SC-Database
Software version = 5.81 Data version = 4.62
Experiment list contains 526 experiments for
 (no ligands specified)
 Metal : Th++++
 (no references specified)
 (no experimental details specified)

****
e- HL Electron (442)
Electron;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Th++++ sp oth/un 25°C 0.00 U 1965MIb (960) 1
K(Th+e=Th+++)=-41, -2400 mV

Th++++ oth none 25°C 0.0 U 1952LAb (961) 2
K(Th+4e=Th(s))=-128.4(-1900 mV
****
Br- HL Bromide CAS 10035-10-6 (19)
Bromide;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Th++++ dis oth/un 25°C 1.00M U K1=-0.1 B2=-0.6 1975RRa (2331) 3
****
BrO3- HL Bromate (6017)
Bromate;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Th++++ dis NaClO4 25°C 1.00M U H K1=0.63 1992CKb (2433) 4
DH(K1)=2.5 kJ mol-1; DS=20 J K-1 mol-1

Th++++ dis NaClO4 25°C 0.50M U K1=0.81 B2=0.91 1950DSa (2434) 5
****
CO3-- H2L Carbonate CAS 465-79-6 (268)
Carbonate;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Th++++ sol none 25°C 0.0 C 1997FRa (3396) 6
K(ThO2(s)+H+H2O+CO3=Th(OH)3CO3)=6.78
K(ThO2(s)+4H+5CO3=Th(CO3)5+2H2O)=37.6

Th++++ sol NaClO4 25°C 0.50M C M 1994OBa (3397) 7
K(ThO2(s)+4H=Th+2H2O)=9.37
K(ThO2(s)+H+H2O+L=Th(OH)3L)6.1
K(ThO2(s)+4H+5L=ThL5+2H2O)42.1

Constants at I=0 also given

Th++++ dis oth/un 20°C 1.00M U I 1987JBa (3398) 8
B5=26.2
When I=2.5 M: B5=26.3

Th++++ sol oth/un 20°C dil U 1960ZMa (3399) 9
Ks(ThOL(s)=ThO+L)=-8.05 ?

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Th++++	dis	NaClO4	25°C	2.00M	U		K1=0.11	B2=-0.19	1975PRb (5782)	10

By extraction from 2M HClO4/HCl with dinonylnaphthalene sulfonic acid

---

Th++++	ISE	none	25°C	0.0	U	TIH	K1=1.57		1968OMa (5783)	11

DH(K1)=0 kJ mol-1, DS=30.1 J K-1 mol-1. Method: Ag electrode

Th++++	ix	NaClO4		4.0M	U		K1=0.20	B2=-0.80	1964NKb (5784)	12
							B3=-0.85			
							B4=-1.46			
							B5=-2.46			

Th++++	dis	NaClO4	25°C	6.0M	U	I	K1=0.32	B2=-0.26	1952WSa (5785)	13
							K3=-0.20			

In 4 M NaClO4 K1=0.23, K2=0.58, K3=-0.15, K4=-0.74. 2 M: K1=0.08, K2=-1.08, K3=0.30. 1 M: K1=0.18. 0.5 M: K1=0.35. I=0 corr.: K1=1.38

Th++++	dis	NaClO4	25°C	4.0M	U		K1=0.11	B2=-0.92	1951ZAa (5786)	14
							K3=-0.51			
							K4=-0.42			

Th++++	dis	NaClO4	25°C	0.50M	U		K1=0.25		1950DSa (5787)	15

****

ClO3- HL Chlorate CAS 7790-93-4 (971)
Chlorate;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Th++++	dis	NaClO4	25°C	1.00M	U	H	K1=0.14		1992CKb (6062)	16

DH(K1)=2.4 kJ mol-1; DS=11 J K-1 mol-1

Th++++	dis	NaClO4	25°C	0.50M	U		K1=0.26		1950DSa (6063)	17

****

CrO4-- H2L Chromate CAS 7738-94-5 (2382)
Chromate;

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

```
--------------------------------------------------------------------------------
Th++++     sp  NaClO4 11°C 0.20M U TIH                  1972BTc  (6511)  18
                                        *K1=0.53
17.8 C; *K1=0.59. 25.7 C; *K1=0.67. DH(*K1)=15.5 kJ mol-1
********************************************************************************
F-                      HL    Fluoride         CAS 7644-39-3  (201)
Fluoride;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Th++++     cal NaClO4 25°C  4.0M U   H                  1990AHa  (7235)  19
DH(Th+HF=ThF+H)=14.3 kJ mol-1; DH(ThF+HF=ThF2+H)=12.8
--------------------------------------------------------------------------------
Th++++     ISE NaClO4 23°C  1.0M C        K1=7.61   B2=13.42  1990SCa  (7236)  20
                                        B3=17.65
                                        B4=23.67
Medium: 1.0 M HClO4/NaClO4. Method: F ion selective electrode.
--------------------------------------------------------------------------------
Th++++     cal NaClO4 25°C 0.50M C   H                  1989GKa  (7237)  21
DH(K1)=1.6 kJ mol-1, DS(K1)=150 J K-1 mol-1; DH(B2)=4.3, DS(B2)=270;
DH(B3)=7.8, DS(B3)=370.
--------------------------------------------------------------------------------
Th++++     ISE NaNO3  25°C 0.10M U   H                  1987SMd  (7238)  22
                                        K(ThA+L)=4.38
                                        K(ThA+2L)=7.96
DH=-25.9 kJ mol-1, DS=67.0 J K-1 mol-1. H3A=HEDTA
--------------------------------------------------------------------------------
Th++++     ISE NaNO3  25°C 0.10M U   H                  1987SMd  (7239)  23
                                        K(ThA+L)=3.81
DH=-6.2 kJ mol-1, DS=52.0 J K-1 mol-1. H5A=DTPA
--------------------------------------------------------------------------------
Th++++     cal KNO3   25°C    4M U TIH    K1=8.65   B2=15.10  1981SMc  (7240)  24
                                        K(ThF+H=ThHF)=3.8
                                        K(ThF2+H=ThF(HL))=3.0
                                        K(ThF3+H=ThF2(HF))=2.2
                                        K(ThF4+H=ThF3(HF))=1.4
ISE also used. 4-13 M HNO3, 25 - 100 C. K(ThF4(s)+4H=Th+4HF)=-12.2
K(ThF4(s)+3H=ThF+3HF)=-9.3, K(ThF4(s)+2H=ThF2+2HF)=-7.0, K(s4)=-5.6
--------------------------------------------------------------------------------
Th++++     ISE KNO3   25°C 0.50M U    M   K1=7.62        1977SSa  (7241)  25
                                        B(Th(EDTA)L)=4.83
                                        B(Th(DTPA)L)=3.81
--------------------------------------------------------------------------------
Th++++     dis NaClO4 25°C 2.00M U        K1=4.70   B2=7.46   1975PRb  (7242)  26
By extraction from 2M HClO4/HCl with dinonylnaphthalene sulfonic acid
--------------------------------------------------------------------------------
Th++++     ISE NaClO4 25°C  4.0M U  I                  1973NOa  (7243)  27
                                        *K1=4.62
                                        *K2=2.81
                                        *K3=2.0
```

Medium: HClO4. *Kn: ThF(n-1)+HF=ThFn+H

Th++++ ISE NaClO4 25°C 3.0M U 1971KMd (7244) 28
*K1=4.52
*B2=7.26
*B3=8.9
*Bn=Th+nHF=ThFn+nH

Th++++ EMF NaClO4 25°C 3.0M U 1971KMd (7245) 29
Kso(ThF4(s))=-15.17
Method: quinhydrone electrode

Th++++ ISE R4N.X 25°C 0.01M U T H K1=8.08 B2=14.44 1970BAc (7246) 30
K3=4.57
K4=3.28
Medium: NH4NO3. K1=8.11(5 C), 7.95(45 C); K2=6.29(5 C), 6.20(45 C); K3=4.64 (5 C), 4.55(45 C); K4=3.33(5 C), 3.71(45 C).

Th++++ ISE none 25°C 0.0 U T K1=8.44 B2=15.06 1970BAc (7247) 31
K3=4.75
K4=3.36
K1=8.46(5 C),8.32(45 C); K2=6.55(5 C),6.48(45 C); K3=4.81(5 C),4.73(45 C); K4=3.41(5 C),3.80(45 C)

Th++++ ISE NaClO4 20°C 4.0M U 1969NOb (7248) 32
*K1=4.68
*K2=2.97
Medium: HClO4. *Kn=ThF(n-1)+HL=ThFn+H. By distribution: *K1=4.62

Th++++ sol NaClO4 25°C var U 1962NLa (7249) 33
K(ThF4(s)+3H=ThF+3HF)=-10.1
Kso(ThF4(s))=-25.3

Th++++ sp oth/un 25°C var U K1=6.0 1959TAa (7250) 34

Th++++ sol oth/un 25°C var U K1=5.9 B2=8.7? 1959TLa (7251) 35

Th++++ dis NaClO4 25°C 0.50M U 1951ZAa (7252) 36
K(Th+HF=ThF+H)=4.70
K(ThF+HF=ThF2+H)=2.76

Th++++ dis oth/un 25°C 0.50M U M 1950DSa (7253) 37
K(Th+HF=ThF+H)=4.63
K(ThF+HF=ThF2+H)=2.86
K(Th+HF+NO3=ThFNO3+H)=4.2
K(Th+2HF+NO3=ThF2NO3+2H)=6.9

Th++++ EMF NaClO4 25°C 0.50M U I 1949DRa (7254) 38
K(Th+HF=ThF+H)=4.65
K(ThF+HF=ThF2+H)=2.81

K(ThF2+HF=ThF3+H)=1.51
*K=-7.23
*K: ThF4(OH)4(s)+2H=ThF2+2HF+4H2O). At I=0 corr. K1=8.65
****
H2O L Water CAS 7732-18-5 (6115)
Water

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Th++++ sp alc/w 25°C 100% U K1=0.18 1953BJa (7612) 39
Medium: EtOH, NO3. Maximum value of n=8 ?
****
IO3- HL Iodate CAS 7782-68-5 (1257)
Iodate;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Th++++ dis NaClO4 25°C 1.00M U H K1=2.49 1992CKb (8559) 40
DH(K1)=6.5 kJ mol-1; DS=70 J K-1 mol-1

Th++++ sol oth/un 25°C 0.50M U K1=2.88 B2=4.81 1961SFa (8560) 41
B3=7.18
B6=11.02
B8=12.96
Kso(ThL4)=-14.62
Medium: LiNO3. K(ThL4(s)+2L=ThL6; K(ThL4(s)+4L=ThL8)=-1.66. B(ThH-1L)=0.40,
B(ThH-1L2)=2.38, Kso(ThH-1L3)=-9.80

Th++++ dis NaClO4 25°C 0.50M U K1=2.88 B2=4.79 1950DSa (8561) 42
K3=2.36
****
NO2- HL Nitrite CAS 7782-77-6 (635)
Nitrite;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Th++++ vlt non-aq 23°C 100% U I K1=2.11 B2=4.03 1968GKd (9406) 43
B3=5.80
B4=7.65 or 7.39 ?
Also spectrophotometry. Medium:Me2NCHO. In MeOH,complex probably Th(OCH3)2Ln
K1=2.23, B2=4.17, B3=5.85
****
NO3- HL Nitrate CAS 7697-37-2 (288)
Nitrate;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Th++++ oth oth/un 25°C var U K1=0.1 B2=0.8 1972ODa (9937) 44
Method:Raman spectra

```
Th++++     ix  NaClO4 25°C  2.0M U        K1=1.22   B2=1.53   1968TRd  (9938)  45
                                         B3=1.1
Medium: HClO4
-------------------------------------------------------------------------------
Th++++     dis oth/un 25°C  1.0M U                    1964DLa  (9939)  46
                                         Kd(Th+4L=ThL4(org))=-2.0
Medium: HNO3. Org=Me(i-Bu)CHOH
-------------------------------------------------------------------------------
Th++++     ix  NaClO4   ?   4.0M U        K1=0.55   B2=0.32   1964NKb  (9940)  47
                                         B3=-0.30
                                         B4=-0.72
-------------------------------------------------------------------------------
Th++++     ix  oth/un 25°C  var  U                    1960DAd  (9941)  48
                                         K4=-0.22
                                         K5=-0.80
                                         k6=-0.90
-------------------------------------------------------------------------------
Th++++     dis NaClO4 20°C  2.0M U                    1960EFa  (9942)  49
Medium: HClO4. Kd(Th+4L+2TBP(C6H6)=ThL4(TBP)2(C6H6))=1.56
-------------------------------------------------------------------------------
Th++++     dis NaClO4   ?  1.70M U    M               1959MFb  (9943)  50
                                         K(Th+HSO4+L=ThSO4L+H)=3.29
                                         K(Th+HSO4+2L=ThSO4L2+H)=3.04
                                         K(Th+HSO4+3L=ThSO4L3+H)=2.07
-------------------------------------------------------------------------------
Th++++     dis NaClO4 20°C  2.0M U        K1=0.78   B2=1.11   1956FMa  (9944)  51
                                         K3=-0.11
                                         K4=-0.26
-------------------------------------------------------------------------------
Th++++     dis NaClO4 25°C 5.97M U        K1=0.45   B2=0.15   1951ZAa  (9945)  52
-------------------------------------------------------------------------------
Th++++     dis NaClO4 25°C 0.50M U        K1=0.67             1950DSa  (9946)  53
*******************************************************************************
OH-                    HL    Hydroxide          (57)
Hydroxide;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Th++++     gl  NaClO4 25°C  3.0M C                      2002TFa (12231)  54
                                         *B(2,2)=-4.96
-------------------------------------------------------------------------------
Th++++     gl  NaClO4 25°C  1.0M C T H                  2000EAa (12232)  55
                                         *K1=-3.3
                                         *B2=-8.6
                                         *B3=-14.2
                                         *B4=-19.4
*B(4,8)=-19.1, *B(6,15)=-39.5. DH(*K1)=38 kJ mol-1, DH(*B2)=36, DH(*B3)=19
DH(*B4)=360. Additional method: solvent extraction. Data at 15 and 35 C.
-------------------------------------------------------------------------------
Th++++     gl  NaClO4 25°C 3.00M C                      1991GLa (12233)  56
```

*B1=-4.35
*B4=-16.65
*B(2,2)=-5.10
*B(2,3)=-7.87
*B(4,8)=-19,6, *B(4,12)=-34.86, *B(6,14)=-33.67, *B(6,16)=-42.90

Th++++ gl NaClO4 25°C 3.00M U 1987BCc (12234) 57
*B(2,2)=-4.74
*B(4,8)=-19.15
*B(6,14)=-33.83
*K1=-4.13, *B4=-15.7

Th++++ sp oth/un 20°C 0.1M U K1=9.81 1986DTa (12235) 58
In 0.1 M HNO3/NaNO3

Th++++ gl KNO3 25°C 0.10M C 1983BEa (12236) 59
*B(1,1)=-2.98
*B(4,12)=-30.55
*B(6,15)=-34.41

Th++++ gl NaNO3 25°C 0.50M C I 1982MSi (12237) 60
*B(2,2)=-5.06
*B(3,5)=-12.59
*B(6,15)=-38.06
Data for 0.50-3.0 M NaNO3. At I=1.0 M, *B(2,2)=-5.08, *B(3,5)=-13.04,
*B(6,15)=-39.5. At I=3.0 M, *B(2,2)=-5.19, *B(3,5)=-14.23, *B(6,15)=-42.32

Th++++ gl oth/un 25°C 2.50M U I 1982SMd (12238) 61
*B(2,2)=-4.90
*B(2,3)=-8.43
Medium: MgCl2. Further data for other chloride media and concentrations

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Th++++ gl oth/un 25°C 3.00M U H 1981MIa (12239) 62
*B(2,2)=-5.23
*B(2,3)=-8.28
In LiCl. DH(*B(2,2))=133.6 kJ mol-1, DS(*B(2,2))=348.3; DH(*B(2,3))=23.1;
DS(*B(2,3))=-80.9

Th++++ gl KCl 25°C 3.00M U H 1981MIa (12240) 63
*B(2,2)=-5.04
*B(2,3)=-8.16
DH(*B(2,2))=101.9 kJ mol-1; DS(*B(2,2))=245.6; DH(*B(2,3))=38.1;
DS(*B(2,3))=-28.2

