GdA+3L)=1.56
                               K(GdB2+3L)=6.23
                               K(Gd(phen)2+3L)=7.43

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Medium: CHCl3. A=tributylphosphate, B=piperidine
*****
C17H15N4O2          L                      CAS 97671-53-9 (5926)
1-Phenyl-3-methyl-4-(2'-methoxyphenylhydrazo)-5-pyrazolone;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++     gl  diox/w 30°C 75% M          K1=8.60  B2=16.84 1987ESa (96007) 993
*****
C17H16N2O3S2        L                      CAS 127335-83-5 (6849)
Sulfafurazole thiophene-2-aldehyde Schiff base; C4H3S.CH:N.C6H4.SO2.NH.C4HO(CH3)2
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++     gl  oth/un 25°C 0.10M U T    K1=4.90          1990TSa (96038) 994
30 C: K=4.70, 35 C: K=4.50
*****
C17H18O4            H2L                      (6188)
1-(2-Furyl)-3-(2-hydroxy-3,4-diethylphenyl)-propan-1,3-dione;
C4H3O.CO.CH2.CO.C6H2(OH)(C2H5)2
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++     gl  diox/w 30°C 50% U          1987DDc (96243) 995

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K(Gd+HL)=7.17

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

Gd+++ gl alc/w 22°C 0.1M U K1=5.66 B2=10.22 2000TBb (96285) 996
Medium: 0.1 M NaClO4 in 70% v/v EtOH/H2O

C17H20N4O6 HL Riboflavin CAS 83-88-5 (1438)
7,8-Dimethyl-10(D-1'-ribityl)isoalloxazine, Vitamin B2, Vitamin H

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

Gd+++ sp mixed 25°C 95% U K1=4.18 1983LRb (96337) 997
Medium: CH3CN, 1 M LiClO4.3H2O

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

Gd+++ sp NaNO3 25°C 0.10M C K1=8.46 19880Ha (96419) 998
K(Gd+HL)=2.79

C17H24N4O6 H3L (7349)
3,6,9,15-Tetraazabicyclo[9.3.1]pentadeca-1(15),11,13-triene-3,6,9-triethanoic acid;

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

Gd+++ nmr oth/un 25°C 0.1M U K1eff=20.8 1997ABa (96456) 999

C17H27N04 L CAS 71089-11-7 (7945)
13-Phenylmethyl-1,4,7,10-tetraoxa-13-azacyclopentadecane;

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

Gd+++ cal non-aq 25°C 100% C H K(GdNO3+L)=3.24 1993LLb (96533)1000
Medium: acetonitrile. DH(GdNO3+L)=-65.02 kJ mol-1.

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

Gd+++ gl KNO3 25°C 0.10M U K1=8.79 1984TPa (96571)1001

K(Gd+HL)=5.67

C17H29N5O8 H3L (6622)
1,4,7-Tris(carboxymethyl)-1,4,7,10,14-pentaazacyclohexadecane-9,15-dione;

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

Gd+++ gl KCl 25°C 0.10M C K1=14.49 1992CKa (96590)1002

Data also for some related ligands

C17H30N4O8 H4L TRITA CAS 60239-20-5 (1018)
1,4,7,10-Tetraazacyclotridecane-1,4,7,10-tetraethanoic acid;

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

Gd+++ gl KCl 25°C 0.10M C K1=19.17 1991CMb (96650)1003

K(GdL+H)=3.2

C17H32N4O6 H3L (6696)
1,4,7,10-Tetraazacyclododecane-1,4,7-tri(2-methyl)ethanoic acid;
C8H17N4(CH(CH3)COOH)3

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

Gd+++ sp R4N.X 25°C 0.10M U K1=25.3 1993KRb (96689)1004

K(GdL+H)=2.24

C17H32N4O7 H3L CAS 120041-08-9 (6702)
10-Hydroxypropyl-1,4,7,10-tetraazacyclododecane-1,4,7-triethanoic acid;

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

Gd+++ gl R4N.X 25°C 0.10M C H K1=24.5 2000BCa (96713)1005

Medium: 0.10 M NMe4Cl. K1 corresponds to 3 weeks equilibration.

Complex formed in minutes has K1=22.9, DH(K1)=-46.9 kJ mol⁻¹.

Gd+++ sp R4N.X 25°C 0.10M C K1=23.8 1994KCa (96714)1006

Medium: Me4NCl

Gd+++ sp R4N.X 25°C 0.10M C K1=23.9 1994KJa (96715)1007

K(Gd+HL)=2.23

Medium: Me4NCl

Gd+++ sp NaCl 25°C 1.00M C 1993KCa (96716)1008

K(GdL+H)=2.38

C17H32N4O9 H3L CAS 124628-01-9 (2013)
1,4,7,10-Tetraazacyclododecane-1,4,7-tri(2-hydroxymethyl)ethanoic acid;

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

Gd+++ gl R4N.X 25°C 0.10M C H K1=18.29 2000BCa (96731)1009
K(GdL+OH)=2.63

Medium: 0.10 M NMe4Cl. Data correspond to 3 weeks equilibration.

Complexes formed in minutes have: K1=15.5, B(Gd+L+2H)=22.1.

C18H15NO3 HL (6196)
8-Formyl-7-hydroxy-4-methyl-2H-[1]-benzopyran-2-one 4-methylanil;
CH3.C6H4.N:CH.C9H3O(OH)(CH3)(O)

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

Gd+++ gl diox/w 30°C 70% U K1=6.61 B2=12.11 1987ECa (96994)1010
B3=16.17

C18H16N2O3 HL (5560)
2-(2-Acetylphenylhydrazone)-1-phenyl-but-1,3-dione;
C6H5.CO.C(CO.CH3):N.NH.C6H4.COCH3

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

Gd+++ gl diox/w 30°C 75% U K1=11.03 B2=19.89 1988ESb (97171)1011

C18H20N2O6 H4L CAS 10328-28-6 (3501)
Ethylenedinitrilo-N,N'-bis(2'-hydroxyphenyl)-N,N'-diethanoic acid;

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

Gd+++ gl KCl 25°C 0.10M C K1=21.18 1993MMa (97402)1012
K(GdL+H)=6.15
K(GdHL+H)=3.71

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

Gd+++ EMF KNO3 25°C 0.10M C T H K1=18.84 1985HWb (97429)1013
K(GdL+H)=7.14

Method: Hg (and glass) electrode, using Hg(II) as competitive indicator
ion. Data for 10-35 C. DH(K1)=-52.0 kJ mol⁻¹, DS(K1)=186 J K⁻¹ mol⁻¹.

