

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 (511) 1		
									K(Gd+3e=Gd(s))=-115.1(-2.27V)	
									K(Gd+e=Gd(II))=-61(-3.6V)	

Method: Literature evaluated data

Gd+++	oth	none	25°C	0.0	U			1952LAb (512) 2		
									K(Gd+3e)=-121.5(-2400 mV)	

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 (1147) 3		
									Kso(GdAsO4)=-21.67	

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 (2689) 4		
									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	

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 2004LBb (3228) 5		
									K(Gd+HCO3=GdHCO3)=1.31	

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
Gd+++ cal none 25°C 0.00 M H K1=3.59 1972SCd (3650) 12
 $\text{DH}(K1)=4.4 \text{ kJ mol}^{-1}$, $\text{DS}=83.3 \text{ J K}^{-1} \text{ mol}^{-1}$

Gd+++ con oth/un 25°C 0.0 U K1=3.74 1963DKb (3651) 13

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

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
Gd+++ dis NaCl 25°C 1.0M C K1=-0.16 1997HTb (4924) 14
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 B2=4.77 1991ITa (4925) 15
K3=1.44
K4=1.11

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
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Gd+++	sol	NaClO4	25°C	?	U	K1=0.33		1982MAa	(4927)	17
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Gd+++	cal	non-aq	25°C	100%	U	K1=1.23	B2=2.94	1980VCa	(4928)	18
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Medium: dimethylacetamide

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

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

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Gd+++	ix	oth/un	25°C	0.02M	C T H		K1=3.71	B2= 6.07	2004LMa	(6914)	21
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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
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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
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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
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Gd+++	ISE	none	25°C	0.0	C H		K1=3.21	B2=6.56	1989MJa	(6918)	25
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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
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Gd+++	cal	NaClO4	25°C	1.00M	C H				1988GBa	(6920)	27
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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
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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
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Gd+++ gl KCl 25°C 1.00M U M 1981KTb (6923) 30
 $K(\text{GdEDTA}+\text{F})=1.73$
 $K(\text{Gd}(\text{EDTA})\text{F}+\text{F})=0.48$

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
 $K(\text{Gd}+\text{HF}=\text{GdF}+\text{H})=0.46$

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

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-		HL	Hydroxide				(57)
Hydroxide;							

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.

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

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*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(GdP04)=-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(GdP04)=-26.92

In synthetic seawater, Ks(GdP04)=-24.26.

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

K(Gd+HP04)=4.11

K(Gd+2HP04)=7.38

K(Gd+H2P04)=1.71

Distribution of 153Gd between 0.68 m NaClO4 and TBP. Calculated for I=0, K1=12.19, K(Gd+HP04)=5.91, K(Gd+2HP04)=9.97, K(Gd+H2P04)=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 K(Gd+HL)=5.10 K(GdL+OH)=4.73	1999BCb (13861)	80
Gd+++	gl	KNO3	25°C	0.10M	U T H			B2=8.9 K(Gd+2HL)=6.6	1974KRa (13862)	81
								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 K(Gd+HL)=4.91 K(Gd+2HL)=8.72	1962RKa (13863)	82

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

CH03F3S 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

$$\begin{aligned} K(\text{Gd}+\text{H}-1\text{L}) &= 8.9 \\ K(\text{Gd}+2\text{H}-1\text{L}) &= 18.4 \\ K(\text{Gd}+3\text{H}-1\text{L}) &= 23 \text{ approx} \end{aligned}$$

Glyoxylic acid; $\text{OHC}\cdot\text{COOH}$

Gd+++	g1	NaClO4	20°C	0.10M	U	K1=2.49	B2=4.53	1964PSd (18422)	97
						K3=1.5			

Ethanedioic acid; (COOH)₂

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

[illegible]

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

2-Amino-5-mercapto-1,3,4-thiadiazole:

Gd+++ g1 NaClO4 25°C 0.10M U T H K1=6.50 B2=11.90 1983SSb (19254) 103
K3=4.18

Ethanoic acid; CH_3COOH

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

Gd+++	gl	NaCl04	25°C	0.50M	C	T	K1=2.52	B2=4.62	1977Cma	(20546)	117
							B3=5.78				
							B4=7.18				

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

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			

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			

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

Gd+++ gl KN03 25°C 0.0 M T H K1=5.89 2003MBa (21561) 123
K(Gd+HL=GdL+H)=-3.75

Gd+++ g1 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	

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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      K(Gd+HL)=3.72  1987RRc (21566) 128
-----
Gd+++      gl  KNO3   35°C 0.10M U    M      K(Gd+HL)=3.72  1986RMb (21567) 129
K(Gd+HL+cytidine)=8.49
-----
Gd+++      gl  NaClO4 25°C 0.10M U      K(Gd+HL)=0.73  1981KBa (21568) 130
-----
Gd+++      EMF KCl    25°C 1.0M U    M      K(GdA+L)=3.70  1977GMa (21569) 131
              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.SO
-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++      sp  non-aq 25°C 100% U      K8=1.0      1992MBb (22100) 132
              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      K(GdH-1L+H)=7.25  1972MCd (22146) 133
*****
C2H6O6P2          H4L          (5706)
Ethene-1,1-diphosphonic acid; H2C:C(P(O3H2)2
-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++      gl  KCl    25°C 0.15M U    I      K(Gd+H2L)=5.25  1989AMa (22171) 134
*****
C2H8N2          L    Ethylenediamine CAS 107-15-7 (23)

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

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 B3=4.98	1992CBa (23162)	135

Medium: DMSO, 0.10 M Et4NClO4. By calorimetry, DH(K1)=-14.0, DH(B2)=-31.3, DH(B3)=-72.1 kJ mol⁻¹.

Gd+++	gl	KNO3	25°C	0.10M	U	TIH		K1=5.34 B2=10.19 B(GdAL)=9.04	1986NSa (23163)	136
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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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	sp	oth/un	25°C	0.70M	U			K(Gd+H2L)=5.64	1987APa (23375)	137

C3H4O2 HL Acrylic acid CAS 79-10-7 (2044)

Propenoic acid; CH2:CH.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	oth/un	25°C	?	U	M		K1=2.08 K(GdL+acac)=5.72 K(Gd(acac)L+acac)=4.33	1998PAa (23987)	138

Additional method: nmr. Medium not stated.

Gd+++	gl	NaClO4	25°C	0.10M	C	H		K1=1.88 B2=3.48 B3=5.0	1996HBa (23988)	139
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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

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	NaClO4	25°C	0.10M	M	M		K1=4.45 K(Gd(nta)+L)=2.74	1987NCa (24460)	141

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 B(GdHL)=6.49 B(GdHL2)=9.78	B2=6.24	1971DGa (24462)	143
Gd+++	ix	NaClO4	25°C	0.15M	U	K(Gd+HL)=1.65 K(GdHL+HL)=1.2		1968KKc (24463)	144
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; H00C.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	1996PJ a (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-Mercaptopropionic 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-Hydroxypropionic 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					CAS 79-33-4	(82)	
L-2-Hydroxypropionic 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	1996PJ a (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 1996PJb (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
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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
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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
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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)
 Nitritotris(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

$$K(\text{GdL}+\text{H})=7.37$$

$$K(\text{GdHL}+\text{H})=5.34$$

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

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 NaCl04 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
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Gd+++	gl	NaClO4	25°C	0.10M	C		K1=2.59 B(GdHL)=6.14 K(Gd+HL)=2.06	1986LCa (29199)	191
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Gd+++	gl	KNO3	25°C	0.10M	U T HM		K1=3.05 B(GdAL)=6.22	1986NSa (29200)	192
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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
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Gd+++	gl	NaClO4	25°C	0.50M	M		K1=3.69 B2=7.37	1991MOa (29267)	194
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Gd+++	gl	oth/un	25°C	?	U		K1=5.5 B2=10.0	1956GNc (29268)	195
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 C4H6O2 HL Methylacrylic (6992)
 2-Methylpropenoic acid; CH2:C(CH3)COOH