Th++++ gl NaCl 25°C 1.00M U IH 1981MIa (12241) 64
*B(2,2)=-4.88
*B(2,3)=-7.93
Range I=0.5-3.0. At I=1.0 DH(*B(2,2))=87.0 kJ mol-1;DS(*B(2,2))=198.7;
DH(*B(2,3))=76.8; DS=106

```
Th++++     gl  oth/un 25°C 1.00M U  I                    1981SMa (12242)  65
                                        *B(2,2)=-5.07 in LiCl.
                                        *B(2,3)=-7.85
--------------------------------------------------------------------------------
Th++++     sol NaClO4 25°C 0.00  U T                     1980ZKa (12243)  66
                                        *Kso(ThO2)=-3.3
                                        *Ks(ThO2(s)+2H2O)=-6.66
--------------------------------------------------------------------------------
Th++++     EMF alc/w  25°C  25%  U  I                    1972USa (12244)  67
                                        *K1=-2.8
                                        *B2=-6.1
Medium: 25% EtOH/H2O, 1.0 M NaClO4. In 50% EtOH: *K1=-2.2, *B2=-5.3
--------------------------------------------------------------------------------
Th++++     EMF NaClO4 25°C 1.00M U  I                    1972USa (12245)  68
                                        *K1=-3.15
                                        *B2=-6.6
I=0(corr), *K1=-2.64, *B2=-5.7
--------------------------------------------------------------------------------
Th++++     gl  oth/un 20°C 0.02M U                       1971KSc (12246)  69
                                        *K1=-3.61
                                        *B2=-7.62
                                        *B3=-11.17
                                        *B4=-14.43
Medium: dilute solution (I=0.01-0.04)
--------------------------------------------------------------------------------
Th++++     gl  oth/un 25°C 3.00M U  I                    1971MIa (12247)  70
                                        *B(2,2)=-5.14
                                        *B(3,5)=-14.23
                                        *B(3,3) < -7.7
Medium: LiNO3. Data also for 3 M KNO3: *B(2,2)=-5.10, *B(2,3)=-8.98,
*B(1,2) < -9.7, *B(6,15)=-40.95
--------------------------------------------------------------------------------
Th++++     gl  oth/un 25°C 3.00M U                       1971MIa (12248)  71
                                        *B(2,2)=-5.17
                                        *B(3,5)=-14.29
                                        *B(6,15)=-43.20
Medium: Mg(NO3)2
--------------------------------------------------------------------------------
Th++++     oth NaNO3  25°C 4.00M U                       1968DMd (12249)  72
                                        *B(2,2)=-5.5
                                        *B(3,6)=-17.92
                                        *B(4,12)=-37.2
                                        *B(2,1)=-2.72
*B(3,5)=-12.42,*B(2,4)=-10.49, *B(4,8)=-19.2, *B(6,14)=-36.2
Method: quinhydrone electrode
--------------------------------------------------------------------------------
Th++++     EMF NaClO4 25°C 1.00M U                       1968HSb (12250)  73
                                        *B(2,2)=-4.44
                                        *B(4,8)=-18.78
                                        *B(6,15)=-36.42
```

```
                                        *K1=-3.71
Method: H electrode
-------------------------------------------------------------------------------
Th++++     EMF NaCl   25°C 3.00M U                      1968HSb (12251)  74
                                        *K1=-5.0
                                        *B(2,2)=-4.76
                                        *B(2,3)=-8.94
                                        *B(2,5)=-16.99
*B(3,1)=-1.36,*B(3,3)=-6.83,*B(4,8)=-21.11,*B(6,14)=-36.58,*B(10,25)=-65.35
Method: H electrode
-------------------------------------------------------------------------------
Th++++     gl  NaClO4 25°C 0.50M U        K1=11.64  B2=22.44  1967BEb (12252)  75
                                        K3=10.62
                                        K4=10.45
-------------------------------------------------------------------------------
Th++++     oth oth/un   ?   2.0M U        K1=7.74        1966LIa (12253)  76
Method:Literature evaluated data
-------------------------------------------------------------------------------
Th++++     gl  NaClO4 25°C 1.00M U                      1965BMb (12254)  77
                                        *B(2,2)=-4.61
                                        *B(4,8)=-19.01
                                        *B(6,15)=-36.53
                                        *K1=-4.12,  *B2=-7.81
m units
-------------------------------------------------------------------------------
Th++++     gl  NaClO4  0°C 1.00M U T H                  1965BMb (12255)  78
                                        *B1=-4.32
                                        *B2=-8.48
                                        *B(2,2)=-5.60
                                        *B(4,8)=-22.79
*B(6,15)=-43.82 (m units). At 95 C: values are:-2.29,-4.50,-2.55,-10.49,
-20.63 respectively. K(ThO2(s)+4H=Th+4H2O)=4.26 by solubility
-------------------------------------------------------------------------------
Th++++     sol NaClO4 25°C 1.00M U   H                  1965BMb (12256)  79
*DH(K1)=-24.7, *DH(B2)=58.1, *DH(2,2)=61.8, *DH(4,8)=241.2, *DH(6,15)=453.5
kJ mol-1. *DS(K1)=3.8,*DS(B2)=46,*DS(2,2)=119,*DS(4,8)=446, " 818 J K-1 mol
-------------------------------------------------------------------------------
Th++++     sol NaClO4  0°C 1.00M U T                    1965BMb (12257)  80
                                        *K1=-4.31
                                        *B2=-8.46
                                        *B(2,2)=-5.59
                                        *B(4,8)=-22.80
*B(6,15)=-43.81. At 25 C: values are respectively: -4.23, -7.69, -4.61,
-19.16, -37.02.  At 95 C: -2.25, -4.51, -2.59, -10.44, -20.61
-------------------------------------------------------------------------------
Th++++     gl  NaCl   25°C 3.00M U                      1964HSa (12258)  81
                                        *B(1,2)=-9.1
                                        *B(2,1)=-2.65
                                        *B(2,2)=-4.70
                                        *B(2,3)=-8.83
```

*B(6,14)=-36.53, *B(6,15)=-40.37.

Th++++ sol NaClO4 17°C 0.10M U K1=9.4 B2=18.30 1964NKc (12259) 82
K3=8.1
K4=8.1
Ks(Th(OH)4(s)=Th(OH)4)=-6.32
Kso=-41.14

Th++++ oth oth/un 20°C var U 1963BFd (12260) 83
Kso(Th(OH)4)=-45.7
Ks(Th(OH)4=Th(OH)2+2OH)=-24.3
*B2=-7.0
method:tyndallometry

Th++++ sp none 22°C 0.0 U 1961KBd (12261) 84
Kso(Th(OH)4)=-44.7

Th++++ EMF NaCl 25°C 2.20M C 1959HSb (12262) 85
*B(2,1)=-2.8
*B(2,2)=-5.02
Method: H electrode. *B(2,2)=-4.95 if no Th2OH

Th++++ EMF NaCl 25°C 3.0M C 1959HSb (12263) 86
*B(2,1)=-2.9
*B(2,2)=-5.09
*B(2,2)=-4.95(if no Th2OH)

Th++++ gl NaClO4 25°C 1.0M U 1958LEb (12264) 87
*B2(Th+2H2O=Th(OH)2+2H)=-7.42
*B(2,2)=-4.56
*B(5,12)=-29.5

Th++++ gl NaClO4 25°C 0.50M U I 1955PHb (12265) 88
*K1=-4.26
*K2=-4.02
At I=0 *K1=-3.89, *K2=-4.20

Th++++ sol none 25°C 0.0 U 1954GLa (12266) 89
*Ks2=4.74
*Ks3=1.51
Ks5=-5.80
Ks6=-5.80
*Ksn: K(M(OH)4(s)+(4-n)H=M(OH)n+(4-n)H2O); Ksn: K(M(OH)4(s)+(n-4)OH=M(OH)n) (n=5,6)

Th++++ EMF NaClO4 25°C 1.0M C 1954HIa (12267) 90
*B(n+1,3n)=-7.50n
*B(n+1,3n)=-7.65n for higher n
*B(n+1,3n): K((n+1)Th+3nH2O=Th(n+1)(OH)3n+3nH). Method: H and quinhydrone el

---

```
Th++++     gl  NaClO4 25°C  1.0M U                          1954KHa (12268)  91
                                        *K1=-4.3
                                        *K2=-3.4
                                        *B(2,2)=-4.7
*B(2,2): K(2Th+2H2O=Th2(OH)2+2H)
-------------------------------------------------------------------------------
Th++++     oth none   25°C  0.0  U                          1952LAb (12269)  92
                                        Kso(Th(OH)4)=-39
Method: combination of thermodynamic data
-------------------------------------------------------------------------------
Th++++     dis oth/un   ?   var  U                          1943KTa (12270)  93
                                        Kso(Th(OH)4)=-42
Method: electrical migration
-------------------------------------------------------------------------------
Th++++     gl  oth/un 25°C  dil  U                          1938OKa (12271)  94
                                        Kso(Th(OH)4)=-44.9
*******************************************************************************
PO4---                H3L    Phosphate        CAS 7664-38-2  (176)
Phosphate;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Th++++     sol none   25°C  0.0  C  I                      1994BFc (13341)  95
                                        Kso(Th3(PO4)4)=-112
Method: 227Th-labelled Th3(PO4)4 dissolved in HClO4 (0.01-1.0M). High
temperature Th3(PO4)4 (1400C). K((1/3)Th3(PO4)4+4H=Th+(4/3)H3PO4)=-8.20.
-------------------------------------------------------------------------------
Th++++     sol NaClO4 25?°C 0.35M U                        1967MEb (13342)  96
                                        K(Th+HL)=10.8
                                        K(Th+2HL)=22.8
                                        K(Th+3HL)=31.3
                                        Ks(Th(HL)2)=-26.89
Medium: HClO4. Other solubility products given
-------------------------------------------------------------------------------
Th++++     sol oth/un 20°C  var  U                          1956CSd (13343)  97
                                        Kso(Th3L4)=-78.59 or -57.61 ?
                                        Ks(Th(HL)2=Th+2HL)=-20.5
-------------------------------------------------------------------------------
Th++++     dis NaClO4 25°C 2.00M U                          1951ZAa (13344)  98
                                        K(Th+H3L)=1.89
                                        B(ThH-1(H3L))=2.18
                                        B(ThH-2(H3L)2)=3.90
                                        B(ThH-1(H2L)2)=4.15
*******************************************************************************
P2O7----              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
-------------------------------------------------------------------------------
Th++++     sol NaClO4 25°C 0.10M U        K1=18.05          1967MSc (13661)  99
```

Kso(ThL(H2O)4)=-24.25

Th++++ con oth/un 25°C dil U K2=5.3 1960FTa (13662) 100

****

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

Thiocyanate;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Th++++	dis	NaClO4	?	3.0M	U		K1=0.85	B2=1.53	1971LFb (15269)	101
							B3=1.16			
							B4=1.51			
Th++++	sp	non-aq		100%	U	I	K1=3.5		1966GKe (15270)	102
							B3=9.57			
							B4=12.55			

Medium: Me2CO. In MeOH: K1=3.37, B2=6.66, B3=9.82, B4=12.89. In Me2NCHO: K1=3.20, B2=6.28, B3=9.26, B4=12.12, B5=14.92, B6=17.7

Th++++	dis	NaClO4	25°C	1.0M	U	T	K1=1.08		1950WSa (15271)	103
							B3=1.78			

****

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

Sulfate;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Th++++	dis	NaNO3	10°C	2.0M	U	T			1972PRb (16583)	104
							*K1=2.34			
							*B2=3.59			

Medium: HClO4. 25 C: *K1=2.26, *B2=3.57; 40 C: *K1=2.24, *B2=3.51

Th++++	dis	none	25°C	0.0	U				1963AMb (16584)	105
							K3=0.76			
							K4=-2.02			
Th++++	dis	NaClO4	?	1.70M	U				1959MFb (16585)	106
							*K1=2.3			
							*K2=1.1			
Th++++	ix	NaClO4	25°C	2.0M	U	H			1959ZIa (16586)	107
							*K1=2.22			
							*K2=1.34			

Medium: HClO4. By calorimetry: DH(*K1)=-2.3 kJ mol-1, DS=35.1 J K-1 mol-1; DH(*K2)=-3.7, DS=13.4

Th++++	dis	NaClO4	25°C	2.0M	U		K1=3.32	B2=5.70	1953WDa (16587)	108
Th++++	dis	NaClO4	25°C	2.0M	U		K1=3.28	B2=5.61	1951ZAa (16588)	109
							*K1=2.20			

*K2=1.25
K(Th+2HL=ThHL2+H)=2.9

****

SeCN- HL Selenocyanate CAS 73102-11-2 (440)
Selenocyanate;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	sp	non-aq	20°C	100%	U	I	K1=3.27 B4=12.12	1967GKd (16995)	110

Medium: Me2CO. In Me2NCHO: K1=3.08, B2=5.92, B3=8.80, B4=11.57, B5=14.36, B6=17.67

****

SeO3-- H2L Selenite CAS 7783-00-8 (2391)
Selenite;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	sol	oth/un	20°C	var	U		Kso(ThL2)=-19.87	1957KCb (17075)	111

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	EMF	NaClO4	20°C	1.00M	U		K1=3.09 B2=5.15 B3=6.73	1972PTb (17654)	112

****

CH4N2S L Thiourea CAS 62-56-6 (51)
Thiocarbamide, Thiourea; (H2N)2CS

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	vlt	KNO3	25°C	1.5M	C		K1=0.46 B2= 0.26	1978DKb (17860)	113

Method: polarography, using Cd as indicator ion.

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	gl	alc/w	25°C	100%	C		*K1=-3.36 *B3=-15.94 *B4=-24.68 *B(2,5)=-22.6	1997ACa (17906)	114

Medium: methanol, 0.01 M NEt4ClO4. *K1: Pr+MeOH=Pr(OMe)+H. *B(2,7)=-36.6, *B(2,9)=-59.2.

```
Th++++     EMF alc/w  20°C 100%  U                        1964GUa (17907) 115
                                        K(Th+H-1L)=12.35
                                        K(Th(H-1L)2+H=ThH-1L+L)=4.35
Method: H electrode. Medium: MeOH, 1.0 M Me4NCl
********************************************************************************
CH6O6P2               H4L    Medronic acid    CAS 1984-15-2  (2384)
Methanediphosphonic acid; CH2(PO3H2)2
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Th++++     dis NaClO4 25°C  2.0M U                        1991NAa (18294) 116
                                        K(Th+H2H+H2L)=8.84
                                        K(Th+H2L)=8.34
                                        K(Th+2H2L)=15.44
--------------------------------------------------------------------------------
Th++++     gl  KCl    25°C 0.10M U        K1=23.9   B2=36.7   1967KLa (18295) 117
********************************************************************************
C2HO2Cl3               HL    Trichloroacetic  CAS 76-03-9  (1205)
Trichloroethanoic acid; Cl3C.COOH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Th++++     dis NaClO4 25°C 0.50M U        K1=1.62   B2=2.82   1950DSa (18335) 118
********************************************************************************
C2H2N2S3              H2L    Bismuthiol I     CAS 1072-71-5  (6261)
2,5-Dimercapto-1,3,4-thiadiazole;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Th++++     gl  NaClO4 25°C 0.15M U  I     K1=12.10  B2=23.00  1977ZIa (18370) 119
********************************************************************************
C2H2O2Cl2              HL                    CAS 79-43-6  (1282)
Dichloroethanoic acid; Cl2CH.COOH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Th++++     dis NaClO4 25°C 0.50M U        K1=2.01   B2=3.71   1950DSa (18400) 120
********************************************************************************
C2H2O4                H2L    Oxalic acid      CAS 144-62-7  (24)
Ethanedioic acid; (COOH)2
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Th++++     cal NaClO4 25°C  1.0M C   H                   1991BGb (19083) 121
DH(K1)=-3.0 kJ mol-1, DS(K1)=140 J K-1 mol-1.
--------------------------------------------------------------------------------
Th++++     oth NaClO4 40°C 0.10M C    M   B2=7.67        1984SIa (19084) 122
                                        B(ThL(nta))=9.74
Method: Paper electrophoresis, pH 10.0.
--------------------------------------------------------------------------------
```

```
Th++++     dis NaClO4 25°C 1.00M U        K1=7.86   B2=14.12  1976BRa (19085) 123
                                          B3=19.94
-------------------------------------------------------------------------------
Th++++     gl  oth/un 25°C 0.05M U        K1=8.81        1973CSd (19086) 124
                                          K(Th+HL)=7.36
-------------------------------------------------------------------------------
Th++++     sp  NaNO3    ?  0.50M U        K1=8.45   B2=15.43  1970GBa (19087) 125
-------------------------------------------------------------------------------
Th++++     sol oth/un 25°C 0.10M U        K1=9.22        1970MKe (19088) 126
-------------------------------------------------------------------------------
Th++++     sol R4N.X  25°C  1.0M U        K1=8.23   B2=16.8   1967MEc (19089) 127
                                          B3=22.8
                                          B4=27.2
                                          Kso=-21.38
Medium: NH4ClO4. At I=0 corr: K1=10.6, B2=20.2, B3=26.4, B4=29.6, Kso=-24.96
-------------------------------------------------------------------------------
Th++++     gl  oth/un 30°C  4.0M U                       1964PCa (19090) 128
                                          B=24.48
-------------------------------------------------------------------------------
Th++++     kin oth/un 25°C  0.0  U        K1=7.16        1962YZa (19091) 129
                                          K(2ThOH+HL)=22.9
*******************************************************************************
C2H3O2Cl               HL    Chloroacetic     CAS 79-11-8  (34)
Chloroethanoic acid; ClCH2.COOH
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Th++++     gl  NaClO4 25°C 1.00M C   H    K1=2.75   B2= 4.64  1978DZa (19384) 130
                                          B3=5.79
                                          B4=6.53
DH(K1)=12.21 kJ mol-1, DS(K1)=93.7 J K-1 mol-1; DH(B2)=13.01, DS(B2)=79.5;
DH(B3)=10.71, DS(B3)=58.2; DH(B4)=7.99, DS(B4)=41.0.
-------------------------------------------------------------------------------
Th++++     EMF NaClO4 20°C 1.00M U        K1=2.77   B2=4.64   1972PTb (19385) 131
                                          B3=5.75
                                          B4=6.79
-------------------------------------------------------------------------------
Th++++     dis NaClO4 25°C 0.50M U        K1=2.98        1949AHa (19386) 132
*******************************************************************************
C2H4O2                 HL    Acetic acid      CAS 64-19-7  (36)
Ethanoic acid; CH3.COOH
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Th++++     gl  NaClO4 25°C 1.00M C T H    K1=3.81   B2= 6.83  2004RZa (20195) 133
                                          B3=8.77
                                          B4=10.25
                                          B5=11.51
Calorimetry: DH(K1)=12.2 kJ mol-1, DS=114 J K-1 mol-1, DH(B2)=16.9, DS=187
DH(B3)=30.8, DS=270, DH(B4)=30.7, DS=298, DH(B5)=38.9, DS=349. Data 10-70C
```

Th++++ dis NaCl 25°C 0.30M C I K1=3.73 B2= 7.47 1999MBb (20196) 134
Method: Solvent extraction into n-heptane,0.05 M dibenzoylmethane
Data for 0.3-5.0 m NaCl. At I=0.0, K1=5.24, B2=9.06.

