SC-Database
Software version = 5.81 Data version = 4.62
Experiment list contains 614 experiments for
 (no ligands specified)
 Metal : Y+++
 (no references specified)
 (no experimental details specified)

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

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ oth none 25°C 0.0 U 1952LAb (1033) 1
K(Y+3e=Y(s))=-120.3(-2.37 V)
Method:combination of thermodynamic data
****
AsO4--- H3L Arsenate CAS 7778-39-4 (1557)
Arsenate;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ sol none 25°C 0.0 C 1992FIa (1166) 2
Kso(YAsO4)=-22.60
Equilibrium monitored by EDTA and iodine titrations.
****
Br- HL Bromide CAS 10035-10-6 (19)
Bromide;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ cal mixed 25°C 50% C IH K1=1.7 B2= 2.00 1999IUa (2377) 3
Medium: 0.5 mole fraction DMA/DMF, 0.2 M Me4NCl. DH(K1)=5 kJ mol-1,
DH(B2)=53. Also data for 0.6-0.85 mole fraction.

Y+++ dis NaClO4 25°C 1.0M U K1=-0.15 1963CUb (2378) 4
Medium: HClO4

Y+++ EMF NaClO4 25°C 0.50M U T H K1=0.45 1962PAb (2379) 5
Method: Ag electrode. K1=0.49(15 C), 0.40(35 C); K1=1.32(25 C, I=0 corr.)
DH(K1)=-3.8 kJ mol-1, DS=-4.2 J K-1 mol-1.
****
CO3-- H2L Carbonate CAS 465-79-6 (268)
Carbonate;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl NaClO4 25°C 0.70M C K1=5.75 2004LBb (3439) 6
K(Y+HCO3=YHCO3)=1.27

Medium: 0.70 m NaClO4. Calculated for I=0, K1=7.48, B2=12.63,
K(Y+HCO3=YHCO3)=2.32, K(Y+HL=YL+H)=-2.85, K(Y+2HL=YL2+2H)=-8.03

Y+++ dis NaClO4 25°C 0.70M C I K1=5.75 B2=10.11 1998LBb (3440) 7
Method: H2O/tributylphosphate distribution and ICP-mass spectrometry.
Values calculated for I=0.0 M, K1=7.73, B2=13.19.

Y+++ dis NaClO4 25°C 0.70M C 1995LBc (3441) 8
B1eff=5.71
B2eff=10.34
Keff(Y+HL)=1.49
By solvent extraction from 0.7 M NaClO4 into tributylphosphate using 88Y.
B1eff=[YL]/[Y]([L]+[NaL]). Keff=[YHL]/[Y]([HL]+[NaHL]).

Y+++ sol NaClO4 25°C 0.0 C I 1992GSc (3442) 9
*Kso=21.55
Extrap. from data for 0.01-3.0 M NaClO4, 0-1.0 M Y(ClO4)3, using SIT and
Pitzer. *Kso: Y2(CO3)3+6H=2Y+3CO2+6H2O. At I=3.0 M: Kso=-28.56, *Kso=24.31

Y+++ sol none 25°C 0.0 C 1986FMa (3443) 10
Kso(Y2(CO3)3)=-31.52

Y+++ sol none 25°C 0.0 C 1986HMa (3444) 11
Kso(Y2(CO3)3)=-31.52
Method: spectrophotometry.

Y+++ gl NaClO4 25°C 3.00M C K1=6.02 1985SPa (3445) 12
B(Y2L)=6.98
K(Y+HL)=1.29

Y+++ sol oth/un 25°C 0.0 U 1966JHa (3446) 13
Kso(Y2L3)=-30.6

****

C6N6Co--- H3L Cyanocobaltate (5470)
Hexacyanocobaltate; [Co(CN)6]---

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

---

Y+++ con diox/w 25°C 10% U I K1=4.06 1960ATb (3507) 14
Medium: 10% w/w dioxan/H2O; K1=3.83(0%), 4.43(20%)

****

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

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

---

Y+++ cal non-aq 25°C 100% U K1=2.20 B2=4.54 1980VCa (5950) 15
Medium: dimethylacetamide

Y+++ dis NaClO4 25°C 1.0M U K1=-0.03 1963CUb (5951) 16

```
--------------------------------------------------------------------------------
Y+++       EMF NaClO4 25°C  2.0M U        K1=-0.3        1963FDa  (5952)  17
                                         B(YCl(CH3CO2))=1.18
Method:quinhydrone electrode
--------------------------------------------------------------------------------
Y+++       EMF NaClO4 25°C 0.50M U TIH    K1=0.36        1962PAb  (5953)  18
Method: Ag electrode. K1=0.38(15 C), 0.32(35). DH(K1)=-1.3 kJ mol-1, DS=-4
At I=0 corr.: K1=1.26
--------------------------------------------------------------------------------
Y+++       sol none   25°C  0.0  U                      1960ASd  (5954)  19
                                         Kso(Y(OH)2.5Cl0.5)=-21.9
                                         Kso(Y(OH)2Cl)=-16.6
--------------------------------------------------------------------------------
Y+++       dis NaClO4 20°C  3.0M U                      1960PBa  (5955)  20
                                         B6=-0.87
                                         Bn=-0.145n + 0.019n(6-n)
********************************************************************************
F-                     HL    Fluoride         CAS 7644-39-3  (201)
Fluoride;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Y+++       ix  oth/un 25°C 0.02M C T H    K1=3.97   B2= 6.35  2004LMa  (7335)  21
Medium: 0.025 M HNO3. Applying Pitzer parameters: at I=0, K1=10.24.
Data for 5 to 45 C. DH(K1)=9.8 kJ mol-1, DH(B2)=20.8.
--------------------------------------------------------------------------------
Y+++       ISE NaClO4 25°C  0.0  C  I     K1=4.46        2000LBa  (7336)  22
Method: Fluoride ISE. Values calc. from data for I=0.015-0.70 M NaClO4.
At I=0.70 M, K1=3.538
--------------------------------------------------------------------------------
Y+++       ix  KNO3   25°C 0.02M C        K1=3.89   B2= 6.50  1999SBc  (7337)  23
Medium: 0.025 M HNO3. Additional method: ICP-MS.
Assumed K1(HF) = 3.03, derived from literature values.
--------------------------------------------------------------------------------
Y+++       cal NaClO4 25°C 1.00M C   H                  1988GBa  (7338)  24
DH(K1)=9.27 kJ mol-1; DS(K1)= 100 J mol-1 K-1
--------------------------------------------------------------------------------
Y+++       ISE KNO3   25°C 0.10M C    M   K1=3.76        1987YHa  (7339)  25
K(YA+F)=2.62(H3A=NTA), 1.8(H3A=HEDTA), 1.5(H4A=EDTA), 1.6(H4A=CDTA)
--------------------------------------------------------------------------------
Y+++       gl  KCl    25°C 1.00M U    M                  1981KTb  (7340)  26
                                         K(YEDTA+F)=1.89
                                         K(Y(EDTA)F+F)=0.48
--------------------------------------------------------------------------------
Y+++       oth NaClO4 25°C 0.10M U        K1=3.43        1973MSg  (7341)  27
method:electromigration or transference number
--------------------------------------------------------------------------------
Y+++       dis NaClO4 25°C 0.50M C        K1=7.89   B2= 7.11  1970ALc  (7342)  28
Method: extraction of 91Y from 0.50 M NaClO4 medium into toluene/
di-(2-ethylhexyl)phosphoric acid. Medium pH 3.6.
```

```
------------------------------------------------------------------------------
Y+++       ISE NaClO4 25°C 0.50M U T H    K1=3.91   B2=7.16   1969ALa  (7343)  29
DH(K1)=5.2 kJ mol-1,DH(B2)=-5.0. K1=3.88,B2=7.19(15 C);K1=3.94,B2=7.16(35 C)
------------------------------------------------------------------------------
Y+++       dis NaClO4 25°C 0.50M U        K1=3.89   B2=7.11   1969ALd  (7344)  30
                                          B3=10.30
------------------------------------------------------------------------------
Y+++       EMF NaClO4 25°C 0.50M U   H                  1967APa  (7345)  31
DH(K1)=9.2 kJ mol-1, DS=104 J K-1 mol-1. At I=0 corr:DH(K1)=9.6, DS=125
------------------------------------------------------------------------------
Y+++       EMF NaClO4 25°C  1.0M U   H    K1=3.60       1967WCa  (7346)  32
By calorimetry: DH(K1)=34.8 kJ mol-1, DS=186.0 J K-1 mol-1
------------------------------------------------------------------------------
Y+++       EMF NaClO4 25°C 0.50M U T H    K1=3.93   B2=7.1    1961PGa  (7347)  33
                                          K3=3.2
                                          K(Y+HF=YF+H)=1.00
                                          K(YF+HF=YF2+H)=0.3
                                          K(YF2+HF=YF3+H)=0.3
At 15 C: *K1=1.02,*K2=0.0,*K3=0. At 35 C:*K1=0.98,*K2=0.7,*K3=0.5
At I=0 corr: K1=4.81,K2=3.73,K3=3.60. DH(*K1)=-4 kJ mol-1,DS=4 J K-1 mol-1
------------------------------------------------------------------------------
Y+++       EMF NaClO4 25°C 0.50M U        K1=3.88       1959SEa  (7348)  34
******************************************************************************
IO3-                    HL    Iodate           CAS 7782-68-5  (1257)
Iodate;
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Y+++       sol oth/un 25°C  0.0  U                      1966FPb  (8574)  35
                                          Kso=-9.96
******************************************************************************
IO4-                    HL    Periodate        CAS 13444-71-8  (6063)
Periodate;
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Y+++       sol oth/un 25°C  dil  U                      1974LOa  (8619)  36
                                          Kso(Y(H2IO6)(H2O)3)=-10.22
******************************************************************************
Mo12O42U--------      H8L                    (2922)
Uranium-12-molybdate;
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Y+++       gl  oth/un 20°C 0.10M U        K1=3.88       1989SBb  (8784)  37
                                          B(YHL)=7.97
                                          B(YH2L)=10.34
******************************************************************************
NH3                      L    Ammonia          CAS 7664-41-7  (414)
Ammonia
```

```
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Y+++       gl  R4N.X  25°C 5.00M U        K1=0.4         1985MMa  (9222)  38
*******************************************************************************
NO3-                   HL    Nitrate          CAS 7697-37-2  (288)
Nitrate;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Y+++       cal NaClO4 25°C  2.0M C   H    K1=-0.92       1998BMb (10009)  39
DH(K1)=9.2 kJ mol-1
-------------------------------------------------------------------------------
Y+++       dis NaClO4 20°C  3.0M U                       1960PBa (10010)  40
                                        B6=-0.46
Bn=-0.77n-0.01n(6-n), n=1 to 6. Kd(Y+3L+3TBP(CCl4)=YL3T3(CCl4)=0
*******************************************************************************
OH-                    HL    Hydroxide          (57)
Hydroxide;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Y+++       gl  NaClO4 25°C  0.0  C  IH                   2000KBa (12494)  41
                                        *K1=-7.80
In 0.7 M NaClO4, *K1=-8.11. DH(*K1)=46 kJ mol-1.
-------------------------------------------------------------------------------
Y+++       gl  NaClO4 25°C 3.00M U                       1973AKa (12495)  42
                                        *B2=-17.0
                                        *B(2,2)=-14.04
Medium: LiClO4
-------------------------------------------------------------------------------
Y+++       gl  NaClO4 25°C 3.00M U                       1973AKb (12496)  43
                                        *B2=-17.0(-16.8?)
                                        *B(2,2)=-14.75
Medium: D2O containing LiClO4. *K2: YOD+D2O=Y(OD)2+D; *B(2,2): 2Y+2D2O=
Y2(OD)2 + 2D
-------------------------------------------------------------------------------
Y+++       gl  oth/un 25°C  3.0M U                      1972MAa (12497)  44
                                        *B2=-16.04
                                        *B(2,2)=-14.08
Medium: LiClO4
-------------------------------------------------------------------------------
Y+++       gl  oth/un 25°C  3.0M U                      1972MAa (12498)  45
                                        *B2=-16.20
                                        *B(2,2)=-14.93
Medium: D2O, 3 M LiClO4
-------------------------------------------------------------------------------
Y+++       oth KNO3   25°C 0.01M U        K1=10.5   B2=19.8   1972SSf (12499)  46
Method: electrical migration or transference number
-------------------------------------------------------------------------------
```

```
Y+++       EMF alc/w  25°C  25%  U  I                    1972USa (12500)  47
                                        *K1=-7.94
Medium: 25% v/v EtOH/H2O, 0.05 M NaClO4. *K1=-8.03(0%), -7.49(50%),
-7.71(0%,I=0)
-------------------------------------------------------------------------------
Y+++       sol oth/un 25°C       U                    1970IEb (12501)  48
                                        K(YL3(s)=L=YL4)=-6.2
                                        K(YL3(s)+2L=YL5)=-7.8
                                        K(YL3(s)+3L=YL6)=-9.3
-------------------------------------------------------------------------------
Y+++       oth oth/un  rt   10%  U                    1967PBb (12502)  49
                                        Kso=-27.4
                                        K(YL3(s)=YL3)=-4.8
Medium: 10% sea water. Method: Tyndall scattering
-------------------------------------------------------------------------------
Y+++       gl  NaClO4 25°C 0.30M U                    1966FKa (12503)  50
                                        *K1=-8.34
-------------------------------------------------------------------------------
Y+++       oth oth/un 20°C  dil  U                    1966OSa (12504)  51
                                        Kso=-25.7
Method: Tyndall scattering
-------------------------------------------------------------------------------
Y+++       gl  oth/un 25°C 3.00M U                    1964BCa (12505)  52
                                        *B(2,2)=-14.30
                                        *B(3,5)=-33.8
                                        *K1=-9.1
-------------------------------------------------------------------------------
Y+++       EMF none   25°C  0.0  M                    1962AEa (12506)  53
                                        Kso=-24.5
Method: H electrode
-------------------------------------------------------------------------------
Y+++       sol none   22°C  0.0  U                    1962KGa (12507)  54
                                        Kso(Y(OH)3)=-24.2
-------------------------------------------------------------------------------
Y+++       gl  oth/un 25°C    ?  U                    1960ASd (12508)  55
                                        Kso=-24.5(aged)
                                        Kso=-23.3(fresh)(see also Cl-)
Kso: K(Y(OH)3(s)=Y+3OH); method:also solubility
-------------------------------------------------------------------------------
Y+++       EMF NaCl   25°C  4.0M C  I                  1959SEb (12509)  56
                                        *Kso=16.46
*Kso: K(Y(OH)3(s)+3H=Y+3H2O); *Kso=17.01(I=3),17.44(I=2). Method:H electrode
-------------------------------------------------------------------------------
Y+++       gl  NaClO4 25°C  var  U                    1951MFb (12510)  57
                                        Kso(Y(OH)3)=-22.80
-------------------------------------------------------------------------------
Y+++       gl  oth/un 25°C  var  U                    1946MOa (12511)  58
                                        *K1=ca.-7
Medium: SO4-- at various concentrations
-------------------------------------------------------------------------------
```

Y+++ gl oth/un 25°C var U 1944MKa (12512) 59
Kso(Y(OH)3)=-22.1

Y+++ gl oth/un 25°C dil U 1938OKa (12513) 60
Kso(Y(OH)3)=-21.45
Method: also solubility
****
O2-- H2L Peroxide CAS 7772-84-1 (2813)
Peroxide; -O.O-

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl NaNO3 25°C 0.10M C 2002MYb (12759) 61
K(2Y+3H2O2=Y2(O2)2(OH)2+6H)=-32.04; K(2Y+2H2O2=Y2(O2)2+4H)=-19.66.
****
PO4--- H3L Phosphate CAS 7664-38-2 (176)
Phosphate;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ sol none 25°C 0.0 M 1997LBd (13383) 62
Kso(YPO4)=-25.02
Calculated from data for 0.10 M HClO4 solution.

Y+++ sol oth/un 25°C 0.0 C I 1993FKb (13384) 63
Kso(YPO4)=-25.60
In synthetic seawater, Ks(YPO4)=-22.92.

Y+++ sol none 25°C 0.0 C 1991FBa (13385) 64
Kso(YPO4)=-24.76

Y+++ ix R4N.X 25°C 0.20M U I 1966BEc (13386) 65
K(Y+H2L)=1.84
Medium: NH4ClO4. K=2.65 (I=0 corr)
****
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
---
Y+++ gl KCl 25°C 0.50M U 1989APd (13672) 66
K(Y+H2L)=4.30
****
P3O10----- H5L CAS 10380-08-2 (1001)
Tripolyphosphate; from (HO)2PO.O.PO(OH).O.PO(OH)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl KNO3 25°C 0.10M U T H B2=9.1 1974KRa (13920) 67
K(Y+2HL)=6.7

K(Y+2HL)=6.8 and B2=9.0 (35 C), K(Y+2HL)=6.5 and B2=8.9 (45 C)
DH(Y+2HL)=-19 kJ mol-1; DH(B2)=-6

Y+++ gl NaClO4 ? 0.10M U B2=17.21 1962RKa (13921) 68
K(Y+HL)=4.97
K(Y+2HL)=8.87

****

P3O9--- H3L CAS 13566-25-1 (235)
Cyclotrimetaphosphate;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Y+++	cal	oth/un	25°C	0.10M	C	H	K1=3.19	1983GGb (13974)	69

Medium: 0.10 M HCl. DH(K1)=32.0 kJ mol-1, DS(K1)=168 J K-1 mol-1.

****

P4O12---- H4L CAS 13598-74-8 (234)
Cyclotetrametaphosphate;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Y+++	cal	oth/un	25°C	0.10M	C	H	K1=3.44	1983GGb (14024)	70

Medium: 0.10 M HCl. DH(K1)=17.8 kJ mol-1, DS(K1)=125 J K-1 mol-1.