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=2.39	1995PAa (29698)	196
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 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
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Gd+++	gl	NaClO4	25°C	0.10M	M M		K1=3.42 K(Gd(nta)+L)=2.25	1987NCa (29976)	197
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Gd+++	gl	NaClO4	25°C	0.10M	M H		K1=3.42	1986CDb (29977)	198
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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 B(GdAL)=7.08	1986NSa (29978)	199
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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
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K(Gd+HL)=1.83

$$K(\text{GdHL}+\text{HL})=1.3$$

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	1996PJ a (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	1996PJ a (30632)	203
Gd+++	gl	KNO3	30°C	0.10M	U	M		1984AI a (30633)	204

$$K(\text{Gd}(\text{EDTA})+\text{L})=2.325$$

Gd+++	gl	NaClO4	25°C	0.10M	C		K1=4.75 B2=7.83	1980KBd (30634)	205
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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
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$$B(\text{GdHL})=7.81$$

Gd+++	gl	KNO3	20°C	0.10M	U		K1=4.57 B2=7.49	1980SDb (30636)	207
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$$K(\text{Gd}+\text{HL})=2.06$$

Gd+++	EMF	NaClO4	25°C	2.00M	U		K1=3.92 B2=6.53	1969JP a (30637)	208
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Gd+++	EMF	KCl	25°C	0.20M	U		K1=4.28	1964DAb (30638)	209
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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

$$K(\text{GdL}+\text{ida})=2.48$$

$$K(\text{GdL}+\text{gly})=2.61$$

$$B(\text{GdLA})=8.77$$

$$B(\text{GdLB})=9.65$$

H2A is tartaric acid, H2B is malic acid. Also data for quaternary systems:
GdLA+ida, GdLA+gly, GdLB+ida, GdLB+gly.

Gd+++ gl KCl 25°C 1.0M U M 1988KTa (30877) 211
K(Gd(edta)+L)=2.35

Gd+++ EMF NaClO4 20°C 1.00M U K1=5.49 B2=10.03 1972G0a (30878) 212
B3=13.22

Gd+++ cal NaClO4 25°C 1.0M C H 1963GRd (30879) 213
DH(K1)=-1.51 kJ mol⁻¹, DS(K1)=98.3 J K⁻¹ mol⁻¹; DH(B2)=-11.18,
DS(B2)=152; DH(B3)=-19.21, DS(B3)=184.

Gd+++ EMF NaClO4 20°C 1.00M U K1=5.40 B2=9.93 1963GTa (30880) 214
B3=13.04

Method: quinhydrone electrode

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Gd+++	sp	oth/un	25°C	0.0	U T H		K1=4.75	1975YBa (31261)	215
DH(K1)=-12.1 kJ mol ⁻¹ , DS=50.2 J K ⁻¹ mol ⁻¹									

Gd+++	gl	alc/w	25°C	40%	U I		K1=5.06	1972SSj (31262)	216
Medium: 0.05, 0-40% ethanol									

Gd+++	gl	alc/w	25°C	40%	U I		K1=6.48	1972SSj (31263)	217
Medium: 0-40% EtOH, I=0									

Gd+++	EMF	NaClO4	25°C	2.00M U			K1=3.54 B2=5.63	1969JPa (31264)	218
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Gd+++	gl	KCl	24°C	0.20M U			K1=3.32	1966DDa (31265)	219
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C4H7NO4 H2L Aspartic acid CAS 56-84-8 (21)
Aminobutanedioic acid; H2N.CH(CH2.COOH).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Gd+++	gl	NaClO4	25°C	0.20M U			K1=5.65 B2=10.87	1996PJa (31860)	220
Gd+++	gl	NaClO4	25°C	0.20M U			K1=5.65 B2=10.87	1996PPa (31861)	221
Gd+++	gl	NaClO4	25°C	0.20M U			K1=5.65 B2=10.87	1990PJb (31862)	222
Gd+++	gl	NaClO4	30°C	0.10M U	I		K1=5.30 B2=9.80	1984YLa (31863)	223
Gd+++	gl	KCl	25°C	0.10M U			K1=5.74 B2=10.50	1968DRb (31864)	224

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		K(Gd(edta)+L)=4.54	1988KTa (32262)	225
Gd+++	gl	NaClO4	25°C	0.20M	U	M		K1=6.78 B2=12.31 K(Gd(HEDTA)+L)=5.68 K(Gd(CDTA)+L)=4.65 K(Gd(DTPA)+L)=4.19	1988VSc (32263)	226
Gd+++	gl	NaClO4	25°C	0.20M	U	M		K1=6.78 B2=12.31 K(Gd(NTA)+L)=5.76 K(Gd(edta)+L)=4.44	1987VSb (32264)	227
Gd+++	gl	KNO3	27°C	0.10M	M	M		K(GdA+L)=5.51 K(GdB+L)=5.38	1984KTb (32265)	228

H2A=Citraconic acid, H2B=Maleic acid

Gd+++	gl	KNO3	27°C	0.10M	U	M		K(GdA+L)=6.01 K(GdB+L)=5.71	1980KTb (32266)	229
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H2A=phthalic acid, H2B=malonic acid

Gd+++	EMF	KCl	25°C	1.0M	U	M		K(GdA+L)=5.07 K(GdA+H2L)=1.02 K(GdA+H3L)=2.39	1977GMA (32267)	230
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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)=4.30	1971GKb (32268)	231
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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
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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 B3=7.19	1964PKb (33476)	243
Gd+++	gl	NaClO4	25°C	0.50M	U		K1=2.71 B3=6.01	1964SPa (33477)	244
Gd+++	gl	NaClO4	25°C	2.0M	U		K1=2.82 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 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 K3=1.90	1976PKb (33699)	247
Gd+++	gl	NaClO4	25°C	0.50M	U		K1=2.69 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 1965DKb (35882) 256
K(Gd+HL)=8.31

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/quinhdrone 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 K(Gd+HL)=1.91	1989MFa (37422)	266

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

Methylacetylglyoxime; 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 K3=3.35	1995PAa (37978)	270

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

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

Gd+++	gl	alc/w	?	50%	U	I	K1=6.98	1971K0a (37981)	273
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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
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Gd+++	gl	oth/un	30°C	0.10M	U		K1=5.90 B2=10.38 K3=3.41	1960GFa (37983)	275
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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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	KN03	25°C	0.10M	U			K1=2.94 K3=1.58	B2=5.28	1969PCa (40254) 291

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	NaCl04	25°C	1.0M	U			K1=2.45	1968GCa (40279)	292

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	NaClO4	25°C	0.10M	U			K1=2.37 K3=1.23	B2=4.00	1970RDa (40297) 293

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	KN03	25°C	0.10M	C			K1=3.08 K3=1.57	B2=5.44	1975PFb (40312) 294

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									

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 KN03 25°C 0.20M U M K1=6.03 1990LSb (40712) 298
K(Gd(phen)+L)=5.77

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				1996ADa (41186)	303
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

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 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

DH=3.7 kJ mol⁻¹, DS=41.5 J K⁻¹ mol⁻¹

$$\begin{aligned} K(\text{Gd}+2\text{H}_3\text{L}=\text{GdL}_2+6\text{H}) &= -14.90, & K(\text{Gd}+2\text{H}_3\text{L}=\text{GdH}-2\text{L}_2+8\text{H}) &= -30.2, \\ K(\text{Gd}+2\text{H}_3\text{L}=\text{GdH}-3\text{L}_2+9\text{H}) &= -29.0, & K(\text{Gd}+2\text{H}_3\text{L}=\text{GdH}-4\text{L}_2+10\text{H}) &= -37.9. \end{aligned}$$

Method: proton relaxation enhancement. A is bovine serum albumin.

Gd+++ gl alc/w 25°C 25% U I K1=8.58 1972BKd (46122) 354
Medium: EtOH/H2O, 0.05 M (NaCl,NaClO4). 0%, K1=7.83, 50%, K1=9.57

Gd+++ sol NaCl04 25°C 0.10M U K1=8.4 1966SSg (46125) 357
Kso=-11.88

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	EMF	NaClO4	25°C	1.00M	U			K1=6.08 B2=10.28	1991WPb (46330)	358

Gd+++ ISE NaClO4 25°C 0.10M C I K1=11.37 1997LBb (46830) 359
Method: Cu ISE and competitive complexation by Cu. Data for 0.1-5.0 M.
At I=0.0 M, K1=13.20.