C18H20N4O4 H2L (7083)
2,11-Diaza[3.3](2,6)pyridinophane-N,N'-diethanoic acid;

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

Gd+++ gl KCl 25°C 0.10M C K1=14.5 1995KHa (97471)1014

C18H22N4O4 H2L CAS 2444-14-6 (3502)

N,N'-Bis(2-pyridylmethyl)diaminoethane-N,N'-diethanoic acid;

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

Gd+++ gl NaCl 25°C 0.16M C K1=12.37 1997CMa (97543)1015
K(Gd+L=GdL(OH)+H)=2.10
K(GdL(OH)+H)=10.25

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

Gd+++ gl KNO3 25°C 0.10M C K1=15.42 1985TPa (97653)1016

C18H26N4O6 H3L (7350)
3,6,10,15-Tetraazabicyclo[10.3.1]hexadeca-1(16),12,14-triene-3,6,10-triethanoic acid;

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

Gd+++ nmr oth/un 25°C 0.1M U 1997ABa (97686)1017

K1eff=19.3 (pH 7)
For 3,7,11,17-Tetraazabicyclo[11.3.1]heptadeca-1(17),13,15-triene-3,7,11-triethanoic acid: K1eff=12.7

C18H26N4O8 H4L CAS 319016-30-3 (7715)
N'-(2-Pyridylmethyl)-diethylenetriamine-N,N,N'',N''-tetraethanoic acid;

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

Gd+++ gl R4N.X 25°C 0.10M M K1=21.59 2000CWa (97691)1018

Medium: 0.1 M NMe4NO3.

C18H26N6 L (6628)
3,6,14,17,23,24-Hexaazatricyclo[17.3.1.1]tetracos-1(23),8,10,12(24),19,21-hexaene;

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

Gd+++ gl KCl 25°C 0.10M M K1=8.1 1996MBb (97713)1019

Gd+++ gl KCl 25°C 0.20M C K1=8.1 1992RMa (97714)1020

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

Gd+++ gl non-aq 25°C 100% U K1=3.02 1982MDa (97805)1021

Medium: propylene carbonate

C18H29N04 L CAS 207603-17-6 (9000)
7-(Phenylmethyl)-1,4,10,13-tetraoxa-7-azacyclohexadecane;

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

Gd+++ cal non-aq 25°C 100% C H K1=2.37 1998LBc (97877)1022
Medium: acetonitrile. DH(K1)=-61.05 kJ mol⁻¹, DS(K1)=-159.5 J K⁻¹ mol⁻¹.

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

Gd+++ gl R4N.X 25°C 0.10M C K1=10.04 1988CCb (97909)1023

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

Gd+++ EMF KNO3 25°C 0.10M C T H K1=23.05 1987Hca (98041)1024
K(GdL+H)=4.73
K(GdHL+H)=2.86

Method: Hg electrode; competitive reaction with Hg(II).
Data for 15-35 C. At 25 C, DH(K1)=-130 kJ mol⁻¹, DS(K1)=6.3 J K⁻¹ mol⁻¹.

Gd+++ vlt R4N.X 30°C 0.01M C K1=19.51 1981GMh (98042)1025

Method: polarography, using Cd as indicator ion. Medium: 0.01 M Et4NBr.

Gd+++ vlt NaClO4 25°C 0.40M C K1=23.83 1978MNB (98043)1026

Medium: 0.40 M NaClO4, pH 4.80. Method: polarography, using Cd as
indicator ion.

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

Gd+++ EMF KCl 25°C 0.10M C K1=13.77 1991CMb (98204)1027
K(GdL+H)=4.52

Gd+++ gl NaNO3 25°C 0.20M C K1=14.73 1991Kka (98205)1028

Gd+++ EMF NaCl 80°C 1.00M C K1=15.75 1986LDb (98206)1029
K(GdL+H)=3.75

C18H33N3O9 H3L (6700)
1,7,13-Trioxa-4,10,16-triazacyclooctadecane-N,N',N''-triethanoic acid;

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

 Gd+++ sp KCl 25°C 0.10M U K1=18.07 1997WHa (98298)1030
 Method: luminescence spectroscopy

Gd+++ gl KCl 25°C 0.10M C K1=18.02 1993DSa (98299)1031

 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

 Gd+++ gl R4N.X 25°C 0.10M C K1=7.02 1988CCc (98337)1032

 C18H34N4O6 H2L (6845)
 1,2-Diaminoethane-N,N'-bis(t-butylethanoamide)-N,N'-diethanoic
 acid;Me3CNHCOCH2N(CH2COOH)CH2)2

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

 Gd+++ gl KCl 25°C 0.10M U K1=12.76 B2=20.35 1999WwA (98364)1033

 C18H34N4O9 H3L D03A-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

 Gd+++ gl NaCl 25°C 0.10M C I K1=18.7 1996TKa (98379)1034
 In 0.1 M Me4NCl K=20.8, in 0.1 M KCl K=21.8

 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

 Gd+++ cal non-aq 25°C 100% C H K1=14.44 2003DCa (98576)1035
 Method: competitive titration calorimetry of AgL+. Medium: acetonitrile.
 DH(K1)=-113.6 kJ mol⁻¹, DS(K1)=-105 J K⁻¹ mol⁻¹.

Gd+++ ISE non-aq 25°C 100% C K1=16.8 1986ALa (98577)1036
 Medium: propylene carbonate, 0.1 M Et4NClO4

Gd+++ gl alc/w 25°C 100% C K1=10.14 1983ANb (98578)1037
 The equilibration took 7-12 days. Medium: MeOH, 0.05 M Et4NClO4

Gd+++ sp non-aq 25°C 100% U K1=3.45 1983PSc (98579)1038
 Medium: DMSO

 C18H36N4O6 H2L (7345)

4,10-Bis(2-hydroxypropyl)-1,4,7,10-Tetraazacyclododecane-1,7-bis(ethanoic acid);

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

Gd+++ gl KCl 25°C 0.10M C K1=22.5 1997HTa (98789)1039

C18H38N4O8P2 H6L CAS 187240-55-7 (7347)
1,4,7,10-Tetraazacyclododecane-1,7-bis(ethanoic
acid)-4,10-bis(methylene-ethylphosphinic acid);