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Y+++	cal	non-aq	25°C	100%	U	H	K1=1.6 B2=2.9 K3=0.5	1992TIa (15340)	71

Medium: DMF, 0.2 M R4NX. DH(K1)=8 kJ mol-1, DH(B2)=4, DH(B3)=25

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Y+++	sp	NaClO4	20°C	0.60M	U	T	K1=-0.07	1964KSe (15341)	72

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Y+++	sol	oth/un	25°C	0.66M	C		K1=1.83	2004SBb (16666)	73

Method: solubility of BaSO4 in 0.117 m YCl3 solution.
Calculated for I=0, K1=3.50.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Y+++	oth	oth/un	15°C	var	U	T H	K1=3.51	1974QAa (16667)	74

Method:ultrasonic absorption. Medium:Y2(SO4)3. K1=3.58(25 C), 3.61(31.6 C)
DH(K1)=17.7 kJ mol-1

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Y+++	cal	oth/un	25°C	0.0	U	H		1969FPa (16668)	75

DH(K1)=13.7 kJ mol-1

```
Y+++       cal oth/un 25°C  0.0  U   H    K1=3.34   B2=5.34   1969IEa (16669)  76
DH(K1)=15.1 kJ mol-1, DH(K2)=3.05; DS(K1)=114.6 J K-1 mol-1, DS(K2)=48.5
-------------------------------------------------------------------------------
Y+++       ISE NaClO4 25°C  2.0M U   H    K1=1.24   B2=1.68   1967CCd (16670)  77
By calorimetry: DH(K1)=16.9 kJ mol-1, DS=80.3 J K-1 mol-1; DH(K2)=6.3, DS=30
-------------------------------------------------------------------------------
Y+++       dis NaClO4 20°C  3.0M U        K1=2.0    B2=3.4    1960PBa (16671)  78
                                         B3=4.36
-------------------------------------------------------------------------------
Y+++       oth oth/un 25°C  0.0  U        K1=3.47        1954SJa (16672)  79
*******************************************************************************
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
-------------------------------------------------------------------------------
Y+++       gl  KCl    25°C 0.50M U                         1989APd (18298)  80
                                         K(Y+H2L)=5.43
*******************************************************************************
C2H2O3                 HL    Glyoxylic acid   CAS 298-12-4  (1142)
Glyoxylic acid; OHC.COOH
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Y+++       gl  NaClO4 20°C 0.10M U        K1=2.56   B2=4.41   1964PSd (18433)  81
                                         K3=1.5
*******************************************************************************
C2H2O4                 H2L    Oxalic acid      CAS 144-62-7  (24)
Ethanedioic acid; (COOH)2
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Y+++       ix  R4N.X  25°C 0.05M C        K1=5.74   B2=10.09  2001SBf (19156)  82
                                         K(Y+HL)=2.08
Medium: 0.05 M NH4NO3. At I=0, K1=6.66, B2=11.27.
-------------------------------------------------------------------------------
Y+++       gl  KCl    25°C  1.0M U    M                    1988KTa (19157)  83
                                         K(Y(edta)+L)=2.90
-------------------------------------------------------------------------------
Y+++       oth oth/un 25°C 0.10M U        K1=5.46   B2=9.29   1971STe (19158)  84
Method: electrical migration or transference number
*******************************************************************************
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
-------------------------------------------------------------------------------
Y+++       oth oth/un   ?     ?  U        B2=3.74        1967MBa (20227)  85
Method: paper electrophoresis
-------------------------------------------------------------------------------
```

```
Y+++       cal NaClO4 25°C  2.0M C   H                    1964GRa (20228)  86
DH(K1)=13.65 kJ mol-1, DS(K1)=75.7 J K-1 mol-1; DH(B2)=22.55, DS(B2)=128;
DH(B3)=21.94, DS(B3)=139.
-------------------------------------------------------------------------------
Y+++       gl  NaClO4 20°C 0.10M U        K1=1.97   B2=3.60   1962KPa (20229)  87
-------------------------------------------------------------------------------
Y+++       EMF NaClO4 20°C  2.0M U        K1=1.53   B2=2.66   1960SOb (20230)  88
                                         B3=3.4
                                         B4=3.3
Method: quinhydrone electrode
*******************************************************************************
C2H4O2S               H2L    Thioglycolic     CAS 68-11-1  (596)
Mercaptoethanoic acid; HS.CH2.COOH
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Y+++       gl  oth/un 25°C .065M U TIH    K1=5.28   B2=8.85   1975GSa (20384)  89
At 35 C: K1=5.22, K2=4.80; 45 C: 5.15, 5.00. At 35  C, I=0.15: K1=4.95,
K2=4.75
-------------------------------------------------------------------------------
Y+++       gl  NaClO4 20°C 0.10M U                    1964PKa (20385)  90
                                         K(Y+HL)=1.91
                                         K(YHL+HL)=1.28
-------------------------------------------------------------------------------
Y+++       gl  NaClO4 25°C  2.0M U                    1962BCa (20386)  91
                                         K(Y+HL)=1.49
                                         K(YHL+HL)=0.7
*******************************************************************************
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
-------------------------------------------------------------------------------
Y+++       cal NaClO4 25°C  2.0M C   H                    1964GRa (20657)  92
DH(K1)=-0.31 kJ mol-1, DS(K1)=46.4 J K-1 mol-1;DH(B2)=-0.724, DS(B2)=82.0;
DH(B3)=-3.75, DS(B3)=96.2; DH(B4)=-3.9, DS(B4)=107.
-------------------------------------------------------------------------------
Y+++       gl  NaClO4 20°C 0.10M U        K1=2.785  B2=4.88   1964PKb (20658)  93
                                         B3=5.78
-------------------------------------------------------------------------------
Y+++       EMF NaClO4 20°C  2.0M U        K1=2.47   B2=4.40   1960SOa (20659)  94
                                         B3=5.7
                                         B4=6.3
                                         B5=6.3
Method: quinhydrone electrode
-------------------------------------------------------------------------------
Y+++       ix  NaClO4 20°C 0.20M U        K1=2.78   B2=4.70   1960SVa (20660)  95
                                         B3=6.0
*******************************************************************************
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
Y+++	gl	NaClO4	30°C	0.2M	U	T	K1=5.06	1977MSf (21759)	96

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Y+++	gl	NaClO4	22°C	0.10M	U		K(YH-1L+H)=6.95	1972MCd (22160)	97

****

C2H6O6P2 H4L (5706)
Ethene-1,1-diphosphonic acid; H2C:C(PO3H2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Y+++	gl	KCl	25°C	0.15M	U	I	K(Y+H2L)=5.00	1989AMa (22178)	98

****

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
Y+++	sp	oth/un	25°C	0.70M	U		K(Y+H2L)=5.51	1987APa (23405)	99

****

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
Y+++	gl	KNO3	25°C	0.10M	U		K1=4.40 B2=7.04	1968PFa (24595)	100

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Y+++	gl	diox/w	20°C	50%	U		K1=5.98	1971MAf (24652)	101

Medium: 50% dioxan, 0.1 M NaClO4

****

C3H6N2O2 L Methylglyoxime CAS 2140-03-6 (2981)
Methylglyoxime; CH3.C(:N.OH).CH:N.OH

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

Y+++ gl diox/w 20°C 50% U K1=6.43 B2=12.17 1971MAf (24814) 102
Medium: 50% dioxan, 0.1 M NaClO4
****
C3H6O2 HL Propionic acid CAS 79-09-4 (35)
Propanoic acid; CH3.CH2.COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl NaClO4 25°C 2.0M U K1=1.61 B2=2.81 1965CGa (25075) 103

Y+++ gl NaClO4 20°C 0.10M U K1=1.88 B2=3.06 1964PKa (25076) 104
****
C3H6O2S H2L Thiolactic acid CAS 79-42-5 (366)
2-Mercaptopropanoic acid; CH3.CH(SH).COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl NaClO4 25°C 2.00M U 1968CMa (25179) 105
K(Y+HL)=1.70

Y+++ gl NaClO4 31°C 2.0M U 1963BCb (25180) 106
K(Y+HL)=1.38
K(YHL+HL)=0.7
****
C3H6O2S H2L CAS 107-96-0 (437)
3-Mercaptopropanoic acid; HS.CH2.CH2.COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl NaClO4 25°C 2.00M U 1968CMa (25233) 107
K(Y+HL)=1.51
****
C3H6O3 HL CAS 81598-26-7 (2521)
3-Hydroxypropanoic acid; HO.CH2.CH2.COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl NaClO4 25°C 2.00M U K1=1.43 1969JCc (25284) 108
****
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
---
Y+++ gl NaClO4 25°C 0.20M U K1=2.80 B2=4.94 1964DVa (25572) 109
K3=1.22
K4=0.55

Y+++ gl NaClO4 20°C 0.10M U K1=3.017 B2=5.33 1964PKb (25573) 110
B3=6.95

```
--------------------------------------------------------------------------------
Y+++       gl  NaClO4 25°C  2.0M U        K1=2.53   B2=4.70   1961CCa (25574) 111
                                         K3=1.42
--------------------------------------------------------------------------------
Y+++       ix  NaClO4 20°C 0.20M U        K1=2.83   B2=4.92   1960SVa (25575) 112
                                         B3=6.8
--------------------------------------------------------------------------------
Y+++       ix  oth/un  rt  0.20M U        B2=4.96        1958PMa (25576) 113
********************************************************************************
C3H6O3                 HL    Methoxyacetic    CAS 625-45-6  (29)
Methoxyethanoic acid; CH3.O.CH2.COOH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Y+++       gl  NaClO4 20°C 0.10M U        K1=2.00   B2=3.11   1964PKa (25610) 114
********************************************************************************
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
--------------------------------------------------------------------------------
Y+++       gl  NaCl   37°C 0.15M U    M   K1=3.92   B2=8.09   1991DWb (26298) 115
                                         B(YH2L(Glu))=23.03
--------------------------------------------------------------------------------
Y+++       gl  KNO3   35°C 0.10M U        K1=5.42        1990RSe (26299) 116
--------------------------------------------------------------------------------
Y+++       gl  KNO3   25°C 0.10M U        K1=5.0         1967EMb (26300) 117
********************************************************************************
C3H7NO3                HL    Serine           CAS 56-45-1  (49)
2-Amino-3-hydroxypropanoic acid; H2N.CH(CH2.OH)COOH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Y+++       gl  KNO3   25°C 0.10M M    M   K1=5.53        1996AEa (27198) 118
Data for ternary complexes with dipicolinic acid.
--------------------------------------------------------------------------------
Y+++       gl  NaNO3  25°C 0.10M M  I M   K1=5.61        1995KDd (27199) 119
                                         K(Y(egta)+L)=3.79
Data for 0.15 and 0.05 M NaNO3. At I=0, K1=5.86, K(Y(egta)+L)=4.08.
--------------------------------------------------------------------------------
Y+++       gl  NaClO4 20°C 0.10M M TIH                   1991ELa (27200) 120
                                         B(YHL)=3.50
Constant independent of I. DH(K1)=23.9 kJ mol-1, DS=149 J K-1 mol-1
--------------------------------------------------------------------------------
Y+++       EMF KCl    22°C 0.10M U        K1=4.51        1968RPa (27201) 121
--------------------------------------------------------------------------------
Y+++       gl  oth/un 25°C 0.10M U        K1=3.50        1965PGe (27202) 122
********************************************************************************
C3H8O2                  L    Propyleneglycol  CAS 57-55-6  (2025)
Propan-1,2-diol; CH3.CH(OH).CH2(OH)
```

```
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Y+++       gl  NaClO4 22°C 0.10M U                        1972MCd (27688) 123
                                        K(YH-1L+H)=6.95
******************************************************************************
C3H8O3                  L    Glycerol         CAS 56-81-5  (2707)
Propane-1,2,3-triol; HO.CH2.CH(OH).CH2.OH
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Y+++       gl  NaClO4 22°C 0.10M U                        1972MCd (27757) 124
                                        K(YH-1L+H)=6.85
------------------------------------------------------------------------------
Y+++       gl  NaCl   25°C 0.10M U                        1970PKe (27758) 125
                                        K(YH-1L+H)=6.79
******************************************************************************
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
------------------------------------------------------------------------------
Y+++       gl  KNO3   25°C 0.10M C                        1991SKb (28596) 126
                                        K(YL+H)=7.15
                                        K(YHL+H)=5.5
------------------------------------------------------------------------------
Y+++       sol oth/un 25°C 0.03M U        K1=22.5         1988BKa (28597) 127
                                        B(YHL)=25.1
                                        B(YH2L)=28.1
                                        B(YH3L)=30.5
                                        B(YH4L)=33.5
B(MH5L) = 33.7
------------------------------------------------------------------------------
Y+++       sol oth/un 25°C 0.03M U        K1=11.0         1979TKc (28598) 128
                                        K(Y+H+L)=19.4
******************************************************************************
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
------------------------------------------------------------------------------
Y+++       cal NaClO4 25°C 0.10M U   H    K1=2.73   B2=4.25   1976OCa (28672) 129
DH(K1)=9.9 kJ mol-1, DS=85 J K-1 mol-1; DH(B2)=13.9, DS=128
------------------------------------------------------------------------------
Y+++       gl  NaClO4 25°C 0.10M C   H    K1=2.727  B2= 4.25  1976OCb (28673) 130
By calorimetry: DH(K1)=9.92 kJ mol-1, DS(K1)=85.4 J K-1 mol-1;
DH(B2)=13.9, DS(B2)=128.
******************************************************************************
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
Y+++	gl	NaNO3	25°C	0.50M	C		K1=4.24	B2=6.32	1977KPa (29160)	131
							B(YHL)=6.3			
							B(Y2H-2L2)=-2.0			
Y+++	gl	NaClO4	25°C	0.10M	U		K1=3.61	B2=5.55	1970RFa (29161)	132

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Y+++	gl	oth/un	25°C	?	U		K1=5.6	B2=9.8	1956GNc (29282)	133

C4H5NO5 H2L (7375)
Oxalohydroxamic acid; HOOC.CO.CH2.CO.NHOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Y+++	gl	KNO3	25°C	0.1M	M		K1=10.50	B2=20.20	1989LWa (29318)	134
							K3=9.09			

C4H6O4S H3L Thiomalic acid CAS 70-49-5 (109)
2-Mercaptosuccinic acid, 2-Sulfanyl-1,4-butanedioic acid; HOOC.CH(SH).CH2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Y+++	gl	NaClO4	25°C	0.20M	U	T	K1=2.92	B2=5.21	1975PMb (30379)	135

35 C: K1=2.95, K2=2.31; 45 C: K1=2.98, K2=2.34

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
Y+++	gl	KNO3	20°C	0.10M	U				1980SDa (30758)	136
							B(YHL)=8.14			
Y+++	gl	KNO3	20°C	0.10M	U		K1=4.60	B2=7.56	1980SDb (30759)	137
							K(Y+HL)=1.85			
Y+++	gl	NaClO4	25°C	0.20M	U	T H	K1=4.63	B2=7.74	1975PMb (30760)	138

35 C: K1=4.65, K2=3.13; 45 C: K1=4.70, K2=3.15

Y+++	gl	NaClO4	25°C	0.10M	U		K1=4.91	B2=8.19	1970RFa (30761)	139

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
---
Y+++ gl KCl 25°C 1.0M U M 1988KTa (30948) 140
K(Y(edta)+L)=1.26

Y+++ cal NaClO4 25°C 1.0M C H 1963GRd (30949) 141
DH(K1)=7.247 kJ mol-1, DS(K1)=126 J K-1 mol-1; DH(B2)=2.046,
DS(B2)=194; DH(B3)=-15.52, DS(B3)=198.

Y+++ EMF NaClO4 20°C 1.00M U K1=5.24 B2=9.76 1963GTa (30950) 142
B3=13.03
Method: quinhydrone electrode
****
C4H6O6 H2L L-Tartaric acid CAS 87-69-4 (92)
L-Tartaric acid, L-2,3-Dihydroxybutanedioic acid; HOOC.CH(OH).CH(OH).COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ oth NaNO3 25°C 0.50M U M K1=2.68 1972PBd (31397) 143
B(YLOH)=11.66
Method: optical rotation

Y+++ ISE NaNO3 25°C 0.50M U M 1972RMa (31398) 144
B(Cu2Y(OH)5L3)=54.40

Y+++ gl alc/w 25°C 50% U I K1=5.52 1972SSj (31399) 145
Medium: 0-50% EtOH, 0.05 M. K1(0%)=4.03; K1(25%)=4.68; K1(40%)=5.12

Y+++ oth oth/un 25°C var U K1=4.07 B2=6.89 1966PBb (31400) 146
K(2Y+L)=5.97
K(Y+H-1L)=12.87
K(Y+HL)=2.82
****
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
---
Y+++ gl KNO3 25°C 0.10M M M K1=8.42 1996AEa (31979) 147
Data for ternary complexes with dipicolinic acid.