Gd+++ gl alc/w 30°C 50% C K1=10.72 1994S0a (46831) 360
Medium: 50% v/v MeOH/H2O, 0.10 M NaClO4.

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 1978SGf (46833) 362
K(GdL+A)=5.34

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 1977GMa (46835) 364
K(GdA+L)=6.09
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 1971GKb (46836) 365
K(GdA+L)=4.86

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 1970VMa (46837) 366
B(GdL)OH)=6.28

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 1957NOa (46842) 371
B(Gd2L3)=36.89

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 1987RRc (47561) 372
K(Gd+HL)=3.76

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

K(Gd+HL+cytidine)=8.57

[illegible]

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Medium: 75% acetone, 0.1 M

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Medium: 75% acetone, 0.1 M NaClO₄

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=3.09 1986CDb (48073) 380
DH=16.5 kJ mol⁻¹, DS=114 J K⁻¹ mol⁻¹

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

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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++      gl  NaCl04 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  NaCl04 25°C 0.20M U      K1=5.21  B2= 9.52  1987PPa (50076) 402
*****
C6H13NO2      HL  Norleucine    CAS 616-06-8 (602)
2-Aminohexanoic acid (2-Aminocaproic acid) CH3.(CH2)3.CH(NH2).COOH
-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++      gl  NaCl04 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-Aminohexanoic acid; H2N.CH2.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)

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

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+++	gl	KNO ₃	15°C	1.0M	U T			K(Gd+HL)=3.02 K(GdHL+HL)=2.76	1989SSg (50823)	411

Also data for 30 C.

Gd+++	gl	NaCl	04	20°C	0.10M	U T H		K1=7.42 B2=14.03	1983SDa (50824)	412
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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+++	gl	KCl	25°C	0.10M	C			B(GdH-6L2)=-18.2	1998HGa (51452)	413

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

Gd+++	gl	KNO ₃	25°C	0.10M	C			K(GdL+H)=7.35	1991SKb (52338)	416
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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	

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

[illegible]

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

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

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			

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

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

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

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Gd+++	gl	diox/w	30°C	50%	M	I	K1=5.11 B2= 9.78 K3=3.58	1978SSi (53544)	427

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 K3=4.82 K4=3.30	1969CMB (53674)	428

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

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

Medium: MeOH

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

Gd+++	gl	alc/w	25°C	99%	U		K1=6.51 B2=11.35 K3=2.73	1974BPb (53835)	431
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 C7H6O3 H2L Salicylic acid CAS 69-72-7 (14)
 2-Hydroxybenzoic acid, Salicylic acid; HO.C6H4.COOH

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

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

Gd+++	gl	NaClO4	25°C	0.10M	C	T	K(Gd+HL)=1.89 K(GdHL+HL)=1.89	1989HMa (54226)	434
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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	1989TMa (54227)	435
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Medium: MeOH

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

Gd+++	ix	mixed	20°C	50%	U		K(Gd+HL)=2.31 K(Gd+2HL)=3.33 K(Gd+2HL)=5.64	1976TRa (54229)	437
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Medium: 50% v/v acetone/H2O, 0.25 M NaClO4

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

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

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

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 NaCl04 25°C 0.10M C H 1988LLa (54418) 442
K(Gd+HL)=2.27

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

Gd+++ gl NaCl04 25°C 0.20M U K1=10.68 1996PJ a (54676) 444

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

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
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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
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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
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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
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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-propene-1,3-dioic acid; HOOCH(CH2CH3)NH2									
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; HOOCH(CH2CH3)N(CH2COOH)2									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Gd+++	gl	KNO3	20°C	0.10M	U		K1=12.24 B2=21.84	1974RMg (56910)	466

C7H12N2O3			HL	Gly-Pro			CAS 704-15-4	(257)	
Glycyl-proline; H2N(CH2CO)2CH2COOH									
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; C4H8N2O3									
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); HOOCC(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 K3=1.39 K4=1.14	1965TVa (57862)	477

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			K1eff=5.031	1978BKd (58504)	482
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Medium pH 5.4 (acetate).

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

Gd+++	sp	KNO3	12°C	0.10M	U			K(Gd+H2L)=4.08	1965GEa (58506)	484
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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
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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
Gd+++	gl	KNO3	25°C	0.10M	U		K1=3.82 B2=6.85	1986NSa (58971)	489

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
Gd+++	cal	NaClO4	25°C	0.10M	U	H	K1=2.73	1982CBc (59053)	491

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
Gd+++	gl	diox/w	20°C	50%	U		K1=6.05 B2=11.45	1971MAf (59101)	492

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
Gd+++	gl	alc/w	25°C	20%	M	I	K1=6.24	1994KDa (59217)	493

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

C8H8N4O5 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)	
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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)	
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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
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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
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Medium: 76% v/v dioxane/H2O, 0.10 M NaClO4.

C8H8O3	HL	Mandelic Acid					CAS 611-72-3	(80)	
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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
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C8H8O3	HL	m-Anisic acid					CAS 586-38-9	(2804)	
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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

$$K(\text{Gd}+\text{HL})=4.37$$

$$K(\text{Gd}+2\text{HL})=7.86$$

Acylnicotinoyl hydrazide; $C_5H_4N.CO.NH.NH.CO.CH_3$

2,5-Dihydroxybenzoquinone bis-thiosemicarbazone;

3-Acetyl-6-methylhydropyrane-2,4-dione;

7-Oxa-bicyclo[2.2.1]-heptan-2,3-dicarboxylic acid;

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

Amino-di(butanedioic acid); $\text{HN}(\text{CH}(\text{COOH})\text{CH}_2.\text{COOH})_2$

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

$$B(\text{GdHL}) = 15.49$$

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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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
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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
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Gd+++ g1 KN03 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
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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 NaCl₀₄

C8H12O4	H2L	CAS 1076-97-9	(2224)
Cyclohexane-1,4-dicarboxylic acid; C6H10.(COOH)2			

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

C8H13N06 H3L (3835)
2-Amino-2-carboxypropane-N,N-diethanoic acid; $\text{HOOCC}(\text{CH}_3)_2\text{N}(\text{CH}_2\text{COOH})_2$

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Gd+++ g1 KN03 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

C9H6N3OClS 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		Kso(GdL3)=-31.38	1981FCa (64276)	547
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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	K(GdA+L)=4.36	1971GKb (64547)	552
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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 K3=1.70 K4=1.33	1966TVa (65438)	560

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.

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Gd+++	gl	NaClO4	24°C	0.10M	U		K1=4.36 K(Gd+HL)=1.40	1986ZBa (65586)	567
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C9H10O5 H2L CAS 54384-22-4 (8406)
1-Methyl-(exo,exo)-7-oxabicyclo[2.2.1]hept-5-ene-2,3-dicarboxylic acid;

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

Gd+++	gl	KCl	30°C	0.10M	U		K1=5.00 B2= 8.04	1996SZa (65603)	568
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C9H10O5 H2L (7233)
1-Methyl-7-oxa-bicyclo[2.2.1]hept-5-en-2-exo,3-cis-dicarboxylic acid;

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

Gd+++	gl	KCl	30°C	0.10M	C		K1=5.00 B2=8.04	1996SZa (65618)	569
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C9H10O8 H4L CAS 3724-52-5 (1264)
cis-1,2,3,4-Cyclopentanetetracarboxylic acid; C5H6.(COOH)4

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

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
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C9H11NO2 HL Phenylalanine CAS 63-91-2 (2)
2-Amino-3-phenylpropanoic acid; H2N.CH(CH2.C6H5)COOH