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

Gd+++ gl KCl 25°C 0.10M C K1=15.8 1997HTa (98867)1040

C18H38N4O10P2 H6L CAS 187240-54-6 (7346)
1,4,7,10-Tetraazacyclododecane-1,7-bis(ethanoic
acid)-4,10-bis(ethylmethylenephosphonic acid);

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

Gd+++ gl KCl 25°C 0.10M C K1=16.8 1997HTa (98871)1041

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

Gd+++ gl R4N.X 25°C 0.10M U K1=7.30 1996BJa (98892)1042
Medium: 0.1 M Me4NCl

C19H15N08 H4L Alizarin Comp. CAS 3952-78-1 (671)
(3,4-Dihydroxy-2-anthraquinonyl-methyl)iminodiethanoic acid;

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

Gd+++ con oth/un 25°C 0.10M U K1=4.54 B2=8.57 1981E1c (99133)1043

C19H28N4O8 H4L TTDA-PY (7933)
N'-(2-Pyridylmethyl)di(carboxymethyl)triazadodecanedioic acid;

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

Gd+++ gl R4N.X 25°C 0.10M M K1=23.48 2001CWa (99416)1044
Medium: 0.10 M Me4NNO3. Method: by competition with EDTA

C19H35N5O7 H3L CAS 118476-80-5 (5886)
1,4,7,10-Tetraazacyclododecane-N-(N-propyl)amide-N',N'',N'''-triethanoic acid;

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

 Gd+++ gl NaCl 25°C 0.10M C K1=20.1 1989SBc (99467)1045

 C20H13N3O7S H3L Eriochrome Bl T CAS 1787-61-7 (997)
 1-(1-Hydroxy-2-naphthylazo)-6-nitro-2-naphthol-4-sulfonic acid;

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

Gd+++ gl NaCl04 30°C 0.10M U M K1=11.4 B2=21.21 1987SOa (99566)1046
 K(GdA+L)=10.14
 K(GdB+L)=9.38

H2A=hydroxyethyliminodiethanoic acid, H3B=nitriilotriethanoic acid

 C20H14N2O5S H3L Solochrome 6B CAS 3564-14-5 (3507)
 1-(1-Hydroxy-2-naphthylazo)-2-naphthol-4-sulfonic acid, Mordant Black3, Eriochrome
 blue-black B;

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

Gd+++ gl alc/w 30°C 50% C M K1=11.91 B2=22.17 1994SOa (99650)1047
 K(GdA+L)=10.34
 K(Gd(nta)+L)=9.69

Medium: 50% v/v MeOH/H2O, 0.10 M NaCl04.
 H2A is hydroxyethyliminodiethanoic acid.

Gd+++ gl NaCl04 30°C 0.10M U T H K1=13.37 1991NNb (99651)1048
 Also data for 40 and 50 C. DH and DS values.

 C20H14N2O5S H3L EriochrBluBlk R CAS 2538-85-4 (3508)
 3-Hydroxy-4-(2-hydroxy-1-naphthylazo)naphthalene-1-sulfonic acid;

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

Gd+++ gl diox/w 30°C 50% U K1=11.52 1976NNa (99691)1049

 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

Gd+++ sp NaCl04 25°C 0.10M C K1=6.03 1979PLb (99711)1050

 C20H14N2O11S3 H2L Hydroxynaphthol CAS 63451-35-4 (2835)
 Hydroxynaphthol blue, 1-(2-Hydroxy-4-sulfo-1-naphthylazo)-2-naphthol-3,

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

Gd+++ sp none 25°C 0.0 U K1eff=3.76 1978BRb (99730)1051

Keff at pH 10

C20H18N4O2 HL (5917)
Pyruvic monohydrazone-3-hydrazino-4-benzyl-6-phenylpyridazine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	diox/w	30°C	75%	U			K(Gd+HL)=5.45 K(Gd+2HL)=11.05	1985RSb (99833)	1052

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
Gd+++	gl	KCl	25°C	0.10M	U			K1=18.89 K(GdL+H)=5.68	1994MMe (99999)	1053
Gd+++	gl	KNO3	20°C	0.10M	U			K1=19.16 K(GdL+H)=5.67 K(GdHL+H)=5.09	1985SNb (100000)	1054

C20H24N2O12S2 H6L CAS 3625-85-3 (5755)
N,N'-Bis(2-hydroxy-5-sulfobenzyl)-diaminoethane-N,N'-diethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	sp	KCl	25°C	0.10M	M			K1=22.27	1990MMa (100033)	1055
Gd+++	gl	KCl	25°C	0.10M	C			K1=23.36 K(GdL+H)=3.86 K(GdHL+H)=5.10 K(GdH2L+H)=4.03 K(GdH3L+H)=1.96	1989MSc (100034)	1056

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
Gd+++	cal	non-aq	25°C	100%	C	H		K1=2.91	1998LHa (100121)	1057
Medium: acetonitrile. DH(K1)=4.10 kJ mol ⁻¹ .										
Gd+++	gl	oth/un	25°C	0.0	U	H		K1=2.57	1991HJa (100122)	1058

C20H24O12S2 H2L CAS 172985-47-6 (7820)
2,3:11,12-Dibenzo-1,4,7,10,13,16-hexaoxacyclooctadeca-2,11-diene-4',4''-disulfonic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Gd+++ dis R4N.X 25°C 0.12M C K1=1.51 1998SUa (100281)1059
Medium: 0.12 M Et4NBr.

Method:solvent extraction into cyclohexane/di(2-ethylhexyl)phosphoric acid

C20H35N5O10 H5L (6545)
1,4,7,10,13-Pentaazacyclopentadecane-N,N',N'',N''',N''''-pentaethanoic acid;

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

Gd+++ gl NaNO3 25°C 0.20M C K1=15.88 1991KKa (100535)1060

Gd+++ gl NaClO4 25°C 0.20M C K1=15.88 1990KMd (100536)1061

C20H35N5O10 H3L (6623)
1,4,7-Tris(carboxymethyl)-13,16-dioxo-1,4,7,10,19-pentaazacycloheneicosa-9,20-dione
;

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

Gd+++ sp KCl 25°C 0.08M U K1=17.4 1994FCa (100556)1062

Gd+++ gl KCl 25°C 0.10M C K1=17.44 1992CKa (100557)1063
Data also for some related ligands

C20H37N5O8 H3L (7381)
Diethylenetriamine-N,N,N',N'',N'''-pentaethanoic acid bis(isopropylamide);

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

Gd+++ gl KCl 25°C 0.10M C K1=17.07 1997WCa (100729)1064

C20H37N5O10 H3L MEA CAS 129009-83-2 (7322)
N,N'-Bis(2-methoxyethylcarbamoylmethyl)diethylenetriamine;

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

Gd+++ gl NaClO4 25°C 0.10M C H K1=16.84 1997ICa (100734)1065
DH(K1)=-27.5 kJ mol⁻¹, DS=230

C20H38N4O10 H3L CAS 214461-75-3 (1659)
10-(2-Hydroxypropyl)-1,4,7,10-tetraazacyclododecane-1,4,7-tris(2-hydroxymethylethanoic acid);

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

Gd+++ gl R4N.X 25°C 0.10M C H K1=19.4 2000BCa (100748)1066
Medium: 0.10 M NMe4Cl. K1 corresponds to 3 weeks equilibration.

