

## SC-Database

Software version = 5.81 Data version = 4.62

Experiment list contains 58 experiments for

(no ligands specified)

3 metals : Pa(IV), Pa(V), Pa++

(no references specified)

(no experimental details specified)

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e- HL Electron (442)

Electron;

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Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo-----  
Pa(IV) oth none rt 0.0 U 1956FEa (770) 1

K(PaF7+5e=Pa(s))=-85(-1000 mV)

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

Chloride;

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Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo-----  
Pa(IV) dis NaCl04 25°C 3.0M U B2=0 1966GUb (5320) 2

B3 &lt; 0

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Pa(IV) dis NaCl04 3.0M U 1965GUc (5321) 3

\*K1 &lt; 0

\*B2=0

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

Fluoride;

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Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo-----  
Pa(IV) dis NaCl04 ? 3.0M U T 1965GUc (7076) 4

K(PaO2+HF=PaO2F+H)=4.73

K(PaO2+2HF=PaO2F2+2H)=8.26

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

Nitrate;

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Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo-----  
Pa(IV) ix NaCl04 25°C 1.0M U K1=0.16 B2=-0.99 1967KRa (9830) 5-----  
OH- HL Hydroxide (57)

Hydroxide;

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

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Pa(IV) dis NaClO4 ? 3.00M U 1970LIa (11842) 6  
\*B(PaO+H2O=PaO2+2H)=0.96

Pa: Pa(V). Kw=-14.22

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Pa(IV) dis NaClO4 25°C 3.00M U 1968GUb (11843) 7  
\*K1=-0.14  
\*B2=-0.52  
\*B3=-1.6 to -2.0  
\*B4=-5.3

Medium: 3 M LiClO4

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O2-- H2L Peroxide CAS 7772-84-1 (2813)  
Peroxide; -0.0-

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Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
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Pa(IV) dis NaClO4 25°C 3.0M U 1969STa (12694) 8  
K(PaOOH+H2L=PaOOH(HL)+H)=2.3  
K(PaOOH+2H2L)=3.25  
K(PaOOH+H2L=PaOHL+H2O)=2  
K(PaOOH+2H2L=PaO(HL)2+H)=3.2

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

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Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
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Pa(IV) dis oth/un 10°C 0.50M U 19690Gb (16431) 9  
K(Pa(OH)2+HL=PaOHL+H2O)=2.50  
-----  
Pa(IV) dis oth/un 10°C 0.50M U 1968MIb (16432) 10  
K(Pa(OH)2+HL=PaLOH+H2O)=2.51

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Pa(IV) dis NaClO4 ? 3.0M U T 1965GUd (16433) 11  
\*K1=1.62  
\*B2=2.18

Medium: HClO4

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

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Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
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Pa(IV) oth oth/un 25°C 0.0 U K1=10.7 B2=20.3 1967MEc (19005) 12  
B3=26.5  
B4=29.2

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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
Pa(IV)	dis	NaClO4	25°C	1.00M	C T H		K1=6.1 B2=6.2 B(PaOL2=PaOL2(org))=2.07	1974LUa (38050)	13

M=PaO++; Organic phase: benzene. DH(Kd)=14 kJ mol<sup>-1</sup>.  
DH(Kd)=30 kJmol<sup>-1</sup>; Kd(PaO+2HL(org))=PaOL2(org)+2H=-4.13

Pa(IV)	dis	NaClO4	25°C	1.00M	C T H			1974LUb (38051)	14
							B'2=12.3 B'3=18.34 K(Pa(OH)L3=Pa(OH)L3(org))=2.54		

Organic phase=benzene; B'n:Pa(OH)SO4+nL=Pa(OH)Ln+SO4

Kd: Pa(OH)SO4+3HL(org)=Pa(OH)L3(org)+3H+SO4

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C6H8O7 H3L Citric acid CAS 77-92-9 (95)  
2-Hydroxypropane-1,2,3-tricarboxylic acid; H00CCH2.CH(OH)(COOH).CH2COOH