Y+++ gl NaClO4 30°C 0.10M U I K1=5.37 1984YLa (31980) 148

Y+++ gl NaClO4 25°C 0.20M U T H K1=4.75 B2=8.07 1975PMb (31981) 149
35 C: K1=4.77, K2=3.34; 45 C: K1=4.80, K2=3.36
****
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
-------------------------------------------------------------------------
Y+++       sp  oth/un 25°C 0.10M U        K1=6.78        1997YSa (32400) 150
-------------------------------------------------------------------------
Y+++       gl  KCl    25°C  1.0M U    M                  1988KTa (32401) 151
                                        K(Y(edta)+L)=3.54
-------------------------------------------------------------------------
Y+++       cal KNO3   20°C 0.10M U   HM                  1971GKb (32402) 152
                                        K(YA+L)=3.24
DH(YA+L)=-27.32 kJ mol-1. DH(YAL)=-27.32, DS=307. H4A=EDTA
-------------------------------------------------------------------------
Y+++       gl  KNO3   25°C 0.10M U    M   K1=6.78   B2=12.03  1962THa (32403) 153
Ternary complexes with N-(2-hydroxyethyl)diaminoethane-triethanoic acid
*************************************************************************
C4H8N2O2              H2L    Dimethylglyoxim  CAS 95-45-4  (2032)
2,3-Butanedione dioxime, Dimethylglyoxime; CH3.(C:NOH).(C:NOH).CH3
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Y+++       gl  diox/w 20°C  50%  U        K1=7.95   B2=14.97  1971MAf (32553) 154
Medium: 50% v/v dioxan, 0.1 M NaClO4
*************************************************************************
C4H8N2O3               HL    Asparagine       CAS 70-47-3  (17)
2-Aminobutanedioic acid 4-amide; H2N.CH(CH2.CO.NH2).COOH
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Y+++       gl  KNO3   25°C 0.10M M    M   K1=5.46        1996AEa (32747) 155
Data for ternary complexes with dipicolinic acid.
-------------------------------------------------------------------------
Y+++       gl  NaClO4 30°C 0.10M U        K1=3.76   B2=6.58   1984YLa (32748) 156
-------------------------------------------------------------------------
Y+++       gl  NaClO4 30°C  0.2M U        K1=4.43        1977MSf (32749) 157
-------------------------------------------------------------------------
Y+++       gl  NaClO4 25°C 0.10M U        B2=8.05        1973TSe (32750) 158
*************************************************************************
C4H8N2O4              H2L                    CAS 39156-77-9  (3008)
Hydrazine-N,N-diethanoic acid; H2N.N(CH2.COOH)2
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Y+++       EMF KCl    25°C 0.10M U        K1=4.1    B2=7.2    1954VIa (33118) 159
                                        K3=0.1
*************************************************************************
C4H8O2                 HL    Isobutyric acid  CAS 79-31-2  (573)
2-Methylpropanoic acid; CH3.CH(CH3).COOH
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Y+++       gl  NaClO4 25°C 2.00M U   H    K1=1.64   B2=2.79   1965CGa (33261) 160
```

By calorimetry: DH(K1)=22.6 kJ mol-1,DS=107 J K-1 mol-1; DH(K2)=12.4,DS=67

Y+++ gl NaClO4 25°C 0.50M U K1=1.60 B2=2.71 1964SPa (33262) 161

****

C4H8O2S HL CAS 627-04-3 (3007)

S-Ethylthioethanoic acid; CH3.CH2.S.CH2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Y+++	gl	NaClO4	31°C	2.0M	U		K1=1.42	B2=2.12	1963BCb (33415)	162

****

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
Y+++	gl	NaClO4	25°C	0.20M	U		K1=2.9	B2=5.60	1964DVa (33538)	163
							K3=1.7			
							K4=1.4			
Y+++	gl	NaClO4	25°C	2.0M	U	I	K1=3.11	B2=5.54	1964DVa (33539)	164
							K3=1.74			
							K4=1.06			

K1=3.22(I=0),3.12(I=0.1),3.05(I=0.5),3.08(I=1.0); K2=2.06(I=0),2.49(I=0.1),
2.45(I=0.5),2.44(I=1.0); K3=1.98(0),1.86(0.1),1.81(1.0); K4=1.37(0),1.22(0.1

Y+++	gl	NaClO4	20°C	0.10M	U		K1=3.204	B2=5.79	1964PKb (33540)	165
							B3=7.51			
Y+++	gl	NaClO4	25°C	0.50M	U		K1=2.88	B2=5.32	1964SPa (33541)	166
							B3=6.75			
Y+++	gl	NaClO4	25°C	2.0M	U		K1=2.86	B2=5.44	1961CCa (33542)	167
							K3=1.86			
Y+++	ix	NaClO4	20°C	0.20M	U		K1=3.11	B2=5.60	1960SVa (33543)	168
							B3=7.3			

****

C4H8O4 HL CAS 21620-60-0 (2326)

2,3-Dihydroxy-2-methylpropanoic acid; HO.CH2.C(OH)(CH3).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Y+++	gl	KNO3	25°C	0.10M	C		K1=3.05	B2=5.49	1975PFb (33688)	169
							K3=1.73			

****

C4H8O5 HL CAS 56309-80-9 (2365)

2,3-Dihydroxy-2-hydroxymethylpropanoic acid; HO.CH2.C(CH2.OH)(OH).COOH

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

---
Y+++ EMF KNO3 25°C 0.10M U K1=2.95 B2=5.33 1976PKb (33717) 170
K3=1.78

Y+++ gl NaClO4 25°C 0.50M U K1=2.65 B2=4.67 1964SPa (33718) 171
B3=5.26
****
C4H9NO2 HL 2-Aminobutyric CAS 2835-81-6 (571)
2-Aminobutanoic acid; CH3.CH2.CH(NH2).COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl KNO3 25°C 0.10M U T K1=5.04 1978SSb (33928) 172
****
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
---
Y+++ gl KCl 20°C 0.10M U K1=3.7 1970RPa (34341) 173
****
C4H11NO3 L Tris buffer CAS 77-86-1 (550)
2-Amino-2-(hydroxymethyl)-propan-1,3-diol; (HO.CH2)3C.NH2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl NaClO4 25°C 0.10M C M K1=2.23 2001GYa (35066) 174
K(2Y+L+5OH)=40.04
****
C4H14N2O6P2 H2L EDDPO CAS 1733-49-9 (2435)
1,2-Diaminoethane-N,N'-bis(methylenephosphonic) acid; (H2O3P.CH2.NH.CH2)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl KCl 25°C 0.10M U 1965DKb (35895) 175
K(Y+HL)=8.79
****
C5H2O5 H2L Croconic acid CAS 488-86-8 (1643)
4,5-Dihydroxycyclopent-4-ene-1,2,3-trione;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ cal NaClO4 25°C 0.10M U H K1=2.78 B2=4.46 1978COa (35952) 176
DH(K1)=11.3 kJ mol-1, DS=91.1; DH(K2)=5.02, DS=48.9
****
C5H7NO3 HL (4313)
Isonitrosoacetylacetone; HO.N:CH.CO.CH2.CO.CH3

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

Y+++ gl diox/w 20°C 50% U K1=5.19 B2=8.87 1971MAf (37535) 177
Medium: 50% v/v dioxan, 0.1 M NaClO4

****

C5H7NO4 HL (6083)
2-Acrylamidoglycolic acid; CH2:CH.CO.NH.CH(OH).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Y+++	gl	NaNO3	25°C	0.50M	C		K1=2.34		1977DPa (37543)	178
							B(YH-1L)=-2.88			
							B(Y2H-3L3)=-9.40			

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Y+++	gl	diox/w	20°C	50%	U		K1=5.63	B2=10.51	1971MAf (37712)	179

****

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
Y+++	dis	NaClO4	25°C	0.10M	C		K1=5.87	B2=10.64	1987SKc (38134)	180
							K3=3.09			
							K4=1.74			

Method: extraction of 88Y into heptane/acac phase.
K1 from literature.

Y+++	gl	NaClO4	20°C	0.10M	U	M			1973TZa (38135)	181
							K(Y(EDTA)+L)=3.60			
Y+++	gl	mixed	30°C	67%	U		K1=7.70	B2=13.62	1964DBb (38136)	182
							K3=4.91			

Medium: 67% acetone, 0.1 M NaClO4

Y+++	gl	NaClO4	25°C	2.0M	U		K1=5.57	B2=10.16	1964YCa (38137)	183
Y+++	gl	oth/un	30°C	0.10M	U		K1=5.87	B2=10.85	1960GFa (38138)	184
							K3=3.25			
Y+++	dis	oth/un	?	0.10M	U		K1=6.4	B2=11.1	1960STb (38139)	185
							B3=13.9			
Y+++	gl	mixed	?	75%	U		K1=7.73	B2=13.73	1956DBa (38140)	186
							K3=4.77			

Medium: acetone

Y+++	gl	oth/un	30°C	0.0	U		K1=6.4	B2=11.1	1955IFa (38141)	187

K3=2.8

****

C5H8O4 H2L CAS 498-21-5 (2234)

Methylsuccinic acid; HOOC.CH2.CH(CH3).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Y+++	gl	NaClO4	25°C	0.10M	U		K1=3.12	B2=4.91	1970RFa (38271)	188

****

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
Y+++	gl	alc/w	25°C	25%	U	I	K1=3.50		1973CSd (38369)	189

Medium: 0-40% (v/v) EtOH, 0.05 M. K1(0%)=3.25, K1(40%)=3.72

****

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
Y+++	EMF	oth/un	25°C	0.10M	U		K1=3.94		1969PSc (38445)	190

****

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
Y+++	gl	NaClO4	25°C	0.10M	U		B2=5.50		1981ZLa (38657)	191

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Y+++	gl	KCl	25°C	0.10M	U	T H	K1=5.40	B2=10.21	1973SCf (38658)	192

Data for 35 C. DH(K1)=26 kJ mol-1, DS(K1)=192 J K-1 mol-1;
DH(K2)=42, DS(K2)=234.

****

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
Y+++	gl	NaClO4	25°C	0.10M	U		B2=5.10		1981ZLa (38760)	193

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Y+++	gl	KCl	25°C	0.10M	U	T H	K1=4.52	B2= 8.92	1973SCf (38761)	194

Data for 35 C. DH(K1)=7 kJ mol-1, DS(K1)=110 J K-1 mol-1;
DH(K2)=14, DS(K2)=131.

****

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

```
--------------------------------------------------------------------------------
Y+++       gl  NaCl   37°C 0.15M U        K1=4.82        1991DWb (39148) 195
                                          B(YHL)=11.77
                                          B(YH2L)=15.13
--------------------------------------------------------------------------------
Y+++       vlt NaClO4 25°C  0.5M C T H    K1=1.60   B2= 2.11  1978ZGb (39149) 196
Method: polarography. Medium: 0.50 M LiClO4, pH 6.3. Also data at 35 C.
DH(K1)=-8.02 kJ mol-1, DS(K1)=3.6 J K-1 mol-1. DH(B2)=-4.80, DS(B2)=24.
********************************************************************************
C5H9NO4               H2L    MIDA            CAS 4408-64-4  (190)
N-Methyliminodiethanoic acid; CH3.N(CH2.COOH)2
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Y+++       gl  KCl    25°C 0.10M U        K1=6.77   B2=12.30  1980MGc (39295) 197
                                          B3=14.64
                                          B(Y+2OH+L)=18.33
********************************************************************************
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
--------------------------------------------------------------------------------
Y+++       gl  NaClO4 30°C  0.2M U        K1=4.72        1977MSf (39848) 198
--------------------------------------------------------------------------------
Y+++       gl  NaClO4 25°C 0.10M U        B2=8.05        1973TSb (39849) 199
********************************************************************************
C5H10N2O5             H2L                    (8080)
3-Hydroxy-2,4-diaminopentane-1,5-dioic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Y+++       gl  KCl    20°C  0.1M U        K1=8.45        1977ABf (40121) 200
********************************************************************************
C5H10O3                HL                     CAS 4026-18-0  (422)
2-Hydroxy-3-methylbutanoic acid; CH3.CH2.C(OH)(CH3).COOH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Y+++       ix  NaClO4 20°C 0.20M U        K1=2.60   B2=4.95   1960SVa (40272) 201
                                          B3 > 6.0
********************************************************************************
C5H10O3                HL                     CAS 617-31-2  (474)
2-Hydroxypentanoic acid; CH3.CH2.CH2.CH(OH).COOH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Y+++       gl  NaClO4 25°C  1.0M U        K1=2.46        1968GCa (40288) 202
********************************************************************************
C5H10O4                HL                     CAS 4767-03-7  (4297)
```

2,2-Bis(hydroxymethyl)propanoic acid; CH3.C(CH2OH)2.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Y+++	gl	NaClO4	25°C	0.10M	U		K1=2.17	B2=3.73	1970RDa (40306)	203

****

C5H10O4 HL CAS 19860-56-1 (2327)
2,3-Dihydroxy-2-methylbutanoic acid; CH3.CH(OH).C(OH)(CH3).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Y+++	gl	KNO3	25°C	0.10M	C		K1=2.91	B2=5.15	1975PFb (40321)	204
							K3=1.43			

****

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
Y+++	gl	KCl	25°C	0.10M	U T H		K1=4.79	B2= 9.06	1973SCf (40773)	205

Data for 35 C. DH(K1)=-35 kJ mol-1, DS(K1)=-26 J K-1 mol-1;
DH(K2)=37, DS(K2)=206.

****

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
Y+++	gl	NaNO3	25°C	0.10M	M I M		K1=5.72		1995KDd (41134)	206
							K(Y(egta)+L)=3.84			

Data for 0.15 and 0.05 M NaNO3. At I=0, K1=5.91, K(Y(egta)+L)=4.08.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Y+++	gl	KCl	20°C	0.10M	U		K1=4.6		1970RPa (41135)	207

****

C6H4O5 H2L Comenic acid CAS 499-78-5 (2544)
3-Hydroxypyran-4-one-6-carboxylic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Y+++	sp	KCl	25°C	0.10M	M I		K1=6.21		1986PEa (42322)	208

****

C6H4O6 H4L CAS 5678-48-2 (871)
Tetrahydroxy-1,4-benzoquinone;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Y+++	EMF	NaClO4	30°C	0.10M	U		K1=6.00	B2=8.30	1981HIa (42329)	209

****

C6H5NO2 HL Picolinic acid CAS 98-98-6 (391)
2-Pyridine-carboxylic acid; C5H4N.COOH

```
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Y+++       gl  NaClO4 25°C 0.50M U        K1=3.68   B2=6.90   1977GGb (42628) 210
                                          B3=9.19
--------------------------------------------------------------------------------
Y+++       gl  KNO3   25°C 0.10M U        K1=4.03   B2=7.36   1964THb (42629) 211
                                          B3=10.0
********************************************************************************
C6H5NO2                HL    Nicotinic acid   CAS 59-67-6  (419)
3-Pyridine-carboxylic acid; C5H4N.COOH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Y+++       gl  NaClO4 25°C 0.20M U        K1=2.39        1973FDa (42691) 212
********************************************************************************
C6H5NO4               H2L    4-Nitrocatechol  CAS 3316-09-4  (890)
1,2-Dihydroxy-4-nitrobenzene; O2N.C6H3(OH)2
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Y+++       gl  NaNO3  25°C  0.0  U    M   K1=9.75        1996KDb (42947) 213
                                          K(Y(egta)+L)=5.81
Extrapolated from data for I=0.05-0.15 M NaNO3.
--------------------------------------------------------------------------------
Y+++       gl  KNO3   25°C 0.10M U        K1=9.36   B2=16.16  1981BDa (42948) 214
********************************************************************************
C6H5O3Cl               HL                     CAS 7599-81-1  (2689)
5-Hydroxy-2-(chloromethyl)-4H-pyran-4-one;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Y+++       sp  KCl    25°C 0.10M M  I     K1=5.85        1986PEa (43092) 215
********************************************************************************
C6H5O3I                HL                     CAS 16065-34-2  (2690)
5-Hydroxy-2-(iodomethyl)-4H-pyran-4-one;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Y+++       sp  KCl    25°C 0.10M M  I     K1=5.97        1986PEa (43098) 216
********************************************************************************
C6H5O4Br                L                     CAS 40838-32-2  (1084)
6-Bromo-5-hydroxy-2-(hydroxymethyl)-4H-pyran-4-one;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Y+++       sp  KCl    25°C 0.10M M  I     K1=5.35        1986PEa (43118) 217
********************************************************************************
C6H5O4Cl               HL    Chlorokojic aci    (3086)
3-Chloro-5-hydroxy-2-hydroxymethyl-4-pyrone;
```

```
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Y+++       gl  oth/un 30°C 0.10M U        K1=6.00   B2=11.32  1972DSd (43139) 218
*******************************************************************************
C6H5O4I                 L                        (1085)
6-Iodo-5-hydroxy-2-hydroxymethyl-4H-pyran-4-one;
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Y+++       sp  KCl    25°C 0.10M M  I     K1=5.43        1986PEa (43160) 219
*******************************************************************************
C6H6O                  HL    Phenol           CAS 108-95-2  (457)
Hydroxybenzene, phenol; C6H5.OH
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Y+++       sp  NaClO4 25°C 0.10M U        K1=2.40        1966PMa (43550) 220
*******************************************************************************
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
-------------------------------------------------------------------------------
Y+++       gl  NaNO3  25°C  0.0  U    M   K1=9.88        1996KDb (43867) 221
                                          K(Y(egta)+L)=5.87
Extrapolated from data for I=0.05-0.15 M NaNO3.
-------------------------------------------------------------------------------
Y+++       gl  KNO3   25°C 0.05M M  I     K1=10.37  B2=19.93  1981BDc (43868) 222
Also data for I=0.2 and 0.35 M. At I=0, K1=11.08, K2=9.56.
-------------------------------------------------------------------------------
Y+++       gl  NaClO4 30°C 0.20M U    M   K1=9.81        1979MSd (43869) 223
                                          K(Y(hedta)+L)=7.35
hedta is N-(hydroxyethyl)diaminoethane-N,N',N'-triethanoic acid.
*******************************************************************************
C6H6O3                H3L    Pyrogallol       CAS 87-66-1  (696)
1,2,3-Trihydroxybenzene; C6H3(OH)3
-------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------------
Y+++       gl  NaClO4 30°C 0.20M U    M   K1=10.68       1979MSd (44001) 224
                                          K(Y(hedta)+L)=6.71
hedta is N-(hydroxyethyl)diaminoethane-N,N',N'-triethanoic acid.
-------------------------------------------------------------------------------
Y+++       gl  NaClO4 30°C 0.20M U    M   K1=10.68       1978MSk (44002) 225
                                          K(Y(nta)+L)=7.34
*******************************************************************************
C6H6O3                 HL    Maltol           CAS 118-71-8  (2442)
3-Hydroxy-2-methyl-4H-pyran-4-one;
-------------------------------------------------------------------------------
```