For complexes formed in minutes: K1=15.2, B(GdHL)=19.8, B(GdH2L)=22.8.

C20H40N8O4 L CAS 219143-29-0 (1185)
 1,4,7,10-Tetrakis(methylcarbamoymethyl)-1,4,7,10-tetraazacyclododecane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	R4N.X	25°C	0.10M	C	H		K1=12.8 K(GdL+H)=3.4 K(GdL+OH)=5.8	2000BCa (100846)	1067

Medium: 0.10 M NMe4Cl. K1 corresponds to 3 weeks equilibration.
 For complexes formed in minutes: K1=8.6, K(Gd+L+H)=13.2.

Gd+++	gl	R4N.X	25°C	0.10M	U			K1=12.8 K(GdL+H)=3.4 K(GdL+OH)=5.8	1998ABd (100847)	1068
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Medium: 0.10 M Me4NNO3.

 C20H43O4P HL CAS 7785-87-1 (2132)
 Didecylphosphoric acid; (C10H21O)2P(O)OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	kin	oth/un	25°C	0.02M	U			K1=4.17	1974GMc (100906)	1069

 C20H48N4O8P4 H4L (6569)
 1,4,7,10-Tetraazacyclododecane-1,4,7,10-tetrakis(methyleneethylphosphinic acid);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	KCl	25°C	0.10M	C			K1=16.5	1997HTa (100994)	1070

Gd+++	gl	KNO3	25°C	0.10M	C			K1=16.50	1991LSc (100995)	1071
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 C20H48N4O12P4 H8L C8-DOTP (7968)
 1,4,7,10-Tetraazacyclododecan-1-(1-octyl-Me-phosphonic acid)-4,7,10-tris(methylene phosphonic ac);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	oth	none	37°C	0.0	C			K(GdL+HSA)=4.16	2001CGb (100997)	1072

Method: ultrafiltration. HSA=human serum albimin. K(GdL+BSA)=3.70.

 C21H17N2O5As H2L ArsenoBDMPH (5931)
 2-Arsonodibenzoylmethanephenylhydrazone; C6H5.CO.C(CO.C6H5):N.NH.C6H4.AsO3H2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	alc/w	27°C	40%	U			K1=14.20 B2=18.66	1990M0c (101078)	1073

Medium: 40% v/v EtOH/H2O, 0.1 M NaClO4

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

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

Gd+++ sp non-aq 20°C 100% U K1=8.5 B2=15.20 1997PBa (101087)1074
K3=6.9

Medium: CH3CN

C21H22N4O HL CAS 56932-30-0 (5308)
1-Hydroxy-2-(2-N-methylanabasiny1-alpha-azo)naphthalene;

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

Gd+++ sp oth/un ? ? U B2=16.44 1967PAa (101201)1075

C21H30N4O10 H5L (7850)
N,N-Bis[2-[N',N'-bis(carboxymethyl)amino]ethyl]-4-amino-L-phenylalanine;

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

Gd+++ gl KCl 25°C 0.10M C K1=22.0 1996DMb (101370)1076

C21H31N3O9 H4L TTDA-H1P (7934)
N'-(2-Hydroxy-1-phenylethyl)di(carboxymethyl)triazadodecanedioic acid;

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

Gd+++ gl R4N.X 25°C 0.10M M K1=17.16 2001Cwa (101398)1077

Medium: 0.10 M Me4NNO3. Method: by competition with EDTA

C21H31N3O9 H4L TTDA-H2P (7935)
N'-(2-Hydroxy-2-phenylethyl)di(carboxymethyl)triazadodecanedioic acid;

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

Gd+++ gl R4N.X 25°C 0.10M M K1=17.44 2001Cwa (101403)1078

Medium: 0.10 M Me4NNO3. Method: by competition with EDTA

C22H14O9 H5L CAS 4431-00-9 (3513)
Aurintricarboxylic acid;

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

Gd+++ sp oth/un 25°C ? U 1967SAa (101500)1079

K(Gd+HL)=4.8(?)

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

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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++     sp  oth/un  ?    ?    U          K1=15.15      1971SSi (101544)1080
*****
C22H18N4O14As2S2      H8L    Arsenazo III      CAS 1668-00-4 (1148)
2,7-Bis(2'-arsonophenylazo)chromotropic acid;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++     sp  oth/un  rt   0.10M C          2004LLa (101621)1081
                                K1eff=4.24
                                B2eff=9.50
                                B(2,2)eff=13.61
Method: spectral deconvolution. Medium: 0.1 M chloroacetate buffer, pH 3.5
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-----
Gd+++     sp  oth/un  25°C  var  U  I          1997HRb (101622)1082
                                K1(eff)=7.495
                                B(GdLCl)eff=7.201
                                B(GdL2Cl)eff=13.650
Conditional constants in chloride medium at pH 3.3. Also data in sulfate
and perchlorate media. K(Gd+Cl)=1.939.
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Gd+++     kin  oth/un  25°C  0.10M U          1994RCb (101623)1083
                                K(GdL+H)=4.51
                                K(GdL2+H)=4.85
Medium: 0.1 M CH3COONa.
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Gd+++     sp  NaClO4  25°C  0.10M U          1975NMa (101624)1084
                                K(Gd+H5L)=7.73
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Gd+++     sp  oth/un  20°C    ?    U          1972SSi (101625)1085
                                K(Gd+H4L)=15.75
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Gd+++     sp  oth/un  ?    ?    U          1967ECa (101626)1086
                                K(Gd+H5L)=5.4    pH 1-4
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Gd+++     sp  NaNO3   20°C  0.20M U          1963BUa (101627)1087
                                B(Gd2L2)=80.5
*****
C22H19N3O4S          HL          CAS 84819-63-6 (8347)
N-(3,4-DiMe-5-isoxazoly1)-4-[[ (2-hydroxy-1-naphthalenyl)methylene]amino]benzenesulf
onamide;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++     gl  NaClO4  25°C  0.10M U          K1=6.64  B2=11.25  1982MBa (101686)1088
*****
C22H20O13          H5L    Carminic acid      CAS 1260-17-9 (714)
Carminic acid;
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Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo

Gd+++ sp oth/un ? 0.10M U 1970PLc (101701)1089
K(GdOH+2H3L)=16.90

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

Gd+++ EMF KNO3 25°C 0.10M C T H K1=10.94 1990HLA (101896)1090
K(GdL+H)=3.54

Method: Competitive reaction with Hg++, using Hg indicator electrode.
Data for 15-35 C. DH(K1)=-31.5 kJ mol⁻¹, DS(K1)=104 J K⁻¹ mol⁻¹.

