

## 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 | NaClO <sub>4</sub> | 25°C | 1.00M | U |  |  | 1971JPa | (598) | 1 |
|--------|-----|--------------------|------|-------|---|--|--|---------|-------|---|

$$K(\text{Ir}^{++++} + e) = 21.5(1.27\text{V})$$

Medium: HClO<sub>4</sub>; also data in 0.18 M H<sub>2</sub>SO<sub>4</sub> and 0.3 M H<sub>3</sub>PO<sub>4</sub>

|        |     |                    |      |       |   |   |  |         |       |   |
|--------|-----|--------------------|------|-------|---|---|--|---------|-------|---|
| Ir(IV) | vlt | NaClO <sub>4</sub> | 25°C | 0.10M | U | I |  | 1971JPa | (599) | 2 |
|--------|-----|--------------------|------|-------|---|---|--|---------|-------|---|

$$K(\text{IrCl}_6^{--} + e) = 15.20(899\text{mV})$$

$K(\text{IrBr}_6^{--} + e) = 14.17(838\text{mV})$ . Background 0 (corr),  $K=13.61(805\text{mV})$

|        |     |        |      |       |   |  |  |         |       |   |
|--------|-----|--------|------|-------|---|--|--|---------|-------|---|
| Ir(IV) | EMF | oth/un | 25°C | 0.40M | U |  |  | 1967EBa | (600) | 3 |
|--------|-----|--------|------|-------|---|--|--|---------|-------|---|

$$K=22.0, 1300 \text{ mV}$$

$$K'=20.6, 1220 \text{ mV}$$

Medium: 0.4 M HClO<sub>4</sub>.  $K: 1, 2, 3, \text{IrCl}_3(\text{H}_2\text{O})_3 + e = 1, 2, 3, \text{IrCl}_3(\text{H}_2\text{O})_3$

$K': \text{trans-IrCl}_4(\text{H}_2\text{O})_2 + e = \text{trans-IrCl}_4(\text{H}_2\text{O})_2^-$

|        |     |                  |      |       |   |   |  |         |       |   |
|--------|-----|------------------|------|-------|---|---|--|---------|-------|---|
| Ir(IV) | EMF | KNO <sub>3</sub> | 25°C | 0.20M | U | H |  | 1965CGb | (601) | 4 |
|--------|-----|------------------|------|-------|---|---|--|---------|-------|---|

$$K(\text{IrCl}_5 + e) = 17, 1000 \text{ mV}$$

$$K(\text{IrCl}_4 + e) = 20, 1200 \text{ mV}$$

Medium: 0.2 M HNO<sub>3</sub>

|        |     |      |      |       |   |   |  |         |       |   |
|--------|-----|------|------|-------|---|---|--|---------|-------|---|
| Ir(IV) | EMF | NaCl | 25°C | 1.00M | U | I |  | 1964KPa | (602) | 5 |
|--------|-----|------|------|-------|---|---|--|---------|-------|---|

$$K(\text{IrCl}_6 + e) = 15.77, 933 \text{ mV}$$

In 1 M HCl,  $K=15.76, 932 \text{ mV}$

|        |     |      |      |      |   |  |  |         |       |   |
|--------|-----|------|------|------|---|--|--|---------|-------|---|
| Ir(IV) | EMF | none | 25°C | 0.00 | U |  |  | 1957GHa | (603) | 6 |
|--------|-----|------|------|------|---|--|--|---------|-------|---|

$$K(\text{IrCl}_6^{--} + e) = 14.65(866.5\text{mV})$$

|        |     |      |      |     |   |  |  |         |       |   |
|--------|-----|------|------|-----|---|--|--|---------|-------|---|
| Ir(IV) | oth | none | 25°C | 0.0 | U |  |  | 1952LAb | (604) | 7 |
|--------|-----|------|------|-----|---|--|--|---------|-------|---|

