

## SC-Database

Software version = 5.81 Data version = 4.62

Experiment list contains 74 experiments for

(no ligands specified)

3 metals : Ir(IV), Ir+, Ir+++

(no references specified)

(no experimental details specified)

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e- HL Electron (442)

Electron;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ir(IV)	vlt	NaClO4	25°C	1.00M	U			1971JPa K(Ir++++ + e)=21.5(1.27V)	(598)	1
Medium: HClO4; also data in 0.18 M H2SO4 and 0.3 M H3PO4										
Ir(IV)	vlt	NaClO4	25°C	0.10M	U	I		1971JPa K(IrCl6-- + e)=15.20(899mV)	(599)	2
K(IrBr6-- + e)=14.17(838mV). Background 0 (corr), K=13.61(805mV)										
Ir(IV)	EMF	oth/un	25°C	0.40M	U			1967EBa K=22.0, 1300 mV K'=20.6, 1220 mV	(600)	3
Medium: 0.4 M HClO4. K: 1,2,3,IrCl3(H2O)3+ + e = 1,2,3,IrCl3(H2O)3 K': trans-IrCl4(H2O)2 + e = trans-IrCl4(H2O)2-										
Ir(IV)	EMF	KNO3	25°C	0.20M	U	H		1965CGb K(IrCl5+e)=17, 1000 mV K(IrCl4+e)=20, 1200 mV	(601)	4
Medium: 0.2 M HNO3										
Ir(IV)	EMF	NaCl	25°C	1.00M	U	I		1964KPa K(IrCl6+e)=15.77, 933 mV	(602)	5
In 1 M HCl, K=15.76, 932 mV										
Ir(IV)	EMF	none	25°C	0.00	U			1957GHa K(IrCl6-- + e)=14.65(866.5mV)	(603)	6
Ir(IV)	oth	none	25°C	0.0	U			1952LAb K=62.6(930 mV)	(604)	7
K: IrO2(s)+4H+4e=Ir(s)+2H2O. From thermodynamic data. K(Ir(IV)Cl6+4e=Ir(s)+6Cl)=56.4(835 mV)										
Ir(IV)	EMF	none	20°C	0.0	U			1947DMa K=17.0(990 mV)	(605)	8
K: Ir(IV)Br6+e=Ir(III)Br6										
Ir(IV)	EMF	oth/un	25°C	1.0M	U			1945PIa	(606)	9

Medium: NaBr. K:  $\text{Ir(IV)Br}_6 + e = \text{Ir(III)Br}_6$

$$K=8.2(485 \text{ mV})$$
$$K(\text{IrCl}_6 + e) = 17.49, \quad 10^{17} \text{ mV}$$
$$K=16.52(977 \text{ mV})$$
$$K=17.36(1026.4 \text{ mV})$$

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$$K(\text{Ba}+\text{IrL6})=2.3$$

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$$K(\text{IrCl}_6 + \text{Br} = \text{IrCl}_5\text{Br} + \text{Cl}) = 0.90$$
$$K(\text{IrCl}_5\text{Br} + \text{Br}) = 0.74$$
$$K(\text{IrCl}_4\text{Br}_2 + \text{Br}) = 0.52$$
$$K(\text{IrCl}_3\text{Br}_3 + \text{Br}) = 0.29$$

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$$K(\text{Ir}(\text{H}_2\text{O})_5\text{OH} + \text{H} = \text{Ir}(\text{H}_2\text{O})_6) = 0.40$$
$$B1' = 7.08$$

B2'=6.45

B3'=6.04

B4'=5.18

Bn':  $\text{IrCl}(7-n)(\text{OH})_{n-1} + \text{OH} = \text{IrCl}(6-n)(\text{OH})_n + \text{Cl}$

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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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Ir(IV) kin oth/un 20°C 2.40M U 1979TZa (16265) 18

$K(\text{Ir}(\text{H}_2\text{O})_5(\text{HSO}_4))=0.92$

$K(\text{Ir}(\text{H}_2\text{O})_4(\text{HSO}_4)_2)=0.15$

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H2 L Hydrogen (6864)

Dihydrogen;

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Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
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Ir+ cal non-aq ??? 100% U HM 1993BSb (7517) 19

Medium: Cyclohexane.  $\text{DH}(\text{IrABC}_2+\text{L}=\text{IrLABC}_2)=-100.4 \text{ kJ mol}^{-1}$

A:Cl. B:CO. C:Triphenylphosphine.