C22H26N4O10 H4L BAPTA (7230)
1,2-Bis(o-aminophenoxy)ethane-N,N,N',N'-tetraethanoic acid;
((HOOCCH2)2NCH(OC6H4NH2)2

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

Gd+++ gl R4N.X 25°C 0.10M C K1=10.6 1993YTa (101977)1091

C22H28O13S2 H2L DSDB21C7 CAS 204931-02-2 (7821)
2,3:11,12-Dibenzo-1,4,7,10,13,16,19-heptaoxacycloheptacosane-2,11-diene-4',4''-disulfo
nic acid;

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

Gd+++ dis R4N.X 25°C 0.12M C K1=1.77 1998SUa (102077)1092
Medium: 0.12 M Et4NBr.

Method: solvent extraction into cyclohexane/di(2-ethylhexyl)phosphoric acid

C22H29N5O6 H3L (6506)
N,N''-2-Bis(2-pyridylmethyl)diethylenetriamine-N,N',N''-triethanoic acid;

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

Gd+++ gl NaCl 25°C 0.10M U K1=16.83 1990CQa (102096)1093

C22H30N4 L CAS 250790-21-7 (7943)
N,N'-Bis(1,1-dimethylethyl)-1,10-phenanthroline-2,9-dimethanamine;

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

Gd+++ gl NaCl04 25°C 0.10M U K1=8.26 2001WZa (102113)1094
B(GdHL)=15.15

Also data for the N,N'-diethyl, isopropyl, butyl and isobutyl derivatives.

C22H31N3O10 H5L CAS 445269-58-9 (8992)
(4S)-4-Benzyl-3,6,10-tris(carboxymethyl)-3,6,10-triazadodecanedioic acid;

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

Gd+++ gl R4N.X 25°C 0.10M M K1=23.79 2002CLb (102181)1095
Medium: 0.1 M Me4NNO3.

C22H31N3O11 H5L BOPTA (7460)
2,5,8-Tris(carboxymethyl)-12-phenyl-11-oxa-2,5,8-triazadodecane-1,9-dicarboxylic
acid;

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

Gd+++ gl NaCl 25°C 0.15M C M K1=22.61 1999BCb (102185)1096
B(GdHL)=24.33
B(GdHL(ATP))=31.76
B(GdH2L(ATP))=35.43
B(GdH3L(ATP))=38.1
B(GdH4L(ATP))=40.8, B(GdH5L(ATP))=43.23, B(GdHL(P3O10))=32.34,
B(GdH2L(P3O10))=37.90, B(GdH3L(P3O10))=40.88, B(GdH4L(P3O10))=43.71.

Gd+++ gl R4N.X 25°C 0.10M C H K1=22.58 1996BCd (102186)1097
B(GdHL)=24.33
Medium: Me4Cl. DH(GdL)=-4.9 kJ mol⁻¹, DS=87 J K⁻¹ mol⁻¹; DH(GdHL)=3.5, DS=100

Gd+++ gl KCl 20°C 0.10M C K1=22.59 1995UAa (102187)1098

C22H35N3O10 H5L CAS 158091-75-9 (7701)
meso-Bis(trans-2-aminocyclohexyl)amine-N,N,N',N'',N''-pentaethanoic acid;

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

Gd+++ gl KCl 25°C 0.10M C K1=20.42 2000SMc (102250)1099
K(GdL+H)=2.38

C22H35N3O10 H5L CAS 158091-75-9 (7700)
rac-Bis(trans-2-aminocyclohexyl)amine-N,N,N',N'',N''-pentaethanoic acid;

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

Gd+++ gl KCl 25°C 0.10M C K1=20.71 2000SMc (102252)1100
K(GdL+H)=1.92

C22H37N5O14 H7L CAS 3234-59-1 (2425)
Tetraethylenepentamineheptaethanoic acid;

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

Gd+++ vlt R4N.X 30°C 0.01M C K1=20.42 1981GMh (102326)1101

Method: polarography, using Cd as indicator ion. Medium: 0.01 M Et4NBr.

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-----
Gd+++      gl  KNO3  25°C 0.10M U      K1=20.41      1968MIc (102327)1102
                      K(Gd+HL)=14.11
                      B(GdH-1L)=5.34
```

```
C22H40N4O8          H4L          CAS 138763-18-5 (8607)
5,7,12,14-Tetramethyl-1,4,8,11-tetraazacyclotetradecane-N,N',N'',N'''-tetraethanoic
acid;
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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++      gl  KNO3  40°C 0.50M U T      K1=18.23      1995BIa (102356)1103
                      K(GdL+H)=4.07
```

Also data for 80 C.