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

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

C9H11NO3 H2L Tyrosine CAS 60-18-4 (4)
2-Amino-3-(4-hydroxyphenyl)propanoic acid; HO.C6H4.CH2.CH(NH2).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Gd+++	gl	KNO3	25°C	0.10M	U	I	K(Gd+HL)=4.92 K(GdHL+HL)=4.43	1976SAc (66222)	574
Gd+++	gl	KNO3	25°C	0.10M	U	T H	K(Gd+H2L)=4.63 K(GdH2L+H2L)=4.17	1976SAe (66223)	575
Gd+++	gl	KCl	25°C	0.10M	U		K(Gd+HL)=4.35 K(GdHL+HL)=4.2	1972BFe (66224)	576

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 K(GdA+L)=4.56 K(GdB+L)=4.43 K(GdC+L)=3.98	1990RSc (66694)	577

H2A=Iminodiethanoic acid, H3B=NTA, H4C=EDTA

Gd+++	gl	KNO3	35°C	0.10M	U	M	K1=4.26 K(GdL+Ala)=9.14 K(GdL+Phe)=8.90 K(GdL+Trp)=9.15	1990RSe (66695)	578
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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 K3=4.98	1994MRa (66796)	580

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
*****
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
*****
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
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C10H5O2F7S L (6996)

1-(2-Thienyl)-3-heptafluoropropylpropane-1,3-dione; C3F7.C(0)CH2C(0)C4H3S

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

Gd+++	gl	alc/w	22°C	80%	U			K1=6.10 B2=11.80	1995MTa (68426)	590
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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
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Gd+++	gl	NaClO4	25°C	0.10M	U	H		K1=4.78	1994CRa (68515)	591
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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
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Gd+++	sp	KCl	25°C	0.10M	M	I		K1=4.44	1976PEa (68577)	592
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Gd+++	sp	oth/un	?	?	U			K1=2.96	1969MSb (68578)	593
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C10H7NO2 HL CAS 132-53-6 (2524)

2-Nitroso-1-naphthol;

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=5.75 B2=11.03	1982LPc (68646)	594
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C10H7NO2 HL Quinaldic acid CAS 93-10-7 (2209)
Quinoline-2-carboxylic acid;

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

Gd+++ gl NaCl04 30°C 0.10M U K1=2.58 B2=5.06 1969DNc (68710) 595

C10H7NO2 HL CAS 86-59-9 (873)
Quinoline-8-carboxylic acid;

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

Gd+++ gl NaCl04 30°C 0.10M U K1=2.61 1969DNc (68761) 596

C10H7NO5S H2L CAS 14090-74-5 (2676)
1-Nitroso-2-hydroxynaphthalene-7-sulfonic acid;

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

Gd+++ gl KCl 25°C 0.10M M K1=4.43 B2=7.98 1979LSb (68812) 597

C10H7NO5S 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

C10H7NO5S H2L CAS 3682-32-4 (1812)
2-Nitroso-1-hydroxynaphthalene-4-sulfonic acid;

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

Gd+++ gl KCl 25°C 0.10M U I K1=3.41 1967MAi (68884) 600
K1=4.50(I=0)

C10H7NO5S H2L CAS 31005-79-9 (1814)
2-Nitroso-1-hydroxynaphthalene-8-sulfonic acid;

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

Gd+++ sp KCl 25°C 0.10M M K1=5.50 1978PPb (68945) 601

C10H7NO8S2 H3L Nitroso-R acid CAS 525-05-3 (1811)
1-Nitroso-2-hydroxynaphthalene-3,6-disulfonic acid;

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

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)
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

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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;
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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;
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++      gl  NaCl04 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;
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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++      gl  NaCl04 35°C 0.20M M      K1=10.13      1982LTa (69847) 615
-----
Gd+++      gl  NaCl04 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;
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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;
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-----
Metal      Mtd Medium Temp Conc Cal Flags Lg K values      Reference ExptNo
-----
Gd+++      gl  NaCl04 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
*****

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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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	NaClO ₄	25°C	0.10M	M			K1=4.48 B2=7.07	1977HCb (70851)	626

C10H11NOS			L					(2831)		
Acetothioacetanilide; CH ₃ .CO.CH ₂ .CS.NH.C ₆ H ₅										

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

C10H11NO ₂			L					CAS 102-01-2 (250)		
Acetoacetanilide; CH ₃ .CO.CH ₂ .CO.NH.C ₆ H ₅										

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

C10H11NO ₃			HL					(1960)		
N-Hydroxyacetoacetanilide; CH ₃ .CO.CH ₂ .CO.N(OH).C ₆ H ₅										

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 K3=5.92	1979KSb (70939)	629

C10H11N ₅ O			L					CAS 105507-56-0 (8131)		
N-Methylisatin-beta-amidinohydrazone;										

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/H ₂ O, 0.10 M NaClO ₄ . Data for 0.02-0.20 M NaClO ₄ and 30-50 C. DH(K ₁)=58.3 kJ mol ⁻¹ , DS=289 J K ⁻¹ mol ⁻¹ ; DH(K ₂)=28.7, DS=174										

C10H11O ₂ F ₇			HL					CAS 17587-22-3 (1252)		
1,1,1,2,2,3,3-Heptafluoro-7,7-dimethyl-4,6-octanedione;										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	dis	R ₄ N.X	25°C	0.10M	U			B2=12.7 B3=18.7 B(GdL ₃ (OH))=25.3	1970SBa (71109)	631

Medium: Et₄NClO₄

C10H12N ₂ O ₄			H ₂ L					CAS 16598-05-3 (967)		
2-Pyridylmethyliminodiethanoic acid; C ₅ H ₄ N.CH ₂ .N(CH ₂ .COOH) ₂										

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	1987GBa (71652)	638

K1(35, 40, 50 C) = 7.69, 7.68, 7.53 respectively. DH(K1)=-41.34 kJ mol⁻¹

C10H12O5 HL CAS 490-64-2 (8492)

2,4,5-Trimethoxybenzoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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			1974STb (73138)	643
							K(Gd+H2L=GdL+2H)=8.00		
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, Sequestic 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			1984BKc (73807)	647
							K(GdL+H)=1.30		
Gd+++	gl	NaClO4	20°C	0.02M	U	M		1982MPd (73808)	648
							K(GdL+PO4)=3.33		
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	1969PJ a (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	1959BD b (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	1958SR a (73822)	662
Gd+++	gl	oth/un	20°C	0.01M	U	K ₁ =17.12 Polarography also used	1955WS a (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	1954SG a (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 K(Gd+HL)=4.28 K(Gd+H2L)=3.57	1999BCb (74732)	666

Gd+++	gl	NaClO4	20°C	0.20M	U T H		K1=7.19 B2=11.04 K(Gd(nta)+L)=4.15 K(Gd(edta)+L)=4.00	1993VL a (74733)	667
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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
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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 K(Gd+HL)=4.17	1988SSd (74735)	669
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Gd+++	kin	oth/un	25°C	0.05M	C		K1=7.06	1983MCc (74736)	670
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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
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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 K3=8.45	1972DSe (74921)	672

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 K(Gd+HL)=9.22 K(GdL+H)=2.76 B(GdHL)=18.48	2001XRa (75022)	673

C10H17N3O6S H3L Glutathione CAS 70-18-8 (333)
Glutamyl-cysteinyglycine;

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 K(GdL+HL)=2.25 K(GdL+H4L)=1.99	1977GMa (75400)	676
Method: Pt/H2 electrode.									
Gd+++	EMF	KCl	25°C	1.0M	U	M	K(Gd(edta)+L)=3.40 K(Gd(edta)+HL)=2.06 K(Gd(edta)+H2L)=1.28	1977GMa (75401)	677
Method: Pt/H2 electrode.									
Gd+++	gl	NaClO4	20°C	0.10M	U		K(GdL+A)=3.58 K(GdL+B)=3.70	1974PJ a (75402)	678
HA=pentane-2,4-dione, B=1-phenylbutane-1,3-dione									
Gd+++	gl	NaClO4	25°C	1.0M	U		K2=3.21 K(GdL+HL)=2.37 K(GdL+H3L)=1.56	1973NMa (75403)	679
Gd+++	gl	oth/un	20°C	?	U		K(GdL+H3L)=0.85 K(GdL+H2L)=0.77 K(GdL+HL)=2.0 K(GdL+L)=3.32	1971MNa (75404)	680
Gd+++	gl	KNO3	25°C	0.10M	U	M	K(GdL+A)=4.96 K(CdL+B)=4.57	1963TLb (75405)	681
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; CH0.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 1984OHa (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 K(Gd(nta)+L)=5.64	1993EEa (77930)	707