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I- HL Iodide CAS 10034-85-2 (20)

Iodide;

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Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
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Ir+ sp non-aq ? 100% U I M 1972FOa (8185) 20

$K=3.7$

Medium: 1,2-dichloroethane.  $K: \text{Ir}(\text{CO})_2\text{Cl}_2+2\text{L}=\text{Ir}(\text{CO})_2\text{L}_2+2\text{Cl}$ .  $K=2.6(\text{MeCN};$

$K=1.3(90\% \text{ MeCN}/\text{H}_2\text{O})$ . Other equilibria reported

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CH03F3S HL CAS 1493-13-6 (6755)

Trifluoromethanesulfonic acid; CF3SO3H

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Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
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Ir+ cal non-aq 25°C 100% U HM 1991SZa (17465) 21

Medium: C2H4Cl2.  $\text{DH}(\text{Ir}(\text{CO})\text{AB}+\text{HL}=(\text{Ir}(\text{CO})\text{ABH})\text{L}(\text{ion pair}))=-122.2 \text{ kJ mol}^{-1}$

A=P(p-ClC6H4)3. B=C5H5. Data also for other complexes

-----  
Ir+ cal non-aq 25°C 100% U HM 1991SZa (17466) 22

Medium: C2H4Cl2.  $\text{DH}(\text{Ir}(\text{CO})_2\text{A}+\text{HL}=(\text{Ir}(\text{CO})_2\text{AH})\text{L}(\text{ion pair}))=-89.5 \text{ kJ mol}^{-1}$

A=C5H5 Data also for complexes with phosphine substituents

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C5H6 HL Cyclopentadiene CAS 542-92-7 (4288)

Cyclopentadiene; cyclo(-CH:CH.CH2.CH:CH-)

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Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
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 Ir+ cal non-aq 25°C 100% U HM 1991SAa (37077) 23  
 Medium:1,2-Dichloroethane. DH(IrLA+CF3SO3)=-95.4 kJ mol-1  
 A:1,5-Cyclooctadiene. Data also for methyl substituted cyclopentadienes  
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 C6H16Si L (6829)  
 Triethylsilane;  
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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ir+	nmr	non-aq	20°C	100%	U	T HM			1992HBa (51797)	24
K(A2TaBIr(CO)2+L)=2.88										
Method:NMR. Medium:toluene. K=4.01(-20C);3.69(0);2.32(40);1.80(60);1.63(70).										
A:C5H5. B:CH2.CH2. DH=-46.9 kJ mol-1; DS=-105. Deuterated ligand K=3.04										
*****										
C9H21P		L							CAS 6476-36-4	(168)
Tri-isopropylphosphine; ((CH3)2CH)3P										

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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ir+	sp	non-aq	80°C	100%	U	M			1969SM1 (68227)	25
K(H2(soln)+Ir(CO)ClL2)=2.79										
K(H2(soln)+Ir(CO)BrL2)=3.21										
K(H2(soln)+Ir(CO)IL2)=4.23										

Medium: Toluene

\*\*\*\*\*  
 C12H8N2 L Phenanthroline CAS 66-71-7 (144)  
 1,10-Phenanthroline;  
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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ir+	sp	oth/un	25°C	u	U	M			1982HLb (80471)	26
K(IrCl(COD)(4-Pic)+L)=1.55										
*****										
C18H15P		L							CAS 603-35-0	(621)
Triphenylphosphine; (C6H5)3P										

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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ir+	sp	non-aq	80°C	100%	U	M			1969SM1 (97140)	27
K(H2(soln)+Ir(CO)ClL2)=2.22										
K(H2(soln)+Ir(CO)BrL2)=3.79										
K(H2(soln)+Ir(CO)IL2)=3.68										