```
C22H41N5O8          H3L          CAS 189687-33-0 (7103)
Diethylenetriamine-N,N',N''-triethanoic acid-N,N''-bis(butylamide);
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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++      gl  KCl   25°C 0.10M C      K1=17.15      1997WCa (102388)1104
```

```
C22H41N5O10        H3L    MMEA          CAS 192631-00-8 (7323)
N,N'-Bis(methyl-2-methoxyethylcarbomoylmethyl)diethylenetriamine;
```

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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++      gl  NaClO4 25°C 0.10M C H      K1=17.69      1997ICa (102392)1105
DH(K1)=-35.3 kJ mol-1, DS=220
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C23H16O9Cl2S      H4L    Chrome azuro1 S CAS 1667-99-8 (711)
Chromazuro1 S;
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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++      sp  oth/un 25°C    ? U          1967SAa (102559)1106
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K(?)=4.4

```
C23H18N2O3          HL          (5561)
2-(2-Acetylphenylhydrazone)-1,3-diphenyl-prop-1,3-dione;
C6H5.CO.C(CO.C6H5):N.NH.C6H4.COCH3
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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++      gl  diox/w 30°C 75% U      K1=11.00 B2=19.75 1988ESb (102594)1107
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```
C23H18O9S          H4L    Eriochrome cyan CAS 3564-18-9 (433)
4'-Hydroxy-3,3'-dimethyl-2''-sulfofuchson-5,5'-dicarboxylic acid;
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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Gd+++	sp	oth/un	25°C	?	U		B2=9.8	1968MDc (102630)	1108

C23H24N4O2		L				Trichachnine	CAS 1251-85-0	(2606)	
4,4'-Diantiprylmethane, 4,4'-phenylmethylene-bis-(1,2-dihydro-1,5-dimethyl-2-phenylpyrazol-3-one									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Gd+++	sp	diox/w	25°C	100%	U		K1=4.23	1995KMa (102672)	1109

C23H33N3O11		H5L					CAS 158599-72-5	(7657)	
S-2-(4-Ethoxybenzyl)-1,4,7-triazaheptane-N,N,N',N'',N'''-pentaethanoic acid;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Gd+++	gl	KCl	25°C	0.10M	C		K1=23.45 K(CdL+H)=2.17	1999SBd (102818)	1110

C23H54N4O12P4		H8L				C11-DOTP	(7969)		
1,4,7,10-Tetraazacyclododeca-1-(1-Undecyl-Me-phosphonic acid)-4,7,10-tris(methylene phosphonic);									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Gd+++	oth	none	37°C	0.0	U		K(GdL+HSA)=5.40	2001CGb (102850)	1111
Method: ultrafiltration. HSA=human serum albimin. K(GdL+BSA)=4.83.									

C24H16O16S8		H8L					CAS 237770-97-7	(8854)	
25,26,27,28-Tetrahydroxy-2,8,14,20-tetrathiacalix[4]arene-5,11,17,23-tetrasulfonic acid;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Gd+++	cal	oth/un	25°C	0.01M	C	H	K1=3.30	2004LWa (102867)	1112
Medium: 0.01 M HCl. DH(K1)=9.0 kJ mol ⁻¹ , DS(K1)=89.3 J K ⁻¹ mol ⁻¹ .									

C24H29N3O12S3		H6L					(7355)		
1,2,3-Tris((2-hydroxy-5-sulfobenzyl)amino)propane;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Gd+++	gl	NaCl	25°C	0.16M	C		K1=14.50 K(GdL+H)=6.38	1998Lca (103016)	1113

C24H32N2O6		H3L				Me4-HBED	(6507)		
N,N'-Bis(2-hydroxy-3,5-dimethylbenzyl)ethylenediamine-N,N'-diethanoic acid;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo	
Gd+++	sp	KCl	25°C	0.10M	M		K1=20.27	1990MMa (103063)	1114	

		C24H32O14S2	H2L				CAS 204931-03-3	(7822)		
2,3:11,12-Dibenzo-1,4,7,10,13,16,19,22-octaoxacyclotetracos-2,14-diene-4',4''-disulfonic acid;										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Gd+++	dis	R4N.X	25°C	0.12M	C		K1=1.84	1998SUa (103193)	1115
Medium: 0.12 M Et4NBr.									
Method:solvent extraction into cyclohexane/di(2-ethylhexyl)phosphoric acid									

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo	
Gd+++	gl	NaNO3	25°C	0.20M	C		K1=22.95 K(Gd+H2L)=17.26	1991KKa (103375)	1116	

		C24H45N5O12	H3L	HEMEA			CAS 185214-83-9	(7324)		
N,N'-Bis(2-hydroxyethyl-2-methoxyethylcarbonylmethyl)diethylenetriamine;										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Gd+++	gl	NaClO4	25°C	0.10M	C	H	K1=17.49	1997ICa (103443)	1117
DH(K1)=-35.1 kJ mol ⁻¹ , DS=217									

		C25H32N2O7	H2L				(7374)		
1,15-Diaza-3,4:12,13-dibenzo-5,8,11-trioxacyclooctadecane-N,N'-diethanoic acid;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Gd+++	gl	KNO3	25°C	0.5M	C		K1=5.55	1993YNa (103730)	1118

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Gd+++	gl	diox/w	30°C	75%	U		K1=12.03 B2=22.54	1985RSb (103880)	1119

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

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

Gd+++ gl R4N.X 25°C 0.10M C K1=13.54 1993YTa (103963)1120

 C26H32N4O14 H4L CAS 372109-77-8 (8980)
 9,20-Dihydroxy-10,21-dioxo-23,24-dioxa-3,6,14,17-tetraazatricyclo-tetracosatetraen-
 etraethanoic:

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

Gd+++ gl NaCl 25°C 0.16M M K1=17.6 2001SKe (104047)1121
 K(GdL+H)=9.36
 K(GdHL+H)=9.04
 K(Gd+H2L)=8.81
 K(Gd+H3L)=6.80
 K(Gd+H4L)=3.90, K(Gd+H5L)=3.7, K(Gd+H6L)=3.6, K(Gd+H7L)=3.0,
 K(Gd+HL)=13.0.

 C26H33N3O12S3 H6L (7354)
 1,1,1-Tris(((2-hydroxy-5-sulfobenzyl)amino)methyl)ethane;

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

Gd+++ gl NaCl 25°C 0.16M C K1=11.86 1998Lca (104063)1122
 K(GdL+H)=6.55

 C26H34N6O8 H4L CAS 132709-65-0 (8941)
 3,6,14,17,23,24-Hexaazatricyclo-tetracos-1,8,10,12,19,21-hexaene-3,6,14,17-tetra-
 tic acid;

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

Gd+++ gl KCl 25°C 0.10M M K1=21.7 1996MBb (104094)1123
 Method: competitive titration with arsenazo-III.

 C26H38N6 L CAS 180684-75-7 (7295)
 1,8,14,17,24,31-Hexaazatricyclo[25.3.1.1.0.0]dotriaconta-10,12,14,26,28,

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

Gd+++ gl KNO3 25°C 0.20M C K1=5.6 1996FJa (104205)1124

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

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

Gd+++ gl diox/w 30°C 75% U K1=8.40 1983RSa (104384)1125

C27H32N6O8 H3L CAS 319430-96-1 (8037)
 4-[2-(2-Hydroxybenzoylamino)ethyl]-1,7-bis[2-(1,2-dihydro-3-hydroxy-1-methyl-2-oxo-
 4-pyridinyl)+;

```

-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++      gl  KCl      25°C 0.10M C          K1=17.3      2000CXa (104522)1126
                                B(GdHL)=23.6
                                B(GdH2L)=27.9

```

Also data for related ligands.