$$K=62.6(930 \text{ mV})$$

$K: \text{IrO}_2(s) + 4\text{H} + 4e = \text{Ir}(s) + 2\text{H}_2\text{O}$ . From thermodynamic data.  $K(\text{Ir(IV)Cl}_6 + 4e = \text{Ir}(s) + 6\text{Cl}^-) = 56.4(835 \text{ mV})$

|        |     |      |      |     |   |  |  |         |       |   |
|--------|-----|------|------|-----|---|--|--|---------|-------|---|
| Ir(IV) | EMF | none | 20°C | 0.0 | U |  |  | 1947DMa | (605) | 8 |
|--------|-----|------|------|-----|---|--|--|---------|-------|---|

$$K=17.0(990 \text{ mV})$$

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

|        |     |        |      |      |   |  |  |         |       |   |
|--------|-----|--------|------|------|---|--|--|---------|-------|---|
| Ir(IV) | EMF | oth/un | 25°C | 1.0M | U |  |  | 1945PIa | (606) | 9 |
|--------|-----|--------|------|------|---|--|--|---------|-------|---|

$$K=16.0(947 \text{ mV})$$

Medium: NaBr. K: Ir(IV)Br<sub>6</sub>+e=Ir(III)Br<sub>6</sub>

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Ir(IV) EMF oth/un 25°C 1.0M U 1945PIa (607) 10  
K=8.2(485 mV)

Medium: KI. K:IrI<sub>6</sub>+e=Ir(III)I<sub>6</sub>

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Ir(IV) EMF none 20°C 0.0 U 1944DMa (608) 11  
K(IrCl<sub>6</sub>+e)=17.49, 1017 mV

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Ir(IV) EMF NaCl 25°C 0.50M U I 1942GSa (609) 12  
K=16.52(977 mV)

K: Ir(IV)Cl<sub>6</sub>+e=Ir(III)Cl<sub>6</sub>. I=2.0 M:K=16.67(986 mV), I=0.01 M:K=16.45(973 mV)

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Ir(IV) EMF KCl 25°C 1.0M U T 1931WOa (610) 13  
K=17.36(1026.4 mV)

Medium: HCl. K: Ir(IV)Cl<sub>6</sub>+e=Ir(III)Cl<sub>6</sub>. 20 C: K=17.74(1031.3 mV)

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

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

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Ir(IV) EMF NaClO<sub>4</sub> 25°C 0.10M U 1971KTh (2066) 14  
K(Ba+IrL<sub>6</sub>)=2.3  
K(Cd+IrL<sub>6</sub>)=1.6

Medium: HClO<sub>4</sub>

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FClBrI HL (541)  
Halides, comparative (for book data under ligand 80)

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

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Ir(IV) sp oth/un 100°C conc U 1965BPF (7407) 15  
K(IrCl<sub>6</sub>+Br=IrCl<sub>5</sub>Br+Cl)=0.90  
K(IrCl<sub>5</sub>Br+Br)=0.74  
K(IrCl<sub>4</sub>Br<sub>2</sub>+Br)=0.52  
K(IrCl<sub>3</sub>Br<sub>3</sub>+Br)=0.29

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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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Ir(IV) kin NaClO<sub>4</sub> 20°C 2.06M U 1976TZa (11653) 16  
K(Ir(H<sub>2</sub>O)<sub>5</sub>OH+H=Ir(H<sub>2</sub>O)<sub>6</sub>)=0.40

Ion exchange also used

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Ir(IV) kin oth/un 25°C 0.10M U 1971KSe (11654) 17  
B1'=7.08