Medium: Toluene

\*\*\*\*\*  
 C18H33P L CAS 2622-14-2 (169)  
 Tri-(cyclohexyl)phosphine; (C6H11)3P  
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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
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Ir+ sp non-aq 80°C 100% U M 1969SM1 (98313) 28  
 K(H2(soln)+Ir(CO)ClL2)=1.98  
 K(H2(soln)+Ir(CO)BrL2)=3.06  
 K(H2(soln)+Ir(CO)IL2)=2.49

Medium: Toluene

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C21H21P L CAS 6163-58-2 (600)  
 Tri(2-methylphenyl)phosphine (or 4-methyl where indicated); (CH3.C6H4)3P

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ir+	sp	non-aq	80°C	100%	U				1969SM1 (101192)	29
									K(H2(soln)+Ir(CO)ClL2)=2.43	

Medium: Toluene. Ligand: tri(4-methylphenyl)phosphine

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e- HL Electron (442)  
 Electron;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ir+++	oth	none	25°C	0.0	U				1968GHa (611)	30
									K(IrCl6+3e=Ir(s)+6Cl)=43.6	

Method:Literature evaluated data.

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Br- HL Bromide CAS 10035-10-6 (19)  
 Bromide;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ir+++	sol	oth/un	25°C	0.1M	C T				1984ISd (2067)	31
									Kout(Ir(phen)3+L)=0.91	
									Kout(Ir(phen)3+2L)=1.52	
Medium: NaF;for I=0.25M K1out=0.92; I=0.5 K1out=0.78;B2out=1.17;B3out=1.56										
I=0.75 K1out=0.80; B2out=1.10; B3out=1.32										

Ir+++	kin	oth/un	90°C	var	U				1972BGc (2068)	32
									K(trans-Ir(en)2Cl2+L)=1.9	

Ir+++	EMF	NaCl04	25°C	0.10M	U				1971KTh (2069)	33
									K(Ba+IrL6)=2.78	
									K(Cd+IrL6)=2.9	

Medium: HCl04

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CO L Carbon monoxide CAS 630-08-0 (551)  
 Carbon monoxide;

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ir+++	sp	non-aq	25°C	100%	U	M			1989KCb (2810)	34
									K(IrA+L)=5.0	

A=octaethylporphyrin(C<sub>3</sub>H<sub>7</sub>). Medium: benzene

\*\*\*\*\*

C03-- H2L Carbonate CAS 465-79-6 (268)

Carbonate;

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

Ir+++ kin NaCl04 25°C 2.0M C 2000KYb (3250) 35

\*K(Ir(NH<sub>3</sub>)<sub>5</sub>HC0<sub>3</sub>)=-6.17

\*K is for loss of proton from HC0<sub>3</sub>-.

-----  
Ir+++ sp NaCl04 25°C 0.10M U 1976MPd (3251) 36

Kout[Ir(en)<sub>3</sub>+L]=0.3

for I=0.5 M Kout=0.1

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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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Ir+++ sol oth/un 25°C 0.0 U I 1989GPa (5106) 37

Kout(cis-Ir(phen)<sub>2</sub>Cl<sub>2</sub>+Cl)=3.26

Medium: NaF. Also Kout=3.28 (I=0.1 M NaF), 2.76 (I=0.25 M),  
2.54 (I=0.50 M), 2.50 (I=0.75 M).

-----  
Ir+++ sol oth/un 25°C 0.1M C T 1984ISd (5107) 38

Kout(Ir(phen)<sub>3</sub>+L)=0.84

Kout(Ir(phen)<sub>3</sub>+2L)=1.34

Medium: NaF;for I=0.25M K<sub>1</sub>out=0.83; I=0.5 K<sub>1</sub>out=0.74;B<sub>2</sub>out=1.06;B<sub>3</sub>out=1.13  
I=0.75 K<sub>1</sub>out=0.77; B<sub>2</sub>out=0.67; B<sub>3</sub>out=1.13