```
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Y+++       gl  NaClO4 30°C 0.10M U    M   K1=5.96   B2=11.10  1989NOb (44111) 226
                                          B(YLA)=13.37
                                          K(YA+L)=6.43
                                          K(YB+L)=5.62
                                          K(YC+L)=4.85
H2A=iminodiacetic acid, H2B=hydroxyethyliminodiethanoic acid, H3C=nitrilo-
triethanoic acid
-------------------------------------------------------------------------
Y+++       sp  KCl    25°C 0.10M C        K1=6.47   B2=11.85  1987PEa (44112) 227
                                          B3=16.07
                                          K(Y+HL=YL+H)=-2.03
                                          K(YL+HL=YL2+H)=-3.12
                                          K(YL2+HL=YL3+H)=-4.28
-------------------------------------------------------------------------
Y+++       sp  KCl    25°C 0.10M M  I     K1=6.50        1986PEa (44113) 228
-------------------------------------------------------------------------
Y+++       gl  NaClO4 30°C 0.10M U        K1=6.70   B2=12.09  1970DSc (44114) 229
                                          K3=3.88
*************************************************************************
C6H6O3                HL    Allomaltol       CAS 644-46-2  (2688)
5-Hydroxy-2-methyl-4H-pyran-4-one;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Y+++       sp  KCl    25°C 0.10M M  I     K1=6.32        1986PEa (44131) 230
*************************************************************************
C6H6O4                HL    Kojic acid       CAS 501-30-4  (1800)
5-Hydroxy-2-(hydroxymethyl)-4H-pyran-4-one;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Y+++       gl  NaClO4 30°C 0.10M U    M   K1=5.32   B2=10.33  1989NOb (44258) 231
                                          B(YLA)=12.51
                                          K(YA+L)=5.83
                                          K(YB+L)=5.21
                                          K(YC+L)=4.54
H2A=iminodiacetic acid, H2B=hydroxyethyliminodiethanoic acid, H3C=nitrilo-
triethanoic acid
-------------------------------------------------------------------------
Y+++       sp  KCl    25°C 0.10M M  I     K1=6.06        1986PEa (44259) 232
-------------------------------------------------------------------------
Y+++       gl  oth/un 30°C 0.10M U        K1=6.18   B2=11.37  1972DSd (44260) 233
                                          K3=4.15
-------------------------------------------------------------------------
Y+++       gl  NaClO4 25°C  2.0M U        K1=5.43   B2=10.81  1964YCa (44261) 234
*************************************************************************
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
--------------------------------------------------------------------------------
Y+++       gl  KNO3   25°C 0.10M U        K1=14.16       2005ATa (44518) 235
                                         B(Y2L3)=43.97
--------------------------------------------------------------------------------
Y+++       gl  KNO3   25°C 0.10M U TIH    K1=14.54  B2=28.34  1980BDd (44519) 236
Data for I=0.05-0.2 M and for I=0.10 M (35 C). Also DH and DS values.
--------------------------------------------------------------------------------
Y+++       gl  NaClO4 30°C 0.20M U    M   K1=14.19       1979MSd (44520) 237
                                         K(Y(hedta)+L)=9.67
hedta is N-(hydroxyethyl)diaminoethane-N,N',N'-triethanoic acid.
--------------------------------------------------------------------------------
Y+++       gl  NaClO4 25°C 0.50M C        K1=12.54  B2=21.71  1976LAf (44521) 238
                                         B(YHL2)=29.32
--------------------------------------------------------------------------------
Y+++       gl  NaClO4 25°C 0.10M U        K1=13.72       1970SSi (44522) 239
                                         K(Y+HL)=5.13
********************************************************************************
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
--------------------------------------------------------------------------------
Y+++       gl  NaNO3  25°C 0.50M C        K1=6.8    B2=10.17  1977KPa (46311) 240
                                         B(YHL)=9.3
                                         B(YH-1L)=0.95
                                         B(Y2H-3L3)=-1.9
--------------------------------------------------------------------------------
Y+++       gl  KNO3   25°C 0.10M U    M                   1975TDa (46312) 241
                                         B(Y(IDA)L)=9.6
--------------------------------------------------------------------------------
Y+++       sp  NaNO3  25°C 0.50M C    M   K1=6.79   B2=10.13  1974RKc (46313) 242
                                         B(YH2L)=10.86
                                         B(YHL)=9.04
                                         B(YH-1L)=0.97
                                         B(Y2H-3L2)=-3.69
B(YCu(H-3/2)L2)=6.40, (i.e. a binuclear complex). Glass electrode also used
--------------------------------------------------------------------------------
Y+++       oth KNO3   32°C 0.10M U                       1973TPa (46314) 243
                                         K(Y+H3L=YL+3H)=-6.86
                                         K(YL=Y(OH)L+H)=-6.30
                                         K(Y(OH)L=Y(OH)2L+H)=-8.91
                                         K(Y+HL=YL+H)=-1.08
--------------------------------------------------------------------------------
Y+++       gl  alc/w  25°C  25%  U  I     K1=8.62        1972BKd (46315) 244
Medium: EtOH/H2O, 0.05 M (NaCl,NaClO4).  0%, K1=7.87,  50%, K1=9.82
--------------------------------------------------------------------------------
Y+++       oth oth/un 25°C 0.10M U        K1=7.75   B2=10.95  1971STe (46316) 245
                                         K(YL+HL)=2.50
```

Constants obtained by survey of literature data

Y+++ sol NaClO4 25°C 0.10M U K1=7.81 1966SSg (46317) 246
Kso=-11.03

Y+++ ix oth/un 25°C 0.14M U 1947TMa (46318) 247
K(Y+H2L)=3.6

****

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

---

Y+++ ISE NaClO4 25°C 0.10M C I K1=11.30 1997LBb (47100) 248
Method: Cu ISE and competitive complexation by Cu. Data for 0.1-5.0 M.
At I=0.0 M, K1=13.18.

Y+++ gl alc/w 30°C 50% C K1=10.78 1994SOa (47101) 249
Medium: 50% v/v MeOH/H2O, 0.10 M NaClO4.

Y+++ ISE KNO3 25°C 0.10M C K1=11.45 1980NSf (47102) 250
Competitive method using Cd ion-selective electrode.

Y+++ gl KNO3 20°C 1.0M C K2=8.02 1978GHb (47103) 251

Y+++ gl diox/w 30°C 50% U 1978SGf (47104) 252
K(YL+A)=5.43
HA=tropolone

Y+++ gl NaClO4 25°C 0.50M U K1=11.09 1977GGb (47105) 253

Y+++ cal KNO3 20°C 0.10M U HM 1971GKb (47106) 254
K(YA+L)=3.73
H4A=EDTA. DH(YA+L)=-29.29 kJ mol-1, SD=-28.5 J K-1 mol-1.
DH(YLA))=-31.8 kJ mol-1, DS=310 J K-1 mol-1

Y+++ gl oth/un 20°C 0.20M U 1970VMa (47107) 255
B(YL(OH))=6.83

Y+++ gl KCl 20°C 0.10M U K1=11.41 B2=20.43 1965ANb (47108) 256

Y+++ gl KNO3 25°C 0.10M U T H T K1=11.48 B2=20.43 1962MFb (47109) 257
15 C: K1=11.46, K2=9.09; 20 C: 11.46, 9.03; 30 C: 11.54, 8.94; 35 C: 11.56,
8.84; 40 C: 11.60, 8.83. DH(K1)=11.3 kJ mol-1, DS=258; DH(K2)=-17.5, DS=113

Y+++ vlt KNO3 20°C 0.10M U 1957NOa (47110) 258
B(Y2L3)=36.8

Y+++ vlt KNO3 20°C 0.10M U K1=11.41 1956SGa (47111) 259

****

C6H10N2O5 H2L ADA CAS 26239-55-4 (2747)
N-(2-Acetamido)iminodiethanoic acid; H2N.CO.CH2.N(CH2.COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Y+++	gl	KNO3	25°C	0.10M	M	M	K1=7.05		1996AEa (47858)	260

Data for ternary complexes with dipicolinic acid

****

C6H10O2 HL CAS 3002-24-2 (2742)
2,4-Hexanedione; CH3.CO.CH2.CO.CH2.CH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Y+++	gl	mixed	30°C	67%	U		K1=7.14	B2=12.94	1964DBb (47934)	261
							K3=5.62			

Medium: 67% acetone, 0.1 M NaClO4

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Y+++	gl	mixed	30°C	75%	U		K1=7.02	B2=13.04	1970DRa (47968)	262
							K3=5.57			

Medium: 75% acetone, 0.1 M

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Y+++	gl	NaClO4	25°C	0.10M	U		K1=2.998	B2=5.43	1966PRb (47999)	263
							K3=1.84			
							K4=1.69			

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Y+++	gl	mixed	30°C	75%	U		K1=6.40	B2=11.93	1969DRa (48020)	264

Medium: 75% acetone, 0.1 M NaClO4

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Y+++	gl	NaClO4	25°C	0.10M	U	M	K1=4.60		1997PPb (48491)	265
							K(Y(edta)+L)=4.19			

****

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
Y+++	gl	alc/w	30°C	50%	C		K1=9.06		1994SOa (48812)	266
Medium: 50% v/v MeOH/H2O, 0.10 M NaClO4.										
Y+++	gl	KNO3	20°C	1.00M	U		K1=8.12	B2=15.82	1974CMd (48813)	267
							K(YL2(OH)+H)=10.15			
Y+++	oth	NaNO3	20°C	0.10M	U	M	K1=8.6	B2=16.20	1966JMc (48814)	268
Method: paper electrophoresis. Ternary complexes with HEDTA										
Y+++	gl	KCl	25°C	0.10M	U		K1=8.38	B2=15.69	1965DTa (48815)	269
Y+++	ISE	KNO3	25°C	0.10M	U		K1=9.22	B2=16.83	1963TLa (48816)	270

****

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
Y+++	gl	KNO3	25°C	0.10M	U		K1=7.78	B2=14.12	1962THb (49285)	271

****

C6H12O4 HL CAS 1112-33-0 (1246)
2,3-Dihydroxy-2,3-dimethylbutanoic acid; (CH3)2.C(OH).C(OH)(CH3).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Y+++	gl	KNO3	25°C	0.10M	U		K1=3.18	B2=5.47	1979PPa (49502)	272
							K3=1.71			

****

C6H12O7 HL Gluconic acid CAS 526-95-4 (904)
D-Gluconic acid, 2,3,4,5,6-Pentahydroxyhexanoic acid; HO.CH2(CHOH)4.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Y+++	gl	KCl	25°C	0.20M	U		K1=2.38	B2=4.52	1963KOc (49768)	273

****

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
Y+++	gl	NaNO3	25°C	0.10M	M	M	K1=6.11		1996KDd (49920)	274
							*K(YL)=-8.29			
							*K(Y(OH)L)=-8.74			
							K(Y(egta)+L)=4.22			

Data for 0.05-0.15 M NaNO3. At I=0, K1=6.29, K(Y(egta)+L)=4.40.
****
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
---
Y+++ gl NaNO3 25°C 0.10M M M K1=6.09 1996KDd (50123) 275
*K(YL)=-8.31
*K(Y(OH)L)=-8.76
K(Y(egta)+L)=4.20
Data for 0.05-0.15 M NaNO3. At I=0, K1=6.29, K(Y(egta)+L)=4.42.

Y+++ gl KCl 25°C 0.10M U T H K1=4.26 B2= 8.16 1973SCf (50124) 276
Data for 35 C. DH(K1)=33 kJ mol-1, DS(K1)=194 J K-1 mol-1;
DH(K2)=53, DS(K2)=252.
****
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
---
Y+++ gl NaNO3 25°C 0.10M M M K1=6.00 1996KDd (50198) 277
*K(YL)=-8.35
*K(Y(OH)L)=-8.79
K(Y(egta)+L)=4.16
Data for 0.05-0.15 M NaNO3. At I=0, K1=6.23, K(Y(egta)+L)=4.39.
****
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
---
Y+++ oth NaNO3 20°C 0.10M U K1=7.2 B2=12.80 1966JMc (50418) 278
Method: paper electrophoresis
****
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
---
Y+++ gl KCl 20°C 0.10M U K1=3.1 1970RPa (50840) 279
****
C6H14N4O2 HL Arginine CAS 74-79-3 (40)
2-Amino-5-guanidopentanoic acid; H2N.CH((CH2)3.NH.C(:NH)(NH2)COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl KCl 20°C 0.10M U K1=3.2 1970RPa (51019) 280
****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Y+++	gl	KCl	25°C	0.10M	C		B(YH-6L2)=-16.4	1998HGa (51455)	281

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Y+++	gl	NaCl	25°C	0.15M	C		K1=11.106 B(YH-1L)=3.935 B(YHL)=17.001 B(YH2L)=22.808	1998DMa (52370)	282
Y+++	gl	KNO3	25°C	0.10M	C		K(YL+H)=7.17 K(YHL+H)=5.9	1991SKb (52371)	283
Y+++	dis	R4N.X	20°C	0.10M	U		K1=15.06	1970TIa (52372)	284

Medium: NH4Cl, method: chromatography
****
C7H4N2O6 HL CAS 2460-59-5 (3139)
3,5-Dinitrosalicylaldehyde; HO.C6H2(NO2)2.CHO

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Y+++	sp	NaClO4	25°C	0.10M	U		K1=1.75	1966PMa (52397)	285

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Y+++	gl	NaNO3	25°C	0.10M	U	I M	K1=5.89 *K(YL)=-6.22 K(Y(egta)+L)=5.24	1996KDc (52509)	286

Data for 0.05 and 0.15 M NaNO3. At I=0, K1=6.31, *K(YL)=-7.40,
K(Y(egta)+L)=5.57.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Y+++	gl	oth/un	24°C	0.20M	U		K1=5.41	1972PSd (52510)	287

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

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

---
Y+++ gl KNO3 25°C 0.10M M M K1=5.56 1996AEa (52822) 288
Data for ternary complexes with aspartic acid, serine, asparagine and N-(2-acetamido)iminodiacetic acid
---
Y+++ cal NaClO4 25°C 0.50M C H 1963GRd (52823) 289
DH(K1)=-6.02 kJ mol-1, DS(K1)=141 J K-1 mol-1; DH(B2)=-22.22, DS(B2)=226; DH(B3)=-51.20, DS(B3)=234.

Y+++ EMF oth/un 20°C 0.50M U K1=8.46 B2=15.73 1961GRa (52824) 290
K3=5.61
****
C7H5NO4 HL CAS 5274-70-4 (3148)
3-Nitrosalicylaldehyde; HO.C6H3(NO2).CHO

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ sp NaClO4 25°C 0.10M U K1=3.27 1966PMa (52884) 291
****
C7H5NO4 HL CAS 97-51-8 (1887)
5-Nitrosalicylaldehyde; O2N.C6H3(OH).CHO

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ sp NaClO4 25°C 0.10M U K1=3.17 1966PMa (52938) 292
****
C7H5O2Cl HL (3747)
2-Hydroxy-6-chlorobenzaldehyde (6-chlorosalicylaldehyde)

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ sp NaClO4 25°C 0.10M U K1=4.87 1966PMa (53160) 293
****
C7H5O2Cl HL CAS 1927-94-2 (3143)
3-Chlorosalicylaldehyde; HO.C6H3(Cl).CHO

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ sp NaClO4 25°C 0.10M U K1=3.77 1966PMa (53191) 294
****
C7H5O2Cl HL CAS 2420-26-0 (3144)
4-Chlorosalicylaldehyde; HO.C6H3(Cl).CHO

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ sp NaClO4 25°C 0.10M U K1=4.09 1966PMa (53209) 295
****
C7H5O2Cl HL CAS 635-93-8 (3145)
5-Chlorosalicylaldehyde; HO.C6H3(Cl).CHO

```
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Y+++       sp  NaClO4 25°C 0.10M U        K1=3.94        1966PMa (53225) 296
*************************************************************************
C7H6OS                 HL    Thiotropolone    CAS 1073-38-7  (8477)
2-Mercapto-2,4,6-cycloheptatrien-1-one;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Y+++       gl  diox/w 30°C  50%  M  I     K1=5.08   B2= 9.70  1978SSi (53549) 297
                                         K3=3.37
Medium: 50% v/v dioxane/H2O, 0.10 M NaClO4. Data for 0.005 and 0.2 M
NaClO4.
*************************************************************************
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
-------------------------------------------------------------------------
Y+++       sp  NaClO4 25°C 0.10M U        K1=4.34        1966PMa (53634) 298
*************************************************************************
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
-------------------------------------------------------------------------
Y+++       dis non-aq 25°C 100%  C                         2001NCa (53699) 299
                                       K(YL3+TOPO)=4.99
                                       K(YL3+2TOPO)=7.39
TOPO is trioctylphosphane oxide. Medium: toluene.
-------------------------------------------------------------------------
Y+++       sp  NaClO4 25°C 0.10M U        K1=7.46        1970HOa (53700) 300
-------------------------------------------------------------------------
Y+++       gl  KNO3   25°C 0.10M U        K1=7.18   B2=13.26  1969CMb (53701) 301
                                         K3=5.01
                                         K4=3.42
*************************************************************************
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
-------------------------------------------------------------------------
Y+++       gl  NaNO3  25°C 0.10M U  I M   K1=8.68        1996KDc (54340) 302
                                         *K(YL)=-7.72
                                         K(Y(egta)+L)=6.91
Data for 0.05 and 0.15 M NaNO3. At I=0, K1=9.03, *K(YL)=-8.81,
K(Y(egta)+L)=6.21.
-------------------------------------------------------------------------
Y+++       gl  alc/w  24°C  20%  C    M                  1996MIa (54341) 303
                                         K(Y(ada)+L)=3.22
```

Medium: 20% w/w EtOH/H2O, 0.10 M KNO3.
ada: N-(acetamido)-iminodiethanoic acid.

Y+++ ix mixed 20°C 50% U 1976TRa (54342) 304
K(Y+HL)=2.56
K(Y+2HL)=4.60
K(Y+3HL)=6.20

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

****

C7H6O5 H4L Gallic acid CAS 149-91-7 (446)
3,4,5-Trihydroxybenzoic acid; C6H2(OH)3.COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Y+++	gl	NaClO4	30°C	0.20M	U	M	K1=12.59	1979MSd (54774)	305
							K(Y(hedta)+L)=7.25		

hedta is N-(hydroxyethyl)diaminoethane-N,N',N'-triethanoic acid.

Y+++	gl	NaClO4	30°C	0.20M	U	M	K1=12.59	1978MSk (54775)	306
							K(Y(nta)+L)=7.68		

****

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
Y+++	gl	KNO3	20°C	0.10M	U	T	K1=7.92	1982DBa (55080)	307
Y+++	gl	KNO3	25°C	0.20M	U	T	K1=6.61	1975PMc (55081)	308

35 C: K=6.61; 45 C: K=6.78

****

C7H6O9S2 H3L CAS 56507-30-3 (2659)
3,5-Disulfosalicylic acid; (HO3S)2.C6H2(OH).COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Y+++	gl	NaClO4	25°C	0.50M	C	T	K1=8.64 B2=14.38	1976LAf (55105)	309
							B(YHL)=12.7		

****

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Y+++	gl	diox/w	30°C	70%	U		K1=7.49 B2=13.10	1981MBb (55157)	310

****

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

---
Y+++ gl alc/w 24°C 20% C M K1=2.505 1996MIa (55271) 311
K(Y(ada)+L)=3.24
Medium: 20% w/w EtOH/H2O, 0.10 M KNO3.
ada: N-(acetamido)-iminodiethanoic acid.

Y+++ gl NaNO3 25°C 0.10M M I M K1=4.22 1995KDc (55272) 312
K(Y(egta)+L)=3.85
Data for 0.05 and 0.15 M NaNO3. At I=0, K1=4.59, K(Y(egta)+L)=4.34.
****
C7H7NO3 H2L CAS 89-73-6 (204)
2-Hydroxybenzohydroxamic acid (salicylhydroxamic acid); HO.C6H4.CO.NHOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl KNO3 25°C 0.1M M K1=11.07 B2=21.27 1989LWa (55618) 313
K=9.45

Y+++ gl mixed 25°C 75% U 1970SEa (55619) 314
K(Y+HL)=7.24
K(YHL+HL)=6.50
Medium: 75% acetone, 0.1 M NaClO4
****
C7H7NO5S H2L CAS 3577-63-7 (3181)
5-Sulfoanthranilic acid; (5-sulfo-2-aminobenzoic acid)

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl NaNO3 25°C 0.10M M I M K1=4.14 1995KDc (55681) 315
K(Y(egta)+L)=3.59
Data for 0.05 and 0.15 M NaNO3. At I=0, K1=4.46, K(Y(egta)+L)=3.86.
****
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
---
Y+++ gl NaNO3 25°C 0.0 U M K1=9.95 1996KDb (56084) 316
K(Y(egta)+L)=6.05
Extrapolated from data for I=0.05-0.15 M NaNO3.
****
C7H8O4 HL Methyl kojic CAS 1506-07-8 (2686)
3-Hydroxy-6-(hydroxymethyl)-2-methyl-4H-pyran-4-one;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ sp KCl 25°C 0.10M M I K1=6.48 1986PEa (56136) 317
****
C7H8O5 HL CAS 2029-29-4 (2687)
3-Hydroxy-2,6-bis(hydroxymethyl)-4H-pyran-4-one;

```
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Y+++       sp  KCl    25°C 0.10M M  I     K1=6.08        1986PEa (56155) 318
********************************************************************************
C7H11NO4              H2L                      CAS 499-82-1  (3163)
Piperidine-2,6-dicarboxylic acid; C5H9N(COOH)2
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Y+++       gl  KNO3   25°C 0.10M U        K1=6.00   B2=11.40  1963THb (56815) 319
********************************************************************************
C7H11NO6              H3L                       (2926)
2-Aminobutanoic-N-propane-1,3-dioic acid; HOOC.CH(C2H5)NH.CH(COOH)2
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Y+++       gl  KNO3   25°C  0.1M U        K1=8.50        1982KKc (56854) 320
********************************************************************************
C7H12N2O3              HL    Gly-Pro          CAS 704-15-4  (257)
Glycyl-proline; H2N.CH2.CO.NC4H7.COOH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Y+++       gl  KNO3   25°C 0.15M M T H    K1=3.80        1979SKd (57130) 321
Data for 35 and 45 C. At 35 C, K1=3.90, DH(K1)=21.9 kJ mol-1,
DS(K1)=145 J K-1 mol-1.
********************************************************************************
C7H12O3                HL                       (4422)
3-Methyl ethylacetoacetate; CH3.CO.CH(CH3).CO.OCH2.CH3
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Y+++       gl  mixed  30°C  75%  U        K1=8.20        1971DRb (57279) 322
Medium: 75% acetone, 0.1 M
********************************************************************************
C7H12O4               H2L                      CAS 510-20-3  (482)
Diethylpropanedioic acid (Diethylmalonic acid); HOOC.C(C2H5)2.COOH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Y+++       gl  KNO3   25°C 0.10M U        K1=4.60   B2=7.05   1968PFa (57375) 323
********************************************************************************
C7H12O6                HL    Quinic acid      CAS 77-95-2  (2578)
1,3,4,5-Tetrahydroxycyclohexane-1-carboxylic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Y+++       gl  NaCl   20°C 0.10M U        K1=2.89        1977SSc (57415) 324
********************************************************************************
```

C7H13NO5 H2L (8081)
4-Hydroxy-2-aminopentane-1,5-dioic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl KCl 20°C 0.1M U K1=7.02 1978KPe (57558) 325
Data for threo isomer. For erythro isomer: K1=6.32
****
C7H14O3 HL CAS 65311-45-1 (6266)
3-Hydroxy-3,4-dimethyl-pentanoic acid; CH3.CH2.C(OH)(CH3).CH(CH3).COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl NaClO4 25°C 0.10M C K1=2.78 B2=4.52 1976SPa (57882) 326
****
C8H5N5O6 H3L Murexide (453)
Purpuric acid (Murexide is ammonium salt);

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ sp KNO3 12°C 0.10M U 1965GEa (58543) 327
K(Y+H2L)=3.36
****
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
---
Y+++ gl alc/w 24°C 20% C M K1=3.81 1996MIa (59037) 328
K(Y(ada)+L)=4.99
Medium: 20% w/w EtOH/H2O, 0.10 M KNO3.
ada: N-(acetamido)-iminodiethanoic acid.

Y+++ gl NaNO3 25°C 0.10M M I M K1=4.85 1995KDb (59038) 329
K(Y(egta)+L)=4.33
Data for 0.05 and 0.15 M NaNO3. At I=0, K1=5.14, K(Y(egta)+L)=4.69.

Y+++ gl NaClO4 30°C 0.10M U K1=4.04 B2=7.12 1966KPb (59039) 330
****
C8H6O4 H2L Isophthalic aci CAS 212-91-5 (1619)
Benzene-1,3-dicarboxylic acid; C6H4(COOH)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ cal NaClO4 25°C 0.10M U H K1=2.51 1982CBc (59063) 331
DH= 15.04 kJ mol-1, DS= 99 J K-1 mol-1
****
C8H7NO2 HL CAS 532-54-7 (4363)
Isonitrosoacetophenone, Phenylglyoxal 2-oxime;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Y+++	gl	diox/w	20°C	50%	U		K1=6.32	B2=11.94	1971MAf (59110)	332

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

****

C8H7NO3 HL (7376)

benzoylhydroxamic acid; C6H5COCONHOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Y+++	gl	KNO3	25°C	0.1M	M		K1=9.66	B2=18.56	1989LWa (59131)	333
							K3=7.62			

****

C8H7O2Cl HL CAS 1450-74-4 (6325)

2-Hydroxy-5-chloro-acetophenone; Cl(HO)C6H3.CO.CH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Y+++	gl	alc/w	25°C	20%	M	I	K1=6.29		1994KDa (59224)	334

Medium: 20% v/v EtOH/H2O, 0.10 M NaNO3. Also data for 0.05 and 0.15 M NaNO3. At I=0 (20% v/v), K1=6.58, *K(YL)=-8.76, *K(Y(OH)L)=-8.90.

****

C8H8N2O L CAS 4856-97-7 (3820)

2-(Hydroxymethyl)benzimidazole;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Y+++	gl	diox/w	30°C	50%	U	T H	B2=16.47		1988NOa (59314)	335

40 C: B2=16.38; 50 C: B2=16.30. DH=-16.3 kJ mol-1, DS=262 J K-1 mol-1

****

C8H8N2O2 HL Phenylglyoxime (3222)

Phenylglyoxime; C6H5.C(:N.OH).CH:N.OH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Y+++	gl	diox/w	20°C	50%	U		K1=6.82	B2=12.79	1971MAf (59345)	336

Medium: 50% dioxan, 0.1 M NaClO4

****

C8H8O2 HL 2-Acetylphenol CAS 118-93-4 (1888)

2-Hydroxyacetophenone; HO.C6H4.CO.CH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Y+++	gl	alc/w	25°C	20%	M	I	K1=6.63		1994KDa (59472)	337

Medium: 20% v/v EtOH/H2O, 0.10 M NaNO3. Also data for 0.05 and 0.15 M NaNO3. At I=0 (20% v/v), K1=6.93, *K(YL)=-8.68, *K(Y(OH)L)=-9.23.

****

C8H8O2 HL CAS 583-80-2 (3191)

beta-Methyltropolone;