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*****
C27H33N7O9          HL          CAS 159356-07-7 (8682)
N,N,N'-(Nitriлотri-2,1-ethanediyl)tris[1,2-dihydro-3-hydroxy-1-methyl-2-oxo)4-pyrid
inecarboxamide

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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++      gl  KCl      25°C 0.10M U          K1=20.3      1995XFa (104542)1127
                                B(GdHL)=23.8

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*****
C27H36N4O6          H6L          CAS 222626-11-1 (8885)
Tris((2,3-dihydroxybenzylamino)ethyl)amine;

```

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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++      gl  NaCl04 25°C 0.10M C          B(GdHL)=27.51
                                B(GdH2L)=34.17
                                B(GdH3L)=40.08
                                B(GdH6L2)=79.10

```

K(Gd+H3L)=8.49, K(GdH3L+H3L)=7.43.

```

*****
C27H36N4O12S3       H6L          (7353)
Tris(((2-hydroxy-5-sulfobenzyl)amino)ethyl)amine;

```

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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++      gl  NaCl    25°C 0.16M C  H    K1=6.67  B2=14.36  1995CHa (104563)1129
By calorimetry: DH(K1)=-12.11 kJ mol-1, DS(K1)=88 J K-1 mol-1; DH(K2)=
-15.15, DS(K2)=97.

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*****
C27H36N10O9          H3L  TrenHOPY          (7967)
Tris[(2,3-dimethyl-5-hydroxy-6-carboxamido-4-pyrimidinone)ethyl]amine;

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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++      gl  KCl      25°C 0.10M U          K1=18.2      2001SBb (104578)1130
                                B(GdHL)=22.4
                                B(GdH2L)=26.6

```

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*****
C27H44O          L  Vitamin D3          CAS 67-97-0 (6103)
7-Dehydrocholesterol, Cholecalciferol
-----

```

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

 Gd+++ gl alc/w 25°C 70% C K1=9.33 2003MYc (104614)1131
 Medium: 70% v/v EtOH/H2O, 0.10 M KNO3.

 C28H24O16S4 H8L CAS 206559-10-6 (7767)
 25,26,27,28-Tetrahydroxycalix[4]arene-5,11,17,23-tetrasulfonic acid;

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

 Gd+++ cal oth/un 25°C 0.10M C H K(Gd+H4L)=3.94 2001BIa (104697)1132
 Medium: 0.10 m Na4H4L, pH=2. DH(Gd+H4L)=9.8 kJ mol-1.

 C28H36N2O14S2 L CAS 84162-07-2 (7948)
 15,15'-Dithiobis[2,3,5,6,8,9,11,12-octahydro-16-nitro-1,4,7,10,13-benzopentaoxacycl
 opentadecin]

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

 Gd+++ sp non-aq 25°C 100% C T H K(GdNO3+L)=2.51 1997LQa (104789)1133
 Medium: acetonitrile. Data for 20-35 C. DH(GdNO3+L)=58.43 kJ mol-1.

 C28H37N5O8 H3L (7382)
 Diethylenetriamine-N,N,N',N'',N''-pentaethanoic acid bis(benzylamide);

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

 Gd+++ gl KCl 25°C 0.10M C K1=16.48 1997WCa (104800)1134
 Medium: acetonitrile. Data for 20-35 C. DH(GdNO3+L)=58.43 kJ mol-1.

 C28H40N4O4 H2L CAS 138110-63-1 (8608)
 7,14-Dimethyl-5,12-diphenyl-1,4,8,11-tetraazacyclotetradecane-1,8-diethanoic acid;

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

 Gd+++ gl KCl 40°C 0.50M M K1=9.53 1997BZa (104824)1135
 Medium: acetonitrile. Data for 20-35 C. DH(GdNO3+L)=58.43 kJ mol-1.

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

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

 Gd+++ gl non-aq 25°C 100% U K1=3.62 1980MDb (104839)1136
 Medium: Propylene carbonate.

Medium: propylene carbonate

 C28H40O10 L DiBz-30-crown10 CAS 104946-67-0 (1776)
 2,3:17,18-Dibenzo-1,4,7,10,13,16,19,22,25,28-decaoxacyclotriaconta-2,17-diene;

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

Gd+++ ISE non-aq 25°C 100% U K1=3.53 1982MDa (104883)1137

Medium: propylene carbonate

C28H64N4O12P4 H4L CAS 154882-99-2 (8222)

1,4,7,10-Tetraazacyclododecane-1,4,7,10-tetramethylenephosphonic acid tetrabutyl ester;

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

Gd+++ gl R4N.X 25°C 0.10M C K1=12.19 2001BKb (105067)1138

Medium: 0.10 M Me4NCl.

C30H41N5O10 H3L (7506)

1,4,7,10,13-Tetraaza-1,13-(2-methoxybenzyl)-tridecane-2,12-dione-4,7,10-triethanoic acid;

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

Gd+++ gl KCl 25°C 0.10M U K1=16.82 1998Wlb (105295)1139

C30H44N2O6 H3L (6508)

N,N'-Bis(2-hydroxy-3-methyl-5-tert-butylbenzyl)diaminoethane-N,N'-diethanoic acid;

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

Gd+++ sp KCl 25°C 0.10M M K1=20.38 1990Mma (105316)1140

C31H24N4O HL CAS 88700-85-0 (1409)

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

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

Gd+++ gl diox/w 30°C 75% U I K1=9.14 1983RRa (105403)1141

In 75% MeOH: K1=7.61; 75% DMF: 6.39

C31H32N2O13S H6L Xylenol orange CAS 63721-85-5 (432)

5,5'-Bis-N,N-bis(carboxymethyl)aminomethyl-4'-hydroxy-3,3'-dimethylfuchstone-2"-sulfonic acid;

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

Gd+++ sp NaNO3 20°C 0.20M U 1963BBb (105471)1142

B(Gd2L2)=43.1

C32H28N8O10S2 H4L Diantipyrylazo CAS 14918-39-9 (5368)

2,7-Bis(antipyrynylphenylazo)chromotropic acid;