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
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C11H12N2O5S HL CAS 56475-09-3 (8410)
3-(4'-Sulfoophenylhydrazo)-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'-sulfoophenylhydrazo-, 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 K(Gd(nta)+L)=7.40	1993EEa (78356)	713

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 K3=5.66	1979KSb (78496)	715

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-Acetylacetyliden-orthanilic acid; HO3S.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; HO.C6H4.CH2.N(CH2.COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Gd+++	gl	KN03	25°C	0.10M	C		K1=13.55 B2=24.13 K(Gd+HL)=5.82 K(Gd+2HL)=12.23	1989YSa (78626)	718

Gd+++ g1 KNO3 20°C 0.10M U K1=12.82 B2=23.36 1983MSc (78627) 719

C11H13NO6 H4L CAS 1911-59-2 (4852)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K	values	Reference	ExptNo
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$$K(\text{Gd}+\text{HL})=14.4$$

C11H13NO6 H4L CAS 59036-09-8 (2111)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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$$K(\text{Gd}+\text{HL})=14.4$$

C11H13N06 H4L CAS 31477-66-7 (4853)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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$$K(Gd+HL)=12.4$$

C11H14N2O3 HL Gly-Phe CAS 3321-03-7 (829)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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C11H14N2O4 H2L Gly-Tyr CAS 658-79-5 (533)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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$$K(Gd+HL)=2.65$$

C11H14N2O4 H2L (1880)

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

C11H26N206 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
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 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
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Gd+++	sp	non-aq	25°C	100%	C	H	K1=1.3	2002KNc (80457)	742
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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
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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
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Gd+++	gl	NaClO4	30°C	0.10M	U	T H	B2=12.60	1982GMb (80782)	744
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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
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Gd+++	gl	diox/w	20°C	75%	U		K1=6.55 B2=11.42	1992SSc (80889)	745
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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
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Gd+++	gl	diox/w	20°C	75%	U	I	K1=9.122 B2=16.541	1992SSc (80917)	746
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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
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Gd+++	kin	oth/un	25°C	0.02M	U		K1=2.38	1974GMc (80949)	747
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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;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	KN03	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-diazayclododecane-5,12-dione-7,10-diethanoic acid;										

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	EMF	KN03	25°C	0.10M	U			K1=13.34	1985SGa (81864)	756

Gd+++	EMF	KN03	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										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	vlt	KN03	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										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	KN03	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										

Gd+++	gl	KN03	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;										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	vlt	KN03	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;										

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									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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									
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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; ((HOOCH₂)₂NCH₂CH₂)₂O

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	EMF	KNO ₃	20°C	0.10M	U			K ₁ =18.13	1962MMc (82537)	772

C ₁₂ H ₂₀ N ₂ O ₁₀		H ₄ L						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+H ₂ L)=13.06		
								K(Gd+HL)=17.15		

C ₁₂ H ₂₀ O ₈ N ₂		H ₄ L						(6908)		
2-Methyl-1,2-diaminopropane-N,N,N',N'-tetraethanoic acid;										
(HOOCH ₂) ₂ NCH ₂ C(CH ₃) ₂ N(CH ₂ COOH) ₂										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	vlt	KNO ₃	20°C	0.10M	C			K ₁ =17.09	1978NLa (82674)	774

C ₁₂ H ₂₁ N ₆ O ₆		H ₃ L						(7209)		
1-Carboxy-1-aminoheptane-N,N-diethanoic acid; HOOCH(C ₆ H ₁₃)N(CH ₂ COOH) ₂										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	alc/w	20°C	40%	U			K ₁ =11.08	1985LBc (82697)	775
Medium: 40% v/v MeOH/H ₂ O, 0.1 M KNO ₃										

C ₁₂ H ₂₁ N ₃ O ₆		H ₃ L		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			K ₁ =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		

C ₁₂ H ₂₃ N ₃ O ₆		H ₃ L						(7085)		
2,5,8-Triazanonane-2,5,8-triethanoic acid;										
CH ₃ N(CH ₂ COOH)CH ₂ CH ₂ N(CH ₂ COOH)CH ₂ CH ₂ N(CH ₂ COOH)CH ₃										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	KCl	25°C	0.10M	C			K ₁ =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
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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
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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
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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
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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
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Gd+++	gl	NaNO3	25°C	0.20M	C		K1=8.40	1991KKa (84329)	788
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Gd+++	gl	NaCl	20°C	0.10M	C		K1=9.8	1988SJb (84330)	789
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C13H502F13S L (6997)
 1-(2-Thienyl)-3-tridecafluorohexylpropane-1,3-dione; C6F13.CO.CH2.CO.C4H3S

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Gd+++	gl	alc/w	22°C	80%	U		K1=5.40 B2=10.56 K3=4.78	1995MTa (84454)	790
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Medium: 0.1 M NaClO4 in 80% (v/v) EtOH/H2O.

C13H8O3 H2L CAS 18931-22-1 (2913)
 peri-Dihydroxynaphthindenone;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Gd+++	sp	alc/w	25°C	50%	U		K1=9.64	1982HMa (84503)	791
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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
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Gd+++	gl	NaClO4	30°C	0.10M	U		K1=5.05	1989SHa (84514)	792
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C13H9N2O4Cl HL CAS 36016-30-5 (182)
 N-(4-Chlorophenyl)-3-nitrobenzohydroxamic acid; O2N.C6H4.CO.N(C6H4Cl).OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Gd+++	gl	diox/w	35°C	50%	A		K1=7.87 B2=14.19 K3=5.29	1977AKa (84602)	793
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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
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Gd+++	gl	alc/w	25°C	70%	U		K1=12.72 B2=24.49	1995IFa (85043)	794
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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-Acetylphenylhydrazon)-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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Gd+++	EMF	alc/w	20°C	50%	U		K1=3.45	1971MAc (85411)	801
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Medium: 50% EtOH, 0.1 M NaClO4

C13H12N4S	L	Dithizone	CAS 60-10-6	(1801)
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Diphenylthiocarbazone; C6H5.NH.NH.CS.N:N.C6H5

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Gd+++	EMF	alc/w	20°C	50%	U		K1=1.80	1971MAc (85458)	802
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Medium: 50% EtOH, 0.1 M NaClO4

C13H14N2O3	HL	(4940)
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3-(2-Acetylphenylhydrazon)pentane-2,4-dione; (CH3.CO)2C:N.NH.C6H4(CO.CH3)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Gd+++	gl	diox/w	30°C	75%	U		K1=11.05 B2=20.48	1988ESb (85609)	803
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C13H15NO6	H3L	(4999)
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2-Benzylnitritotriethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Gd+++	oth	oth/un	25°C	0.10M	U		K2=8.97	1962HKa (85737)	804
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C13H19NO3	H2L	(2031)
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2-(1-(2-Hydroxyphenyl)-ethylimine)-3-methylbutanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Gd+++	gl	NaClO4	25°C	0.10M	U	TIH	K1=11.10 B2=20.55	1980SSc (86054)	805
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C13H20N2O8	H4L	CAS 123064-92-6	(7929)
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trans-1,3-Cyclopentanediarninotetraethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Gd+++	gl	KCl	25°C	1.0M	U		K1=12.67 K(GdHL+H)=3.73 K(GdL+H)=4.29	1989CMb (86120)	806
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C13H22N2O8	H4L	CAS 1798-14-7	(921)
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(Pentamethylenedinitrilo)tetraethanoic acid; ((HOOCH2)2N.CH2.CH2)2CH2

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; (HOOCCCH2)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 1974NL a (86227) 808

C13H22N2O8 H4L (7164)
2,4-Diaminopentane-N,N,N',N'-tetraethanoic acid;
(HOOCCCH2)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 B(GdH-1L)=7.64 B(GdH-2L)=0.27	2004NJa (86533)	814

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	1981EIa (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	NaCl04	25°C	0.20M	U	M		K1=10.18	1987VSa (86730)	816

K(Gd(cdta)+L)=6.03, K(Gd(dtpa)+L)=5.02.