Th++++ gl NaClO4 20°C 0.10M U K1=3.88 1985SAa (20197) 135

Th++++ cal NaClO4 25°C 1.00M U H K1=3.86 B2=6.97 1975PBa (20198) 136
B3=8.94
B4=10.29
B5=10.99
DH(K1)=11.30, DH(B2)=7.69, DH(B3)=13.68, DH(B4)=5.19, DH(B5)=37.24 kJ mol-1
DS(K1)=111.7, DS(B2)=74.5, DS(B3)=83.7, DS(B4)=43.5, DS(B5)=25.9 J mol-1 K-1

Th++++ EMF NaClO4 20°C 1.00M U K1=3.88 B2=6.91 1972PTb (20199) 137
B3=9.05

Th++++ sp oth/un 25°C 1.00M U K1=1.15 1972PTb (20200) 138
pH=2

Th++++ EMF oth/un 25°C 1.00M U K1=1.02 1972TAa (20201) 139

Th++++ EMF KNO3 25°C 0.50M U K1=3.12 B2=3.17 1970SAd (20202) 140

Th++++ oth none ? 0.00 U K1=2.68 B2=5.03 1969MOc (20203) 141
B3=6.60
Survey of literature data.
****
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
---
Th++++ gl NaClO4 25°C 1.0M C H K1=3.22 B2= 5.69 1978DRa (20376) 142
B3=7.20
B4=8.54
By calorimetry: DH(K1)=10.2 kJ mol-1, DS=95.8 J K-1 mol-1; DH(B2)=7.99,
DS=74.0; DH(B3)=10.9, DS=65.7; DH(B4)=3.3, DS=37.
****
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
---
Th++++ gl NaClO4 25°C 3.0M C K1=4.27 B2= 7.66 2002TFa (20635) 143
B3=10.4
B4=12.2
B(Th2H-2L2)=4.48
B(Th2H-2L4)=11.0
B(Th2H-2L6)=15.7, B(Th4H-6L8)=21.6, B(Th4H-8L8)=8.63, B(Th4H-9L8)=2.03,

B(Th4H-10L8)=-5.97, B(Th4H-11L8)=-14.8, B(Th4H-12L8)=-24.8; other values

---

Th++++ gl NaClO4 25°C 1.0M C H K1=4.11 B2= 7.45 1978DRa (20636) 144
B3=10.18
B4=11.97
B5=13.36
By calorimetry: DH(K1)=2.1 kJ mol-1, DS=85.8 J K-1 mol-1; DH(B2)=-0.84, DS=61.1; DH(B3)=-2.97, DS=42.3; DH(B4)=-3.9, DS=21; DH(B5)=-2.4, DS=19.

Th++++ EMF NaClO4 20°C 1.00M U T K1=3.98 B2=7.36 1973MBc (20637) 145
B3=9.95
B4=11.95

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	gl	NaClO4	20°C	0.10M	U		K1=9.68	1985SAa (21729)	146
Th++++	oth	NaClO4	35°C	0.01M	U		K1=7.82 B2=11.64	1984YSa (21730)	147

Method: paper electrophoresis.

Th++++ gl NaClO4 25°C 1.00M C H K1=2.55 B2=4.21 1983BRa (21731) 148
K3=1.33
DH1=4.2, DH(K2)=4.5, DH(K3)=2.3 kJ mol-1

Th++++ ix KNO3 20°C 0.50M U T K1=8.90 1980SEa (21732) 149

Th++++ gl KNO3 30°C 0.10M U M 1976PTc (21733) 150
K(ThA+L)=6.06
K(ThB+L)=5.16
H4A=EDTA, H4B=CDTA

****

C2H5O5P H3L CAS 4408-78-0 (4225)
Phosphonoethanoic acid; HOOC.CH2.PO3H2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	dis	NaClO4	25°C	2.0M	U		K(Th+H+H2L)=8.50	1991NAa (21895)	151
							K(Th+2H+2H2L)=16.05		

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	gl	NaClO4	10°C	0.10M	U	T	K1=8.62 B2=17.11	1977SKe (22083)	152
							K3=8.33		

At 20 C: K1=8.60, K2=8.46, K3=8.25; 30 C: K1=8.56, K2=8.41, K3=8.30

****

C2H6O6P2 H4L (5706)

Ethene-1,1-diphosphonic acid; H2C:C(PO3H2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	dis	NaClO4	25°C	2.0M	U		K(Th+H+H2L)=8.83 K(Th+H2L)=8.64 K(Th+2H+2H2L)=15.78	1991NAa (22176)	153

****

C2H7O4P HL CAS 813-78-5 (1754)

Dimethylphosphoric acid; (CH3O)2P(O)OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	kin	none	25°C	0.00	U		K(ThOH+L)=3.81	1966SSb (22577)	154

****

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
Th++++	dis	NaClO4	25°C	2.0M	U		K(Th+H2L)=9.72 K(Th+H+3H2L)=25.10 K(Th+2H+2H2L)=17.65	1991NAa (23400)	155
Th++++	gl	KCl	25°C	0.10M	U		K(Th+H-1L))=27.8 K(Th+2H-1L))=39.9	1967KLa (23401)	156

****

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
Th++++	gl	NaClO4	25°C	0.10M	M	M	K1=8.35 K(Th(nta)+L)=4.81	1987NCa (24565)	157
Th++++	gl	NaClO4	25°C	1.00M	U		K1=7.47 B2=12.79 B3=16.28	1977BNa (24566)	158
Th++++	EMF	NaClO4	20°C	1.00M	U		K1=7.42 B2=12.68	1972TMa (24567)	159
Th++++	kin	oth/un	25°C	0.0	U		K1=7.25 B(Th2L(OH))=22.46	1963YZa (24568)	160

****

C3H5O2Cl HL CAS 107-94-8 (1436)
3-Chloropropanoic acid; Cl.CH2.CH2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Th++++	EMF	NaClO4	20°C	1.00M	U		K1=3.50	B2=5.98	1972PTb (24735)	161
							B5=8.17			

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
Th++++	EMF	NaClO4	20°C	1.00M	U		K1=3.94	B2=7.25	1972PTb (25059)	162
							B3=9.44			
							B4=11.20			
Th++++	sp	oth/un	25°C	1.00M	U		K1=1.31		1972TAa (25060)	163
pH 2										
Th++++	EMF	oth/un	25°C	1.00M	U		K1=1.42		1972TAa (25061)	164

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Th++++	dis	NaCl	25°C	0.30M	C	I	K1=3.85	B2= 7.08	1999MBb (25551)	165
Method: Solvent extraction into n-heptane, 0.05 M dibenzoylmethane.										
Data for 0.3-5.0 m NaCl. At I=0.0, K1=5.12, B2=9.12.										
Th++++	gl	NaClO4	20°C	0.10M	U		K1=4.16		1985SAa (25552)	166
Th++++	EMF	alc/w	25°C	20%	U	I	K1=6.27		1973LSa (25553)	167
Also in 0% and 40.3% EtOH and in 0.05 M NaClO4 in 0%, 20% and 40% EtOH										
Th++++	EMF	NaClO4	20°C	1.00M	U	T	K1=4.21	B2=7.78	1973MBc (25554)	168
							B3=10.54			
							B4=12.90			

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
Th++++	gl	KNO3	25°C	0.20M	U	M	K1=8.51	B2=16.91	1992SSf (26275)	169
							K(Th(ida)+L)=8.47			
							K(Th(nta)+L)=8.37			
							K(Th(edta)+L)=7.23			
							K(Th(cdta)+L)=6.81			

K(Th(dtpa)+L)=5.89; K(Th(hedta)+L)=8.27.
hedta is N-(2-hydroxyethyl)-1,2-diaminoethane-N,N',N'-triethanoic acid

---

Th++++ gl KNO3 25°C 0.10M C T K1=7.18 B2=14.51 1983NMb (26276) 170

Th++++ ix KNO3 20°C 0.50M U T K1=8.80 1980SEa (26277) 171

Th++++ gl KNO3 30°C 0.10M U M 1976PTc (26278) 172
K(ThA+L)=5.90
K(ThB+L)=5.07
H4A=EDTA, H4B=CDTA

****

C3H7NO2 HL B-Alanine CAS 107-95-9 (575)
3-Aminopropanoic acid; H2N.CH2.CH2.COOH

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

---

Th++++ gl KNO3 25°C 0.20M U M K1=8.37 B2=17.66 1992SSf (26480) 173
K(Th(ida)+L)=8.36
K(Th(nta)+L)=8.34
K(Th(edta)+L)=6.79
K(Th(cdta)+L)=6.64
K(Th(dtpa)+L)=5.88; K(Th(hedta)+L)=8.25.
hedta is N-(2-hydroxyethyl)-1,2-diaminoethane-N,N',N'-triethanoic acid

---

Th++++ ix KNO3 20°C 0.50M U T K1=9.80 1980SEa (26481) 174

Th++++ EMF KNO3 25°C 0.50M U T K1=9.76 1971KSb (26482) 175

****

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

---

Th++++ gl KNO3 35°C 0.10M U 1997RVa (26841) 176
K(Th+HL)=8.40

Th++++ gl NaNO3 15°C 0.10M U T K1=14.30 1984IDa (26842) 177
At 30 C, K1=14.05.

Th++++ gl KNO3 25°C 0.10M C K1=7.51 B2=14.80 1983NMb (26843) 178

****

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

---

Th++++ oth NaClO4 35°C 0.10M C K1=7.91 1986SGd (27182) 179
Method: electrophoresis

```
Th++++     gl  KNO3   25°C 0.10M C        K1=8.25   B2=16.75  1983NMb (27183) 180
--------------------------------------------------------------------------------
Th++++     ix  KNO3   20°C 0.50M U        K1=8.10        1980SEa (27184) 181
--------------------------------------------------------------------------------
Th++++     EMF oth/un 25°C 0.50M U        K1=8.07        1973SKb (27185) 182
********************************************************************************
C3H12NO9P3            H6L    NTPA             CAS 6419-19-8  (2920)
Nitrilotris(methylenephosphonic acid); N(CH2PO3H2)3
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Th++++     gl  R4N.X  20°C  0.1M C        K1=12.6        1967HEa (28592) 183
                                         K(Th+HL)=9.3
                                         K(Th+H2L)=6.2
********************************************************************************
C4H2O4                H2L    Squaric acid     CAS 2892-51-5  (439)
3,4-Dihydroxy-3-cyclobutene-1,2-dione;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Th++++     ix  R4N.X  25°C 1.00M U        K1=4.08   B2=7.32   1972CSb (28667) 184
Medium: NH4ClO4
********************************************************************************
C4H3N3O4              H3L    Violuric acid    CAS 26351-19-9  (1208)
2,4,5,6-(1H,3H)Pyrimidinetetrone-5-oxime,  5-isonitrosobarbituric acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Th++++     sp  oth/un  rt   dil  U        K1=2.90   B2=5.30   1970PBe (28752) 185
                                         K3=2.40
                                         K4=2.30
********************************************************************************
C4H4N6                  L    8-Azaadenine     CAS 1123-54-2  (1884)
8-Aza-6-aminopurine;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Th++++     gl  KNO3   35°C 0.10M U    M   K1=6.40        1982RKa (28955) 186
                                         K(Th(EDTA)+L)=3.12
                                         K(Th(EDTA)L+H)=5.59
********************************************************************************
C4H4O4                H2L    Maleic acid      CAS 110-16-7  (111)
cis-Butenedioic acid; HOOC.CH:CH.COOH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Th++++     gl  NaClO4 25°C 1.00M C   H                    1985BSc (29141) 187
                                         B(-2,1,1)=-0.80
                                         B(-6,1,3)=-7.58
                                         B(-6,1,2)=-13.65
```

B(-6,1,1)=-23.0
B(p,q,r); pH+qTh+rH2L=HpThq(H2L)r

Th++++ EMF NaClO4 20°C 1.00M U K1=6.34 B2=10.55 1972TMa (29142) 188
****
C4H5N3O HL Cytosine CAS 71-30-7 (1096)
2-Oxy-6-aminopyrimidine;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Th++++ gl KNO3 35°C 0.10M U M K1=12.40 1982RKa (29419) 189
K(Th+HL)=5.50
K(Th(EDTA)+L)=3.27
K(Th(EDTA)L+H)=5.90
****
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
---
Th++++ gl NaClO4 25°C 0.10M M M K1=7.00 1987NCa (30052) 190
K(Th(nta)+L)=4.68

Th++++ cal NaClO4 25°C 1.0M U H K1=6.44 1983BCa (30053) 191
K(Th+HL)=3.60
K(Th+HL+L)=8.94
DH(K1)=18.6 kJ mol-1, DS=186 J K-1 mol-1; DH(ThHL)=8.5, DS=97

Th++++ EMF NaClO4 20°C 1.00M U K1=6.23 1972TMa (30054) 192

Th++++ sol oth/un 25°C 0.50M U K1=8.38 1970MKe (30055) 193

Th++++ kin oth/un 25°C 0.0 U 1963YKa (30056) 194
K(2Th+L)=11.78
****
C4H6O4S H2L Thiodiacetic CAS 123-93-3 (140)
2,2'-Thiodiglycolic acid, Thiodiethanoic acid; HOOC.CH2.S.CH2.COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Th++++ cal NaClO4 25°C 1.0M U H K1=5.60 B2=9.85 1983BCa (30234) 195
K(Th+HL)=3.29
DH(K1)=20.5 kJ mol-1, DS=176 J K-1 mol-1; DH(K2)=14.9, DS=131; DH(ThHL)=12.4
****
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
---
Th++++ kin oth/un 25°C 0.0 U 1963YKa (30738) 196

B(Th2L)=13.34

Th++++ ix oth/un ? 0.30M U K1=5.15 B2=6.70 1962GLa (30739) 197
****
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
---
Th++++ cal NaClO4 25°C 1.0M U H K1=8.15 B2=14.82 1983BCa (30938) 198
K3=3.34
DH(K1)=8.4 kJ mol-1,DS=184 J K-1 mol-1; DH(K2)=-11.5, DS=89; DH(K3)=35.9
DS=184
****
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
---
Th++++ oth NaClO4 40°C 0.10M C 1982SYb (31370) 199
B3=9.14
K(Th+4HL)=12.23
Method: paper electrophoresis. Medium: 0.1 M HClO4.