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Pa(IV)	dis	NaClO4	25°C	3.00M	U M			1968GUa (46209)	15
							K(MO(OH)+H3L=MO(OH)H2L+H)=1.30 K(MO(OH)+2H3L=MO(H2L)2+H)=1.80 K(MO(OH)+H3L=MO(OH)HL+2H)=0.0 K(MO(OH)2+H3L=MO(OH)HL+H)=1.11		

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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
Pa(IV)	dis	NaClO4	25°C	1.00M	C			1975LUa (70760)	16
							Kd(Pa)=-0.7		

Organic phase=benzene

Kd(Pa): PaO+4HL(org)=PaL4(org)+2H+H2O

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C10H16N2O8 H4L EDTA CAS 60-00-4 (120)  
1,2-Diaminoethane-N,N,N',N'-tetraethanoic acid, Sequestic acid;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Pa(IV)	dis	NaClO4	25°C	1.00M	C			1974LUc (74036)	17
							K(PaO+L)=19.0 K(PaO+H+L)=20.5		

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e- HL Electron (442)  
Electron;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Pa(V)	oth	oth/un	25°C	6.0M	U			1962HPb (771)	18

K(Pa+e=Pa(IV))=-4.9(-290 mV)

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

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Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
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Pa(V) oth oth/un ? 6.0M U 1966DMg (1155) 19

K(Pa+H3L)=1.65

K(Pa+2H3L)=2.75

Method:sorption on silica gel. Medium:HN03

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

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Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
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Pa(V) dis NaCl04 25°C 1.0M U K1=0.21 B2=-0.68 1967KR a (5322) 20  
Medium:HCl04

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Pa(V) dis oth/un 20?°C 0.0 U 1966Snd (5323) 21

K(Pa(OH)3+L)=0.0

K(Pa(OH)3+2H+6L=PaCl6)=-11.26

K(Pa(OH)3+3H+6L=PaCl6)=-13.70

Kd values into benzene also given

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Pa(V) dis NaCl04 ? 3.0M U 1965GUc (5324) 22

K(Pa(OH)3+L)=0.08

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

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Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
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Pa(V) dis NaCl04 25°C 1.0M U 1967KR a (7077) 23

\*K1=3.95

\*K2=3.48

\*K3=3.04

\*Kn: K(PaF(n-1)+HL=PaFn+H)

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Pa(V) EMF NaCl04 25°C 1.0M U K1=5.4 B2=10.40 1966BFb (7078) 24

K3=4.9

K4=4.8

K5=4.5

K6=4.4

K7=3.7, K8=1.7. Method:quinhydrone electrode.

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Pa(V) dis NaCl04 25°C 3.0M U 1966GUb (7079) 25

K(PaOOH+HF=PaOF+H2O)=3.56

K(PaOOH+2HF-H)=7.65

$$K(PaO_0H+3HF-2H)=10.91$$

Pa(V)	dis	NaClO4	?	3.0M	U	1965GUC	(7080)	26
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$$K(\text{Pa}(\text{OH})_3 + \text{HF}) = 3.56$$
$$K(\text{Pa}(\text{OH})_3 + 2\text{HF} - \text{H}) = 7.65$$
$$K(\text{Pa}(\text{OH})_3 + 3\text{HF} - 2\text{H}) = 10.90$$

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Pa(V)      dis NaClO<sub>4</sub> 25°C 1.0M U      1967KRa (8542) 27

\*K1=2.11

\*K2=1.54

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N03-	HL	Nitrate	CAS 7697-37-2 (288)
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Nitrate;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Pa(V)	dis	NaClO4	?	5.0M U	K1=1.23	B2=2.10	1966KDa	(9831)	28
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B3=2.73

B4=3.14

Medium: HClO<sub>4</sub>. Probably Pa(OH)<sub>2</sub>+++ .  $K_d(\text{Pa(OH)}_2+2\text{H}+5\text{L}+2\text{TPB(in C}_6\text{H}_6))=$

$$\text{PaL5(TBP)}_2(\text{in C}_6\text{H}_6)+2\text{H}_2\text{O})=3.73$$

Pa(V) ix NaClO4 20°C 4.0M U I K1=-0.20 B2=-0.68 1963NPa (9832) 29

Medium: HClO<sub>4</sub>. I=2.0: K<sub>1</sub>=-0.10, B<sub>2</sub>=-0.13; I=1.0: K<sub>1</sub>=-0.17, B<sub>2</sub>=0.48, B<sub>4</sub>=1.08