-----  
Ir+++ EMF NaCl04 30°C 0.10M U T HM 1973KTc (5108) 39

K(Ba+IrCl<sub>6</sub>)=-2.19

Medium: HCl04; DH=21 kJ mol<sup>-1</sup>. K=-2.16(35 C), -2.06(42 C), -1.98(50 C)

-----  
Ir+++ EMF NaCl04 42°C 3.0M U T M 1973LKa (5109) 40

K(K+IrCl<sub>6</sub>)=-0.34

Medium: LiCl. K=-0.11(50 C)

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Ir+++ kin NaCl 90°C var U 1972BGc (5110) 41

K(trans-Ir(en)<sub>2</sub>+Cl)=1.4

-----  
Ir+++ kin oth/un 35°C 1.0M U TI 1970KTb (5111) 42

K<sub>6</sub>=-1.37

Medium: 1 M HCl04. K<sub>6</sub>=-1.29(42 C), -1.22(50 C), -1.13(60 C)

In 3M HCl04: K<sub>6</sub>=-0.72(35 C), -0.68(42 C), -0.64(50 C), -0.59(60 C)

-----  
Ir+++ kin NaCl04 25°C 1.03M U H 1969DDb (5112) 43

K<sub>6</sub>=-1.08

Medium: HCl04. DS(K<sub>6</sub>)=-20.5 J K<sup>-1</sup> mol<sup>-1</sup>

-----  
 Ir+++ kin NaClO4 45°C 3.70M U TI 1965CGb (5113) 44  
 K5=0.67  
 Medium: Na,HClO4. At I=2.2 M: K5=0.55(50 C)  
 -----

Ir+++ gl oth/un 25°C var U 1965CGb (5114) 45  
 K(IrCl4(H2O)OH+H)=8.5, 10.1  
 -----

Ir+++ sp NaClO4 50°C 2.20M U I 1962PGa (5115) 46  
 K6=-0.9  
 K6=-0.4 (I=3.7).  
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\*\*\*\*\*  
 ClO4- HL Perchlorate CAS 7001-90-3 (287)  
 Perchlorate;  
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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ir+++	sol	oth/un	25°C	0.1M	C T		1984ISd (6251) 47 Kout(Ir(phen)3+L)=1.21 Kout(Ir(phen)3+2L)=2.36		

Medium: NaF;for I=0.25M K1out=1.22; I=0.5 K1out=1.27;B2out=1.61;B3out=2.50  
 I=0.75 K1out=1.16; B2out=1.47; B3out=2.24  
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\*\*\*\*\*  
 H2 L Hydrogen (6864)  
 Dihydrogen;  
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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ir+++	nmr	non-aq	20°C	100%	U T HM		1994HGa (7518) 48		

Method: NMR. Medium: Toluene-d8. T:-10 to 20C. K: IrA2BC2+L. A:H, B:Cl, C:PtBu2Me. DH=-28.5 kJ mol-1; DS=-80.3. Data also for D2 complexes  
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\*\*\*\*\*  
 I- HL Iodide CAS 10034-85-2 (20)  
 Iodide;  
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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ir+++	sol	oth/un	25°C	0.1M	C T		1984ISd (8186) 49 Kout(Ir(phen)3+L)=0.98 Kout(Ir(phen)3+2L)=1.66		

Medium: NaF;for I=0.25M K1out=0.98; I=0.5 K1out=1.1;B2out=1.95;B3out=1.96  
 I=0.75 K1out=1.22; B2out=1.59  
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\*\*\*\*\*  
 NH3 L Ammonia CAS 7664-41-7 (414)  
 Ammonia  
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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ir+++	sol	R4N.X	25°C	1.00M	U		1995MPa (9171) 50 Kout(Ir(NH3)6+L)=1.09		