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

Gd+++ sp KNO3 ? 0.20M U 1968BBa (105570)1143
K(?)=80.3

C32H34N4O2 L CAS 163892-66-8 (7329)
1-Phenyl-1,1-di(2,3-dimethyl-1-phenyl-3-pyrazolyl-5-one)butane;C6H5C(C3H7)((C2N2(O)
(CH3)2(C6H5))2

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

Gd+++ sp diox/w 25°C 100% C 1997KMa (105630)1144
K(La(NO3)2+L)=4.00

C32H45N5O10 H3L (7507)
1,4,7,10,13-Pentaaza-1,13-di(2-ethyl-(2-methoxyphenyl))tridecane-2,12-dione-4,7,10-
triethanoic a;

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

Gd+++ gl KCl 25°C 0.10M U K1=16.91 1998Wlb (105784)1145

C33H44N3O14P H6L CAS 193901-91-6 (7981)
(4,4-Diphenylcyclohexyl)(methylene-2-dien pentaethanoic acid) phosphoric acid;

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

Gd+++ gl NaClO4 25°C 0.10M C K1=22.06 2001CCa (105938)1146
K1 from competitive titration using EDTA. In 0.10 M Me4NCl, K1=23.2.

C33H45N7O12 H3L CAS 282529-02-6 (7690)
Tris[3-hydroxy-1-(methoxyethyl)-2-oxo-1,2-didehydropyridine-4-carboxamido]ethyl]ami
ne;

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

Gd+++ gl KCl 25°C 0.10M C K1=19.69 2000JOa (105979)1147
B(GdHL)=22.80
B(GdH2L)=25.88

Additional method: spectrophotometry.

C34H53N5O8 H3L (7508)
1,4,7,10,13-Pentaaza-1,13-bis(adamantanyl)tridecane-2,12-dione-4,7,10-triethanoic
acid;

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

Gd+++ gl KCl 25°C 0.10M U K1=16.85 1998Wlb (106092)1148

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


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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++      gl  alc/w  25°C 100% M          K1=8.3      B2=15.3     1989TMa (106135)1149
                               B3=18.7

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Medium: MeOH

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C36H32O24S4          H8L          CAS 171798-10-0 (9139)
25,26,27,28-Tetrakis(hydroxycarbonylmethoxy)calix[4]arene-5,11,17,23-tetrasulfonic
acid;

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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++      cal oth/un 25°C 0.01M C  H   K1=3.86      2004LWa (106227)1150
Medium: 0.01 M HCl. DH(K1)=5.5 kJ mol-1, DS(K1)=93.0 J K-1 mol-1.

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C36H40O20S4          L          CAS 851791-27-0 (9149)
Sulfonatomethylated calix[4]resorcinarene;

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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++      nmr oth/un 25°C 100% C   C   K1=3.1      2004AMb (106310)1151
Medium: D2O, pH 2 (HCl). Method: 1H nmr.

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C36H54O12          L          (6732)
1,8-Dioxooctamethylenebis(4'-2,3-benzo-1,4,7,10,13-pentaoxacyclopentadecane);

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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++      dis non-aq 25°C 100% U          B(Gd+3P+2L)=8.83
                               1993INa (106422)1152

```

By solvent extraction into dichloromethane. B is the extraction constant
 $Gd(aq)+picrate(aq)+L(org)=GdL2P3(org)$.

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C36H60O30          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
-----
Gd+++      gl  NaCl  25°C 0.10M U  I   K1=2.5      1999FBa (106464)1153
In 0.1 M Me4NCl, K1=2.78.

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C37H33N5O4          L          (7366)
2,6-Bis(1-(3,5-dimethoxybenzyl)benzimidazol-2-yl)pyridine

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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++      gl  non-aq 25°C 100% C          K2=4.8      1997PBa (106548)1154
                               K3=3.2

```

Medium: CH3CN; 0.1 M Et4NC104

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	NaClO4	30°C	0.10M	U			K(Gd+H3L)=4.30 K(Gd+H2L)=6.70 K(GdH2L+H)=4.74	1980NAb (106601)	1155

Also data for GdHnL(OH) species

C47H46N6O4 L (7367)
2,6-Bis(1-(3,5-dimethoxybenzyl)benzimidazol-2-yl)-4-(4-diethylamino)phenylpyridine
;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	non-aq	25°C	100%	C			K3=6.1	1997PBa (107315)	1156

Medium: CH3CN; 0.1 M Et4NClO4

C52H69NO7 L CAS 178626-47-6 (8569)
5,11,17,23-Tetra-t-butyl-25-(diethylcarbamoyl)methoxy-27-carboxymethoxy-26,28-dihydroxycalix[4]ar

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	sp	non-aq	25°C	100%	C			K1=6.02	2002BBc (107512)	1157

Method: uv/vis spectroscopy. Medium: DMSO. Also data for the 25-methoxy-ethyl(carbamoylmethoxy)- and 25-di-(n-hexyl-carbamoyl)methoxy- derivatives

C62H94N2O4S2 L (8109)
5,11,17,23-Tetrakis(1,1-dimethylethyl)-25-27-bis[2-methylthio]ethoxy]...calix(4)arene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	cal	non-aq	25°C	100%	U	H		K1=5.06	2001NJa (107703)	1158

Method: microcalorimetry. Medium: MeCN.. DH(K1)=-146 kJ mol⁻¹

C76H116N4O8 L (8156)
p-tert-Butylcalix(4)arene tetradiisopropylethanoamide;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	cal	non-aq	25°C	100%	U	H		K1=5.24	2001NJa (107880)	1159

Method: microcalorimetry. Medium: MeCN.. DH(K1)=-79.1 kJ mol⁻¹

Polymer HL Bleomycin (2324)

Bleomycin A2, B2 etc.

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

Gd+++ sp oth/un 25°C ? U 1980LPb (108089)1160
K1eff=4.34 pH 6.8

Method: fluorescence

Polymer (1526)
Bovine serum albumin protein

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

Gd+++ nmr NaCl 27°C 0.15M C M K1=4.35 1985JAa (108103)1161
B(Gd(CO3)L)=>8.0
B(GdH(CO3)L)=>16.0

Method: proton relaxation enhancement.

Polymer L (3532)
Human transferrin;

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

Gd+++ sp oth/un 25°C 0.10M U 1992HCa (108214)1162
Keff(Gd+L)=7.96
Keff(GdL+Gd)=5.94

Medium: N-(2-Hydroxyethyl)piperazine-N'-2-ethanesulfonic acid, pH 7.4

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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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