|  |   |
|--|---|
| Bn': IrCl(7-n)(OH)n-1 + OH = IrCl(6-n)(OH)n + Cl           | B2'=6.45<br>B3'=6.04<br>B4'=5.18  |
| *****  |   |
| SO4--  | H2L Sulfate CAS 7664-93-9 (15)  |
| Sulfate;   |   |
| -----  |   |
| Metal  | Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo   |
| -----  |   |
| Ir(IV)   | kin oth/un 20°C 2.40M U 1979TZA (16265) 18  |
|  | K(Ir(H2O)5(HSO4))=0.92  |
|  | K(Ir(H2O)4(HSO4)2)=0.15   |
| *****  |   |
| H2   | L Hydrogen (6864)   |
| Dihydrogen;  |   |
| -----  |   |
| Metal  | Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo   |
| -----  |   |
| Ir+  | cal non-aq ??? 100% U HM 1993BSb (7517) 19  |
| Medium:  | Cyclohexane. DH(IrABC2+L=IrLABC2)=-100.4 kJ mol-1   |
| A:C1. B:CO. C:Triphenylphosphine.                          |   |
| *****  |   |
| I-   | HL Iodide CAS 10034-85-2 (20)   |
| Iodide;  |   |
| -----  |   |
| Metal  | Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo   |
| -----  |   |
| Ir+  | sp non-aq ? 100% U I M 1972FOa (8185) 20  |
|  | K=3.7   |
| Medium:  | 1,2-dichloroethane. K: Ir(CO)2Cl2+2L=Ir(CO)2L2+2Cl). K=2.6(MeCN; K=1.3(90% MeCN/H2O). Other equilibria reported |
| *****  |   |
| CH03F3S  | HL CAS 1493-13-6 (6755)   |
| Trifluoromethanesulfonic acid; CF3SO3H                     |   |
| -----  |   |
| Metal  | Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo   |
| -----  |   |
| Ir+  | cal non-aq 25°C 100% U HM 1991SZa (17465) 21  |
| Medium:  | C2H4Cl2. DH(Ir(CO)AB+HL=(Ir(CO)ABH)L(ion pair)=-122.2 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. DH(Ir(CO)2A+HL=(Ir(CO)2AH)L(ion pair)=-89.5 kJ mol-1   |
| A=C5H5 Data also for complexes with phosphine substituents |   |
| *****  |   |
| 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   |

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 Ir+ cal non-aq 25°C 100% U HM 1991SAa (37077) 23  
 Medium:1,2-Dichloroethane. DH(IrLA+CF<sub>3</sub>SO<sub>3</sub>)=-95.4 kJ mol<sup>-1</sup>  
 A:1,5-Cyclooctadiene. Data also for methyl substituted cyclopentadienes  
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C6H16Si L (6829)  
 Triethylsilane;

| 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     |
|  |     |        |      |      |     |       |    |               | $K(A_2TaB\bar{I}r(CO)_2+L)=2.88$ |        |
| Method:NMR. Medium:toluene. K=4.01(-20C);3.69(0);2.32(40);1.80(60);1.63(70).<br>A:C5H5. B:CH <sub>2</sub> .CH <sub>2</sub> . DH=-46.9 kJ mol <sup>-1</sup> ; DS=-105. Deuterated ligand K=3.04 |     |        |      |      |     |       |    |               |                                  |        |
| *****  |     |        |      |      |     |       |    |               |                                  |        |
| C9H21P   |     | L      |      |      |     |       |    | CAS 6476-36-4 | (168)                            |        |
| Tri-isopropylphosphine; ((CH <sub>3</sub> ) <sub>2</sub> CH) <sub>3</sub> P  |     |        |      |      |     |       |    |               |                                  |        |

| Metal | Mtd | Medium | Temp | Conc | Cal | Flags | Lg | K values | Reference                       | ExptNo |
|-------|-----|--------|------|------|-----|-------|----|----------|---------------------------------|--------|
| Ir+   | sp  | non-aq | 80°C | 100% | U   |       | M  |          | 1969SM1 (68227)                 | 25     |
|       |     |        |      |      |     |       |    |          | $K(H_2(soln)+Ir(CO)ClL_2)=2.79$ |        |
|       |     |        |      |      |     |       |    |          | $K(H_2(soln)+Ir(CO)BrL_2)=3.21$ |        |
|       |     |        |      |      |     |       |    |          | $K(H_2(soln)+Ir(CO)IL_2)=4.23$  |        |