Ir+++	gl	NaClO4	25°C	1.00M	C	H			1992GMb	(9172)	51
									*K(trans-IrL4(H2O)2)=-5.214		
									*K(trans-IrL4(OH)(H2O))=-8.052		
									*K(trans-IrL4(H2O)Cl)=-6.532		
DH(*K(trans-IrL4(H2O)2))=44.6 kJ mol-1; DH(*K(trans-IrL4(H2O)Cl))=43.4.											
DH(*K(trans-IrL4(OH)(H2O))=46.1 kJ mol-1.											
-----											
Ir+++	sp	NaClO4	25°C	1.00M	C	T	H		1992GSb	(9173)	52
									*K(cis-IrL4(H2O)2)=-6.265		
									*K(cis-IrL4(OH)(H2O))=-8.088		
									*K(trans-IrL4(H2O)2)=-5.214		
									*K(trans-IrL4(OH)(H2O))=-8.052		
K(Ir2L8(OH)2+H2O=Ir2L8(OH)2(H2O)) = 0.52											
*K(Ir2L8(OH)(H2O)2)=-3.115; *K(Ir2L8(OH)2(H2O))=-9.012											
*****											
N02-		HL		Nitrite				CAS	7782-77-6	(635)	
Nitrite;											
-----											
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo	
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Ir+++	kin	oth/un	90°C	var	U				1972BGc	(9383)	53
									K(Ir(en)2Cl2+L)=2.3		
*****											
N3-		HL		Azide				CAS	7782-79-8	(441)	
Azide;											
-----											
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo	
-----											
Ir+++	kin	oth/un	22°C	var	U				1972LMa	(10238)	54
									K(Ir(NH3)5L+H)=2.1		
*****											
OH-		HL		Hydroxide					(57)		
Hydroxide;											
-----											
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo	
-----											
Ir+++	gl	NaClO4	25°C	1.0M	C	T			1990GHa	(11655)	55
									*K(Ir(NH3)5H2O)=-6.716		
At 40 C, *K=-6.323											
-----											
Ir+++	gl	NaClO4	25°C	1.05M	U	T	H		1979GBa	(11656)	56
									*K1=-4.37		
									*K2=-5.20		
									*Kso=10.22		
-----											
Ir+++	gl	oth/un	?25	dil	U				1959GVa	(11657)	57
									*K1(Ir(en)3) < -12		



Ir+++ gl oth/un rt var U 1957J0a (11658) 58  
 \*K1(IrCl5(H2O))=-10.1  
 \*K1(cis-Ir(py)2Cl3H2O)=-6.7  
 \*K1(trans-Irpy2(NH3)3H2O)=-5.1

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S-- H2L Sulfide CAS 7783-06-4 (705)  
 Sulfide;

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 Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
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Ir+++ oth none 25°C 0 U 1988LIa (14405) 59  
 Kso(Ir2S3)=-196.3  
 \*Kso(Ir2S3)=-144.4

Derived from thermodynamic data and K(H+S=HS)=17.3.

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S03-- H2L Sulfite CAS 7782-99-2 (801)  
 Sulfite;

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 Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
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Ir+++ sp NaCl04 25°C 0.10M U 1976MPd (15464) 60  
 Kout[Ir(en)3+L]=0.32

for I=0.5 M Kout=0.10

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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  
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Ir+++ sp NaCl04 25°C 0.10M U 1976MPd (16266) 61  
 Kout[Ir(en)3+L]=0.26

for I=0.5 M Kout=-0.09

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S203-- H2L Thiosulfate CAS 73686-28-7 (177)  
 Thiosulfate;

-----  
 Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
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Ir+++ sp NaCl04 25°C 0.10M U 1976MPd (16861) 62  
 Kout[Ir(en)3+L]=0.33

for I=0.5 M Kout=0.13

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Se03-- H2L Selenite CAS 7783-00-8 (2391)  
 Selenite;

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

Ir+++ sp NaCl04 25°C 0.10M U 1976MPd (17065) 63  
 Kout[Ir(en)3+L]=0.30

for I=0.5 M Kout=0.01

\*\*\*\*\*  
 TeO3--                      H2L      Tellurite                      CAS 10049-23-7    (1165)  
 Tellurate(IV)  
 -----

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ir+++	sp	NaClO4	25°C	0.10M	U				1976MPd (17283)	64

Kout[Ir(en)3+L]=0.28

for I=0.5 M Kout=-0.03

\*\*\*\*\*  
 CH2O2                      HL      Formic acid                      CAS 64-18-6    (37)  
 Methanoic acid; H.CO2H  
 -----

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ir+++	sol	oth/un	25°C	0.0	U	I			1989GPa (17619)	65

Kout(cis-Ir(phen)2Cl2+L)=0.93

Medium: NaF. Also Kout=0.66 (I=0.1 M NaF), 0.23 (I=0.25 M),  
 0.14 (I=0.50 M).