Th++++ oth oth/un 40°C 0.10M U M 1981YSa (31371) 200
B(ThL2(NTA))=9.74
Method: paper electrophoresis

Th++++ kin oth/un 25°C 0.0 U 1963YKa (31372) 201
K(2ThOH+L)=13.2

Th++++ ix oth/un ? 0.30M U K1=4.64 1962GLa (31373) 202
****
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
---
Th++++ gl NaClO4 25°C 1.00M U H K1=4.21 1989BRc (31952) 203
DH(K1)=10.9 kJ mol-1; DS(K1)=117 J mol-1 K-1

Th++++ EMF oth/un 25°C 0.50M U K1=10.49 1973SKb (31953) 204

Th++++ gl NaClO4 25°C 0.10M U K1=9.23 B2=17.80 1972SSg (31954) 205
K3=4.55
K4=3.87
****
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
-------------------------------------------------------------------------
Th++++     gl  NaClO4 20°C 0.10M U        K1=11.15       1985SAa (32373) 206
-------------------------------------------------------------------------
Th++++     cal NaClO4 25°C  1.0M U   H    K1=9.69        1983BCa (32374) 207
                                         K(Th+HL)=2.91
DH(K1)=6.5 kJ mol-1, DS=207 J K-1 mol-1; DH(ThHL)=7.41, DS=81
-------------------------------------------------------------------------
Th++++     gl  KNO3   25°C 0.10M U        K1=10.66  B2=19.73  1982NBa (32375) 208
-------------------------------------------------------------------------
Th++++     gl  KNO3   35°C 0.10M U    M                   1977PTb (32376) 209
                                         K(ThA+L)=3.73
H5A=DTPA
-------------------------------------------------------------------------
Th++++     gl  KCl    25°C 0.10M U        K1=10.15       1974KPd (32377) 210
-------------------------------------------------------------------------
Th++++     EMF oth/un 25°C 0.50M U        K1=9.32        1973SKb (32378) 211
*************************************************************************
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
-------------------------------------------------------------------------
Th++++     ix  KNO3   20°C 0.50M U        K1=10.53       1980SEa (32732) 212
-------------------------------------------------------------------------
Th++++     gl  NaClO4 25°C 0.10M U        K1=8.28   B2=16.05  1973TSe (32733) 213
                                         K3=7.72
*************************************************************************
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
-------------------------------------------------------------------------
Th++++     gl  NaClO4 25°C  1.0M C   H    K1=3.10   B2= 5.40  1992BIa (33055) 214
                                         B3=6.89
By calorimetry DH(K1)=6.7 kJ mol-1, DS=82 J K-1 mol-1; DH(B2)=13.4, DS=148
DH(B3)=19.2, DS=196
*************************************************************************
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
-------------------------------------------------------------------------
Th++++     EMF NaClO4 20°C 1.00M U        K1=3.85   B2=7.30   1972PTb (33250) 215
*************************************************************************
C4H8O2                 HL                     CAS 107-92-6  (1118)
n-Butanoic acid; CH3.CH2.CH2.COOH
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
```

```
Th++++     EMF NaClO4 20°C 1.00M U        K1=3.90   B2=7.00   1972PTb (33352) 216
                                          B3=9.74
**************************************************************************
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
--------------------------------------------------------------------------
Th++++     EMF NaClO4 20°C 1.00M U        K1=4.43   B2=8.15   1973MBc (33527) 217
                                          B3=11.06
                                          B4=13.60
--------------------------------------------------------------------------
Th++++     ix  oth/un   ?  0.20M U        K1=3.56   B2=5.53   1962GLa (33528) 218
                                          B3=7.08
**************************************************************************
C4H8O3                HL                      CAS 300-85-6  (30)
3-Hydroxybutanoic acid; CH3.CH(OH).CH2.COOH
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Th++++     EMF NaClO4 20°C 1.00M U        K1=3.87   B2=6.85   1973MBc (33630) 219
                                          B3=9.01
**************************************************************************
C4H8O3                HL                      CAS 591-81-1  (39)
4-Hydroxybutanoic acid; HO.CH2.CH2.CH2.COOH
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Th++++     EMF NaClO4 20°C 1.00M U        K1=3.80   B2=6.65   1973MBc (33659) 220
**************************************************************************
C4H9NO2S              HL    Methylcysteine   CAS 1187-84-4  (84)
2-Amino-3-methylmercaptopropanoic acid; H2N.CH(CH2.S.CH3)COOH
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Th++++     dis NaClO4 35°C 0.10M U    M   K1=8.37        1995TKa (34107) 221
Method: Paper electrophoresis; Ternary complexes with NTA.
**************************************************************************
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
--------------------------------------------------------------------------
Th++++     oth NaClO4 35°C 0.10M C        K1=8.16        1986SGd (34327) 222
Method: electrophoresis
--------------------------------------------------------------------------
Th++++     gl  KNO3   25°C 0.10M C        K1=7.21   B2=14.01  1983NMb (34328) 223
--------------------------------------------------------------------------
Th++++     EMF oth/un 25°C 0.50M U        K1=7.97        1973SKb (34329) 224
**************************************************************************
```

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	kin	oth/un	25°C	0.02M	U		K(ThOH+L)=4.56	1971MGb (35268)	225
Estimated for Th+++, K1=1.86									
Th++++	kin	none	25°C	0.00	M		K(ThOH+L)=4.70	1966SSb (35269)	226

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	gl	NaClO4	25°C	0.50M	C		K1=3.04 B2=5.69 B(ThH-1L)=0.39 B(ThH2L3)=14.16 B(ThH2L4)=18.00	1995PSb (36265)	227

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	gl	NaClO4	25°C	0.50M	C		K1=2.85 B2=5.11 B(ThH2L3)=12.78 B4=10.07 B(ThH2L4)=15.14	1995PSb (36299)	228

****

C5H5N5 L Adenine CAS 73-24-5 (237)
6-Aminopurine; H2N.C5H3N4

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	gl	KNO3	35°C	0.10M	U	M	K1=10.30 K(Th(EDTA)+L)=3.21 K(Th(EDTA)L+H)=5.88	1982RKa (36983)	229

****

C5H6N6 HL Diaminopurine CAS 1904-98-9 (4290)
2,6-Diaminopurine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	gl	KNO3	35°C	0.10M	U	M	K1=11.98 K(Th(EDTA)+L)=3.41 K(Th(EDTA)L+H)=5.86	1982RKa (37339)	230

****

C5H7NO3 HL 5-Oxoproline CAS 149-87-1 (2110)
2-Pyrrolidone-5-carboxylic acid, Pyroglutamic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Th++++	ix	KNO3	20°C	0.50M	U		K1=8.20		1980SEa (37518)	231

****

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
Th++++	gl	NaClO4	25°C	1.0M	C	T H	K1=9.0 B3=22.8 B4=27.4	B2=16.70	2000EAa (38097)	232

Additional method: solvent extraction. Also data at 15 and 35 C
DH(K1)=-60 kJ mol-1, DH(B2)=50, DH(B3)=110, DH(B4)=102.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Th++++	dis	NaClO4	25°C	0.01M	U		K2=7.43 K3=5.83 K4=5.35		1960RYa (38098)	233
Th++++	dis	NaClO4	25°C	0.01M	U		B2=15.57 K3=6.15 K4=5.14		1959RSa (38099)	234
Th++++	gl	oth/un	30°C	0.0	U		K1=8.8 K3=6.3 K4=4.2	B2=16.2	1955IFa (38100)	235
Th++++	dis	oth/un	25°C	0.01M	U		K1=7.85 K3=6.28 K4=5.00	B2=15.59	1955RYb (38101)	236
Th++++	dis	NaClO4	25°C	0.01M	C		K1=7.84 K3=6.28 K4=5.0	B2=15.57	1950RYa (38102)	237

Method: distribution. Aqueous medium: 0.01 M HClO4.

****

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
Th++++	gl	NaClO4	25°C	0.10M	M	M	K1=6.60 K(Th(nta)+L)=4.10		1987NCa (38360)	238
Th++++	gl	alc/w	25°C	40%	U	I	K1=8.24		1973CSd (38361)	239

Medium: 0-50% (v/v) EtOH, 0.05 M. K1(0%)=7.44, K1(50%)=8.96

```
Th++++     EMF NaClO4 20°C 1.00M U                        1972TMa (38362) 240
                                        K(Th+HL)=3.48
                                        K(Th+2HL)=6.14
-------------------------------------------------------------------------------
Th++++     sol oth/un 25°C 0.50M U        K1=8.76         1970MKe (38363) 241
*******************************************************************************
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
-------------------------------------------------------------------------------
Th++++     ix  oth/un   ?  0.30M U        K1=4.52         1962GLa (38442) 242
-------------------------------------------------------------------------------
Th++++     gl  oth/un 20°C 0.06M U        K1=3.70         1961ZKa (38443) 243
*******************************************************************************
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
-------------------------------------------------------------------------------
Th++++     ix  KNO3   20°C 0.50M U        K1=9.36         1980SEa (38646) 244
-------------------------------------------------------------------------------
Th++++     EMF KNO3   25°C 0.50M U        K1=9.30         1971KSb (38647) 245
*******************************************************************************
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
-------------------------------------------------------------------------------
Th++++     EMF oth/un 25°C 0.50M U        K1=8.23         1973SKb (38755) 246
*******************************************************************************
C5H9NO4               H2L    Glutamic acid    CAS 56-86-0  (22)
2-Aminopentanedioic acid; H2N.CH(CH2.CH2.COOH)COOH
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Th++++     ix  KNO3   20°C 0.50M U        K1=11.40        1980SEa (39130) 247
-------------------------------------------------------------------------------
Th++++     gl  NaClO4 25°C 0.10M U        K1=9.11   B2=17.63  1972SSg (39131) 248
                                        K3=4.18
                                        K4=3.62
*******************************************************************************
C5H10N2O3              HL    Glutamine        CAS 56-85-9  (18)
2-Aminopentanedioic acid 5-amide; H2N.CH(CH2.CH2.CO.NH2)COOH
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Th++++     gl  NaClO4 25°C 0.10M U        K1=8.30   B2=15.91  1973TSe (39839) 249
                                        K3=7.55
*******************************************************************************
```

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	ix	KNO3	20°C	0.50M	U	T	K1=8.60	1980SEa (40762)	250
Th++++	EMF	KNO3	25°C	0.50M	U	T	K1=8.58	1971KSb (40763)	251

****
C5H11NO2 HL DL-Valine CAS 516-06-3 (186)
DL-2-Amino-3-methylbutanoic acid; H2N.CH(CH(CH3)2).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	gl	KNO3	25°C	0.10M	C		K1=8.30 B2=14.23	1983NMb (40896)	252

****
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
Th++++	oth	oth/un	25°C	0.10M	C		K1=8.08	1998TEb (41127)	253

Method: electrophoresis. Medium: 0.1 M HClO4.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	gl	KNO3	25°C	0.10M	C		K1=6.82 B2=13.48	1983NMb (41128)	254

****
C5H11NO2S H2L Penicillamine CAS 52-66-4 (350)
DL-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
Th++++	oth	NaClO4	35°C	0.10M	C		K1=13.61	1996TKb (41283)	255

Method: paper electrophoresis.
****
C5H12NO4P HL CAS 51276-47-2 (5704)
2-Amino-4-(methylhydroxyphosphoryl)butanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	gl	NaClO4	23°C	0.10M	U		K1=9.37	1990YTa (41446)	256

****
C6H3N3O7 HL Picric acid CAS 88-89-1 (593)
2,4,6-Trinitrophenol; HO.C6H2(NO2)3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	sp	oth/un	21°C	0.40M	U		B2=2.66	1955BKa (42152)	257

Medium:0.2-0.9(some EtOH)
****
C6H4N2O5 HL CAS 50-28-5 (505)

2,4-Dinitrophenol; HO.C6H3(NO2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	gl	KCl	21°C	0.10M	U		K1=3.2	1978KUb (42240)	258

C6H4N2O5 HL CAS 329-71-5 (1941)

2,6-Dinitrophenol; HO.C6H3(NO2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	gl	KCl	21°C	0.10M	U		K1=3.23	1978KUb (42249)	259

C6H4O6 H4L CAS 5678-48-2 (871)

Tetrahydroxy-1,4-benzoquinone;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	EMF	NaClO4	30°C	0.10M	U		K1=7.30 B2=10.50	1981HIa (42327)	260

C6H5NO3 HL 2-Nitrophenol CAS 88-75-5 (510)

2-Nitrohydroxybenzene; HO.C6H4.NO2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	gl	KCl	21°C	0.10M	U		K1=6.3	1978KUb (42740)	261

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
Th++++	gl	KCl	21°C	0.10M	U		K1=6.04	1978KUb (42817)	262

C6H6N2O2 HL Cupferron CAS 135-20-6 (637)

N-Nitrosophenylhydroxylamine; C6H5.N(OH).NO

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	dis	NaClO4	25°C	0.10M	U		B2=14.58	1960RYa (43423)	263

Extraction into CHCl3

Th++++	dis	NaClO4	25°C	0.10M	U		B4=27.00	1954DYa (43424)	264
Th++++	dis	oth/un	25°C	0.10M	U		K1=7.35 B2=14.30 K3=6.55 K4=6.15	1953DYa (43425)	265

C6H6O HL Phenol CAS 108-95-2 (457)

Hydroxybenzene, phenol; C6H5.OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	gl	KCl	25°C	0.10M	U		K1=8.44	1978KUb (43545)	266

****

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
Th++++	gl	KNO3	25°C	0.20M	U	M	K1=16.17 B2=30.90	1990SSc (43842)	267
							K(UO2(IMDA)+L)=15.61		
							K(UO2(NTA)+L)=15.09		
							K(UO2(HEDTA)+L)=14.79		
							K(UO2(EDTA)+L)=12.03		
							K(UO2(CDTA)+L)=11.74, K(UO2(DTPA)+L)=11.21		
Th++++	gl	KCl	25°C	0.10M	U		K1=18.1	1978KUb (43843)	268
Th++++	gl	KNO3	30?°C	0.10M	U	M	K1=17.72	1962AMb (43844)	269

Ternary complexes with EDTA and CDTA

****

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
Th++++	gl	KNO3	32°C	0.10M	U			1965AMa (43984)	270
							K(Th+H3L=ThL+3H)=-6.32		
							K(Th+2H3L=ThH2L2+4H)=-7.30		

****

C6H6O5S H3L CAS 7134-09-0 (3687)
3,4-Dihydroxybenzenesulfonic acid; (HO)2.C6H3.SO3H

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	gl	oth/un	20°C	?	U			1970BGb (44286)	271
							K(Th+H2L=ThL+2H)=-3.50		
							K(Th+H2L=ThHL+H)=-1.37		

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	gl	KNO3	25°C	0.20M	U	M	K1=17.30 B2=33.69	1990SSc (44499)	272
							K(UO2(IMDA)+L)=15.93		
							K(UO2(NTA)+L)=15.39		
							K(UO2(HEDTA)+L)=15.21		

```
                                        K(UO2(EDTA)+L)=12.75
K(UO2(CDTA)+L)=12.48, K(UO2(DTPA)+L)=12.01
--------------------------------------------------------------------------
Th++++     gl  KNO3   25°C 0.10M U    M                  1966MMa (44500) 273
                                        K(Th2L3(OH)2+2H)=12.8
                                        K(Th2L3(OH)2+4H=2ThL+H2L)=11.9
Ternary complexes with EDTA and CDTA
--------------------------------------------------------------------------
Th++++     dis KNO3   25°C 0.10M U                     1960BMa (44501) 274
                                        K(Th2L3+8HB=2ThB4+3H2L+2H)=4.1
HB=trifluorothenoylacetone
**************************************************************************
C6H7O3As              H2L    Phenylarsonic    CAS 98-05-5  (3690)
Benzenearsonic acid, phenylarsonic acid; C6H5AsO3H2
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Th++++     sol oth/un 18°C 0.10M U        K1=3.8         1960MIa (45178) 275
15-21 C
**************************************************************************
C6H8O7                H3L    Citric acid      CAS 77-92-9  (95)
2-Hydroxypropane-1,2,3-tricarboxylic acid; HOOCCH2.CH(OH)(COOH).CH2COOH
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Th++++     gl  NaCl   25°C 0.10M C        K1=11.611 B2=21.139 1987RDa (46277) 276
                                        B(ThHL2)=23.637
--------------------------------------------------------------------------
Th++++     gl  oth/un 25°C 0.50M U        K1=13.0   B2=20.97  1966NUa (46278) 277
**************************************************************************
C6H9NO6               H3L    NTA              CAS 139-13-9  (191)
Nitrilotriethanoic acid; N(CH2.COOH)3
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Th++++     cal KNO3   25°C 0.10M U   H                   1989KGa (47046) 278
DH(K1)=5.7 kJ mol-1; DS(K1)=260 J mol-1 K-1
--------------------------------------------------------------------------
Th++++     gl  NaNO3  25°C 0.50M U    M                  1981NAb (47047) 279
                                        K(ThL+H5A=ThH2LA+3H)=-1.85
                                        K(ThL+H2A)=7.57
                                        K(ThH2LA=ThHA+HL)=24.81
                                        K(Th+H3L+H5B=ThHLB+7H)=-9.16
K(Th+L+HB)=29.58, *K(ThLHB)=-9.72.H5A=1-(o-arsono-phenylazo)-2-naphthol-3,6-
disulphonic acid (thorin) and H5B=methyl thymol blue.
--------------------------------------------------------------------------
Th++++     gl  KNO3   35°C 0.10M U    M                  1977PTb (47048) 280
                                        K(ThA+L)=3.89
H5A=DTPA
--------------------------------------------------------------------------
```