Gd+++	sp	oth/un	25°C			?	U		1967SAa (86731)	817
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K(?)=8.6

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 NaCl04.

C14H10N02F 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	NaCl04	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 K3=7.36	1983AGb (87046)	822

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 K3=7.38	1983AGb (87072)	823

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 K3=7.65	1983AGb (87081)	824

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 K3=7.04	1983AGb (87242)	826

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		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	1981RSb (87404)	831

Medium: 50% v/v EtOH, 0.1 M KNO3. K1=7.77(I=0), 7.02(I=0.05)

C14H13NO2 HL CAS 1503-92-0 (1817)
N-(4-Tolyl)benzohydroxamic acid; C6H5.CO.N(C6H4.CH3).OH

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

C14H13NO4S H2L (3660)
 2-Aminobenzenesulfonic acid 2-hydroxyacetophenone Schiff base;
 HS03.C6H4.N:C(CH3).C6H4.OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Gd+++	gl	NaCl04	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	1997E1a (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	NaCl04	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

C14H19NO7 HL (6775)
16-Nitro-3,6,9,12-tetraoxabicyclo[12.3.1]octadeca-1(18),14,16-trien-18-ol;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Gd+++	gl	R4N.X	25°C	0.10M	C		K1=3.18	1990CBe (88148)	839

C14H20O5 L Benzo15-crown-5 CAS 14098-44-3 (608)
2,3-Benzo-1,4,7,10,13-pentaoxacyclopentadeca-2-ene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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
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C14H20O8S HL CAS 127461-53-4 (7818)
2,3-Benzo-1,4,7,10,13-pentaoxacyclopentadeca-2-ene-4'-sulfonic acid;

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

C14H22N2O8 H4L cis-1,2-CDTA CAS 92761-75-6 (2846)
cis-1,2-Diaminocyclohexane-N,N,N',N'-tetraethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Gd+++	gl	KCl	25°C	1.0M	U		K1=4.37	1987CMe (88430)	843

K(GdL+H)=7.00

C14H22N2O8 H4L cis-1,3-CDTA CAS 92681-23-7 (2847)
cis-1,3-Diaminocyclohexane-N,N,N',N'-tetraethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Gd+++	gl	KCl	25°C	1.0M	U		K1=7.28	1987CMe (88442)	844

K(GdHL+H)=5.36
K(GdL+H)=7.91

C14H22N2O8 H4L cis-1,4-CDTA CAS 92681-25-9 (2848)
cis-1,4-Diaminocyclohexane-N,N,N',N'-tetraethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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 K(GdL+H)=1.66	1987CMe (88667)	846
Gd+++	gl	KCl	25°C	1.00M	U			K1=18.97	1984MFa (88668)	847
Gd+++	gl	KNO3	27°C	0.10M	U	M		K(Gd+L+HA)=13.17 K(GdL+HA)=5.83	1981KSe (88669)	848

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 DH(K1)=24.3 kJ mol ⁻¹ , DS=439 J K ⁻¹ mol ⁻¹ . At 20 C: K(GdL+H)=2.23	1962MHa (88671)	850

Gd+++	vlt	KNO3	20°C	0.10M	U			K1=18.77	1954SGa (88672)	851
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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 K(GdHL+H)=5.12 K(GdL+H)=7.48	1987CMe (88836)	852

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 K(GdHL+H)=5.95 K(GdL+H)=6.41	1987CMe (88856)	853

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)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Gd+++	gl	NaClO4	25°C	0.10M	C		K1=22.39	2001CCa (89256)	855
K1 from competitive titration using EDTA. In 0.10 M Me4NCl, K1=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		K1=22.52	1999SBd (89260)	859
Gd+++	sp	NaClO4	25°C	0.15M	U		K1=21.04	1996GMA (89261)	860
Arsenazo III used as indicator. Also data for several DTPA-bis-anilides									
Gd+++	sp	R4N.X	25°C	0.10M	C		K1=22.2	1994KCa (89262)	861
Medium: Me4NCl									
Gd+++	cal	KNO3	25°C	0.10M	C T			1988MIa (89263)	862
DH(K1)=-30.7 kJ mol-1, DS=324.5 J mol-1 K-1. Also data for 283 and 313 K									
Gd+++	cal	NaClO4	25°C	0.10M	C	H		1987YJa (89264)	863
DH(K1)=-27.0 kJ mol-1, DS(K1)=339 J K-1 mol-1.									
Gd+++	cal	NaClO4	25°C	0.50M	U	H		1977CGc (89265)	864
DH(K1)=-47.5 kJ mol-1									
Gd+++	gl	NaClO4	25°C	0.50M	U		K1=20.73	1977GGb (89266)	865
Gd+++	sp	oth/un	20°C	dil	U		K1=22.46	1969KAF (89267)	866
Gd+++	cal	KNO3	27°C	0.10M	U	H		1968CLd (89268)	867
DH(K1)=-32.6 kJ mol-1, DS=321 J K-1 mol-1									
Gd+++	EMF	KNO3	25°C	0.10M	U	H	K1=22.46	1962MTc (89269)	868
DH(K1)=-31.4 kJ mol-1, DS=325 J K-1 mol-1									
Gd+++	gl	oth/un	25°C	0.10M	U		K1=23.01	1959HCa (89270)	869

C14H24N2O8 H4L (5075)									
1,2-Diaminoethane-N,N'-diethanoic-N,N'-di-2-butyric acid;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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; (H00CCH2)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; ((H00C.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;									
(H00CCH2)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'-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; (H00C.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-CH2O(CH2)2COOH-
derivatives.

C14H25N3O6 H3L (6556)

9-Methyl-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=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	1968VL a (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
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Medium: Me4NCl

Gd+++	sp	R4N.X	25°C	0.10M	C		K1=21.0	1994KCa (90250)	889
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Medium: Me4NCl

Gd+++	sp	NaCl	25°C	1.00M	C		K(GdL+H)=2.06	1993KCa (90251)	890
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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 Et4NCl04

Gd+++	sp	non-aq	25°C	100%	U		K1=3.87	1983PSc (90368)	892
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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
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Gd+++	gl	R4N.X	25°C	0.10M	C		K1=7.29	1988CCc (90480)	893
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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
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Gd+++	gl	R4N.X	25°C	0.10M	U		K1=12.71	1996BJa (90764)	894
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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
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Gd+++	gl	KCl	25°C	0.10M	C		K1=9.81	1998BRa (90843)	895
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C15H11NO4 HL CAS 1776-18-7 (955)
3-Phenyl-1-(2'-hydroxy-5'-nitrophenyl)-2-propen-1-one;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Gd+++	gl	alc/w	35°C	70%	U		K1=6.46 B2=12.86	1982SLb (91077)	896
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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
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Gd+++	sp	alc/w	21°C	50%	U		K1=9.29	1988CMD (91217)	897
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Gd+++	sp	alc/w	21°C	50%	U	I	K1=8.80	1981MCb (91218)	898
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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
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Gd+++	gl	alc/w	35°C	70%	U		K1=7.10	1982SLb (91370)	899
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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

C15H12O5 HL (1261) mono-Thiodibenzoylmethane; C6H5.CO.CH2.CS.C6H5									
Gd+++	gl	NaCl04	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									
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									
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									
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;									
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

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

C15H15NO2 HL (1167)
N-(4-Tolyl)-4'-tolylhydroxamic acid; CH₃.C₆H₄.CO.N(C₆H₄.CH₃)OH

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

35 C: $K_1=10.26$, $K_2=8.75$, $K_3=7.77$

C15H18N2O3 HL CAS 116822-13-0 (6743)
5,5-Dimethylcyclohexane-2-(2-hydroxy-4'-methylphenyl)-hydrazono-1,3-dione;

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-Benzylldiaminoethane-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 B(GdHL)=23.55 B(GdH2L)=26.38	1995MMa (92169)	920

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 B3=22.6	1997RPb (92283)	922