```
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Y+++       sp  alc/w    ?    3%  U        K1=7.38        1967GDb (59606) 338
Medium: 3% EtOH, 0.2 M NaClO4
*************************************************************************
C8H8O3               H2L                      CAS 490-78-8  (6324)
2,5-Dihydroxyacetophenone; (HO)2C6H3.CO.CH3
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Y+++       gl  alc/w  25°C  20%  M  I                     1994KDa (59685) 339
                                        K(Y+HL)=6.44
Medium: 20% v/v EtOH/H2O, 0.10 M NaNO3. Also data for 0.05 and 0.15 M
NaNO3. At I=0 (20% v/v), K1=6.70, *K(YHL)=-8.59, *K(Y(OH)HL)=-9.02.
*************************************************************************
C8H8O3                 HL    o-Anisic acid    CAS 579-75-9  (2337)
2-Methoxybenzoic acid; CH3O.C6H4.COOH
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Y+++       gl  NaClO4 25°C 0.10M M   H    K1=1.66        1988CLb (59757) 340
DH=9.32 kJ mol-1, DS=63 J K-1 mol-1
*************************************************************************
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
-------------------------------------------------------------------------
Y+++       gl  NaClO4 25°C 0.10M M   H    K1=1.87        1988CLb (59923) 341
DH=11.6 kJ mol-1, DS=75 J K-1 mol-1
*************************************************************************
C8H8O3                 HL                       CAS 148-52-8  (3193)
3-Methoxysalicylaldehyde; CH3O.C6H3(OH).CHO
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Y+++       gl  NaNO3  25°C 0.10M M  I M   K1=4.853       1995KDd (59933) 342
                                        K(Y(egta)+L)=3.645
Data for 0.15 and 0.05 M NaNO3. At I=0, K1=5.076, K(Y(egta)+L)=3.938.
*************************************************************************
C8H8O3                 HL    p-Anisic acid    CAS 100-09-4  (1373)
4-Methoxybenzoic acid; CH3O.C6H4.COOH
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Y+++       gl  NaClO4 25°C 0.10M M   H    K1=2.01        1988CLb (59966) 343
DH=14.2 kJ mol-1, DS=86 J K-1 mol-1
*************************************************************************
C8H8O4                 HL                       CAS 520-45-6  (4478)
3-Acetyl-2-hydroxy-6-methylpyran-4-one, Dehydroethanoic acid;
```

```
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Y+++       gl  diox/w 35°C  50%  U        K1=4.80   B2=8.78   1971MAa (60101) 344
Medium: 50% dioxan, 0.1 M NaClO4
******************************************************************************
C8H9NO2                HL                      CAS 4389-45-1  (3226)
3-Methyl-2-aminobenzoic acid; CH3.C6H3(NH2).COOH
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Y+++       gl  NaNO3  25°C 0.10M M  I M   K1=5.56        1995KDc (60237) 345
                                         K(Y(egta)+L)=5.18
Data for 0.05 and 0.15 M NaNO3. At I=0, K1=5.78, K(Y(egta)+L)=5.30.
******************************************************************************
C8H9NO4               H2L                       (4520)
Dehydroethanoic acid oxime;
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Y+++       gl  diox/w 35°C  50%  U                        1971MAa (60507) 346
                                         K(Y+HL)=4.16
                                         K(Y+2HL)=7.38
Medium: 50% dioxan, 0.1 M NaClO4
******************************************************************************
C8H10O4                 L                      CAS 34241-51-5  (5701)
3-Acetyl-6-methylhydropyrane-2,4-dione;
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Y+++       gl  alc/w  22°C  20%  U        K1=4.57   B2=8.24   1988ZTa (60857) 347
                                         K3=3.12
******************************************************************************
C8H10O5               H2L                      CAS 145-73-7  (138)
7-Oxa-bicyclo[2.2.1]-heptan-2,3-dicarboxylic acid;
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Y+++       gl  KCl    30°C 0.10M C        K1=5.77   B2=9.85   1996SZa (60878) 348
For the -5-en-2-exo isomer, K1=6.03, B2=10.84.
******************************************************************************
C8H12N2O8             H4L                      CAS 35039-85-1  (4537)
1,2-Diaminoethane-N,N'-dimalonic acid; (HOOC)2.CH.NH.CH2.CH2.NH.CH(COOH)2
------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
------------------------------------------------------------------------------
Y+++       vlt KNO3   25°C 0.10M U        K1=10.47       1972GBd (61532) 349
******************************************************************************
C8H12O2                HL                      CAS 874-23-7  (3203)
2-Acetylcyclohexanone;
```

```
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Y+++       gl  mixed  25°C  75%  U        K1=8.46   B2=16.05  1971DRa (61678) 350
Medium: 75% acetone, 0.1 M NaClO4
********************************************************************************
C8H12O2                HL    Dimedone         CAS 126-81-8  (1137)
5,5-Dimethyl-1,3-cyclohexanedione;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Y+++       gl  oth/un 30°C 0.10M U        K1=2.78   B2=5.37   1975DSa (61692) 351
********************************************************************************
C8H12O4              H2L                      CAS 1076-97-9  (2224)
Cyclohexane-1,4-dicarboxylic acid; C6H10.(COOH)2
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Y+++       gl  NaClO4 25°C 0.10M M   H    K1=4.24        1986CDb (61718) 352
DH(K1)=17.2 kJ mol-1, DS=141 J K-1 mol-1
********************************************************************************
C8H13NO6S            H3L                        (5675)
2-Mercapto-1-aminoethane-N,N,S-triethanoic acid; HOOC.CH2.S.CH2.CH2.N(CH2COOH)2
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Y+++       gl  NaClO4 25°C 0.10M U        K1=8.36        1975POa (61834) 353
                                         K(Y+HL)=2.63
********************************************************************************
C8H14O3                HL                       CAS 607-97-6  (4489)
3-Ethylethylacetoacetate; CH3.CO.CH(C2H5).CO.OC2H5
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Y+++       gl  mixed  30°C  75%  U        K1=9.03        1971DRb (62083) 354
Medium: 75% acetone, 0.1 M
********************************************************************************
C8H18N2O10P2         H6L    EDDADPO          CAS 2310-83-0  (2436)
1,2-Diaminoethane-N,N'-diethanoic-N,N'-dimethylphosphonic acid;
(-CH2.N(CH2.COOH)(CH2.PO3H2))2
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Y+++       gl  KCl    25°C 0.10M U                        1965DKb (62908) 355
                                         K(Y+HL)=17.7
                                         K(Y+H2L)=9.2
--------------------------------------------------------------------------------
Y+++       ix  oth/un 25°C 0.10M U        K1=24.04       1965TIc (62909) 356
********************************************************************************
C8H18N2O10P2         H6L                      CAS 2310-83-0  (5667)
```

1,2-Diaminoethane-N,N-diethanoic-N',N'-dimethylphosphonic acid;
(HOOC.CH2)2NCH2CH2N(CH2.PO3H2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Y+++	ix	R4N.X	20°C	0.10M	U		K1=18.82		1970TIc (62922)	357
							K(Y+HL)=13.80			
							K(Y+H2L)=11.92			

****

C8H19NO5 L Bis-tris CAS 6976-37-0 (2827)
Bis-(2-hydroxyethyl)imino-tris(hydroxymethyl)methane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Y+++	gl	NaCl	30°C	0.10M	C		K1=5.76	B2= 9.01	2002NWa (63070)	358
							B(Y2L)=6.01			

Constants expressed on the molality scale.

****

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
Y+++	dis	oth/un	20°C	?	U		K1=1.91		1961SSa (63196)	359

****

C8H22N2O6P2 H4L CAS 13516-59-1 (3850)
2,2'-(Ethylenedi-imino)bis(propylphosphonic acid);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Y+++	gl	KCl	25°C	0.10M	U		K1=12.87		1965DKb (63346)	360
							K(Y+HL)=6.48			

****

C8H24N2O12P4S H8L CAS 33424-58-7 (2648)
1,7-Diaza-4-thiaheptane-1,1,7,7-tetra(methylphosphonic acid);
S(CH2.CH2.N(CH2.PO3H2)2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Y+++	ix	KCl	20°C	0.10M	U		K1=13.01		1971TIa (63488)	361
							K(Y+HL)=10.14			

****

C8H24N2O13P4 H8L CAS 25007-19-4 (2647)
1,7-Diaza-4-oxaheptane-1,1,7,7-tetra(methylphosphonic acid);
O(CH2.CH2.N(CH2.PO3H2)2)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Y+++	dis	oth/un	20°C	0.10M	U		K1=15.30		1969TIa (63496)	362

Method: chromatography

****
C9H5NO4 HL CAS 22308-86-7 (4607)
3-Nitroso-4-hydroxycoumarin (oximidobenzotetronic acid);

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ sp diox/w 20°C 50% U K1=2.76 B2=4.65 1977MBb (63617) 363
****
C9H6NO4BrS H2L CAS 3062-37-1 (3889)
7-Bromo-8-hydroxyquinoline-5-sulfonic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl NaClO4 25°C 0.10M U K1=5.50 B2=10.36 1973MAa (63707) 364
K3=4.2
****
C9H6NO4IS H2L Ferron CAS 547-91-1 (275)
7-Iodo-8-hydroxyquinoline-5-sulfonic acid; (HO)(HO3S)C9H4NI

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl oth/un 20°C 0.10M U K1=6.23 1977SKd (63836) 365

Y+++ gl KNO3 25°C 0.20M U T K1=5.23 1975PMc (63837) 366
35 C: K=5.16; 45 C: K=4.92
****
C9H6N2O5S H2L CAS 5263-74-1 (2738)
7-Nitroso-8-hydroxyquinoline-5-sulfonic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl alc/w 27°C 50% C H K1=5.99 B2=11.0 1986EAa (63878) 367
****
C9H6O6 H3L Hemimellitic ac CAS 569-51-7 (1621)
1,2,3-Benzenetricarboxylic acid; C6H3.(COOH)3

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl NaClO4 25°C 0.10M U H K1=4.76 1994CRa (63979) 368
K(Y+HL)=2.81
DH(K1)=18.5 kJ mol-1; DS=153 J K-1 mol-1
****
C9H7NO HL Oxine CAS 148-24-3 (504)
8-Hydroxyquinoline (8-quinolinol);

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ sol none RT 0.0 U 1981FCa (64375) 369
Kso(YL3)=-32.64
Method: spectrophotometry.

Y+++ gl diox/w 30°C 50% U K1=9.09 B2=17.24 1970GMb (64376) 370
Medium: 50% dioxan, 0.3 M NaClO4
****
C9H7NO2 HL CAS 1127-45-3 (4614)
8-Hydroxyquinoline-N-oxide;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl diox/w 30°C 50% U K1=7.21 1970GMb (64414) 371
Medium: 50% dioxan, 0.3 M NaClO4
****
C9H7NO4S H2L Sulfoxine CAS 84-88-8 (448)
8-Hydroxyquinoline-5-sulfonic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl KNO3 30°C 0.20M U T K1=5.77 1975PMc (64590) 372
40 C: K=5.71; 50 C: K=5.62

Y+++ cal KNO3 20°C 0.10M U HM 1971GKb (64591) 373
K(YA+L)=4.31
DH(YA+L)=-21.11 kJ mol-1, DS=10.45 J K-1 mol-1
DH(YAL): DH=-23.57, DS=347.8. H4A=EDTA
****
C9H8O4 H2L CAS 97652-17-0 (3855)
3-Carboxy-4-methyltropolone;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ sp NaClO4 ? 0.20M U K1=8.47 1967GDc (64958) 374
K(YHL)=10.61

Y+++ gl NaClO4 25°C 0.20M U K1=8.26 B2=14.88 1966GDa (64959) 375
K3=3.96
****
C9H8O4 H2L CAS 15872-28-3 (8407)
Bicyclo[2.2.1]hepta-2,5-diene-2,3-dicarboxylic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl KCl 30°C 0.10M U K1=4.16 1996SZa (64984) 376
****
C9H10O4 H2L (7232)
Bicyclo[2.2.1]hept-5-en-2-endo,3-cis-dicarboxylic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl KCl 30°C 0.10M C K1=4.03 B2=6.91 1996SZa (65580) 377
for the -2,5-dien-2-exo isomer, K1=4.16.

****
C9H10O5 H2L CAS 54384-22-4 (8406)
1-Methyl-(exo,exo)-7-oxabicyclo[2.2.1]hept-5-ene-2,3-dicarboxylic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl KCl 30°C 0.10M U K1=5.13 B2= 8.00 1996SZa (65612) 378
****
C9H10O5 H2L (7233)
1-Methyl-7-oxa-bicyclo[2.2.1]hept-5-en-2-exo,3-cis-dicarboxylic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl KCl 30°C 0.10M C K1=5.13 B2=8.00 1996SZa (65627) 379
****
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
---
Y+++ gl NaCl 25°C 0.15M U H K1=3.49 1992ZNa (65988) 380
By calorimetry: DH(K1)=6.38 kJ mol-1, DS(K1)=88.22 J K-1 mol-1.

Y+++ gl KNO3 35°C 0.10M U K1=5.27 1990RSe (65989) 381
****
C9H11NO3 H2L Tyrosine CAS 60-18-4 (4)
2-Amino-3-(4-hydroxyphenyl)propanoic acid; HO.C6H4.CH2.CH(NH2).COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl KNO3 25°C 0.10M U 1977SAb (66244) 382
K(Y+HL)=4.43
K(Y+2HL)=8.48
At 35 C, I=0: K(Y+HL)=5.09, K(Y+2HL)=9.69
****
C9H11N3O2S HL CAS 51146-75-9 (6170)
N-(2-Hydroxy-3-methoxybenzylidene)thiosemicarbazide; CH3O(OH)C6H3.CH:N.CS.NH.NH2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl diox/w 30°C 75% U K1=6.96 1988MKd (66512) 383
****
C9H11N3O3 HL CAS 58336-41-7 (6169)
N-(2-Hydroxy-3-methoxybenzylidene)semicarbazide; CH3O(OH)C6H3.CH:N.CO.NH.NH2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl diox/w 30°C 75% U K1=10.50 1988MKd (66519) 384
****
C9H12N2O6 HL Uridine CAS 58-96-8 (828)

Uracil-1-beta-D-ribofuranoside;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Y+++	gl	KNO3	35°C	0.10M	U	M	K1=5.20	1990RSc (66717)	385
							K(YA+L)=4.89		
							K(YB+L)=4.72		
							K(YC+L)=4.47		

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Y+++	gl	KNO3	35°C	0.10M	U	M	K1=4.49	1990RSc (66718)	386
							K(YL+Ala)=9.59		
							K(YL+Phe)=9.41		
							K(YL+Trp)=9.60		

****

C9H12N2O10 H5L CAS 80921-06-8 (2924)

2,3-Diaminopropanoic-N,N'-di-1,3-propanedioic acid;
(HOOC)2CH.NH.CH(COOH).CH2.NH.CH(COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Y+++	ISE	KNO3	25°C	0.10M	U		K1=11.34	1983KBd (66749)	387

Hg-electrode.

****

C9H13NO6 H3L (3881)

2,6-Dicarboxypiperidyl-N-ethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Y+++	gl	KNO3	25°C	0.10M	U		K1=10.83 B2=18.58	1968TKe (66897)	388

****

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
Y+++	gl	KNO3	35°C	0.10M	U	M	K1=3.30	1990RSc (67087)	389
							K(Y+HA+L)=8.32		
							B(YBL)=15.69		
							B(YCL)=20.50		

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Y+++	gl	KNO3	35°C	0.10M	U	M	K1=2.70	1990RSe (67088)	390
							K(YL+Ala)=5.20		
							K(YL+Phe)=5.35		
							K(YL+Trp)=5.29		

****

C9H16N2O6 H3L MEDTA CAS 40423-02-7 (5717)

N-Methyldiaminoethane-N,N',N'-triethanoic acid; HOOC.CH2.N(CH3)CH2.CH2.N(CH2.COOH)2