```
Th++++     gl  KNO3   25°C 0.10M U                        1968BMa (47049) 281
                                        K(Th(OH)L+H)=8.6
-------------------------------------------------------------------------------
Th++++     EMF NaClO4 20°C 0.10M U      T K1=16.9         1967BAc (47050) 282
-------------------------------------------------------------------------------
Th++++     ISE NaClO4 25°C 0.10M U        K1=13.3         1967SKe (47051) 283
-------------------------------------------------------------------------------
Th++++     gl  KNO3   25°C 0.10M U        K1=12.4         1958CGa (47052) 284
                                        K(Th(OH)2L+2H)=8.2
*******************************************************************************
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
-------------------------------------------------------------------------------
Th++++     gl  KNO3   35°C 0.10M U                        1997RVa (47621) 285
                                        K(Th+HL)=6.46
*******************************************************************************
C6H10O4                H2L    Adipic acid      CAS 124-04-9  (401)
1,6-Hexanedioic acid; HOOC.(CH2)4.COOH
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Th++++     gl  NaClO4 25°C 0.10M M    M   K1=6.50          1987NCa (48090) 286
                                        K(Th(nta)+L)=4.13
-------------------------------------------------------------------------------
Th++++     oth NaClO4 40°C 0.10M U        K1=5.2           1981SSe (48091) 287
                                        B4=15.3
Method: Paper electrophoresis.
-------------------------------------------------------------------------------
Th++++     sol oth/un 25°C 0.50M U        K1=8.42          1970MKe (48092) 288
*******************************************************************************
C6H10O6                H2L                     CAS 23243-68-7  (242)
1,2-Bis(carboxymethoxy)ethane; HOOC.CH2.O.CH2.CH2.O.CH2.COOH
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Th++++     gl  NaClO4 25°C  1.0M U   H    K1=6.86   B2=12.70  1988BSb (48356) 289
By calorimetry: DH(K1)=13.4 kJ mol-1, DS(K1)=176 J K-1 mol-1.
DH(B2)=25.4, DS(B2)=328.
*******************************************************************************
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
-------------------------------------------------------------------------------
Th++++     gl  KNO3   25°C 0.10M U        K1=10.7          1958CGa (48798) 290
                                        K(Th(OH)2L+2H)=7.8
*******************************************************************************
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
Th++++	gl	NaClO4	25°C	1.0M	U	H	B(ThHL)=16.23 B(ThH2L)=18.78	1988BSb (49274)	291

By calorimetry: DH(ThHL)=-43.6 kJ mol-1, DS(ThHL)=165 J K-1 mol-1.
DH(ThH2L)=-60.2, DS(ThH2L)=158

****

C6H12N2O4 H2L CAS 4726-83-4 (5911)
N,N-Dihydroxyhexanediamide; HN(OH).CO.(CH2)4.CO.NH(OH)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	gl	NaNO3	25°C	0.10M	C		K1=16.36	1989EHa (49336)	292

****

C6H13NO2 HL Isoleucine CAS 73-32-5 (424)
2-Amino-3-methylpentanoic acid; CH3.CH2.CH(CH3).CH(NH2).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	gl	KNO3	25°C	0.10M	C		K1=8.26 B2=14.22	1983NMb (49917)	293

****

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
Th++++	oth	NaClO4	35°C	0.10M	C		K1=8.81	1986SGd (50110)	294

Method: electrophoresis

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	gl	KNO3	25°C	0.10M	C	T	K1=8.25 B2=14.14	1983NMb (50111)	295
Th++++	EMF	KNO3	25°C	0.50M	U	T	K1=8.70	1971KSb (50112)	296

Ligand: D-leucine

****

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
Th++++	gl	NaClO4	20°C	0.10M	U	T H	K2=8.52 K3=8.20 K4=4.99	1983SDc (50195)	297

Data for 30 and 40 C. DH(B4)=102 kJ mol-1, DS(B4)=765 J K-1 mol-1.

****

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
-------------------------------------------------------------------------
Th++++     oth NaNO3  20°C 0.10M U        K1=7.8    B2=13.80  1966JMc (50413) 298
Method: paper electrophoresis
*************************************************************************
C6H13NO5               HL    Tricine          CAS 5704-04-1  (1239)
N-(Tris(hydroxymethyl)methyl)glycine; (HO.CH2)3C.NH.CH2.COOH
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Th++++     gl  KNO3   25°C  0.1M M  I     K1=8.05   B2=15.74  1997EAa (50510) 299
Also values in 40% w/w ethanol, DMF, dioxane, acetonitrile.
*************************************************************************
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
-------------------------------------------------------------------------
Th++++     gl  NaClO4 20°C 0.10M U T      K2=8.50        1986SHa (50837) 300
                                         K3=8.20
                                         K4=5.00
Data for 20-40 C.
*************************************************************************
C6H15O4P               HL                    CAS 1611-31-0  (4393)
Dipropylphosphoric acid; (CH3.CH2.CH2.O)2.PO.OH
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Th++++     kin none   25°C 0.00  M                      1966SSb (51516) 301
                                         K(ThOH+L)=4.77
*************************************************************************
C7H5NO5               H2L    Nitrosalicylic   CAS 96-97-9  (148)
2-Hydroxy-5-nitrobenzoic acid; HO.C6H3(NO2).COOH
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Th++++     gl  alc/w  25°C  80%  U        K1=4.46   B2=8.01   1985ISa (53055) 302
*************************************************************************
C7H6N2S                HL                    CAS 583-39-1  (2043)
2-Mercaptobenzimidazole;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Th++++     gl  alc/w  25°C  50%  U        K1=10.17  B2=20.04  1978ZIa (53532) 303
*************************************************************************
C7H6O2                 HL    Salicylaldehyde  CAS 90-02-8  (193)
2-Hydroxybenzaldehyde, Salicylaldehyde; HO.C6H4.CHO
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
```

```
Th++++     dis NaClO4 25°C 0.10M U        B2=7.67        1960RYa (53632) 304
                                          B4=11.61
**************************************************************************
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
--------------------------------------------------------------------------
Th++++     dis NaClO4 25°C 0.10M U        K2=7.43        1960RYa (53694) 305
                                          K3K4=13.96
                                          K5K6=4.34
--------------------------------------------------------------------------
Th++++     dis NaClO4 25°C 0.10M U        K1=9.61   B2=18.24  1955DYa (53695) 306
                                          K3=7.65
                                          B4=32.56
                                          K5=2.29
                                          K6=1.87
**************************************************************************
C7H6O2S               H2L    Thiosalicylic    CAS 147-93-3  (236)
2-Mercaptobenzoic acid; HS.C6H4.COOH
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Th++++     gl  alc/w  25°C  40%  U        K1=4.45   B2=8.35   1988ISc (53917) 307
Medium: 40% EtOH/H2O, 0.1 M NaClO4
--------------------------------------------------------------------------
Th++++     gl  alc/w  25°C  40%  U    M   K1=4.45   B2=8.35   1986SIa (53918) 308
**************************************************************************
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
--------------------------------------------------------------------------
Th++++     gl  alc/w  25°C  40%  U        K1=4.41   B2=8.15   1988ISc (54305) 309
--------------------------------------------------------------------------
Th++++     gl  alc/w  25°C  80%  U        K1=4.48   B2=8.22   1985ISa (54306) 310
Medium: 80% EtOH/H2O, 0.1 M NaClO4
--------------------------------------------------------------------------
Th++++     gl  NaClO4 20°C 0.10M U      T K1=15.45       1985SAa (54307) 311
--------------------------------------------------------------------------
Th++++     dis NaClO4 25°C 0.10M U        K1=4.25   B2=7.60   1956HOa (54308) 312
                                          K3=2.45
                                          K4=1.55
**************************************************************************
C7H6O5S               H2L                    CAS 2745-13-3  (3755)
Tropolone-5-sulfonic acid;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Th++++     sp  NaClO4 25°C  2.0M U        K1=7.95   B2=14.09  1963OUa (54802) 313
```

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C7H6O6S H3L CAS 5965-83-3 (399)
5-Sulfosalicylic acid, 2-Hydroxy-5-sulfobenzoic; HO3S.C6H3(OH).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	gl	alc/w	25°C	80%	U		K1=4.35 B2=7.90	1985ISa (55052)	314
Th++++	gl	NaClO4	20°C	0.10M	U		K1=11.97	1985SAa (55053)	315
Th++++	gl	NaClO4	20°C	1.0M	U		K1=12.30	1972CBb (55054)	316
Th++++	con	oth/un	28°C	0.01M	U	H	K(Th+HL=ThL+H)=2.42(?)	1962SBc (55055)	317

Ternary complexes with EDTA and CDTA

****

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
Th++++	gl	KNO3	30°C	0.20M	C	M	K(Th(nta)+L)=3.20 K(Th(edta)+L)=3.28	1985KMd (55266)	318

****

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
Th++++	gl	diox/w	37°C	30%	C	M	B2=10.18 B(Th(bpy)L)=11.91	1983MAd (55516)	319
Th++++	gl	KNO3	25°C	.025M	U		K1=9.60 B2=19.81 B3=28.76	1966BBf (55517)	320

Medium: HNO3

****

C7H7NO6S H2L CAS 35379-88-5 (4464)
3-Nitro-p-cresol-5-sulfonic acid; (CH3)(HO).C6H2(NO2).SO3H

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	dis	NaCl	25°C	1.0M	U		K1=7.20	1972BEa (55699)	321

****

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
Th++++	gl	KNO3	25°C	0.20M	U	M	K1=16.35 B2=31.08	1990SSc (56079)	322

K(UO2(IMDA)+L)=15.73
K(UO2(NTA)+L)=15.22
K(UO2(HEDTA)+L)=14.94
K(UO2(EDTA)+L)=12.12
K(UO2(CDTA)+L)=11.87, K(UO2(DTPA)+L)=11.33

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Th++++	gl	R4N.X	25°C	0.50M	U		K1=16.4		1985GMb (56171)	323

Medium: 0.5 M Me4NCl

****

C8H2O4Cl4 H2L CAS 632-58-6 (3214)
Tetrachlorophthalic acid; Cl4.C6(COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Th++++	gl	oth/un	20°C	0.10M	U				1960WKa (58393)	324
							Kso=6.71			

****

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
Th++++	sp	NaCl	25°C	5.0M	C		K1=7.14		1996XCa (58683)	325
Th++++	sp	oth/un	25°C	0.11M	U		K1=7.4		1964PCa (58684)	326
Th++++	sol	none	25°C	0.0	U		K1=1.01		1960GMb (58685)	327

****

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
Th++++	EMF	NaClO4	20°C	1.0M	U		K1=5.92	B2=10.05	1972TMa (59019)	328

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Th++++	dis	NaClO4	25°C	0.25M	M	M	K1=3.0	B2= 5.0	1985CAb (59878)	329
							B3=6.0			
							B4=6.5			
Th++++	EMF	NaClO4	20°C	1.0M	U	T	K1=3.88	B2=6.89	1973MBc (59879)	330

B3=9.69
B4=11.98

Th++++ ix oth/un ? 0.20M U K1=2.94 B2=4.98 1962GLa (59880) 331
B3=5.91
****
C8H8O3 HL m-Anisic acid CAS 586-38-9 (2804)
3-Methoxybenzoic acid; CH3O.C6H4.COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Th++++ dis NaClO4 25°C 0.10M U K1=3.7 B2=6.8 1956HOa (59920) 332
B3=9.3
B4=11.2
****
C8H8O3 HL Phenoxyacetic CAS 122-59-8 (1153)
Phenoxyethanoic acid; C6H5.O.CH2.COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Th++++ dis NaClO4 25°C 0.25M M K1=3.8 B2= 7.20 1985CAb (60041) 333
B3=9.8
****
C8H12N2O3 H2L Barbital CAS 57-44-3 (2744)
5,5-Diethylbarbituric acid, Veronal, Barbitone;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Th++++ gl alc/w 20°C 50% C TIH K1=7.35 B2=12.97 1987EAa (61444) 334
K3=3.95
DH(K1)=-74.65 kJ mol-1
****
C8H19O4P HL CAS 107-66-4 (2130)
Dibutylphosphoric acid; (C4H9O)2P(O)OH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Th++++ kin none 25°C 0.0 M M 1966SSb (63193) 335
K(ThOH+L)=5.06
****
C9H5NOCl2 HL CAS 773-76-2 (3278)
5,7-Dichloro-8-hydroxyquinoline;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Th++++ dis NaClO4 25°C 0.10M U 1960RYa (63546) 336
K4=8.12
K2K3=19.80

Th++++ dis NaClO4 25°C 0.10M U K1=11.40 B2=21.80 1956DDb (63547) 337

K3=9.40
K4=8.40

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Th++++	sp	NaCl	25°C	5.0M	C		K1=10.46		1996XCa (64355)	338
Th++++	gl	oth/un	20°C	0.10M	U		K1=11.70		1977SKd (64356)	339
Th++++	dis	NaClO4	25°C	0.10M	U		B2=21.3		1960RYa (64357)	340
							K3=9.422			
							K4=8.41			
							K5=3.18			
Th++++	dis	oth/un	25°C	0.10M	U		K1=10.45	B2=20.40	1953DYa (64358)	341
							K3=9.45			
							K4=8.95			

****

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
Th++++	gl	KNO3	25°C	0.10M	U		K1=9.56	B2=18.29	1959RGa (64582)	342
							K3=7.62			
							K4=6.12			
							K(ThL3(OH)+H)=6.2			
							K((ThL3OH)2+2H=2ThL3)=8.9			

****

C9H8N2O4S2 HL CAS 219931-32-5 (8394)
3-Phenylsulfonamidorhodanine;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Th++++	sp	alc/w	30°C	20%	C T H		K1=10.3	B2=19.44	1998EGa (64833)	343

Medium: 20% v/v EtOH/H2O, 0.10 M KCl. Also data for 35 and 45 C.
DH and DS values reported

****

C9H8O2 HL CAS 140-10-3 (3245)
trans-Cinnamic acid; C6H5.CH:CH.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Th++++	dis	NaClO4	25°C	0.10M	U				1960RYa (64871)	344
							K2K3=7.15			
Th++++	dis	NaClO4	25°C	0.10M	U		K1=4.2	B2=8.0	1956HOa (64872)	345

K3=3.4
K4=3.0

****

C9H9N3O2S2 HL Sulfathiazole CAS 72-14-0 (8357)
4-Amino-N-2-thiazolyl-benzenesulfonamide;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Th++++	gl	alc/w	25°C	50%	C		K1=8.26	B2=16.16	1999GAa (65135)	346

Medium: 50% EtOH/H2O, 0.10 M NaNO3.

****

C9H10O2 HL CAS 1450-72-2 (4596)
2-Hydroxy-5-methylacetophenone; HO(CH3).C6H3.CO.CH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	sp	oth/un	30°C	?	U			1970GMe (65336)	347
							K(Th+HL)=2.42		

****

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
Th++++	gl	KNO3	25°C	0.10M	C		K1=7.84	B2=14.51	1983NMb (65978)	348
Th++++	gl	KNO3	30°C	0.10M	U	M			1976PTc (65979)	349
							K(ThA+L)=5.56			
							K(ThB+L)=4.81			
Th++++	EMF	KNO3	25°C	0.50M	U		K1=8.18		1971KSb (65980)	350

H4A=EDTA, H4B=CDTA

****

C9H13N3O5 L Cytidine CAS 65-46-3 (2152)
Cytidine, Cytosine-1-beta-D-ribofuranoside;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Th++++	gl	KNO3	35°C	0.10M	U	M	K1=4.6		1982RKa (67083)	351
							K(Th(EDTA)+L)=2.85			

****

C9H16O4 H2L Azelaic acid CAS 123-99-9 (3255)
Nonanedioic acid; HOOC.(CH2)7.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	dis	oth/un	25°C	0.50M	U		K1=9.60	1970MKe (67798)	352

****

C10H6O3 HL CAS 83-72-7 (3294)
2-Hydroxy-1,4-naphthoquinone;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Th++++ dis oth/un 25°C 0.10M U K1=4.77 B2=8.99 1959ZPa (68463) 353
K3=4.11
K4=3.13
****
C10H6O4 H2L CAS 475-38-7 (6120)
5,8-Dihydroxy-1,4-naphthoquinone;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Th++++ sp alc/w 25°C 40% C 1994HAa (68488) 354
K(Th+H2L=ThHL+H)=-2.0
K(Th+HL=ThHL)=12.9
K(Th+2HL=Th(HL)2)=23.3
K(ThHL=Th(OH)2HL+2H)=-15.2
Medium: 40% v/v EtOH/H2O, 0.10 M NaClO4.
****
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
---
Th++++ dis NaClO4 25°C 0.10M U K2=9.02 1960RYa (68594) 355
K3=7.89
K4=6.26

Th++++ dis NaClO4 25°C 0.10M U K1=8.50 B2=16.13 1956DDa (68595) 356
****
C10H7NO2 HL CAS 132-53-6 (2524)
2-Nitroso-1-naphthol;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Th++++ dis NaClO4 25°C 0.10M U 1960RYa (68662) 357
K3=7.50
K4=6.22

Th++++ dis NaClO4 25°C 0.10M U K1=8.30 B2=15.54 1956DDa (68663) 358
****
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
---
Th++++ gl NaClO4 25°C 0.10M U K2=6.19 1966BDa (69031) 359
K3=5.50
K4=3.30
****

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
Th++++	gl	alc/w	25°C	80%	U		K1=4.75 B2=8.70	1985ISa (69651)	360
Th++++	gl	diox/w	37°C	30%	C	M	B2=6.78 B(Th(bha)L)=11.91	1983MAd (69652)	361

bha: benzohydroxamic acid

****

C10H8N2O2S2 L (7069)
3-Benzamidorhodanine; C6H5.CO.NH.C3H2NS2:O

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	gl	alc/w	25°C	20%	U T H		K1=11.35 B2=20.58 K3=6.29	1994BSd (69695)	362

Medium: 20% v/v EtOH/H2O, 0.1 M KCl. Also at 35 C, 45 C.
DH(K1)=-35 kJ mol-1, DH(K2)=-25, DH(K3)=-13

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	gl	KNO3	25°C	0.20M	U	M	K1=16.81 B2=32.48 K(UO2(IMDA)+L)=15.74 K(UO2(NTA)+L)=15.26 K(UO2(HEDTA)+L)=15.07 K(UO2(EDTA)+L)=12.55	1990SSc (69780)	363

K(UO2(CDTA)+L)=12.05, K(UO2(DTPA)+L)=11.93

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	gl	NaNO3	25°C	0.10M	U		K1=17.39 B2=31.71 B3=39.12	1984NHa (69864)	364

****

C10H8O8S2 H4L Chromotropic ac CAS 148-25-4 (1875)
1,8-Dihydroxynaphthalene-3,6-disulfonic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	gl	KNO3	25°C	0.20M	U	M	K1=17.36 B2=34.46 K(UO2(IMDA)+L)=16.81 K(UO2(NTA)+L)=16.45 K(UO2(HEDTA)+L)=16.02	1990SSc (69969)	365

K(UO2(EDTA)+L)=14.48
K(UO2(CDTA)+L)=14.08, K(UO2(DTPA)+L)=13.51

Th++++ gl NaClO4 25°C 0.10M U M K1=16.46 B2=29.14 1968BDe (69970) 366
Ternary complexes with EDTA and CDTA

Th++++ sp NaClO4 20°C 0.10M U 1963SMa (69971) 367
Keff(Th+H2L=ThHL+H)=4.11, 4.70
Keff varied with pH
****
C10H12N2O4 HL (6004)
N-Benzyloxycarbonylglycyl hydroxamic acid; C6H5.CH2.O.CO.NH.CH2.CO.NHOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Th++++ gl KNO3 25°C 0.10M U K1=9.1 1987CSb (71305) 368
****
C10H12O2 HL CAS 1946-74-3 (202)
3-Isopropyltropolone;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Th++++ sp alc/w 25°C 50% U 1961HSa (71608) 369
B4=31.17
Medium: 50% EtOH, 0.01 M
****
C10H13N5O4 L Adenosine CAS 58-61-7 (2154)
Adenosine, Adenine-9-beta-D-ribofuranoside;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Th++++ gl KNO3 35°C 0.10M U M K1=5.6 1982RKa (71953) 370
K(Th(EDTA)+L)=2.57
****
C10H13N5O5 HL Guanosine CAS 118-00-3 (1402)
2-Aminopurin-6-one-9-riboside;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Th++++ gl KNO3 35°C 0.10M U M 1997RVa (72018) 371
K(Th+HL)=3.40
K(Th+HL+HA)=11.41
K(Th+HL+HC)=13.40
H2A is histidine, H2C is cysteine.

Th++++ gl KNO3 35°C 0.10M U M K1=3.4 1982RKa (72019) 372
K(Th(EDTA)+L)=2.81
K(Th(EDTA)L+H)=5.62

Th++++ gl NaNO3 20°C 1.0M U 1965FBa (72020) 373