Medium: acetonitrile.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Gd+++	EMF	KCl	?	0.10M	U		K1=16.71	1966VL a (92371)	923

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+++	vlt	oth/un	?	?	U		K1=18.4	1966VL a (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 K(Gd+HL)=13.38	1989SPa (92393)	925

C15H26N4O9 H4L (7685)									

Diethylenetriamine-N,N,N',N'',N''-pentaethanoic acid N'-methylester;

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-methylester;										

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 K(Gd+HL=GdL+H)=-3.47	1991BCa (92467)	928

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

C15H33N6O6				L				CAS 70384-51-9	(838)	
Tris(3,6-dioxahexyl)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'-Sulfofenylazo)chromotropic acid,
2-(4-sulfofenylazo)-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 NaCl04. 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-Acetylphenylhydrazon)-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 B(GdHL)=14.62	2001WZa (93842)	949

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-pentaazacyclpentadeca-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	KN03	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	KN03	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	KN03	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
Medium: Me4NCl										

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: Me4NCI									

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
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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
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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
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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
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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
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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)

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 B3=13.64	1987ECa (95738)	989

C17H13N4O3 HL (5927)									
1-Phenyl-3-methyl-4-(2'-carboxyphenylhydrazo)-5-pyrazolone;									

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;									

Gd+++	gl	NaNO3	20°C	0.10M	U	M		1981GCa (95883)	991
B(Gd+3L+3TBP)=25.65									
B(Gd+3L=4TBPoxide)=32.8									

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									
Medium: CHCl3. A=tributylphosphate, B=piperidine									

C17H15N4O2 L CAS 97671-53-9 (5926)									
1-Phenyl-3-methyl-4-(2'-methoxyphenylhydrazo)-5-pyrazolone;									

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.C4H0(CH3)2									

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									

Gd+++	gl	diox/w	30°C	50%	U			1987DDc (96243)	995

$$K(\text{Gd}+\text{HL})=7.17$$

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 K(GdL+H)=2.38 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-hydroxymethylethanoic acid);

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

N,N'-Bis(2-pyridylmethyl)diaminoethane-N,N'-diethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Gd+++	gl	NaCl	25°C	0.16M	C			K1=12.37 K(Gd+L=GdL(OH)+H)=2.10 K(GdL(OH)+H)=10.25	1997CMa (97543)	1015
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C18H25N3O8 H4L BEATA CAS 87732-99-8 (5600)

N,N-Bis(2-aminoethyl)aniline-N',N',N'',N''-tetraethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Gd+++	gl	KNO3	25°C	0.10M	C			K1=15.42	1985TPa (97653)	1016
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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
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Gd+++	nmr	oth/un	25°C	0.1M	U			K1eff=19.3 (pH 7)	1997ABa (97686)	1017
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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
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Gd+++	gl	R4N.X	25°C	0.10M	M			K1=21.59	2000Cwa (97691)	1018
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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
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Gd+++	gl	KCl	25°C	0.10M	M			K1=8.1	1996MBb (97713)	1019
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Gd+++	gl	KCl	25°C	0.20M	C			K1=8.1	1992RMa (97714)	1020
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C18H28O5 L CAS 15196-73-3 (2359)

2,3-(4'-Dimethylethylbenzo)-1,4,7,10,13-pentaoxacyclopentadeca-2-ene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Gd+++	gl	non-aq	25°C	100%	U			K1=3.02	1982MDa (97805)	1021
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Medium: propylene carbonate

C18H29NO4 L CAS 207603-17-6 (9000)
7-(Phenylmethyl)-1,4,10,13-tetraoxa-7-azacyclohexadecane;

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

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;((HOOCH₂)₂NCH₂CH₂N(CH₂COOH)₂)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
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C18H34N2O8 H2L CAS 68670-15-5 (5851)

1,4,10,13-Tetraoxa-7,16-diazacyclooctadecane-7,16-di-(3-propanoic acid);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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
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Medium: propylene carbonate, 0.1 M Et4NCl04

Gd+++	gl	alc/w	25°C	100%	C		K1=10.14	1983ANb (98578)	1037
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The equilibration took 7-12 days. Medium: MeOH, 0.05 M Et4NCl04

Gd+++	sp	non-aq	25°C	100%	U		K1=3.45	1983PSc (98579)	1038
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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	1981Eic (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
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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
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C20H24O12S2 H2L CAS 172985-47-6 (7820)
2,3:11,12-Dibenzo-1,4,7,10,13,16-hexaoxacyclooctadeca-2,11-diene-4',4''-disulfonic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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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 1990K Md (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(methylcarbamoylmethyl)-1,4,7,10-tetraazacyclododecane;

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	H	K1=12.8 K(GdL+H)=3.4 K(GdL+OH)=5.8	2000BCa (100846)	1067
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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
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Gd+++	kin	oth/un	25°C	0.02M	U		K1=4.17	1974GMc (100906)	1069
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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
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Gd+++	gl	KCl	25°C	0.10M	C		K1=16.5	1997HTa (100994)	1070
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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
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Gd+++	oth	none	37°C	0.0	C			2001CGb (100997)	1072
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K(GdL+HSA)=4.16

Method: ultrafiltration. HSA=human serum albumin. K(GdL+BSA)=3.70.

C21H17N2O5As H2L ArsenoBDMPH (5931)

2-Arsenodibenzoylmethanephnylhydrazone; C6H5.CO.C(CO.C6H5):N.NH.C6H4.AsO3H2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Gd+++	gl	alc/w	27°C	40%	U		K1=14.20 B2=18.66	1990M0c (101078)	1073
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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 K3=6.9	1997PBa (101087)	1074

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;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Gd+++	sp	oth/un	?	?	U		K1=15.15	1971SSi (101544)	1080
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 C22H18N4O14As2S2 H8L Arsenazo III CAS 1668-00-4 (1148)
 2,7-Bis(2'-arsonophenylazo)chromotropic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Gd+++	sp	oth/un	rt	0.10M	C			2004LLa (101621)	1081
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K1eff=4.24
 B2eff=9.50
 B(2,2)eff=13.61

Method: spectral deconvolution. Medium: 0.1 M chloroacetate buffer, pH 3.5

Gd+++	sp	oth/un	25°C	var	U	I		1997HRb (101622)	1082
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K1(eff)=7.495
 B(GdLC1)eff=7.201
 B(GdL2C1)eff=13.650

Conditional constants in chloride medium at pH 3.3. Also data in sulfate and perchlorate media. K(Gd+Cl)=1.939.

Gd+++	kin	oth/un	25°C	0.10M	U			1994RCb (101623)	1083
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K(GdL+H)=4.51
 K(GdL2+H)=4.85

Medium: 0.1 M CH3COONa.

Gd+++	sp	NaClO4	25°C	0.10M	U			1975NMa (101624)	1084
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K(Gd+H5L)=7.73

Gd+++	sp	oth/un	20°C	?	U			1972SSi (101625)	1085
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K(Gd+H4L)=15.75

Gd+++	sp	oth/un	?	?	U			1967ECa (101626)	1086
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K(Gd+H5L)=5.4 pH 1-4

Gd+++	sp	NaNO3	20°C	0.20M	U			1963BUa (101627)	1087
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B(Gd2L2)=80.5

C22H19N3O4S HL CAS 84819-63-6 (8347)
 N-(3,4-DiMe-5-isoxazolyl)-4-[[(2-hydroxy-1-naphthalenyl)methylene]amino]benzenesulfonamide;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Gd+++	gl	NaClO4	25°C	0.10M	U		K1=6.64 B2=11.25	1982MBa (101686)	1088
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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
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Gd+++      sp  oth/un  ?  0.10M U                                1970PLc (101701)1089
                                         K(GdOH+2H3L)=16.90

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*****
C22H24N2O10      H4L      CAS 132796-79-3 (8113)
1,2-Bis(2-aminophenoxy)ethane-N,N,N',N'-tetraethanoic 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 C T H      K1=10.94      1990HLA (101896)1090
                                         K(GdL+H)=3.54

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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.