\*\*\*\*\*  
 C2H4O2                      HL      Acetic acid                      CAS 64-19-7    (36)  
 Ethanoic acid; CH3.CO2H  
 -----

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ir+++	sol	oth/un	25°C	0.0	U	I			1989GPa (20010)	66

Kout(cis-Ir(phen)2Cl2+L)=1.67

Medium: NaF. Also Kout=1.38 (I=0.1 M NaF), 1.01 (I=0.25 M),  
 0.60 (I=0.50 M), 0.36 (I=0.75 M).

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

Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ir+++	sp	non-aq	25°C	100%	U	M			1989KCb (22102)	67

K(IrA+L)=3.8

A=octaethylporphyrin(C3H7). Medium: benzene

\*\*\*\*\*  
 C4H6N2                      L      N-Me-Imidazole                      CAS 616-47-7    (354)  
 N-Methyl-1,3-diazole; C3H3N2.CH3  
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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg	K values	Reference	ExptNo
Ir+++	sp	non-aq	25°C	100%	U	M			1989KCb (29601)	68

K(IrA+L)=5.6

A=octaethylporphyrin(C3H7). Medium: benzene

\*\*\*\*\*  
 C5H5N                      L      Pyridine                      CAS 110-86-1    (31)  
 Pyridine, Azine;  
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Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ir+++	sp	non-aq	25°C	100%	U	M	K(IrA+L)=4.8 A=octaethylporphyrin(C3H7). Medium: benzene *****	1989KCb (36647)	69
C5H6		HL		Cyclopentadiene			CAS 542-92-7 (4288) Cyclopentadiene; cyclo(-CH:CH.CH2.CH:CH-)		
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ir+++	sp	NaClO4	25°C	0.20M	C	M	*K(IrL(H2O)3)=-3.86 K(2IrL(OH)=(IrL)2(u-OH)3)=-1.6 K(IrL+Cl)=2.7 K(IrL+Br)=3.5 K(IrL(py)+py)=4.9, K(IrL(dms)+dms)=>6, K(IrL(tu)+tu)=>6. dms: dimethylsulfide; tu: thiourea. *****	1999CEa (37078)	70
C6H15N		L		Triethylamine			CAS 121-44-8 (1340) N,N,N-Triethylamine; (C2H5)3N		
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ir+++	sp	non-aq	25°C	100%	U	M	K(IrA+L)=1.6 A=octaethylporphyrin(C3H7). Medium: benzene *****	1989KCb (51179)	71
C6H15O3P		L					CAS 122-52-1 (1723) Triethylphosphite; (C2H5O)3P		
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ir+++	sp	non-aq	25°C	100%	U	M	K(IrA+L)=8.2 A=octaethylporphyrin(C3H7). Medium: benzene *****	1989KCb (51513)	72
C7H7NO		L		Benzamide			CAS 55-21-0 (2328) Benzamide; C6H5.CO.NH2		
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo
Ir+++	sp	NaClO4	25°C	1.0M	U		K(Ir(NH3)5+H-1L)=2.4 *****	1975ZFa (55149)	73
C18H15P		L					CAS 603-35-0 (621) Triphenylphosphine; (C6H5)3P		
Metal	Mtd	Medium	Temp	Conc	Cal	Flags	Lg K values	Reference	ExptNo

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Ir+++ sp non-aq 25°C 100% U M 1989KCb (97141) 74  
K(IrA+L)=6.1

A=octaethylporphyrin(C<sub>3</sub>H<sub>7</sub>). Medium: benzene

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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