Pa(V)      dis NaClO<sub>4</sub> 20°C    6.0M U      1963SIIa    (9833)    30

$$K6 = -0.85$$
$$K7=0.04$$

Medium: HCl04.  $K_d(\text{PaL5}+2\text{TBP}(\text{C6H6})=\text{PaL5}(\text{TBP})_2(\text{C6H6}))=0.7$

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OH-	HL	Hydroxide	(57)
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Hydroxide;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Pa(V)      dis NaClO4 25°C 0.10M C I      2002TLa (11844) 31

$$K(\text{PaOOH} + \text{H}_2\text{O} = \text{PaO}(\text{OH})_2 + \text{H}) = -2.0$$

Extraction of 233Pa with thenoyltrifluoroacetone from HClO<sub>4</sub>/NaClO<sub>4</sub> into toluene.  $K(\text{PaO}(\text{OH})_2 + 2\text{H}_2\text{O} = \text{PaO}(\text{OH})_5 + \text{H}) = -7.0$ . Data for 1.05 and 3.52 m.

Pa(V)      dis NaCl04 25°C    0.0   C   I                          2002TLA (11845)    32

$$K(\text{PaOOH} + \text{H}_2\text{O} = \text{PaO}(\text{OH})_2 + \text{H}) = -1.26$$

Extraction of  $^{233}\text{Pa}$  with TTA from  $\text{HClO}_4/\text{NaClO}_4$  into toluene.

K(PaO(OH)<sub>2</sub>+2H<sub>2</sub>O=PaO(OH)<sub>5</sub>+H)= -7.15. SIT analysis of data for 0.1-3.52 m.

Pa(V) dis NaClO4 25°C 3.00M U 1968GUb (11846) 33

$K(\text{PaO}_3(\text{OH})+\text{H})=5.55$

$K(\text{PaO}_2+\text{H})=1.05$

Medium: 3 M LiClO4

Pa(V) dis NaClO4 25°C 3.00M U 1965GUa (11847) 34

$K(\text{PaO}(\text{OH})_3+\text{H})=1.05$

Medium: 3 M LiClO4

Pa(V) dis NaNO3 20°C 6.0M U 1959MIb (11848) 35

\* $K_1(\text{PaA}(\text{H}_2\text{O})_3)=2.1$

\* $K_2(\text{PaA}(\text{OH}))=1.46$

\* $K_3(\text{PaA}(\text{OH})_2)=1.32$

Medium: LiNO3. HA=(CHMeEtO)2PO2H

Pa(V) oth oth/un ? var U 1959SSc (11849) 36

$K_{\text{so}}(\text{Pa}(\text{OH})_5)=-55(?)$

Method: adsorption studies

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

Phosphate;

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

Pa(V) dis NaClO4 25°C 1.00M U 1973CGd (13283) 37

$K(\text{PaOOH}+\text{H}_3\text{L}=\text{PaOOHH}_2\text{L}+\text{H})=1.75$

$K(\text{PaOOH}+2\text{H}_3\text{L}=\text{PaOH}_3\text{LH}_2\text{L})=3.04$

$K(\text{PaOOH}+2\text{H}_3\text{L}=\text{PaO}(\text{H}_2\text{L})_2+\text{H})=1.91$

$K(\text{PaOOH}+\text{H}_2\text{O}=\text{PaO}(\text{OH})_2+\text{H})=-1.05$

Medium: LiClO4,  $K(\text{PaOOH}+3\text{H}_3\text{L}+\text{HSO}_4=\text{PaO}(\text{H}_2\text{L})_3\text{HSO}_4+2\text{H})=5.11$