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*****
C22H26N4O10      H4L      BAPTA      (7230)
1,2-Bis(o-aminophenoxy)ethane-N,N,N',N'-tetraethanoic acid;
((HOOCCH2)2NCH(OC6H4NH2)2
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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

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*****
C22H28O13S2      H2L      DSDB21C7      CAS 204931-02-2 (7821)
2,3:11,12-Dibenzo-1,4,7,10,13,16,19-heptaoxacycloheicosa-2,11-diene-4',4''-disulfo
nic acid;
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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.

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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;

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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

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*****
C22H30N4      L      CAS 250790-21-7 (7943)
N,N'-Bis(1,1-dimethylethyl)-1,10-phenanthroline-2,9-dimethanamine;
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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

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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
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Gd+++	gl	R4N.X	25°C	0.10M	M		K1=23.79	2002CLb (102181)	1095
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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
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Gd+++	gl	NaCl	25°C	0.15M	C	M	K1=22.61 B(GdHL)=24.33 B(GdHL(ATP))=31.76 B(GdH2L(ATP))=35.43 B(GdH3L(ATP))=38.1	1999BCb (102185)	1096
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B(GdH4L(ATP))=40.8, B(GdH5L(ATP))=43.23, B(GdHL(P3010))=32.34,
B(GdH2L(P3010))=37.90, B(GdH3L(P3010))=40.88, B(GdH4L(P3010))=43.71.

Gd+++	gl	R4N.X	25°C	0.10M	C	H	K1=22.58 B(GdHL)=24.33	1996BCd (102186)	1097
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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
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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
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Gd+++	gl	KCl	25°C	0.10M	C		K1=20.42 K(GdL+H)=2.38	2000SMc (102250)	1099
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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
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Gd+++	gl	KCl	25°C	0.10M	C		K1=20.71 K(GdL+H)=1.92	2000SMc (102252)	1100
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C22H37N5O14 H7L CAS 3234-59-1 (2425)
Tetraethylenepentamineheptaethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Gd+++	vlt	R4N.X	30°C	0.01M	C		K1=20.42	1981GMh (102326)	1101
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Gd+++	gl	KNO ₃	25°C	0.10M U	K ₁ =20.41	1968MIc (102327)1102
					K(Gd+HL)=14.11	
					B(GdH-1L)=5.34	

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	KN03	40°C	0.50M	U	T		K1=18.23 K(GdL+H)=4.07	1995BIa	(102356)1103

C22H41N5O8 H3L CAS 189687-33-0 (7103)
Diethylenetriamine-N,N',N''-triethanoic acid-N,N''-bis(butylamide);

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									

C23H16O9Cl2S			H4L		Chrome	azuro1 S	CAS 1667-99-8	(711)	
Chromazurol S;									

C23H18N2O3 HL (5561)
2-(2-Acetylphenylhydrazon)-1,3-diphenyl-prop-1,3-dione;
C6H5.CO.C(CO.C6H5):N.NH.C6H4.COCH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	diox/w	30°C	75%	U			K1=11.00 B2=19.75	1988ESb (102594)	1107

C23H18O9S		H4L			Eriochrome cyan			CAS 3564-18-9	(433)	
4'-Hydroxy-3,3'-dimethyl-2''-sulfofuchstone-5,5'-dicarboxylic acid;										

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Gd+++	sp	oth/un	25°C	?	U		B2=9.8	1968MDc (102630)	1108
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C23H24N4O2		L			Trichachnine		CAS 1251-85-0	(2606)	
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4,4'-Diantiprylmethane,

4,4'-phenylmethylen-bis-(1,2-dihydro-1,5-dimethyl-2-phenylpyrazol-3-one

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Gd+++	sp	diox/w	25°C	100%	U		K1=4.23	1995KMa (102672)	1109
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C23H33N3O11		H5L					CAS 158599-72-5	(7657)	
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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
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Gd+++	gl	KCl	25°C	0.10M	C		K1=23.45	1999SBd (102818)	1110
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K(CdL+H)=2.17

C23H54N4O12P4		H8L			C11-DOTP		(7969)		
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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
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Gd+++	oth	none	37°C	0.0	U			2001Cgb (102850)	1111
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K(GdL+HSA)=5.40

Method: ultrafiltration. HSA=human serum albimin. K(GdL+BSA)=4.83.

C24H16O16S8		H8L					CAS 237770-97-7	(8854)	
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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
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Gd+++	cal	oth/un	25°C	0.01M	C	H	K1=3.30	2004LWa (102867)	1112
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Medium: 0.01 M HCl. DH(K1)=9.0 kJ mol⁻¹, DS(K1)=89.3 J K⁻¹ mol⁻¹.

C24H29N3O12S3		H6L					(7355)		
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1,2,3-Tris((2-hydroxy-5-sulfobenzyl)amino)propane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
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Gd+++	gl	NaCl	25°C	0.16M	C		K1=14.50	1998LCa (103016)	1113
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K(GdL+H)=6.38

C24H32N2O6		H3L			Me4-HBED		(6507)		
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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-methoxyethylcarbamoylmethyl)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-tetraazatricyclotetracosatetraen-
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-Hexaazatricyclotetracos-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-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=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 B(GdHL)=23.6 B(GdH2L)=27.9	2000CXa (104522)	1126

Also data for related ligands.

C27H33N7O9 HL CAS 159356-07-7 (8682)
N,N'N'-(Nitrilotri-2,1-ethanediyl)tris[1,2-dihydro-3-hydroxy-1-methyl-2-oxo)4-pyridinecarboxamide

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	KCl	25°C	0.10M	U			K1=20.3 B(GdHL)=23.8	1995XFa (104542)	1127

C27H36N4O6 H6L CAS 222626-11-1 (8885)
Tris((2,3-dihydroxybenzylamino)ethyl)amine;

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	2002BDc (104557)	1128

K(Gd+H3L)=8.49, K(GdH3L+H3L)=7.43.

C27H36N4O12S3 H6L (7353)
Tris(((2-hydroxy-5-sulfobenzyl)amino)ethyl)amine;

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.

C27H36N10O9 H3L TrenHOPY (7967)
Tris[(2,3-dimethyl-5-hydroxy-6-carboxamido-4-pyrimidinone)ethyl]amine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Gd+++	gl	KCl	25°C	0.10M	U			K1=18.2 B(GdHL)=22.4 B(GdH2L)=26.6	2001SBb (104578)	1130

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		2001BIa (104697)	1132

K(Gd+H4L)=3.94

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		1997LQa (104789)	1133

K(GdNO3+L)=2.51

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

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

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'-dimethylfuchsone-2"-sulfonic acid;									

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Gd+++	sp	NaNO3	20°C	0.20M	U		B(Gd2L2)=43.1	1963BBb (105471)	1142

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
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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
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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          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

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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

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Medium: CH3CN; 0.1 M Et4NClO4

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

Also data for $\text{GdHnL}(\text{OH})$ species

C47H46N6O4 L (7367)
2,6-Bis(1-(3,5-dimethoxybenzyl)benzimidazol-2-yl)-4-(4-diethylamino)phenylpyridine
;

Medium: CH₃CN; 0.1 M Et₄NClO₄

C52H69N07 L CAS 178626-47-6 (8569)
5,11,17,23-Tetra-*t*-butyl-25-(diethylcarbamoyl)methoxy-27-carboxymethoxy-26,28-dihydroxycalix[4]ar

C62H94N2O4S2 L (8109)
5,11,17,23-Tetrakis(1,1-dimethylethyl)-25-27-bis[2-methylthio]ethoxy]...calix(4)are
ne;

C76H116N4O8 L (8156)
p-tert-Butylcalix(4)arene tetradiisopropylethanoamide;

Polymer	HL	Bleomycin	(2324)
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Bleomycin A2, B2 etc.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Gd+++	sp	oth/un	25°C	?	U		K1eff=4.34 pH 6.8	1980LPb (108089)	1160

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 B(Gd(CO3)L)=>8.0 B(GdH(CO3)L)=>16.0	1985JAa (108103)	1161

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		Keff(Gd+L)=7.96 Keff(GdL+Gd)=5.94	1992HCa (108214)	1162

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

END