Medium: Toluene

|                      |     |        |                |      |             |       |    |          |                              |        |
|----------------------|-----|--------|----------------|------|-------------|-------|----|----------|------------------------------|--------|
| *****                |     |        |                |      |             |       |    |          |                              |        |
| C12H8N2              |     | L      | Phenanthroline |      | CAS 66-71-7 | (144) |    |          |                              |        |
| 1,10-Phenanthroline; |     |        |                |      |             |       |    |          |                              |        |
| 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; (C<sub>6</sub>H<sub>5</sub>)<sub>3</sub>P

|       |     |        |      |      |     |       |    |          |                                 |        |
|-------|-----|--------|------|------|-----|-------|----|----------|---------------------------------|--------|
| Metal | Mtd | Medium | Temp | Conc | Cal | Flags | Lg | K values | Reference                       | ExptNo |
| Ir+   | sp  | non-aq | 80°C | 100% | U   | M     |    |          | 1969SM1 (97140)                 | 27     |
|       |     |        |      |      |     |       |    |          | $K(H_2(soln)+Ir(CO)ClL_2)=2.22$ |        |
|       |     |        |      |      |     |       |    |          | $K(H_2(soln)+Ir(CO)BrL_2)=3.79$ |        |
|       |     |        |      |      |     |       |    |          | $K(H_2(soln)+Ir(CO)IL_2)=3.68$  |        |

Medium: Toluene

|   |  |   |  |  |               |       |  |  |  |  |
|---|--|---|--|--|---------------|-------|--|--|--|--|
| *****   |  |   |  |  |               |       |  |  |  |  |
| C18H33P   |  | L |  |  | CAS 2622-14-2 | (169) |  |  |  |  |
| Tri-(cyclohexyl)phosphine; (C <sub>6</sub> H <sub>11</sub> ) <sub>3</sub> P |  |   |  |  |               |       |  |  |  |  |

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

Ir+ sp non-aq 80°C 100% U M 1969SM1 (98313) 28  
 K(H<sub>2</sub>(soln)+Ir(CO)ClL<sub>2</sub>)=1.98  
 K(H<sub>2</sub>(soln)+Ir(CO)BrL<sub>2</sub>)=3.06  
 K(H<sub>2</sub>(soln)+Ir(CO)IL<sub>2</sub>)=2.49

Medium: Toluene

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 C21H21P L CAS 6163-58-2 (600)  
 Tri(2-methylphenyl)phosphine (or 4-methyl where indicated); (CH<sub>3</sub>.C<sub>6</sub>H<sub>4</sub>)<sub>3</sub>P

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

Ir+ sp non-aq 80°C 100% U 1969SM1 (101192) 29  
 K(H<sub>2</sub>(soln)+Ir(CO)ClL<sub>2</sub>)=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(IrCl<sub>6</sub>+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  
 K<sub>out</sub>(Ir(phen)3+L)=0.91  
 K<sub>out</sub>(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)2Cl<sub>2</sub>+L)=1.9

Ir+++ EMF NaClO<sub>4</sub> 25°C 0.10M U 1971KTh (2069) 33  
 K(Ba+IrL<sub>6</sub>)=2.78  
 K(Cd+IrL<sub>6</sub>)=2.9

Medium: HClO<sub>4</sub>

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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

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CO<sub>3</sub>-- H<sub>2</sub>L Carbonate CAS 465-79-6 (268)  
Carbonate;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Ir+++ kin NaClO<sub>4</sub> 25°C 2.0M C 2000KYb (3250) 35  
\*K(Ir(NH<sub>3</sub>)<sub>5</sub>HC<sub>03</sub>)=-6.17

\*K is for loss of proton from HC<sub>03</sub>-.