```
                                          K(Th+HL)=0.9
********************************************************************************
C10H16N2O8            H4L    EDTA             CAS 60-00-4  (120)
1,2-Diaminoethane-N,N,N',N'-tetraethanoic acid, Sequestric acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Th++++     cal KNO3   25°C 0.10M U   H                    1989KGa (74211) 374
DH(K1)=-11.5, DH(ThHL)=-11.9 kJ mol-1
DS(K1)=406, DS(B(ThHL))=443 J mol-1 K-1
--------------------------------------------------------------------------------
Th++++     gl  NaClO4 20°C 0.10M U        K1=21.17       1985SAa (74212) 375
--------------------------------------------------------------------------------
Th++++     sp  NaClO4 21°C 0.20M U        K1=25.1        1983KDa (74213) 376
--------------------------------------------------------------------------------
Th++++     gl  KNO3   30°C 0.15M U    M                  1980LMa (74214) 377
                                          K(ThL+Ser)=4.23
                                          K(ThL+Thr)=4.30
                                          K(ThL+Leu)=5.10
                                          K(ThL+A)=5.31
HA=2-Aminoisobutanoic acid
--------------------------------------------------------------------------------
Th++++     cal NaClO4 25°C  0.1M U   H                    1978DOd (74215) 378
DH(K1)=-12.9 kJ mol-1, DH(ThL+H)=0.3
--------------------------------------------------------------------------------
Th++++     gl  KNO3   35°C 0.10M M    M                  1976PTb (74216) 379
                                          K(ThL+glycolate)=4.64
                                          K(ThL+malate)=3.90
At 30 C: K(ThL+glycolate)=4.62, K(ThL+malate)=3.87
--------------------------------------------------------------------------------
Th++++     gl  oth/un 25°C    ?  U                       1970BGb (74217) 380
                                          K(ThL+H2L=ThHL2+H)=-1.9
--------------------------------------------------------------------------------
Th++++     EMF NaClO4 20°C 0.10M U        K1=25.3        1967BAc (74218) 381
                                          K(ThL+H)=1.98
                                          K(2ThL+2OH)=7.92
--------------------------------------------------------------------------------
Th++++     gl  KNO3   25°C 0.10M U                       1966MCa (74219) 382
                                          K(ThLOH+ThLOH=Th2L2(OH)2)=4.3
--------------------------------------------------------------------------------
Th++++     gl  KNO3   25°C 0.10M U    M                  1964CBa (74220) 383
                                          K(ThLA+H)=4.46
                                          K(ThL+HA)=5.35
                                          K(ThL+A)=13.4
                                          K(ThL+B)=13.66
H4A=1,2-dihydroxybenzene-3,5-disulfonic acid, H4B=1,8-dihydroxynaphthalene-
-3,6-disulfonic acid.
--------------------------------------------------------------------------------
Th++++     gl  KNO3   25°C 0.10M U    M                  1964CBa (74221) 384
                                          K(ThL+A)=9.29
```

K(ThL+B)=12.90
K(ThL+C)=6.98
K(ThL+D)=6.70
K(ThL+E)=3.09. H3A=5-sulfosalicylic acid, H2B=catachol, H2C=8-hydroxyquinol-ine-5-sulfonic acid, H2D=iminodiethanoic acid, H2E=2-phthalic acid

---

Th++++ gl KNO3 25°C 0.10M U M 1964PCa (74222) 385
K(ThL+H2A=ThLHA+H)=-2.26
K(ThLA+H)=4.46
B(ThLA)=36.7

Th++++ gl KNO3 25°C 0.10M U 1958BMa (74223) 386
K(ThLOH+H)=7.04
K((ThLOH)2+2H=2ThL)=9.82

Th++++ vlt KNO3 20°C 0.10M U T K1=23.2 1954SGa (74224) 387

****

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

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

---

Th++++ gl NaClO4 25°C 1.0M U H K1=4.27 1990BRa (75147) 388
B(Th2L)=5.30
By calorimetry: DH(K1)=11.1 kJ mol-1, DS(K1)=119 J K-1 mol-1.

****

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

---

Th++++ cal KNO3 25°C 0.10M U H 1989KGa (75515) 389
DH(K1)=-4.4 kJ mol-1; DS(K1)=340 J mol-1 K-1

Th++++ gl KNO3 25°C 0.10M U 1968BMa (75516) 390
K(Th(OH)L+H)=5.4
K((Th(OH)L)2+2H)=5.6
By spectrophotometry: K1=18.5

Th++++ ix R4N.X 20°C 0.10M U K1=19.24 1965RVb (75517) 391

Th++++ sp KNO3 25°C 0.10M U K1=18.5 1964PCa (75518) 392

****

C10H18O4 H2L Sebacic acid CAS 111-20-6 (3308)
Decanedioic acid; HOOC.(CH2)8.COOH

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

---

Th++++ gl oth/un 20°C 0.10M U 1960WKa (75607) 393
Kso=-17.78

****
C10H20N2O4 H2L CAS 5578-84-7 (5914)
N,N-Dihydroxydecanediamide; HN(OH).CO.(CH2)8.CO.NH(OH)

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Th++++ gl NaNO3 25°C 0.10M C K1=18.44 1989EHa (75803) 394
****
C10H20N2O6 H2L CAS 5616-21-7 (570)
N,N'-Bis(2-hydroxyethyl)diaminoethane-N,N'-diethanoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Th++++ gl KNO3 25°C 0.10M U K1=12.8 1958CGa (75859) 395
K(ThL(OH)2+2H)=7.8
****
C11H8N6O7S2 H4L CAS 35322-95-7 (909)
3-Hydroxy-4-(1H-tetrazol-5-ylazo)-2,7-naphthalenedisulfonic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Th++++ gl NaClO4 25°C var U 1992PPa (76942) 396
K(Th+H2L=ThL+2H)=1.50
****
C11H8N6O8S2 H5L CAS 74385-48-1 (897)
2-(1H-Tetrazol-5-ylazo)chromotropic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Th++++ gl NaClO4 25°C var U 1992PPa (76955) 397
K(Th+H3L=ThH2L+H)=1.73
****
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
---
Th++++ sp KCl 21°C 0.10M U 1978KUb (77586) 398
K(Th+HL)=7.06
****
C11H11NO6 H3L CAS 1147-65-5 (425)
N-(2'-Carboxyphenyl)iminodiethanoic acid; HOOC.C6H4.N(CH2.COOH)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Th++++ gl KNO3 25°C 0.10M U K1=12.93 B2=21.33 1982NBa (77837) 399
****
C12H8N2 L Phenanthroline CAS 66-71-7 (144)
1,10-Phenanthroline;

```
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Th++++     sp  NaCl   25°C  5.0M C        K1=3.81        1996XCa (80520) 400
-------------------------------------------------------------------------
Th++++     gl  alc/w  25°C  80%  U        K1=5.14   B2=9.26   1985ISa (80521) 401
*************************************************************************
C12H10N2O              HL                     CAS 1823-47-8  (3969)
2-Salicylideneaminopyridine; (2-OH).C6H4.CH:N.C5H4N
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Th++++     sp  alc/w  20°C 100%  U   H    K1=5.76        1984EAb (80677) 402
Data also for related hydroxybenzylidene-aminopyridines, -aminopyrimidines,
and amino-1,2,4-triazines
*************************************************************************
C12H12N4O2             HL    AHMP             CAS 62201-49-4  (7697)
4-(4-Acetophenyl)hydrazono-3-methyl-2-pyrazolin-5-one;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Th++++     gl  alc/w  25°C  50%  U T H    K1=7.62   B2=14.88  1999EEa (81129) 403
Medium: 50%(v/v) EtOH/H2O, 0.10 M KCl. DH(K1)=-30.3 kJ mol-1,
DS(K1)=44.4 J K-1 mol-1; DH(K2)=-35.0 kJ mol-1, DS(K2)=21.5 J K-1 mol-1.
*************************************************************************
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
-------------------------------------------------------------------------
Th++++     gl  alc/w  25°C  50%  C        K1=8.30   B2=16.02  1999GAa (81373) 404
Medium: 50% EtOH/H2O, 0.10 M NaNO3.
*************************************************************************
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
-------------------------------------------------------------------------
Th++++     EMF NaClO4 20°C 0.10M U        K1=19.8        1967BAc (82476) 405
                                        K(ThL+H)=2.43
                                        K(ThL+OH)=7.24
*************************************************************************
C12H20N2O9             H4L    EEDTA            CAS 923-73-9  (2112)
Oxa-bis(ethyleneimino)diethanoic acid; ((HOOC.CH2)2N.CH2.CH2)2O
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Th++++     gl  KNO3   25°C 0.10M U                        1968BMa (82567) 406
                                        K(Th(OH)L+H)=6.35
-------------------------------------------------------------------------
Th++++     EMF NaClO4 20°C 0.10M U        K1=24.9        1967BAc (82568) 407
```

K(ThL+H)=2.09
K(ThL+OH)=7.44

****

C13H8N2O3Cl2 HL (6202)
2-Carboxy-2'-hydroxy-3',5'-dichloroazobenzene; HOOC.C6H4.N:N.C6H2(OH)Cl2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Th++++	gl	diox/w	25°C	70%	U	I	K1=15.46	B2=29.70 B3=41.42	1987KBc (84472)	408

****

C13H8O3 HL CAS 719-41-5 (3397)
1-Hydroxyxanthone (1-Hydroxy-9-xanthenone)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	sp	alc/w	25°C	50%	U		K1=11.89	1968GDb (84498)	409

Medium: 50% EtOH, 0.1 M NaClO4

****

C13H10NOBr HL CAS 886-34-0 (2729)
Salicylidene-4-bromo aniline; HO.C6H4.CH:N.C6H4.Br

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Th++++	sp	alc/w	20°C	100%	U	H	K1=5.54	B2=9.80	1983EAb (84677)	410

Data also for salicylidene-3-anisidine

****

C13H10N2O6S H2L MordentYellow10 CAS 21542-82-5 (1390)
5-(4'-Sulfophenylazo)salicylic acid; HO3S.C6H4.N:N.C6H3(OH).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Th++++	gl	oth/un	20°C	0.10M	M	T H	K1=9.4	B2=16.60	1978MBe (84942)	411

Medium: 0.10 M KClO4. Data for 44 C. DH and DS values reported.

****

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
Th++++	dis	KCl	20°C	0.10M	U		K1=10.90	B2=20.93	B3=29.68 B4=37.70	1967ZOa (85179)	412
Th++++	oth	NaClO4	25°C	0.10M	U		B2=7.67			1960RYa (85180)	413

****

C13H12N2O HL (2728)
Salicylidene phenyl hydrazone; HO.C6H4.CH:N.NH.C6H5

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

```
------------------------------------------------------------------------------
Th++++     sp  alc/w  20°C 100%  U   H    K1=4.34   B2=7.06   1983EAb (85346) 414
******************************************************************************
C14H8O4              H2L    Alizarin         CAS 72-48-0  (1058)
1,2-Dihyhroxyanthraquinone;
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Th++++     sp  non-aq 25°C 100%  U        K1=4.76        1970DSd (86651) 415
Medium: BuOH
******************************************************************************
C14H8O4              H2L    Quinizarin       CAS 81-64-1  (1060)
1,4-Dihydroxyanthraquinone;
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Th++++     gl  alc/w  25°C  40%  U        K1=6.26   B2=10.53  1988ISc (86667) 416
------------------------------------------------------------------------------
Th++++     sp  alc/w  20°C  50%  U                          1982KMd (86668) 417
                                        K(Th+HL)=10.2
Medium: 50% v/v EtOH/H2O
******************************************************************************
C14H8O6              H4L    Quinalizarin     CAS 81-61-8  (1056)
1,2,5,8-Tetrahydroxyanthraquinone;
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Th++++     sp  non-aq 25°C 100%  U                          1970DSd (86684) 418
                                        K(?)=5.43
Medium: BuOH
******************************************************************************
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
------------------------------------------------------------------------------
Th++++     EMF oth/un   ?  0.10M U        K1=11.52  B2=18.15  1972GBc (86761) 419
------------------------------------------------------------------------------
Th++++     sp  NaNO3  30°C 0.10M U                          1963SDa (86762) 420
                                        K(?)=8.2
------------------------------------------------------------------------------
Th++++     sp  R4N.X  25°C 0.10M U T      B2=8.23        1960SDa (86763) 421
Medium:NH4NO3. B2=8.24(30 C)
------------------------------------------------------------------------------
Th++++     sp  oth/un 25°C    ?  U        B2=8.2         1959DBb (86764) 422
******************************************************************************
C14H8O7S             H3L                    (4037)
1,4-Dihydroxyanthraquinone-2-sulfonic acid, quinizarin-2-sulfonic acid;
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
```