```
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Y+++       cal NaClO4 25°C 0.50M M  IH    K1=12.89       1986RCa (67647) 391
DH=-10.1 kJ mol-1, DS=213 J K-1 mol-1
*************************************************************************
C9H16O4               H2L                    CAS 1636-27-7  (485)
Dipropylpropanedioic acid (Di-n-propylmalonic acid);
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Y+++       gl  KNO3   25°C 0.10M U        K1=4.74   B2=7.36   1968PFa (67781) 392
*************************************************************************
C9H28N3O15P5          10L    DTPPH           CAS 15827-60-8  (2921)
Diethylenetriamine-N,N,N',N",N"-penta(methylphosphonic acid);
H2O3PCH2.N(CH2CH2.N(CH2PO3H2)2)2  H
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Y+++       dis KCl    20°C 0.10M U                        1968TIa (68417) 393
                                        K(Y+H4L)=9.48
*************************************************************************
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
-------------------------------------------------------------------------
Y+++       sp  alc/w  25°C  50%  U                        1993ISb (68489) 394
                                        K(Y+HL)=6.904
                                        K(Y+HL+L)=16.3
                                        B(Y(OH)2L)=24.72
Medium: 50% v/v EtOH/H2O; 0.1 M NaClO4
-------------------------------------------------------------------------
Y+++       sp  alc/w  25°C  50%  M                        1993ISc (68490) 395
                                        K(Y+HL)=6.904
                                        B(YL(OH)2)=24.72
                                        K(Y+H2L=YHL+H)=-1.47
                                        K(Y+L+HL)=16.3
Medium: 50%. v/v ethanol/H2O, 0.1 M NaClO4. K(YHL+H2L=YHL2+2H)=-10.2,
K(YHL=YL(OH)2+3H)=-21.4, K(YHL2=YL(OH)2+H2L+H)=-11.22.
*************************************************************************
C10H6O8               H4L    Pyromellitic Ac  CAS 89-05-4  (519)
Benzene-1,2,4,5-tetracarboxylic acid; C6H2.(COOH)4
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Y+++       gl  NaClO4 25°C 0.10M U   H    K1=4.57        1994CRa (68532) 396
                                        K(Y+HL)=3.62
DH(K1)=20.2 kJ mol-1, DS=155 J K-1 mol-1; DH(Y+HL)=15.3, DS=121
*************************************************************************
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
Y+++	sp	KCl	25°C	0.10M	M	I	K1=4.09		1976PEa (68598)	397
Y+++	gl	diox/w	30°C	75%	U		K1=9.02 B3=25.04	B2=17.74	1957CFa (68599)	398

C10H7NO2 HL CAS 132-53-6 (2524)
2-Nitroso-1-naphthol;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Y+++	gl	diox/w	30°C	75%	U		K1=8.3 B3=23.3	B2=15.9	1957CFa (68666)	399

C10H7NO2 HL Quinaldic acid CAS 93-10-7 (2209)
Quinoline-2-carboxylic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Y+++	gl	NaClO4	30°C	0.10M	U		K1=2.58	B2=5.04	1969DNc (68724)	400

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Y+++	gl	NaClO4	30°C	0.10M	U		K1=2.60		1969DNc (68773)	401

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Y+++	gl	KCl	25°C	0.10M	M		K1=4.28		1979LSb (68821)	402

C10H7NO5S H2L (4766)
1-Nitroso-2-hydroxynaphthalene-6-sulfonic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Y+++	sp	KCl	25°C	0.10M	C		K1=4.24		1973PMb (68857)	403

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

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

```
Y+++       gl  KCl    25°C 0.10M U  I     K1=2.87        1967MAi (68898) 404
K1=3.97(I=0)
**************************************************************************
C10H7NO5S             H2L                     CAS 31005-79-9  (1814)
2-Nitroso-1-hydroxynaphthalene-8-sulfonic acid;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Y+++       sp  KCl    25°C 0.10M U        K1=4.82        1978PPb (68955) 405
**************************************************************************
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
--------------------------------------------------------------------------
Y+++       gl  KNO3   25°C 0.20M U T      K1=3.44        1975PMc (69038) 406
35 C: K=3.43; 45 C: K=3.37
--------------------------------------------------------------------------
Y+++       gl  KCl    25°C 0.10M U  I     K1=4.48   B2=7.83   1967MAi (69039) 407
                                        B3=11.29
K1=6.24(I=0)
**************************************************************************
C10H8O2               H2L                     CAS 92-44-4  (1658)
2,3-Dihydroxynaphthalene;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Y+++       gl  NaClO4 20°C 0.10M U    M                   1973PAc (69785) 408
                                        K(YA+L)=7.70, H4A=EDTA
**************************************************************************
C10H8O5S              H3L    DHNSA              (877)
2,3-Dihydroxynaphthalene-6-sulfonic acid;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Y+++       gl  NaClO4 30°C 0.20M U    M   K1=10.09       1979MSd (69869) 409
                                        K(Y(hedta)+L)=8.06
hedta is N-(hydroxyethyl)diaminoethane-N,N',N'-triethanoic acid.
--------------------------------------------------------------------------
Y+++       gl  NaClO4 30°C 0.20M U    M   K1=10.06       1978MSl (69870) 410
                                        K(Y(edta)+L)=6.81
--------------------------------------------------------------------------
Y+++       gl  NaClO4 25°C 0.50M C        K1=10.14  B2=18.22  1976LAf (69871) 411
                                        B3=24.0
                                        B(YHL2)=24.8
--------------------------------------------------------------------------
Y+++       gl  KNO3   30°C 0.20M U T      K1=8.64        1975PMc (69872) 412
40 C: K=8.21; 50 C: K=7.89
**************************************************************************
C10H10OS               HL                      CAS 13522-48-0  (4722)
```

3-Mercapto-1-phenylbut-2-en-1-one; C6H5.CO.CH:CH.C(SH).CH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Y+++	gl	mixed	30°C	75%	U		K1=3.85 K3=3.18	B2=7.27 1969DNb (70641)	413

Medium: 75% acetone, 0.1 M NaClO4

****

C10H10O2 HL Benzoylacetone CAS 93-91-4 (197)

1-Phenylbutane-1,3-dione; C6H5.CO.CH2.CO.CH3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Y+++	gl	alc/w	25°C	80%	U		K1=8.29 K3=4.42	B2=14.64 1967DZa (70784)	414

Medium: 80% MeOH, 0.1 M NaCl

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Y+++	gl	alc/w	24°C	80%	U		K1=8.29 K3 = 4.42	B2=14.64 1967DZb (70785)	415

Medium: 80% v/v MeOH/H2O, 0.1 M NaCl

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Y+++	gl	mixed	30°C	67%	U		K1=8.21 K3=5.68	B2=14.89 1964DBb (70786)	416

Medium: 67% acetone, 0.1 M NaClO4

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Y+++	dis	oth/un	?	0.10M	U		K1=6.55 B3=14.4	B2=11.4 1960STb (70787)	417
Y+++	gl	none	?	0.0	U		K1=8.24 K3=5.59	B2=14.98 1958DBa (70788)	418

****

C10H10O6 H2L CAS 5411-14-3 (2394)

1,2-Phenylenedioxodiethanoic acid; C6H4(O.CH2.COOH)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Y+++	gl	NaClO4	25°C	0.10M	M		K1=3.78	1977HCb (70864)	419

****

C10H11NO3 HL (1960)

N-Hydroxyacetoacetanilide; CH3.CO.CH2.CO.N(OH).C6H5

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Y+++	gl	diox/w	20°C	82%	U		K1=7.44 K3=6.22	B2=13.73 1979KSb (70946)	420

****

C10H12N2O4 H2L CAS 16598-05-3 (967)

2-Pyridylmethyliminodiethanoic acid; C5H4N.CH2.N(CH2.COOH)2

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

```
--------------------------------------------------------------------------------
Y+++       gl  KNO3   25°C 0.10M U        K1=8.63   B2=16.01  1964THa (71283) 421
********************************************************************************
C10H12O2               HL                     CAS 1946-74-3  (202)
3-Isopropyltropolone;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Y+++       gl  diox/w 30°C  50%  U    M   K1=7.85   B2=15.28  1980SGa (71612) 422
                                         K3=5.95
                                         K(Y(NTA)+L)=6.41
--------------------------------------------------------------------------------
Y+++       gl  alc/w  25°C  80%  U        K1=9.0    B2=16.50  1968DZb (71613) 423
                                         K3=6.2
                                         K4=4.8
Medium: 80% MeOH, 0.1 M NaCl
--------------------------------------------------------------------------------
Y+++       sp  alc/w    ?    3%  U        K1=7.28        1967GDb (71614) 424
Medium: 3% EtOH, 0.2 M NaClO4
********************************************************************************
C10H14N5O7P            H2L    AMP-5            CAS 18422-05-4  (842)
Adenosine-5'-monophosphoric acid, 5-Adenylic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Y+++       gl  R4N.X  25°C 0.10M C      T K1=4.48        1991SMa (72501) 425
                                         K(Y+HL)=2.76
IUPAC evaluation
--------------------------------------------------------------------------------
Y+++       ix  NaCl   25°C 0.15M U        K1=5.7         1960OLa (72502) 426
********************************************************************************
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
--------------------------------------------------------------------------------
Y+++       sp  R4N.X  25°C 0.10M C        K1=18.5        1994KCa (74310) 427
Medium: Me4NCl
--------------------------------------------------------------------------------
Y+++       cal NaClO4 25°C 0.10M C   H                   1987YJa (74311) 428
DH(K1)=-1.68 kJ mol-1, DS(K1)=327 J K-1 mol-1.
--------------------------------------------------------------------------------
Y+++       gl  NaClO4 20°C 0.02M U    M                  1982MPd (74312) 429
                                         K(YL+PO4)=3.40
--------------------------------------------------------------------------------
Y+++       gl  NaClO4 25°C 0.50M U        K1=16.58       1977GGb (74313) 430
--------------------------------------------------------------------------------
Y+++       gl  KCl    25°C 1.00M U        K2=2.24        1976BKa (74314) 431
                                         K(YL+HL)=1.39
                                         K(2YL+L)=4.81
```

```
--------------------------------------------------------------------------------
Y+++       sp  KCl    25°C 0.10M U        K2=2.24        1975BKa (74315) 432
                                          K(2YL+L)=4.81
                                          K(YL+HL)=1.39
--------------------------------------------------------------------------------
Y+++       gl  KCl    25°C  1.0M C        K2=2.24        1974BKe (74316) 433
                                          K(YL+HL)=1.39
                                          K(2YL+L=Y2L3)=4.81
--------------------------------------------------------------------------------
Y+++       gl  KNO3   25°C 0.10M U T  M                  1973TRb (74317) 434
                                          K(YL+HA)=4.02
                                          K(YL+H)=5.43
K(YL+HA)(2 C)=4.10, K(35 C)=3.86, K(45 C)=3.80;  K(YL+H)(2 C)=5.86,
K(35 C)=5.24, K(45 C)=5.22,  H5A=tripolyphosphoric acid
--------------------------------------------------------------------------------
Y+++       gl  KNO3   25°C 0.10M U T  M                  1973TRb (74318) 435
                                          K(YL+A)=5.3
K(2 C)=5.4, K(35 C)=5.2, K(45 C)=5.0,  H4A=adenosine triphosphate
--------------------------------------------------------------------------------
Y+++       gl  KNO3   25°C 0.10M U    M                 1970OZa (74319) 436
                                          K(YL+A)=7.63
                                          K(YL+B)=7.05
                                          K(YL+C)=7.32
                                          K(YL+D)=3.15
H4A=tiron; H3B=2,3-dihydroxynaphthalene-6-sulphonic acid, H2C=catechol,
H2D=iminodiacetic acid, K(YL+E)=2.95,H2E=hydroxyethyl iminodiacetic acid
--------------------------------------------------------------------------------
Y+++       gl  NaClO4 25°C 0.10M U    M                 1969AIb (74320) 437
                                          K(YL+A)=7.19, A4A=tiron
--------------------------------------------------------------------------------
Y+++       nmr oth/un 40°C 0.10M U                      1969MGc (74321) 438
                                          K(Y(OH)L(H2O)n-1+H)=11.9
                                          K(YL(H2O)n+H) < 2
--------------------------------------------------------------------------------
Y+++       sp  oth/un 19°C 0.10M U        K1=16.9       1965VAa (74322) 439
--------------------------------------------------------------------------------
Y+++       sol oth/un 20°C 0.15M U  I     K1=18.21      1963TTa (74323) 440
Kso=-25.13(I=0.1)
--------------------------------------------------------------------------------
Y+++       ix  R4N.X  22°C 0.50M U        K1=17.70      1962TIa (74324) 441
--------------------------------------------------------------------------------
Y+++       cal KNO3   20°C 0.10M U   H                 1958SRa (74325) 442
DH(K1)=1.33 kJ mol-1, DS=350 J K-1 mol-1
--------------------------------------------------------------------------------
Y+++       gl  oth/un 20°C 0.01M U        K1=17.98      1955WSa (74326) 443
Polarography also used
--------------------------------------------------------------------------------
Y+++       gl  KCl    20°C 0.10M U  I   T K1=17.38      1954SGa (74327) 444
By polarography K1=17.8. In 0.1 M KNO3 K1=18.08
--------------------------------------------------------------------------------
```

```
Y+++       vlt KNO3   20°C 0.10M U      T K1=17.56       1953WSa (74328) 445
--------------------------------------------------------------------------------
Y+++       gl  KCl    20°C 0.10M U        K1=18.0        1952VIa (74329) 446
********************************************************************************
C10H16N5O13P3         H4L    ATP              CAS 56-65-5  (403)
Adenosine-5'-triphosphoric acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Y+++       gl  R4N.X  25°C 0.10M C      T K1=6.64        1991SMa (74840) 447
                                          K(Y+HL)=3.64
IUPAC evaluation
--------------------------------------------------------------------------------
Y+++       gl  KNO3   35°C 0.10M U    M                  1972TRc (74841) 448
                                       K(Y(EDTA)+L)=5.2
--------------------------------------------------------------------------------
Y+++       ix  NaCl   25°C 0.15M U        K1=11.1        1960OLa (74842) 449
********************************************************************************
C10H16O2               HL                    CAS 100563-25-5  (4706)
2-Butanoylcyclohexanone; CH3.CH2.CH2.CO.C6H9O
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Y+++       gl  oth/un 30°C 0.10M U        K1=9.13   B2=17.15  1972DSe (74926) 450
********************************************************************************
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
--------------------------------------------------------------------------------
Y+++       gl  NaClO4 25°C 0.50M U        K1=14.32       1977GGb (75535) 451
--------------------------------------------------------------------------------
Y+++       gl  KNO3   25°C 0.10M U    M                  1970OZa (75536) 452
                                          K(YL+A)=8.70
                                          K(YL+B)=8.45
                                          K(YL+C)=8.20
                                          K(YL+D)=4.85
H4A=tiron;  H3B=2,3-dihydroxynaphthalene-6-sulphonic acid;  H2C=catechol,
H2D=iminodiacetic acid.  K(YL+E)=4.48, H2E=hydroxyethyl iminodiacetic acid
--------------------------------------------------------------------------------
Y+++       gl  KNO3   25°C 0.10M U    M                  1963TLb (75537) 453
                                          K(YL+A)=5.10
                                          K(YL+B)=4.39
Id=iminodiacetic acid
--------------------------------------------------------------------------------
Y+++       EMF oth/un 20°C 0.10M U        K1=15.03       1962PMa (75538) 454
--------------------------------------------------------------------------------
Y+++       gl  KNO3   15°C 0.10M U T H    K1=14.69       1961MFb (75539) 455
K1=14.67(20 C), 14.65(25 C), 14.62(30 C), 14.71(35 C), 14.65(40 C)
DH(K1)=-1.2 kJ mol-1(25 C), DS1=277 J K-1 mol-1
```

Y+++ gl KNO3 25°C 0.10M U K1=14.49 1956SPa (75540) 456
By polarography K1=14.8
****
C10H19N3O4 HL Leu-Gly-Gly CAS 1187-50-4 (1230)
Leucyl-glycyl-glycine; H2N.CH(CH2.CH(CH3)2).CO.NH.CH2.CO.NH.CH2.COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl KNO3 25°C 0.10M U T H K1=3.30 1981SKg (75697) 457
Data for 35 and 45 C. DH(K1)=5.44 kJ mol-1, DS(K1)=81.4 J K-1 mol-1.
****
C10H20N2O4 H2L (4753)
N,N'-Diethylethylenedinitrilo-N,N'-diethanoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl KNO3 25°C 0.10M U K1=6.8 1973PSb (75787) 458
****
C11H8O3 H2L CAS 86-48-6 (1129)
1-Hydroxy-2-naphthoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl KNO3 30°C 0.05M U I K1=8.76 B2=17.05 1976SSb (77022) 459

Y+++ gl diox/w 25°C 75% U K1=4.97 1975DJa (77023) 460
****
C11H8O3 H2L CAS 2083-08-1 (1131)
2-Hydroxy-1-naphthoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl diox/w 25°C 75% U K1=4.72 1975DJa (77067) 461
****
C11H8O3 HL CAS 483-35-6 (3347)
2-Hydroxy-3-methyl-1,4-naphthoquinone;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl diox/w 35°C 75% M K1=4.81 B2=8.37 1986SSc (77081) 462
****
C11H8O3 H2L CAS 92-70-6 (1130)
2-Hydroxy-3-naphthoic acid (3-Hydroxy-2-naphthoic acid);

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl KNO3 20°C 0.10M U T H K1=8.70 B2=17.07 1977SKc (77135) 463
Further data at 30, 40 C. DH(B2)=-70.3 kJ mol-1

Y+++ gl diox/w 25°C 75% U K1=5.28 1975DJa (77136) 464
****
C11H8O4 HL CAS 7555-37-5 (4812)
3-Acetyl-4-hydroxycoumarin

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl diox/w 35°C 50% U K1=4.02 B2=7.10 1971MAa (77189) 465
Medium: 50% dioxan, 0.01 M NaClO4
****
C11H9NO2 H2L CAS 7470-09-9 (8481)
2-Hydroxy-1-naphthaldoxime;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl diox/w 25°C 75% U K1=8.24 B2=15.59 1978MCd (77320) 466
Medium: 75% v/v dioxane/H2O, 0.10 M NaClO4.
****
C11H9NO4 H2L CAS 4321-82-7 (4829)
3-Acetyl-4-hydroxycoumarin oxime;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl diox/w 35°C 50% U 1971MAa (77432) 467
K(Y+HL)=3.35
K(Y+2HL)=5.91
Medium: 50% dioxan, 0.01 M NaClO4
****
C11H9N3O2 H2L PAR CAS 1141-59-9 (636)
4-(2'-Pyridylazo)-1,3-dihydroxybenzene; C5H4N.N:N.C6H3(OH)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ sp NaClO4 20°C 0.10M U K1=9.1 1967SNb (77604) 468
K(Y+HL)=10.2
****
C11H12N2O2 HL Tryptophan CAS 73-22-3 (3)
2-Amino-3-(3-indolyl)propanoic acid; H2N.CH(CH2.C8H6N)COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl KNO3 35°C 0.10M U K1=5.48 1990RSe (78240) 469
****
C11H12O3 HL CAS 94-02-0 (3351)
Ethyl benzoylacetate; C6H5.CO.CH2.CO2.C2H5

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl mixed 25°C 75% U K1=8.56 B2=15.74 1971DRa (78405) 470
Medium: 75% acetone, 0.1 M NaClO4

****
C11H13NO3 H2L CAS 63467-38-9 (1961)
4-Methyl-N-hydroxyacetoacetanilide; CH3.CO.CH2.CO.N(OH).C6H4.CH3

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl diox/w 20°C 82% U K1=7.16 B2=13.67 1979KSb (78503) 471
K3=6.09
****
C11H13NO4 L CAS 15658-60-3 (4587)
Diethyl 2,6-pyridinedicarboxylate; Dipicolinic acid diethyl ester;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ sp non-aq 20°C 100% C K1=6.9 B2=13.50 1997RPa (78540) 472
B3=17.3
Medium: acetonitrile.
****
C11H13NO5 H3L HBIDA CAS 7372-13-6 (1603)
N-(2-Hydroxybenzyl)iminodiethanoic acid; HO.C6H4.CH2.N(CH2.COOH)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl KNO3 25°C 0.10M C K1=13.63 B2=24.17 1989YSa (78645) 473
K(Y+HL)=5.85
K(Y+2HL)=12.32
****
C11H13NO6 H4L CAS 59036-09-8 (2111)
2,5-Dihydroxybenzyliminodiethanoic acid; (HO)2.C6H3.CH2.N(CH2.COOH)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ sp oth/un 25°C ? U 1974VKa (78683) 474
K(Y+HL)=13.41
****
C11H14N2O4 H2L (1880)
N-(6-Methyl-2-pyridylmethyl)iminodiethanoic acid; CH3C5H3NCH2N(CH2COOH)2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl KNO3 25°C 0.10M U K1=6.84 B2=11.58 1964THa (78895) 475
****
C11H15NO5 HL CAS 1429-25-0 (2696)
3-Hydroxy-6-(hydroxymethyl)-2-(4-morpholinylmethyl)-4H-pyran-4-one;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ sp KCl 25°C 0.10M M I 1986POa (79054) 476
B(YHL)=11.57
****