Ir+++ sp NaClO<sub>4</sub> 25°C 0.10M U 1976MPd (3251) 36  
Kout[Ir(en)3+L]=0.3

for I=0.5 M Kout=0.1

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

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
Ir+++ sol oth/un 25°C 0.0 U I 1989GPa (5106) 37  
Kout(cis-Ir(phen)2Cl<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)3+L)=0.84  
Kout(Ir(phen)3+2L)=1.34

Medium: NaF; for I=0.25M K1out=0.83; I=0.5 K1out=0.74; B2out=1.06; B3out=1.13  
I=0.75 K1out=0.77; B2out=0.67; B3out=1.13

Ir+++ EMF NaClO<sub>4</sub> 30°C 0.10M U T HM 1973KTc (5108) 39  
K(Ba+IrCl<sub>6</sub>)=-2.19

Medium: HClO<sub>4</sub>; DH=21 kJ mol-1. K=-2.16(35 C), -2.06(42 C), -1.98(50 C)

Ir+++ EMF NaClO<sub>4</sub> 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)

Ir+++ kin NaCl 90°C var U 1972BGc (5110) 41  
K(trans-Ir(en)2+Cl)=1.4

Ir+++ kin oth/un 35°C 1.0M U TI 1970KTb (5111) 42  
K6=-1.37

Medium: 1 M HClO<sub>4</sub>. K6=-1.29(42 C), -1.22(50 C), -1.13(60 C)

In 3M HClO<sub>4</sub>: K6=-0.72(35 C), -0.68(42 C), -0.64(50 C), -0.59(60 C)

Ir+++ kin NaClO<sub>4</sub> 25°C 1.03M U H 1969DDb (5112) 43  
K6=-1.08

Medium: HClO<sub>4</sub>. DS(K6)=-20.5 J K-1 mol-1

|  |     |        |             |       |     |                             |         |                         |                   |
|--|-----|--------|-------------|-------|-----|-----------------------------|---------|-------------------------|-------------------|
| 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).   |     |        |             |       |     |                             |         |                         |                   |
| *****  |     |        |             |       |     |                             |         |                         |                   |
| C1O4-  |     | HL     | Perchlorate |       | CAS | 7001-90-3                   | (287)   |                         |                   |
| Perchlorate;   |     |        |             |       |     |                             |         |                         |                   |
| 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  |     |        |             |       |     |                             |         |                         |                   |
| *****  |     |        |             |       |     |                             |         |                         |                   |
| H2   |     | L      | Hydrogen    |       |     |                             | (6864)  |                         |                   |
| Dihydrogen;  |     |        |             |       |     |                             |         |                         |                   |
| 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 |     |        |             |       |     |                             |         |                         |                   |
| *****  |     |        |             |       |     |                             |         |                         |                   |
| I-   |     | HL     | Iodide      |       | CAS | 10034-85-2                  | (20)    |                         |                   |
| Iodide;  |     |        |             |       |     |                             |         |                         |                   |
| 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  |     |        |             |       |     |                             |         |                         |                   |
| *****  |     |        |             |       |     |                             |         |                         |                   |
| NH3  |     | L      | Ammonia     |       | CAS | 7664-41-7                   | (414)   |                         |                   |
| Ammonia  |     |        |             |       |     |                             |         |                         |                   |
| 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   |                   |

Medium: NH4ClO4

-----  
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

\*\*\*\*\*

NO2- HL Nitrite CAS 7782-77-6 (635)  
Nitrite;

Metal Mtd Medium Temp Conc Cal Flags Lg K values Reference ExptNo  
-----  
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(IrCl<sub>5</sub>(H<sub>2</sub>O))=-10.1  
     \*K1(cis-Ir(py)Cl<sub>3</sub>H<sub>2</sub>O)=-6.7  
     \*K1(trans-Irpy<sub>2</sub>(NH<sub>3</sub>)<sub>3</sub>H<sub>2</sub>O)=-5.1  
\*\*\*\*\*