```
--------------------------------------------------------------------------------
Th++++     sp  oth/un 20°C    ?  U                      1970JJa (86781) 423
                                        K(Th+H2L=ThHL+H)=(?)3.0
                                        K(Th+2H2L=Th(HL)2+2H)=(?)6.1
********************************************************************************
C14H9NO4              H2L    Alizarin Maroon  CAS 3963-78-8  (1052)
3-Amino-1,2-dihydroxyanthraquinone;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Th++++     gl  NaClO4 25°C 0.10M U        K1=6.30   K2=4.75   1986SIa (86814) 424
********************************************************************************
C14H11NO4              HL                        (2727)
Salicylidene-4-amino salicylic acid; HO.C6H4.CH:N.C6H3(OH).COOH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Th++++     gl  alc/w  27°C  40%  M        K1=10.75  B2=17.00  1993MRa (86979) 425
Medium: 40% v/v EtOH/H2O, 0.10 M NaCl.
--------------------------------------------------------------------------------
Th++++     sp  alc/w  20°C 100%  U   H    K1=4.94        1983EAb (86980) 426
********************************************************************************
C14H11NO5             H4L                      CAS 245062-92-4  (8423)
4-[(E)-[(2,4-Dihydroxyphenyl)methylene]amino-2-hydroxybenzoic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Th++++     gl  alc/w  27°C  40%  M        K1=7.39   B2=13.57  1993MRa (86984) 427
Medium: 40% v/v EtOH/H2O, 0.10 M NaCl.
********************************************************************************
C14H12O3               HL    Benzilic acid    CAS 76-93-7  (710)
Diphenylglycolic acid, (benzilic acid); (C6H5)2C(OH).COOH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Th++++     dis NaClO4 25°C 0.25M M        K1=6.0    B2=11.20  1985CAb (87351) 428
                                        B3=16.2
********************************************************************************
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
--------------------------------------------------------------------------------
Th++++     gl  KNO3   35°C 0.10M M    M                 1976PTb (88792) 429
                                        K(ThL+glycolate)=5.88
                                        K(ThL+malate)=4.79
At 30 C: K(ThL+glycolate)=5.70; K(ThL+malate)=4.72
--------------------------------------------------------------------------------
Th++++     EMF NaClO4 20°C 0.10M U        K1=29.95       1967BAc (88793) 430
                                        K(ThL+H)=2.50
```

```
                                        K(2ThL+2OH)=5.70
--------------------------------------------------------------------------------
Th++++     ISE KNO3   30°C 0.10M U T H    K1=23.77       1965HWa (88794) 431
K1=23.79(10 C),23.78(20 C). DH(K1)=-2.1 kJ mol-1, DS=447 J K-1 mol-1
--------------------------------------------------------------------------------
Th++++     gl  KNO3   25°C 0.10M U    M                  1964CBa (88795) 432
                                        K(ThL+A)=12.67
                                        K(ThL+B)=13.13
                                        K(ThL+C)=8.87
                                        K(ThL+D)=12.26
H4A=dihydroxybenzene-3,5-disulfonic acid, H4B=1,8-dihydroxynaphthalene-3,6-
disulfonic acid, H3C=5-sulfosalicylic acid, H2D=catechol, also other ligands
--------------------------------------------------------------------------------
Th++++     gl  KNO3   25°C 0.10M U                       1958BMa (88796) 433
                                        K(ThLOH+H)=7.85
                                        K(Th2L2(OH)2+2H=2ThL)=10.84
                                        K(2ThLOH=Th2L2(OH)2)=4.3
********************************************************************************
C14H22N4O10           H3L                     CAS 29725-87-9  (5074)
Ethylenedinitrilo-N,N'-bis(methylenecarbonyliminoethanoic)-N,N'-diethanoic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Th++++     gl  KNO3   25°C 0.10M U        K1=12.0        1970MMc (88934) 434
********************************************************************************
C14H22N4O10           H4L    DGENTA           CAS 29725-86-8  (2371)
N,N-Diglycyldiaminoethane-tetraethanoic acid;(-CH2.HNCOCH2N(CH2COOH)2)2
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Th++++     gl  KNO3   25°C 0.10M U        K1=14.0        1970MMc (88952) 435
********************************************************************************
C14H23N3O10           H5L    DTPA             CAS 67-43-6  (238)
Diethylenetriamine-pentaethanoic acid; HOOC.CH2.N(CH2.CH2.N(CH2.COOH)2)2
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Th++++     cal KNO3   25°C 0.10M U   H                   1989KGa (89403) 436
DH(K1)=-12.3, DH(ThHL)=-12.3 kJ mol-1
DS(K1)=510, DS(B(ThHL))=550 J mol-1 K-1
--------------------------------------------------------------------------------
Th++++     sp  oth/un 25°C 0.10M C T H    K1=26.39       1983SPb (89404) 437
DH1=-45 kJ/mol
--------------------------------------------------------------------------------
Th++++     gl  KNO3   30°C 0.10M U    M                  1976PTa (89405) 438
                                        K(ThL+lactate)=6.09
                                        K(ThL+mandelate)=5.92
                                        K(ThL+A)=5.41
                                        K(ThL+B)=5.40
A=1-Hydroxy-2-naphthol, B=2-Hydroxy-3-naphthol
```

```
--------------------------------------------------------------------------------
Th++++     gl  KNO3   35°C 0.10M M    M                  1976PTb (89406) 439
                                       K(ThL+glycolate)=6.48
                                       K(ThL+malate)=5.93
At 30 C: K(ThL+glycolate)=6.42; K(ThL+malate)=5.89
--------------------------------------------------------------------------------
Th++++     gl  KNO3   30°C 0.10M U    M                  1975PTb (89407) 440
                                       K(ThL+A)=10.82
                                       K(ThL+B)=10.01
                                       K(ThL+C)=8.83
H4A=tiron, H2B=chromotropic acid, H2C=catechol
--------------------------------------------------------------------------------
Th++++     EMF NaCl   20°C 0.50M U        K1=26.64       1972PRc (89408) 441
--------------------------------------------------------------------------------
Th++++     gl  KNO3   25°C 0.10M U                       1968BMa (89409) 442
                                       K(Th(OH)L+H)=8.9
--------------------------------------------------------------------------------
Th++++     EMF NaClO4 20°C 0.10M U        K1=28.78       1967BAc (89410) 443
                                       K(ThL+H)=2.16
                                       K(ThL+OH)=4.9
--------------------------------------------------------------------------------
Th++++     ix  R4N.X  20°C 0.10M U        K1=30.34       1965RVb (89411) 444
********************************************************************************
C14H24N2O8            H4L    HMDTA            CAS 1633-00-7  (920)
1,6-Diaminohexane-N,N,N',N'-tetraethanoic acid; ((HOOC.CH2)2N.CH2.CH2.CH2)2
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Th++++     gl  KCl    25°C 0.10M U                       1974KPd (89608) 445
                                       K(Th+HL)=10.92
********************************************************************************
C14H24N2O10                  EGTA             CAS 67-42-5  (349)
Ethyleneglycol-O,O'-bis(2-aminoethyl ether)-N,N,N',N'-tetraethanoic acid; H4L
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Th++++     gl  KNO3   25°C 0.10M U        K1=9.89        1982NBa (89947) 446
--------------------------------------------------------------------------------
Th++++     gl  KNO3   25°C 0.10M U                       1968BMa (89948) 447
                                       K(Th(OH)L+H)=7.30
********************************************************************************
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
--------------------------------------------------------------------------------
Th++++     dis R4N.X  25°C 0.10M U                       1990MMe (90210) 448
                                       K(Th+H4L=ThL+4H)=16.26
********************************************************************************
C14H30N2O4              L                        (6566)
```

N,N,N',N'-Tetrakis(2-hydroxyethyl)-trans-1,2-diaminocyclohexane;
C6H10(N(CH2.CH2OH)2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	gl	NaNO3	25°C	0.10M	C			1991DCa (90598)	449
							B(ThLOH)=19.36		
							K(ThLOH+OH)=9.46		

****

C15H10O6S H2L CAS 17356-57-5 (4058)
Flavonol-2'-sulfonic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	sp	NaClO4	25°C	0.50M	U		K1=10.28 B2=18.06	1964OYb (90998)	450

****

C15H10O7 H5L Melanoxetin CAS 27696-41-9 (4054)
3,3',4',7,8-Pentahydroxyflavone;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	sp	alc/w	20°C	40%	U			1966KPa (91007)	451
							K(ThO+H5L=ThO(H4L)+H)=3.68(?)		

****

C15H10O8 H6L Myricetin CAS 529-44-2 (4055)
3,3',4',5,5',7-Hexahydroxyflavone;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	sp	oth/un	20°C	?	U			1965GKa (91027)	452
							K(ThO+H6L=ThO(H5L)+H)=4.55(?)		

****

C15H13NO2 HL CAS 7369-44-0 (4066)
N-3-Diphenylpropenohydroxamic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	dis	NaClO4	20°C	0.10M	U		K1=12.76 B2=24.70	1967ZSa (91644)	453
							B3=35.72		

****

C15H14N2O3 HL (6201)
2-Carboxy-2'-hydroxy-3',5'-dimethylazobenzene; HOOC.C6H4.N:N.C6H2(OH)(CH3)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	gl	diox/w	25°C	70%	U	I	K1=16.24 B2=30.84	1987KBc (91715)	454
							B3=43.69		

****

C15H23N3O12 H6L CAS 21979-64-6 (4069)
1,2,3-Tris(N,N-bis(carboxymethyl)amino)propane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Th++++ gl KNO3 25°C 0.10M U 1968MMb (92321) 455
K(ThL+H)=5.99
****
C16H9NO5 HL (6257)
1-Anthraquinonyloxamic acid; C14H7O2.NH.CO.COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Th++++ sp none 25°C 0.0 U K1=4.5 B2=13.30 1979ISa (92636) 456
Data also for 4-nitro analogue
****
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
---
Th++++ kin oth/un 25°C 0.02M U 1972GSe (92666) 457
K(ThOH+L)=6.45
****
C16H11NO3 HL HPBI CAS 41836-94-6 (7740)
3-Phenyl-4-benzoyl-5-isoxazolone;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Th++++ dis non-aq 30°C 100% U 2000SCa (92686) 458
Kd=8.71
Kd: Th+4HL(org)=ThL4(org)+4H.
Method: Solvent extraction, H2O(0.5 M NaNO3)/chloroform.
****
C16H11N2O8ClS2 H4L Solochrome FN CAS 25747-11-9 (8527)
6-[(5-Chloro-2-hydroxy-3-sulfophenyl)azo]-5-hydroxy-1-naphthalenesulfonic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Th++++ gl oth/un 20°C 0.10M M T H K1=18.0 B2=31.30 1978MBe (92779) 459
Medium: 0.10 M KClO4. Data for 44 C. DH and DS values reported.
****
C16H11N3O10S2 H4L Chromotrope 2B CAS 548-80-1 (896)
2-((4-Nitrophenyl)azo)chromotropic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Th++++ gl NaClO4 25°C var U 1992PPa (92866) 460
K(Th+H2L=ThHL+H)=1.81
K(2Th+H2L=Th2L+2H)=4.85

Th++++ sp KCl 20°C 0.10M U K1=24.34 1979BGa (92867) 461

```
--------------------------------------------------------------------------------
Th++++     sp  oth/un 25°C 0.10M U                        1967TMc (92868) 462
                                        K(Th+H2L=ThHL+H)=4.0
--------------------------------------------------------------------------------
Th++++     sp  oth/un 25°C    ?  U        B2=10.1         1961BDb (92869) 463
********************************************************************************
C16H11N3O10S2         H4L                      CAS 2103-69-0  (4091)
2-(2'-Nitrophenylazo)chromotropic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Th++++     sp  oth/un 25°C 0.10M U                        1967TMc (92874) 464
                                        K(Th+H2L=ThHL+H)=3.8
********************************************************************************
C16H11N3O10S2         H4L                      CAS 21908-70-3  (4092)
2-(3'-Nitrophenylazo)chromotropic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Th++++     sp  oth/un 25°C 0.10M U                        1967TMc (92876) 465
                                        K(Th+H2L=ThHL+H)=4.1
********************************************************************************
C16H11N5O4            H2L                        (5153)
1,5-Bis(2-carboxyphenyl)-3-cyanoformazan;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Th++++     sp  NaClO4 25°C 0.10M U                        1971BSf (92900) 466
                                        K(Th+2H+2L)=33.6
********************************************************************************
C16H12N2O3             HL                       CAS 49747-16-2  (8340)
7-Hydroxy-4-methyl-8-(phenylazo)coumarin;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Th++++     gl  alc/w  25°C  60%  U        K1=9.39   B2=17.54  1992IOa (92979) 467
Medium: 60% v/v EtOH/H2O, 0.1 M NaCl. Data for a range of aryl-substituted
derivatives.
********************************************************************************
C16H12N2O8S2          H4L    Chromotrope 2R   CAS 4197-07-3  (2604)
2-(Benzeneazo)-chromotropic acid, Acid Red 29
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Th++++     sp  KCl    20°C 0.10M U        K1=26.18        1979BGa (93069) 468
--------------------------------------------------------------------------------
Th++++     sp  NaClO4 25°C 0.10M U                        1963MIa (93070) 469
                                        Keff(Th+H2L=ThHL+H)=3.61
Keff at pH 2.0
********************************************************************************
```

C16H12N2O9S2 H5L CAS 26197-92-2 (4094)
2-(2'-Hydroxyphenylazo)chromotropic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	sp	oth/un	25°C	0.10M	U			1967TMb (93077)	470
							Keff(Th+H3L=ThHL+2H)=3.42		

Kee at pH 1.95

****

C16H12N2O11S3 H5L (4095)
2-(2'-Sulphophenylazo)chromotropic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	sp	NaClO4	25°C	0.10M	U			1963MIa (93084)	471
							Keff(Th+H2L=ThHL+H)=3.36		

Keff at pH 2.0

****

C16H12O5 H2L CAS 4431-41-8 (4072)
5,7-Dihydroxy-8-methoxyflavone;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	sp	alc/w	20°C	50%	U			1965KSd (93152)	472
							K(?)=4.54		

Medium: 50% EtOH, 0.001 M

****

C16H13N2O10AsS2 H5L Thorin I CAS 3688-92-4 (2609)
1-((2-Arsonophenyl)azo)-2-hydroxy-3,6-naphthalyldisulfonic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	sp	oth/un	?	0.50M	U		B2=8.72	1970GBa (93213)	473

Medium: HNO3

Th++++	sp	oth/un	25°C	?	U			1963SDc (93214)	474
							K(?)=9.8		

****

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
Th++++	gl	KNO3	35°C	0.10M	U			1974NDb (93269)	475
							K(Th+HL)=13.60, K(ThL+H)=6.00		
							K(Th+H5L=ThHL+4H)=6.35		
							K(ThL+OH)=4.45		
							K(ThL(OH)+OH)=3.45		
Th++++	sp	oth/un	20°C	?	U			1960KPa (93270)	476

K(Th+H4L)=6.8

****

C16H14N4O2 H2L (3467)

5-Hydroxy-4-(2-hydroxyphenylazo)-3-methyl-1-phenylpyrazole;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Th++++	sp	alc/w	25°C	100%	U		K1=6.88	B2=12.67	1991EHa (93477)	477

Medium: EtOH. Data also for other analogues

****

C16H30N2O8 H2L CAS 72912-01-7 (1568)

1,4,10,13-Tetraoxa-7,16-diazacyclooctadecane-N,N'-diethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	EMF	R4N.X	25°C	0.10M	U			1990MMe (95060)	478

K(Th+H4L=ThL+4H)=13.98

****

C17H12N2O10S2 H5L CAS 3440-76-4 (4119)

2-(2'-Carboxyphenylazo)chromotropic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	sp	NaClO4	25°C	0.10M	U			1967TMa (95723)	479

Keff(Th+H3L=ThHL+2H)=3.8

Keff at pH 2.0

****

C17H13NO4 H2L CAS 216243-24-2 (8612)

5,7-Dihydroxy-2-methyl-6-[(phenylimino)methyl]-4H-1-benzopyran-4-one;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Th++++	gl	alc/w	25°C	70%	U	TIH	K1=7.30	B2=14.06	1998ISd (95753)	480

Medium: 70% v/v EtOH/H2O, 0.106 M NaCl. Data for 60-100% EtOH/H2O,
0.15-0.03 M NaCl and 0-55 C. At 25 C, I=0 M: K1=9.29, B2=17.40. DH and DS.

****

C17H13NO5 H3L CAS 216243-25-3 (8613)

5,7-Dihydroxy-6-[[(2-hydroxyphenyl)imino]methyl]-2-methyl-4H-1-benzopyran-4-one;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Th++++	gl	alc/w	25°C	70%	U	TIH	K1=7.98	B2=15.74	1998ISd (95756)	481

Medium: 70% v/v EtOH/H2O, 0.106 M NaCl. Data for 60-100% EtOH/H2O,
0.15-0.03 M NaCl and 0-55 C. At 25 C, I=0 M: K1=9.68, B2=18.48. DH and DS.

****

C17H14N2O2 L CAS 4551-69-3 (698)

4-Benzoyl-3-methyl-1-phenyl-2-pyrazolin-5-one;

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