C11H18N2O8 H4L PDTA CAS 4408-81-5 (1655)
1,2-Diaminopropane-N,N,N',N'-tetraethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Y+++	vlt	KNO3	20°C	0.10M	U		K1=18.78		1964ICb (79348)	477

****
C11H18N2O8 H4L CAS 38539-29-0 (2573)
1,3-Diaminopropane-N,N'-di(1,4-butanedioic acid)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Y+++	gl	KNO3	25°C	0.10M	U		K1=10.18		1976GKd (79376)	478

****
C11H18N2O8 H4L CAS 4408-81-5 (923)
1,3-Diaminopropane-N,N,N',N'-tetraethanoic acid; ((HOOC.CH2)2N.CH2.)2.CH2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Y+++	gl	KNO3	20°C	0.10M	U		K1=14.40		1964LAa (79478)	479

Also K1=14.26

****
C11H18N2O9 H4L HDPTA CAS 3148-72-9 (431)
1,3-Diamino-2-hydroxypropane-N,N,N',N'-tetraethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Y+++	gl	KNO3	25°C	0.10M	M		K1=14.15		1986PLc (79580)	480

****
C11H18N2O9 H4L CAS 668-21-1 (2562)
2-Hydroxy-1,3-diaminopropane-N,N'-di(1,4-butanedioic) acid

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Y+++	gl	KNO3	25°C	0.10M	U		K1=11.05		1976GKd (79609)	481

****
C11H18O2 HL CAS 40072-58-3 (4820)
2-(3'-Methylbutanoyl)cyclohexanone (2-isovaleryl cyclohexanone);

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Y+++	gl	mixed	30°C	75%	U		K1=9.56	B2=18.16	1972DSd (79658)	482

Medium: 75% acetone

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Y+++	gl	mixed	30°C	75%	U		K1=10.58	B2=20.48	1972DSd (79669)	483

Medium: 75% acetone
****
C11H18O9 H3L CAS 64020-00-4 (8225)
1,1,1-Tris(carboxymethoxymethyl)ethane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl R4N.X 25°C 0.10M C K1=6.6 2001VSa (79678) 484
Medium: 0.10 M Me4NCl. Also data for N-ethyl-, N-phenyl-, N-NH2-,
N,N-dibenzyl- and N-CH2OCH2COOH- derivatives.
****
C11H20O4 H2L CAS 2283-16-1 (2854)
2,2-Dibutylpropanedioic acid; HOOC.C(C4H9)2.COOH

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl KNO3 25°C 0.10M U K1=4.67 B2=7.23 1968PFa (79774) 485
****
C11H26N2O6 L Bistris-propane CAS 64431-96-5 (7920)
1,3-Bis[tris(hydroxmethyl)methylamino]propane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl NaClO4 25°C 0.10M C M K1=3.55 2001GYa (79959) 486
K(2Y+L+2OH)=18.66
K(2Y+L+4OH)=31.87
K(2Y+L+5OH)=36.55
K(2Y+L+6OH)=40.66
****
C12H10N6O4S H2L CAS 77327-19-6 (8343)
2-[4-Amino-3-(1,2,4-triazolylazo)]napthol-4-sulphonic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl NaClO4 30°C 0.10M U T H B2=13.13 1982GMb (80790) 487
B3=18.66
Data for 40 and 50 C. Also DH and DS values.
****
C12H11N3OS HL (6787)
2-Hydroxy-1-naphthaldehyde thiosemicarbazone;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl diox/w 20°C 75% U I K1=7.64 B2=14.77 1992SSc (80898) 488
Medium: 75% v/v dioxan/H2O; 0.1 M NaClO4
****
C12H11N3O2 HL CAS 50536-09-5 (6323)
2-Hydroxy-1-naphthaldehyde-semicarbazone; HO.C10H6.CH:N.NH.CO.NH2

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

```
--------------------------------------------------------------------------------
Y+++       gl  diox/w 20°C  75%  U  I     K1=9.214  B2=16.715 1992SSc (80927) 489
Medium: 75% v/v dioxan/H2O; 0.1 M NaClO4
********************************************************************************
C12H12NO3Cl            HL                          (1055)
2-Chloro-4-dimethylamino-benzylidenepyruvic acid; (CH3)2N.C6H3Cl.CH:CH.CO.COOH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Y+++       sp  NaClO4 25°C 0.50M U        K1=1.942       1987MSa (80977) 490
********************************************************************************
C12H13NO3              HL                          (1054)
4-Dimethylamino-benzylidenepyruvic acid; (CH3)2N.C6H4.CH:CH.CO.COOH
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Y+++       sp  NaClO4 25°C 0.50M U        K1=2.062       1987MSa (81207) 491
********************************************************************************
C12H16N2O8            H4L                          (6460)
1,4-Diaminobut-2-yne-N,N,N',N'-tetraethanoic acid;
(HOOC.CH2)2N.CH2.CC.CH2.N(CH2.COOH)2
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Y+++       gl  KCl    25°C 0.10M U        K1=8.12        1979TSa (81605) 492
                                         K(Y+HL)=6.05
                                         K(Y+YL)=5.5
********************************************************************************
C12H17NO4              HL                          (2695)
3-Hydroxy-6-(hydroxymethyl)-2-(1-piperidinylmethyl)-4H-pyran-4-one;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Y+++       sp  KCl    25°C 0.10M M  I                     1986POa (81719) 493
                                         B(YHL)=14.16
********************************************************************************
C12H18N2O5S           H2L                      CAS 80459-15-0  (1595)
2-Nitroso-5-(N-propyl-3-sulfopropylamino)phenol;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Y+++       gl  KNO3   25°C 0.10M C        K1=5.52   B2=10.06  1988YSa (81822) 494
********************************************************************************
C12H18N2O8            H4L                      CAS 76079-31-7  (2587)
trans-1,2-Diaminocyclohexane-N,N'-di(propanedioic acid)
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Y+++       EMF KNO3   25°C 0.10M U        K1=13.85       1985SGa (81883) 495
--------------------------------------------------------------------------------
```

```
Y+++       EMF KNO3   25°C 0.10M U        K1=15.02  B2=19.22  1980SGb (81884) 496
**************************************************************************
C12H18N2O8            H4L                        (8011)
trans-1,4-Diaminobuten-2-N,N,N',N'-tetraethanoic acid
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Y+++       gl  KCl    20°C 0.10M U        K1=9.10        1976TTb (81895) 497
                                         K(Y+HL)=6.34
                                         K(YL+Y)=4.9
**************************************************************************
C12H20N2O8            H4L                      CAS 40623-42-5  (1101)
1,2-Diaminoethane-N,N'-di(2-pentane-1,5-dioic acid); (CH2NHCH(COOH)CH2CH2COOH)2
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Y+++       gl  KNO3   25°C 0.10M U        K1=8.50        1973GBd (82109) 498
**************************************************************************
C12H20N2O8            H4L                      CAS 40623-42-5  (3388)
1,2-Diaminoethane-N,N'-diethanoic-N,N'-dipropanoic acid;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Y+++       gl  NaClO4 25°C 0.10M U  IH    K1=13.52       1988RNa (82182) 499
                                         B(Y+HL)=6.29
DH(K1)=6.81 kJ mol-1, DH(Y+HL)=30.6, DS(K1)=282 J K-1 mol-1
**************************************************************************
C12H20N2O8            H4L                      CAS 2458-58-4  (922)
1,4-Diaminobutane-N,N,N',N'-tetraethanoic acid; (HOOC.CH2)2N.(CH2)4.N(CH2.COOH)2
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Y+++       gl  NaClO4 25°C 0.50M M   H    K1=10.11       1985CBa (82241) 500
                                         K(YL+H)=6.63
                                         K(YHL+H)=5.48
DH(K1)=23.9 kJ mol-1, DS=274 J K-1 mol-1 (by calorimetry)
**************************************************************************
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
--------------------------------------------------------------------------
Y+++       EMF KNO3   20°C 0.10M U        K1=17.54       1962MMc (82573) 501
--------------------------------------------------------------------------
Y+++       ix  R4N.X  20°C 0.10M U  I     K1=17.92       1962STc (82574) 502
At pH 3.0. At pH 3.5, K1=17.77. At I=0.5 M, pH 2.6: K=17.66
**************************************************************************
C12H26N2O4              L    Cryptand 2,2     CAS 23978-55-4  (925)
4,7,13,16-Tetraoxa-1,10-diazacyclooctadecane;
--------------------------------------------------------------------------
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Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Y+++       gl  alc/w  25°C 100%  C        K1=8.66        1983ANb (83916) 503
The equilibration took 7-12 days. Medium: MeOH, 0.05 M Et4NClO4
*************************************************************************
C12H30N6               L                     CAS 296-35-5  (143)
1,4,7,10,13,16-Hexaazacyclooctadecane; cyclo(-(NH.CH2.CH2)6-)
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Y+++       gl  NaNO3  25°C 0.20M C        K1=8.52        1991KKa (84362) 504
*************************************************************************
C13H11NOS            H2L                      (7306)
2-(Salicylideneamino)thiophenol, Salicylaldehyde-2-mercaptoanil;
HO.C6H4.CH:N.C6H4.SH
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Y+++       gl  alc/w  25°C  70%  U        K1=14.17  B2=25.59  1995IFa (85050) 505
Medium: 70% v/v EtOH/H2O, 0.10 M NaCl.
*************************************************************************
C13H11NO2             HL                     CAS 304-88-1  (181)
N-Phenylbenzohydroxamic acid; C6H5.CO.N(C6H5).OH
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Y+++       gl  diox/w 25°C  50%  U        K1=7.73   B2=14.73  1972GDb (85185) 506
                                        B3=20.81
Medium: 50% dioxan, 0.25 M NaClO4
-------------------------------------------------------------------------
Y+++       gl  mixed  25°C  75%  U        K1=8.0    B2=14.32  1969DSb (85186) 507
Medium: 75% dioxan, 0.1 M NaClO4
*************************************************************************
C13H11NO5S           H2L                     CAS 23117-22-8  (6287)
N-Benzoyl-4-hydroxylaminobenzene sulfonic acid; C6H5.CO.N(OH).C6H4HSO3
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Y+++       gl  NaNO3  30°C 0.50M U        K1=5.58   B2=10.47  1976GMc (85223) 508
                                        B3=14.05
*************************************************************************
C13H11NS              HL                     CAS 42152-36-3  (8401)
2-[(Phenylmethylene)amino]benzenethiol;
-------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
-------------------------------------------------------------------------
Y+++       gl  alc/w  25°C  70%  U        K1=11.31  B2=20.94  1995IFa (85234) 509
Medium: 70% v/v EtOH/H2O, 0.10 M NaCl. Also data for p-Cl, p-NMe2, p-OH,
p-OCH3, p-CH3, p-NO2 substituted benzaldehyde Schiff bases.
*************************************************************************
```

C13H15NO6 H3L (660)
2-(Carboxymethyl)benzylamine-N,N-diethanoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl KNO3 30°C 0.10M U K1=9.55 1985ZXa (85725) 510
****
C13H15NO6 H3L (4999)
2-Benzylnitrilotriethanoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ oth oth/un 25°C 0.10M U K2=8.94 1962HKa (85746) 511
****
C13H22N2O8 H4L CAS 1798-14-7 (921)
(Pentamethylenedinitrilo)tetraethanoic acid; ((HOOC.CH2)2N.CH2.CH2)2CH2

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl KNO3 25°C 0.10M C K1=10.36 1982PPd (86211) 512
K(Y+HL)=6.82
****
C13H22N2O9 H4L DETAP CAS 36829-96-6 (5602)
Bis(2-aminoethyl)ether-N,N,N'-triethanoic acid-N'-(3-propanoic acid);

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl KNO3 25°C 0.10M C K1=14.28 1985PLa (86313) 513
K(Y+HL)=8.77
****
C14H8O4 H2L Alizarin CAS 72-48-0 (1058)
1,2-Dihyhroxyanthraquinone;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl oth/un 25°C 0.10M U K1=12.55 1981EIa (86653) 514
****
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
---
Y+++ gl alc/w 25°C 20% U M K1=5.78 B2=10.43 1988SIa (86816) 515
Medium: 20% EtOH/H2O (v/v), 0.1 NaClO4. Ternary complexes with salicylic
acid, sulfosalicylic acid, nitrosalicylic acid, phen and bpy
****
C14H11N5O8S2 H5L CAS 1105-53-9 (5084)
1,5-Bis(2-hydroxy-5-sulfophenyl)-3-cyanoformazan;

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

---
Y+++ gl NaNO3 20°C 0.10M U K1=14.57 1971SEa (87022) 516
****
C14H14N2O2 HL (6168)
N-(2-Hydroxy-3-methoxybenzylidene)phenylhydrazine; C6H5.NH.N:CH.C6H3(OH)OCH3

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl diox/w 30°C 75% U K1=9.03 B2=17.65 1988MKd (87660) 517
****
C14H20O5 L Benzo15-crown-5 CAS 14098-44-3 (608)
2,3-Benzo-1,4,7,10,13-pentaoxacyclopentadeca-2-ene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ ISE R4N.X 25°C 0.10M C K1=2.38 1986XJa (88386) 518
****
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
---
Y+++ gl NaClO4 25°C 0.50M U K1=18.83 1977GGb (88818) 519

Y+++ EMF KNO3 25°C 0.10M U T H K1=19.14 1962MHa (88819) 520
DH(K1)=17.6 kJ mol-1, DS=431 J K-1 mol-1. At 20 C: K(YL+H)=2.18

Y+++ vlt KNO3 20°C 0.10M U K1=19.15 1954SGa (88820) 521
****
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
---
Y+++ sp R4N.X 25°C 0.10M C K1=22.5 1994KCa (89433) 522
Medium: Me4NCl

Y+++ cal NaClO4 25°C 0.10M C H 1987YJa (89434) 523
DH(K1)=-14.2 kJ mol-1, DS(K1)=374 J K-1 mol-1.

Y+++ cal NaClO4 25°C 0.50M U H 1977CGc (89435) 524
DH(K1)=-36.3 kJ mol-1

Y+++ gl NaClO4 25°C 0.50M U K1=20.39 1977GGb (89436) 525

Y+++ sp oth/un 20°C dil U K1=21.95 1969KAf (89437) 526

Y+++ EMF KNO3 25°C 0.10M U H K1=22.05 1962MTc (89438) 527
DH(K1)=-21.8 kJ mol-1, DS=349 J K-1 mol-1

Y+++ ix R4N.X 20°C 0.10M U K1=22.28 1962STc (89439) 528

Y+++ gl oth/un 25°C 0.10M U K1=22.40 1959HCa (89440) 529
****
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
---
Y+++ gl KCl 25°C 1.00M U M 1976BKa (89616) 530
K(YEDTA+L)=2.8
K(YEDTA+HL)=2.6
K(2YEDTA+L)=5.6

Y+++ gl KCl 25°C 0.10M U 1974KPd (89617) 531
K(Y+HL)=6,87
****
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
---
Y+++ gl NaNO3 25°C 0.0 U K1=17.10 1996KDb (89963) 532
Extrapolated from data for I=0.05-0.15 M NaNO3.

Y+++ gl NaNO3 25°C 0.10M U I K1=17.01 1996KDc (89964) 533
Data for 0.05 and 0.15 M NaNO3. At I=0, K1=17.18.

Y+++ gl NaNO3 25°C 0.10M M K1=16.95 1996KDd (89965) 534
Data for 0.05-0.15 M NaNO3. At I=0, K1=17.10.

Y+++ gl NaNO3 25°C 0.10M M I K1=16.95 1995KDb (89966) 535
Data for 0.05 and 0.15 M NaNO3. At I=0, K1=17.10.

Y+++ gl NaNO3 25°C 0.10M M I K1=16.95 1995KDc (89967) 536
Data for 0.05 and 0.15 M NaNO3. At I=0, K1=17.10.

Y+++ gl NaNO3 25°C 0.10M M I K1=16.951 1995KDd (89968) 537
Data for 0.15 and 0.05 M NaNO3. At I=0, K1=17.183.

Y+++ EMF KNO3 20°C 0.10M U K1=16.82 1962MMc (89969) 538
****
C14H24O9 H3L CAS 64020-01-5 (8224)
1,1,1-Tris[(2-carboxyethoxy)methyl]ethane;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl R4N.X 25°C 0.10M C K1=3.65 2001VSa (90055) 539
K(YL+H)=4.30
Medium: 0.10 M Me4NCl. Also data for N-ethyl-, N-CH2OH-, N-CH2O(CH2)2COOH-

derivatives.
****
C14H25N3O8 H4L DEATA CAS 97315-55-4 (5601)
N,N-Bis(2-aminoethyl)ethylamine-N',N',N",N"-tetraethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Y+++	gl	KNO3	25°C	0.10M	C		K1=17.13		1985TPa	(90109) 540

****
C14H25N3O9 H4L CAS 4454-15-3 (5078)
((N-(2-Hydroxyethyl)-2,2'-iminodiethylene)dinitrilo)tetraethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Y+++	vlt	KCl	?	0.10M	U		K1=13.21		1968VLa	(90120) 541

****
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
Y+++	gl	R4N.X	25°C	0.10M	M		K1=10.85		1986COb	(90212) 542

****
C14H26N4O6 H3L DOTRA (6701)
1,4,7,10-Tetraazacyclododecane-1,4,7-triethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Y+++	sp	R4N.X	25°C	0.10M	C		K1=21.1		1994KCa	(90256) 543

Medium: Me4NCl
****
C15H12OS HL (1261)
mono-Thiodibenzoylmethane; C6H5.CO.CH2.CS.C6H5

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Y+++	gl	NaClO4	30°C	0.05M	U		K1=7.34	B2=14.04	1979VMa	(91507) 544
							K3=6.34			

****
C15H13N3O HL CAS 104992-04-3 (6852)
2-((1H-Benzimidazo-2yl-methyl)-iminomethyl)phenol;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Y+++	gl	alc/w	30°C	60%	U	M	K1=6.57	B2=12.70	1990DOb	(91667) 545
							K(YA+L)=5.27			
							K(YB+L)=5.07			
							K(YC+L)=4.66			

H2A=iminodiethanoic acid, H3B=hydroxyethyliminodiethanoic acid, H3C=NTA.
Data also for 3-chloro and 3-methoxysalicylidene analogues

****
C15H14NOCl HL CAS 268214-29-5 (8398)
4-Chloro-3,5-dimethyl-2-[(phenylimino)methyl]phenol;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl diox/w 30°C 75% M K1=7.42 2000ANa (91697) 546
Medium: 75% v/v dioxan/H2O, 0.10 M NaClO4. Data for an extensive series of
4'-substituted phenylimino derivatives.
****
C15H20N2O6 H3L BEDTA CAS 65311-06-0 (2944)
N-Benzyldiaminoethane-N,N',N'-triethanoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl KNO3 25°C 0.10M C K1=12.69 1978MPb (92160) 547
****
C15H23N3O2 L CAS 36763-33-4 (5176)
N,N,N',N'-Tetraethyl-2,6-pyridinedicarboxamide;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ sp non-aq 25°C 100% M K1=7.6 B2=14.60 1997RPb (92292) 548
B3=22.4
Medium: acetonitrile.
****
C15H25N3O10 H5L (5127)
Diethylenetriamine-N,N,N",N"-tetraethanoic acid-N'-propanoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ EMF KCl ? 0.10M U K1=16.52 1966VLa (92386) 549
****
C15H36N3O9P3 H3L (6749)
1,4,7-Triazacyclononane-N,N'N''-tris(methylenephosphonatemonoethylester)

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl R4N.X 25°C 0.10M C K1=10.4 1992LRa (92614) 550
****
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
---
Y+++ sp oth/un 25°C ? U 1964MDc (92871) 551
K1eff=4.7 (pH 6.0)
****
C16H12N3O4ClS H2L CAS 133131-00-7 (8468)
7-Amino-8-[(4-chlorophenyl)azo]-4-hydroxy-2-naphthalenesulfonic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl NaCl 25°C 0.10M U K1=6.53 B2=12.56 1997IHa (93122) 552
B3=18.21
Also data for the 4'-fluoro-, 4'-nitro-, 4'-methoxy-, 4'-dimethylamino-,
4'-hydroxy-, 4'-carboxy-, 4'-AsO(OH)2-, 2'-hydroxy- analogue
****
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
---
Y+++ gl NaClO4 30°C 0.10M U 1976NDa (93218) 553
K(Y+H2L=YH2L)=5.66
K(YHL+H)=7.21
K(YL+H)=9.57
K(YL+OH)=2.81
****
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
---
Y+++ sp oth/un 20°C 0.10M U 1971SSd (93272) 554
K(Y+H2L)=9.60
****
C16H14O4 HL BHMMA (5929)
omega-Benzoyl-2-hydroxy-4-methoxy-3-methylacetophenone;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl alc/w 30°C 25% M K1=6.70 B2=12.82 1987DGb (93587) 555
Medium: 25% v/v EtOH/H2O
****
C16H23NO8 L CAS 53408-96-1 (1765)
2,3-(4'-Nitrobenzo)-1,4,7,10,13,16-hexaoxacyclooctadeca-2-ene;
4'-Nitrobenzo-18-crown-6

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ ISE R4N.X 25°C 0.10M C K1=3.26 1986XJa (94275) 556
****
C16H27N3O9 H4L (5673)
N'-(Allyloxyethyl)diethylenetriamine-N,N,N",N"-tetraethanoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl KCl 20°C 0.10M U K1=18.81 1982TIa (94653) 557
****

C16H28N4O8 H4L DOTA CAS 60239-18-1 (1017)
1,4,7,10-Tetraazacyclododecane-1,4,7,10-tetraethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Y+++	gl	R4N.X	25°C	0.10M	U		K1=24.9		1991BCc (94936)	558

Medium: 0.1 M Me4NNO3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Y+++	gl	R4N.X	25°C	0.10M	U		K1=24.9		1989CJa (94937)	559

Medium: 0.10 M Me4NNO3.