$K(\text{PaOOH}+3\text{H}_3\text{L}=\text{PaO}(\text{H}_2\text{L})_3+2\text{H})=4.07$

Pa(V) oth KNO3 ? 6.0M U 1966DMg (13284) 38

$K(\text{Pa}+\text{H}_3\text{L})=1.54$

$K(\text{Pa}+2\text{H}_3\text{L})=2.20$

Method: sorption on silica gel. Medium: HNO3

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

Sulfate;

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

Pa(V) dis NaClO4 25°C 1.0M U 1973CGd (16434) 39

$K(\text{PaOOH}+\text{HL})=1.49$

$K(\text{PaOOH}+2\text{HL}+\text{H}=\text{PaO}(\text{HL})_2)=2.40$

Medium: LiClO4

Pa(V) dis NaClO4 25°C 1.0M U 1967KRd (16435) 40

$K(\text{Pa}+\text{HL}=\text{PaL}+\text{H})=2.08$

$K(\text{PaHL}+\text{HL}=\text{PaL}_2+\text{H})=0.23$



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Pa(V) ix oth/un 25°C 0.25M U 1966GAa (31324) 49  
K(Pa20(OH)3.5+HL)=2.34 ?  
K(Pa20(OH)4.5+2HL)=4.96 ?  
\*\*\*\*\*

C4H8O3 HL CAS 594-61-6 (81)  
2-Hydroxy-2-methylpropanoic acid; (CH3)2C(OH).COOH  
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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Pa(V) ix oth/un ? 0.25M U 1962GLa (33501) 50  
K(?)=3.47  
K(?)=7.00  
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C5H8O7 H2L CAS 40120-71-6 (3022)  
2,3,4-Trihydroxypentanedioic acid, Trihydroxyglutaric acid; HOOCH(CH(OH))3.COOH  
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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Pa(V) ix oth/un 25°C 0.25M U 1966GAa (38433) 51  
K(Pa20(OH)3+HL)=2.80 ?  
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C6H6O6 H3L Aconitic acid CAS 449-12-7 (3647)  
1,2,3-Propenetricarboxylic acid;  
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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Pa(V) ix oth/un 25°C 0.25M U 1966GAa (44291) 52  
K(?)=2.39  
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C6H8O7 H3L Citric acid CAS 77-92-9 (95)  
2-Hydroxypropane-1,2,3-tricarboxylic acid; HOOCCCH2.CH(OH)(COOH).CH2COOH  
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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Pa(V) ix oth/un 25°C 0.25M U 1966GAa (46210) 53  
K(?)=3.43  
K(?)=5.92  
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C8H5O2F3S HL TTA CAS 326-91-0 (165)  
4,4,4-Trifluoro-1-(2-thienyl)butane-1,3-dione; F3C.CO.CH2.CO.C4H3S  
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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Pa(V) dis NaClO4 25°C 3.0M U 1965GUa (58663) 54  
K(Pa(OH)3+L)=2.26  
K(Pa(OH)3+2L)=2.2  
K(Pa(OH)3+OH+L)=-0.9  
K(Pa(OH)3+OH+L+2HL)=6.2  
Medium: LiClO4. K(Pa(OH)3+2L+2HL=Pa(OH)3L2(HL)2) < 9.6



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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Pa(V)	ix	oth/un	?	0.25M	U		K(?)=2.85	1962GLa (59860)	55

\*\*\*\*\*  
 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
Pa(V)	dis	oth/un	20°C	1.0M	U		K(Pa(OH)2+L)=22.1    pH 0-2	1969SKa (74037)	56
Pa(V)	ix	oth/un	25°C	0.25M	U		K(?)=8.19 K(?)=11.96	1966GAa (74038)	57

\*\*\*\*\*  
 C8H5O2F3S                      HL      TTA                      CAS 326-91-0    (165)  
 4,4,4-Trifluoro-1-(2-thienyl)butane-1,3-dione; F3C.CO.CH2.CO.C4H3S

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Pa++	dis	NaCl04	20°C	1.0M	U		K1=8.3      B2=15.44	1968DKb (58664)	58

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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

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END