```
Th++++     dis oth/un 25°C  1.0M U                          1973BKc (95901) 482
                                          B4=32.76
**************************************************************************
C17H14N2O8S2          H4L                       CAS 15475-90-8  (2605)
2-(2-Tolylazo)-chromotropic acid;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Th++++     sp  KCl    20°C 0.10M U        K1=25.34       1979BGa (95940) 483
**************************************************************************
C18H12N2O11S2         H5L                         (5251)
2-(2'-Oxalophenylazo)chromotropic acid;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Th++++     sp  KNO3   25°C 0.10M U                          1970TMa (96870) 484
                                        K(Th+HL)=13.56
**************************************************************************
C18H13NO4             H3L                       CAS 698-51-6  (8424)
2-Hydroxy-4-[[2-hydroxy-1-naphthalenyl)methylene]amino]benzoic acid;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Th++++     gl  alc/w  27°C  40%  M        K1=6.52   B2=11.94  1993MRa (96897) 485
Medium: 40% v/v EtOH/H2O, 0.10 M NaCl.
**************************************************************************
C18H13NO6             H3L                       CAS 216243-28-6  (8614)
5,7-Dihydroxy-6-[[(2-carboxyphenyl)imino]methyl]-2-methyl-4H-1-benzopyran-4-one;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Th++++     gl  alc/w  25°C  70%  U TIH    K1=5.85   B2=11.42  1998ISd (96900) 486
Medium: 70% v/v EtOH/H2O, 0.106 M NaCl. Data for 60-100% EtOH/H2O,
0.15-0.03 M NaCl and 0-55 C. At 25 C, I=0 M: K1=7.51, B2=14.01. DH and DS.
**************************************************************************
C18H13N5O3S4           HL                       CAS 683787-43-1  (9097)
4-[(4-Oxo-3-phenyl-2-thioxo-5-thiazolidinyl)azo]-N-2-thiazolyl-benzenesulfonamide;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Th++++     gl  alc/w  25°C  30%  U T H    K1=8.00   B2=12.80  2003EEa (96905) 487
Medium: 30% v/v EtOH/H2O, 0.10 M KCl. Data for 25-45 C. DH(K1)=45 kJ mol-1
DS=270 J K-1 mol-1. DH(K2)=52, DS=267. Protonation constants not reported.
**************************************************************************
C18H14N2O2             HL                       CAS 15017-21-7  (6859)
2-Hydroxynaphthalidene benzoyl hydrazone; C6H5.CO.NH.N:CH.C10H6.OH
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Th++++     gl  diox/w 20°C  75%  U T      K1=8.77   B2=15.05  1992MCb (96909) 488
```

K(Th(NTA)+L+)=3.72
K(Th(HEDTA)+L)=3.53
K(Th(EDTA)+L)=3.42
30 C: B1=8.72, B2=14.97; 40 C: B1=8.66, B2=14.90
****
C18H14N2O3 H2L CAS 54009-54-0 (6860)
2-Hydroxynaphthalidene salicylic hydrazone; HO.C6H4.CO.NH.N:CH.C10H6.OH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Th++++ gl diox/w 20°C 75% U T M K1=8.18 B2=14.26 1992MCb (96919) 489
K(Th(NTA)+L)=3.67
K(Th(HEDTA)+L)=3.37
K(Th(EDTA)+L)=3.17
30 C: B1=8.10, B2=14.10; 40 C: B1=8.00, B2=13.91
****
C18H14N2O11S2 H5L (4132)
2-(2'-(Carboxyhydroxymethyl)phenylazo)chromotropic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Th++++ sp oth/un 25°C 0.10M U 1967MIb (96947) 490
Keff(Th+H3L=ThHL+2H)=5.91
Keff at pH 2.0. Values given for pH 1.1 to 3.2
****
C18H14N2O11S2 H5L (4133)
2-(2'-(Carboxymethoxy)phenylazo)chromotropic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Th++++ sp NaClO4 25°C 0.10M U 1967MIa (96954) 491
K(Th+H3L=ThHL+2H)=3.6
K varies with pH: 3.6 - 7.6
****
C18H30N4O12 H6L TTHA CAS 869-52-3 (694)
Triethylenetetraaminehexaethanoic acid;((HOOC.CH2)2N.CH2.CH2.N(CH2.COOH).CH2)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Th++++ EMF KNO3 25°C 0.10M U K1=31.9 1970HAa (98095) 492
By glass electrode: K(ThL+H)=3.05

Th++++ gl KNO3 25°C 0.10M U K1=>27 1965BMf (98096) 493
****
C18H34N6O8 H4L CAS 253273-56-2 (5455)
2,2',2",2"'-(1,2-Cyclohexanediyldinitrilo)tetrakis[N-hydroxy-N-methyl] acetamide;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Th++++ gl KNO3 25°C 0.10M C 2000ARa (98389) 494

B(ThHL)=30.0
B(ThH2L)=36.23
B(ThH3L)=41.99
B(ThH4L)=46.37

****

C19H10O5Br4S H2L Bromophenol Blu CAS 115-39-9 (2109)
3,3',5,5'-Tetrabromophenolsulfonephthalein, Bromophenol blue

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	sp	KCl	21°C	0.10M	U		K1=3.63	1978KUb (98987)	495

****

C19H12O9Br2S H6L Bromo Pyrog.Red CAS 16574-43-9 (706)
5',5"-Dibromopyrogallolsulfonephthalein;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	sp	oth/un	?	?	U			1967VSa (99013)	496
							K(Th+H3L=ThH2L+H)=4.36		

****

C19H14N6O3S3 HL CAS 364325-73-5 (9096)
4-[(4-Oxo-3-phenyl-2-thioxo-5-thiazolidinyl)azo]-N-2-pyrimidinyl-benzenesulfonamide
;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	gl	alc/w	25°C	30%	U	T H	K1=8.38 B2=13.71	2003EEa (99070)	497

Medium: 30% v/v EtOH/H2O, 0.10 M KCl. Data for 25-45 C. DH(K1)=37 kJ mol-1
DS=284 J K-1 mol-1. DH(K2)=38, DS=238. Protonation constants not reported.

****

C19H15N5O4S3 HL CAS 403480-96-6 (9095)
N-(5-Methyl-3-isoxazolyl)-4-[(4-oxo-3-phenyl-2-thioxo-5-thiazolidinyl)azo]-benzenes
ulfonamide;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	gl	alc/w	25°C	30%	U	T H	K1=8.00 B2=12.85	2003EEa (99148)	498

Medium: 30% v/v EtOH/H2O, 0.10 M KCl. Data for 25-45 C. DH(K1)=64 kJ mol-1
DS=268 J K-1 mol-1. DH(K2)=35, DS=210. Protonation constants not reported.

****

C20H13N3O7S H3L Eriochrome Bl T CAS 1787-61-7 (997)
1-(1-Hydroxy-2-naphthylazo)-6-nitro-2-naphthol-4-sulfonic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	gl	oth/un	20°C	0.10M	M	T H	K1=14.6 B2=25.70	1978MBe (99575)	499

Medium: 0.10 M KClO4. Data for 44 C. DH and DS values reported.

****

C20H14N2O5S H3L Solochrome 6B CAS 3564-14-5 (3507)
1-(1-Hydroxy-2-naphthylazo)-2-naphthol-4-sulfonic acid, Mordant Black3, Eriochrome

blue-black B;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Th++++ gl oth/un 20°C 0.10M M T H K1=14.7 B2=23.60 1978MBe (99664) 500
Medium: 0.10 M KClO4. Data for 44 C. DH and DS values reported.
****
C20H14N2O11S3 H5L Chromotrope 8B CAS 5850-64-6 (2674)
3-(4'-Sulfonaphthylazo)chromotropic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Th++++ sp NaClO4 25°C 0.10M C K1=9.56 1979PLa (99717) 501
****
C20H16N2 L CAS 63283-05-6 (2734)
N,N'-Bis(benzylidene)-1,2-diaminobenzene; (C6H5.CH:N)2.C6H4

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Th++++ sp alc/w 20°C 100% U K1=4.99 1984EAa (99755) 502
Data for other related benzylidene-1,2-diaminobenzenes also included
****
C20H16N2O2 H2L CAS 3946-91-6 (2733)
N,N'-Bis(2'-hydroxybenzylidene)-1,2-diaminobenzene; (HOC6H4CH:N)2.C6H4

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Th++++ sp alc/w 20°C 100% U K1=5.88 1984EAa (99775) 503
****
C20H16N2O2 H2L (2730)
N,N'-Bis(salicylidene)-1,4-phenylenediamine; (HO.C6H4.CH:N)2C6H4

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Th++++ sp alc/w 20°C 100% U H K1=4.18 B2=6.96 1983EAb (99784) 504
****
C21H18N6O3S3 HL CAS 364325-74-6 (9094)
N-(4,6-Dimethyl-2-pyrimidinyl)-4-[(4-oxo-3-phenyl-2-thioxo-5-thiazolidinyl)azo]-ben
zenesulfonamid

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Th++++ gl alc/w 25°C 30% U T H K1=8.20 B2=13.10 2003EEa (101122) 505
Medium: 30% v/v EtOH/H2O, 0.10 M KCl. Data for 25-45 C. DH(K1)=36 kJ mol-1
DS=280 J K-1 mol-1. DH(K2)=38, DS=222. Protonation constants not reported.
****
C21H18N6O5S3 HL CAS 412024-79-4 (9093)
N-(5,6-Dimethoxy-4-pyrimidinyl)-4-[(4-oxo-3-phenyl-2-thioxo-5-thiazolidinyl)azo]-be
nzenesulfonami

```
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Th++++     gl  alc/w  25°C  30%  U T H    K1=9.74   B2=17.57  2003EEa (101126) 506
Medium: 30% v/v EtOH/H2O, 0.10 M KCl. Data for 25-45 C. DH(K1)=35 kJ mol-1
DS=303 J K-1 mol-1. DH(K2)=38, DS=278. Protonation constants not reported.
*************************************************************************
C22H14O9             H5L                    CAS 4431-00-9  (3513)
Aurintricarboxylic acid;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Th++++     gl  NaClO4 25°C 0.10M U                         1968BDa (101509) 507
                                      K(Th+HL)=8.26
                                      K(ThHL+HL)=3.07
                                      K(Th(HL)2+HL)=2.80
-------------------------------------------------------------------------
Th++++     sp  oth/un 25°C    ?  U        K1=5.04        1958MDa (101510) 508
*************************************************************************
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
-------------------------------------------------------------------------
Th++++     sp  none   25°C  0.0  U        K1=11.33       1989LIa (101554) 509
*************************************************************************
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
-------------------------------------------------------------------------
Th++++     sp  oth/un  RT   6.0M U                         1997RRc (101651) 510
                                     K1eff=5.84
                                     B2eff=11.56
Medium: 6 M HCl
-------------------------------------------------------------------------
Th++++     sp  oth/un 25°C    ?  C        K1=5.0    B2=10.4   1987SLa (101652) 511
                                     B3=16.0
Medium: HCl, pH=2.0
*************************************************************************
C23H16O9Cl2S         H4L    Chrome azurol S  CAS 1667-99-8  (711)
Chromazurol S;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Th++++     sp  R4N.X  30°C 0.15M U                         1963SSb (102574) 512
                                     K1eff=4.2 (pH 4.5)
Medium: NH4NO3
*************************************************************************
C25H48N6O8           H3L    Desferrioxamine  CAS 70-51-9  (2488)
```

Desferrioxamine B; NH2.((CH2)5.NOH.CO.C2H4.CO.NH)2.(CH2)5.NOH.CO.CH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	gl	KCl	25°C	0.10M	C		K1=18.9 B(ThHL)=26.6 B(ThH2L)=29.3 B(ThH3L)=31.1 B(ThH-1L)=8.6	1996WNa (103823)	513

K(ThH-1L+H)=10.2. Data also for N-(2,3-dihydroxy-4-carbobenzoyl)desferrioxamine B: K1=37.2, B(ThHL)=46.1

****

C27H29NO10 H2L Daunorubicine CAS 23541-50-6 (5660)
Daunomycin;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	sp	oth/un	20°C	0.15M	U		K(Th+HL)=10.3	1982KMd (104444)	514

****

C27H30N4O18S3 H9L TRENCAMS CAS 252906-93-7 (7599)
3,3',3"-[Nitrilotris(2,1-ethanediyliminocarbonyl)]tris(4,5-dihydroxybenzenesulfonic acid);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	gl	NaClO4	25°C	0.10M	C		K1=37.72 B(ThHL)=41.29 B(ThH2L)=45.74 B(ThH3L)=49.12	1999BCa (104481)	515

****

C28H52N4O10 H5L CAS 137203-80-6 (8096)
1-N-Dodecyltriethylenetetramine-N,N',N", N'",N"'-pentaethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	gl	alc/w	25°C	50%	C		K1=24.5 K(ThL+H)=4.8 K(ThL+OH)=4.6	2001SYb (104992)	516

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

****

C29H26N2O13Br2S H6L BrCresol orange CAS 34352-52-8 (7742)
Bromocresol orange, o-Bromophthalexon S;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	sp	oth/un	25°C	0.1M	U	M	Keff(Th+L+A)=12.04	1998KHb (105074)	517

A: Cetylpyridinium bromide

****

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
Th++++	gl	NaNO3	25°C	0.50M	U		K1=24.58 K(Th+HL)=19.63 K(ThL+H)=6.13 K(Th+OH+L)=28.87 K(Th+2OH+L)=32.12 K(ThL+OH)=4.29, K(Th(OH)L+OH)=3.25	1977NDa (105496)	518
Th++++	gl	KNO3	35°C	0.10M	U		K(Th+HL)=19.54 K(Th+H6L=ThHL+5H)=8.66 K(ThL+H)=6.10 K(ThL+OH)=4.30 K(Th(OH)L+OH)=3.20	1974NDb (105497)	519
Th++++	sp	NaClO4	25°C	0.10M	U		B(ThH2L)=34.93 B(ThH4L2)=64.47 K(Th2H2L)=39.25	1972BSa (105498)	520
Th++++	sp	NaNO3	20?°C	0.20M	U		B(Th2L2)=52.5	1963BGa (105499)	521

****

C34H55N7O12 H5L CAS 153502-63-7 (7187)
N-(2,3-Dihydroxy-4-(methylamido)benzoyl)desferrioxamine B;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	sp	KCl	25°C	0.10M	C		K1=38.55 B(ThHL)=44.24	1996WNa (106166)	522

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Th++++	sp	NaClO4	?	1.0M	U		K(Th+H3L)=6.7 K(Th+2H3L)=10.8 K(2Th+HL)=25.3	1973CPb (106621)	523

****

C46H58O6 HL (6716)
Calix[4]arene-O(1)-ethanoic acid;

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

```
--------------------------------------------------------------------------------
Th++++     gl  alc/w  25°C 0.01M C        K1=34.4        1997ACa (107299) 524
                                        B(ThHL)=40.2
                                        B(ThH2L)=44.0
                                        B(ThH-1L)=27.4
                                        B(ThH-2L)=14.9
Medium: methanol, 0.01 M NEt4ClO4.  Also data for many other calixarenes
with mixed functionalities.
********************************************************************************
Polymer                       Fulvic acid        (1523)
Fulvic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Th++++     dis NaClO4 25°C 0.10M C TIH                  1980NCa (108182) 525
                                        K1eff=9.80
                                        B2eff=13.50
Medium: 0.10 M NaClO4, 0.05 M acetate, pH 4.0. Data for 5-50 C. Method:
solvent extraction. Soil fulvic acid. DH(K1)=18.9, DH(B2)=46.4 kJ mol-1.
********************************************************************************
Polymer                       Humic acid         (1524)
Humic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Th++++     dis NaClO4 25°C 0.10M C TIH                  1980NCa (108243) 526
                                        K1eff=11.14
                                        B2eff=16.17
Medium: 0.10 M NaClO4, 0.05 M acetate, pH 4.0. Data for 5-50 C. Method:
solvent extraction. Lake sediment humic acid. DH(K1)=32.6, DH(B2)=42.2.

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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