****

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
Y+++	dis	NaClO4	21°C	0.10M	C	I	K1=5.7 B3=14.9	B2=10.70	1978NMb (95907)	560

Method: distribution of 90Y between 0.10 M NaClO4 solution and benzene.
Data for 1.0 M NaClO4 and for distribution into CHCl3 and toluene.

****

C17H14N2O5S H3L Calmagite CAS 3147-14-6 (2875)
1-(1-Hydroxy-4-methyl-2-phenylazo)-2-naphthol-4-sulfonic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Y+++	gl	NaClO4	25°C	0.10M	M		K1=15.70 K3=5.90	B2=23.55	1978MPd (95932)	561

****

C17H16O4 H2L CAS 58134-82-0 (6193)
Benzoyl-2-hydroxy-4-methoxy-3-methylacetophenone;
C6H5.CO.CH2.CO.C6H2(OH)(OCH3)(CH3)

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Y+++	gl	alc/w	30°C	75%	U	M	B2=14.00		1991GDd (96165)	562

Medium: 75% v/v EtOH/H2O, 0.1 M NaClO4. K(Y(Acetylacetone)+L)=12.00

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Y+++	gl	alc/w	30°C	75%	U T H		K1=7.75	B2=14.70	1987DGd (96166)	563

20 C:K1=7.64, K2=7.14; 40 C:K1=8.02, K2=7.12; 50 C:K1=8.40, K2=8.06
DH(K1)=-31 kJ mol-1, DS=50 J K-1 mol-1

****

C17H30N4O8 H4L TRITA CAS 60239-20-5 (1018)
1,4,7,10-Tetraazacyclotridecane-1,4,7,10-tetraethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values		Reference	ExptNo
Y+++	gl	R4N.X	25°C	0.10M	U		K1=19.6		1991BCc (96663)	564

Medium: 0.1 M Me4NNO3

Y+++ gl R4N.X 25°C 0.10M U K1=19.6 1989CJa (96664) 565
Medium: 0.10 M Me4NNO3.
****
C17H32N4O6 H3L (6696)
1,4,7,10-Tetraazacyclododecane-1,4,7-tri(2-methyl)ethanoic acid;
C8H17N4(CH(CH3)COOH)3

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ sp R4N.X 25°C 0.10M U K1=25.2 1993KRb (96690) 566
****
C17H32N4O7 H3L CAS 120041-08-9 (6702)
10-Hydroxypropyl-1,4,7,10-tetraazacyclododecane-1,4,7-triethanoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ sp R4N.X 25°C 0.10M C K1=22.2 1994KCa (96721) 567
Medium: Me4NCl
****
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
---
Y+++ gl diox/w 20°C 75% U T HM K1=8.99 B2=17.64 1994MCa (96912) 568
B3=24.48
K(Y(edta)+L)=3.36
K(Y(Hedta)+L)=3.44
K(Y(nta)+L)=3.58
Medium: 75% v/v dioxane/H2O, 0.10 M NaClO4. Data for 30 and 40 C.
DH and DS values.
****
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
---
Y+++ gl diox/w 20°C 75% U T HM 1994MCa (96922) 569
K(Y+HL)=7.64
K(Y+2HL)=14.92
K(Y+3HL)=20.83
K(Y(nta)+L)=3.54
Medium: 75% v/v dioxane/H2O, 0.10 M NaClO4. Data for 30 and 40 C.
K(Y(edta)+L)=3.02, K(Y(Hedta)+L)=3.23. DH and DS values.

Y+++ gl diox/w 20°C 75% U T HM 1994MCa (96923) 570
K(Zr+HL)=6.94
K(Zr+2HL)=13.53
K(Zr+3HL)=18.74
K(Zr(nta)+L)=4.08

Medium: 75% v/v dioxane/H2O, 0.10 M NaClO4. Data for 30 and 40 C.
K(Zr(edta)+L)=3.33, K(Zr(Hedta)+L)=3.68. DH and DS values.

****

C18H20N2O6 H4L EHPG CAS 10328-28-6 (429)
N,N'-Ethylene-bis-(2-(2'-hydroxyphenyl))glycine; (HOOCCH(C6H4OH)NHCH2.)2

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Y+++	EMF	KNO3	25°C	0.10M	C	T H	K1=19.48 K(YL+H)=7.25	1985HWb (97443)	571

Method: Hg (and glass) electrode, using Hg(II) as competitive indicator
ion. Data for 10-35 C. DH(K1)=-48.7 kJ mol-1, DS(K1)=210 J K-1 mol-1.

****

C18H26N6 L (6628)
3,6,14,17,23,24-Hexaazatricyclo[17.3.1.1]tetracosa-1(23),8,10,12(24),19,21-hexaene;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Y+++	gl	KCl	25°C	0.10M	M		K1=7.1	1996MBb (97725)	572

****

C18H32N4O8 H4L TETA CAS 60239-22-7 (1019)
1,4,8,11-Tetraazacyclotetradecane-1,4,8,11-tetraethanoic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Y+++	gl	R4N.X	25°C	0.10M	U		K1=16.1	1991BCc (98233)	573

Medium: 0.1 M Me4NNO3

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Y+++	gl	NaNO3	25°C	0.20M	C		K1=14.77	1991KKa (98234)	574

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Y+++	gl	R4N.X	25°C	0.10M	U		K1=16.3	1989CJa (98235)	575

Medium: 0.10 M Me4NNO3.

****

C18H36N2O6 L Cryptand 2,2,2 CAS 23978-09-8 (514)
1,10-Diaza-4,7,13,16,21,24-hexaoxabicyclo[8.8.8]hexacosane;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Y+++	cal	non-aq	25°C	100%	C	H	K1=11.16	2003DCa (98764)	576

Method: competitive titration calorimetry of AgL+. Medium: acetonitrile.
DH(K1)=-198.3 kJ mol-1, DS(K1)=-451 J K-1 mol-1.

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Y+++	gl	alc/w	25°C	100%	C		K1=10.34	1983ANb (98765)	577

The equilibration took 7-12 days. Medium: MeOH, 0.05 M Et4NClO4

****

C19H14O7S H4L Pyrocatechol Vi CAS 369596-29-2 (709)
Pyrocatechol Violet,
3-[3,4-Dihydroxyphenyl-3-hydroxy-4-oxo-2,5-cyclohexadien-1-ylidenemethyl-b.;

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

---
Y+++ gl NaClO4 30°C 0.20M U M K1=9.81 1978MSk (99118) 578
K(Y(nta)+L)=7.74
****
C19H15NO8 H4L Alizarin Comp. CAS 3952-78-1 (671)
(3,4-Dihydroxy-2-anthraquinonyl-methyl)iminodiethanoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ con oth/un 25°C 0.10M U K1=4.13 B2=8.30 1981EIc (99142) 579

Y+++ sp KNO3 22°C 0.1M U 1975PTf (99143) 580
K(Y+H+L)=28.0
K(Y+HL)=16.84
K((Y+2H+L)=31.31
K(YHL+H)=3.28
****
C19H16N4O L LAMI (5930)
2-(2'-Lepidylazo)-N-methylisatin

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl diox/w 30°C 75% M I K1=9.87 B2=19.19 1987DGc (99170) 581
Medium: 75% v/v dioxan/H2O, 0.15 M NaClO4
****
C19H19NO7 H2L (7003)
3-Methoxy-5-(N,N-dicarboxymethyl)aminomethyl-4-hydroxybenzophenone;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl KCl 20°C 0.10M U K1=12.5 1981SYa (99259) 582
K(Y+HL)=6.5
****
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
---
Y+++ gl NaClO4 25°C 0.10M M K1=10.70 B2=19.87 1978MPd (99578) 583
K3=5.35
****
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
---
Y+++ gl alc/w 30°C 50% C M K1=11.99 B2=22.25 1994SOa (99668) 584
K(YA+L)=10.40
K(Y(nta)+L)=9.63

Medium: 50% v/v MeOH/H2O, 0.10 M NaClO4.
H2A is hydroxyethyliminodiethanoic acid.

Y+++ gl NaClO4 30°C 0.10M U T H K1=13.55 1991NNb (99669) 585
Also data for 40 and 50 C. DH and DS values.

Y+++ gl NaClO4 25°C 0.10M M K1=11.15 B2=21.15 1978MPd (99670) 586
K3=6.85
****
C20H35N5O10 H5L (6545)
1,4,7,10,13-Pentaazacyclopentadecane-N,N',N",N"',N""-pentaethanoic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ gl NaNO3 25°C 0.20M C K1=16.07 1991KKa (100549) 587
****
C21H14O3 HL CAS 26073-81-4 (5306)
6,7-Dihydroxy-2,4-diphenylbenzopyranol,
6-hydroxy-2,4-diphenyl-7H-1-Benzopyran-7-one;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ sp oth/un ? ? U 1969PSf (101038) 588
K(YOH+L)=9.36
****
C22H14O9 H5L CAS 4431-00-9 (3513)
Aurintricarboxylic acid;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ sp oth/un 25°C ? U 1966MSc (101515) 589
K(Y+HL)=4.5(?)
****
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
---
Y+++ sp NaClO4 25°C 0.1M U 1975MBa (101557) 590
K(Y+H4L)=10.19
Room temperature

Y+++ sp oth/un ? ? U K1=15.59 1971SSi (101558) 591
****
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
---

```
Y+++       sp  NaClO4 25°C 0.10M U                        1975NMa (101659) 592
                                        K(Y+H5L)=7.36
--------------------------------------------------------------------------------
Y+++       dis KCl      ?  0.30M U                        1973AGb (101660) 593
                                        K(2Y+2H4L)=22.56
--------------------------------------------------------------------------------
Y+++       sp  oth/un 20°C    ?  U                        1972SSi (101661) 594
                                        K(Y+H4L)=16.07
********************************************************************************
C22H19N3O4S            HL                    CAS 84819-63-6  (8347)
N-(3,4-DiMe-5-isoxazolyl)-4-[[(2-hydroxy-1-naphthalenyl)methylene]amino]benzenesulf
onamide;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Y+++       gl  NaClO4 25°C 0.10M U        K1=4.91   B2= 9.52  1982MBa (101690) 595
********************************************************************************
C22H20O13             H5L    Carminic acid    CAS 1260-17-9  (714)
Carminic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Y+++       sp  oth/un   ?  0.10M U                        1970PLc (101708) 596
                                        K(YOH+2H3L)=17.76
********************************************************************************
C23H16O9Cl2S          H4L    Chrome azurol S  CAS 1667-99-8  (711)
Chromazurol S;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Y+++       sp  oth/un   ?     ?  U    M                   1973GAb (102579) 597
                                        K(YOH+phen+2H3L)=12.50
--------------------------------------------------------------------------------
Y+++       sp  oth/un 25°C    ?  U                        1967SSi (102580) 598
                                        K1eff=4.3 (pH 6.0)
********************************************************************************
C24H18N4O18As2S2      10L                   CAS 2604-69-5  (4164)
2,7-Bis(2'-arsono-5'-carboxyphenylazo)chromotropic acid;
           H
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
Y+++       sp  KNO3   20°C 0.20M U                        1965BMd (102877) 599
                                        B(YH12L2)=96.4
********************************************************************************
C24H42N6O12           H6L                     (6546)
1,4,7,10,13,16-Hexaazacyclooctadecane-N,N',N",N"',N"",N""'-hexaethanoic acid;
--------------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------------
```

```
Y+++       gl  NaNO3  25°C 0.20M C        K1=24.04       1991KKa (103390) 600
                                         K(Y+H2L)=15.93
**************************************************************************
C25H28N2O13           H6L                    CAS 42281-29-8  (5335)
(Carbonylbis((6-hydroxy-5-methoxy-3-phenylene)methylenenitrilo))tetraethanoic acid;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Y+++       gl  KCl    20°C 0.10M U        K1=22.1        1973VIb (103667) 601
                                         K(Y+HL)=16.1
                                         K(Y+H2L)=10.2
                                         K(Y+H3L)=6.4
                                         K(YOH+L)=4.4
**************************************************************************
C26H34N6O8            H4L                    CAS 132709-65-0  (8941)
3,6,14,17,23,24-Hexaazatricyclotetracosa-1,8,10,12,19,21-hexaene-3,6,14,17-tetraace
tic acid;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Y+++       gl  KCl    25°C 0.10M M        K1=ca. 20      1996MBb (104102) 602
                                         K(YL+H)=4.2
                                         K(YHL+H)=2.4
**************************************************************************
C26H38N6                L                    CAS 180684-75-7  (7295)
1,8,14,17,24,31-Hexaazatricyclo[25.3.1.1.0.0]dotriaconta-10,12,14,26,28,
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Y+++       gl  KNO3   25°C 0.20M C        K1=5.0         1996FJa (104210) 603
**************************************************************************
C28H24N2O2            H2L    Solvent Green 3  CAS 128-80-3  (1021)
1,4-Bis(4'-methylanilino)anthraquinone;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Y+++       sp  mixed  20°C  40%  U                      1984IHa (104669) 604
                                         K(Y+H3L=YHL+2H)=-7.03
Medium: 40% DMF, 0.1 M NaClO4
**************************************************************************
C31H32N2O13S          H6L    Xylenol orange   CAS 63721-85-5  (432)
5,5'-Bis-N,N-bis(carboxymethyl)aminomethyl-4'-hydroxy-3,3'-dimethylfuchsone-2"-sulf
onic acid;
--------------------------------------------------------------------------
Metal      Mtd Medium Temp Conc Cal Flags Lg K values       Reference ExptNo
--------------------------------------------------------------------------
Y+++       sp  NaClO4 20°C 0.20M U                      1966KSd (105511) 605
                                         K(Y+HL)=12.81
--------------------------------------------------------------------------
Y+++       sp  oth/un 25°C    ?  U                      1962TOa (105512) 606
```

K(?)=5.5
Acetate buffer
****
C36H48O6 L CAS 76543-12-9 (7372)
p-tert-Butyloxacalix[3]arene;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ nmr non-aq 25°C 100% U 1997HDa (106392) 607
Keff(YA3+H3L=YL+3H+3A)=-23.2
Medium: DMSO; 0.2 M 1,4-Diazabicyclo[2.2.2]octane, pH 8.5. A=triflate.
For p-chlorooxacalix[3]arene, Keff(YA3+H3L=YL+3H+3A)=-17.57
****
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
---
Y+++ gl NaClO4 30°C 0.10M U 1980NAb (106625) 608
K(Y+H3L)=4.39
K(Y+H2L)=6.92
K(YH2L+H)=4.61
Also data for YHnL(OH) species

Y+++ sp NaNO3 ? 0.20M U 1965TRa (106626) 609
B(Y2H2L2)=50.4
K(Y2HL2+H)=8.0
K(Y2L2+H)=9.5
****
C37H54N6O14S L CAS 357165-79-8 (8003)
1-[5-Dimethylaminonaphthalene-1-sulfonyl-aminoethyl]-4,7,10-tris[3'-carboxyl-1'-car
boxypropyl]cyc

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ sp NaCl 22°C 0.10M C 2001LPc (106638) 610
K(YL+H)=6.21
K(YHL+H)=3.73
****
C45H66N10O6 L CAS 362613-35-2 (7912)
Tris[3-(6-diethylcarbamoylpyridine-2-carboxamide)propyl]amine;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo
---
Y+++ sp non-aq 25°C 100% C I K1=7.1 2001RDa (107234) 611
K(Y+HL)=6.5
Medium: CH3CN. In 95% v/v CH3CN/H2O, K1=4.9, K(Y+HL)=5.1.
****
C62H94N2O4S2 L (8109)
5,11,17,23-Tetrakis(1,1-dimethylethyl)-25-27-bis[2-methylthio)ethoxy]...calix(4)are

ne;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Y+++	cal	non-aq	25°C	100%	U	H	K1=4.42	2001NJa (107710)	612

Method: microcalorimetry. Medium: MeCN.. DH(K1)=-94 kJ mol-1

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Y+++	cal	non-aq	25°C	100%	U	H	K1=4.57	2001NJa (107711)	613

Method: microcalorimetry. Medium: MeCN.. DH(K1)=-188 kJ mol-1

****

C76H116N4O8 L (8156)

p-tert-Butylcalix(4)arene tetradiisopropylethanoamide;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Y+++	cal	non-aq	25°C	100%	U	H	K1=4.96	2001NJa (107887)	614

Method: microcalorimetry. Medium: MeCN.. DH(K1)=-70.8 kJ mol-1

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EXPLANATORY NOTES

DATA Flags are :-

T Data at other TEMPERATURES
I Data with various BACKGROUNDS
H Data for THERMOCHEMICAL quantities
M Data for TERNARY Complexes

EVALUATION Flags are :-

T or IUP=T signifies EVALUATION RATING = Tentative by IUPAC

END