S-- H<sub>2</sub>L Sulfide CAS 7783-06-4 (705)  
 Sulfide;  
-----

| Metal | Mtd | Medium | Temp | Conc | Cal | Flags | Lg | K values  | Reference       | ExptNo |
|-------|-----|--------|------|------|-----|-------|----|---|-----------------|--------|
| Ir+++ | oth | none   | 25°C | 0    | U   |       |    |   | 1988LIA (14405) | 59     |
|       |     |        |      |      |     |       |    | K <sub>so</sub> (Ir <sub>2</sub> S <sub>3</sub> )=-196.3  |                 |        |
|       |     |        |      |      |     |       |    | *K <sub>so</sub> (Ir <sub>2</sub> S <sub>3</sub> )=-144.4 |                 |        |

Derived from thermodynamic data and K(H<sub>2</sub>S=HS)=17.3.  
\*\*\*\*\*

SO<sub>3</sub>-- H<sub>2</sub>L Sulfite CAS 7782-99-2 (801)  
 Sulfite;  
-----

| Metal | Mtd | Medium             | Temp | Conc  | Cal | Flags | Lg | K values                                       | Reference       | ExptNo |
|-------|-----|--------------------|------|-------|-----|-------|----|--|-----------------|--------|
| Ir+++ | sp  | NaClO <sub>4</sub> | 25°C | 0.10M | U   |       |    |  | 1976MPd (15464) | 60     |
|       |     |                    |      |       |     |       |    | K <sub>out</sub> [Ir(en) <sub>3</sub> +L]=0.32 |                 |        |

for I=0.5 M Kout=0.10  
\*\*\*\*\*

SO<sub>4</sub>-- H<sub>2</sub>L Sulfate CAS 7664-93-9 (15)  
 Sulfate;  
-----

| Metal | Mtd | Medium             | Temp | Conc  | Cal | Flags | Lg | K values                                       | Reference       | ExptNo |
|-------|-----|--------------------|------|-------|-----|-------|----|--|-----------------|--------|
| Ir+++ | sp  | NaClO <sub>4</sub> | 25°C | 0.10M | U   |       |    |  | 1976MPd (16266) | 61     |
|       |     |                    |      |       |     |       |    | K <sub>out</sub> [Ir(en) <sub>3</sub> +L]=0.26 |                 |        |

for I=0.5 M Kout=-0.09  
\*\*\*\*\*

S<sub>2</sub>O<sub>3</sub>-- H<sub>2</sub>L Thiosulfate CAS 73686-28-7 (177)  
 Thiosulfate;  
-----

| Metal | Mtd | Medium             | Temp | Conc  | Cal | Flags | Lg | K values                                       | Reference       | ExptNo |
|-------|-----|--------------------|------|-------|-----|-------|----|--|-----------------|--------|
| Ir+++ | sp  | NaClO <sub>4</sub> | 25°C | 0.10M | U   |       |    |  | 1976MPd (16861) | 62     |
|       |     |                    |      |       |     |       |    | K <sub>out</sub> [Ir(en) <sub>3</sub> +L]=0.33 |                 |        |

for I=0.5 M Kout=0.13  
\*\*\*\*\*

SeO<sub>3</sub>-- H<sub>2</sub>L Selenite CAS 7783-00-8 (2391)  
 Selenite;  
-----

| Metal | Mtd | Medium             | Temp | Conc  | Cal | Flags | Lg | K values                                       | Reference       | ExptNo |
|-------|-----|--------------------|------|-------|-----|-------|----|--|-----------------|--------|
| Ir+++ | sp  | NaClO <sub>4</sub> | 25°C | 0.10M | U   |       |    |  | 1976MPd (17065) | 63     |
|       |     |                    |      |       |     |       |    | K <sub>out</sub> [Ir(en) <sub>3</sub> +L]=0.30 |                 |        |

for I=0.5 M Kout=0.01

\*\*\*\*\*
TeO<sub>3</sub>- H<sub>2</sub>L Tellurite CAS 10049-23-7 (1165)  
Tellurate(IV)

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| Metal | Mtd | Medium             | Temp | Conc  | Cal | Flags | Lg K values          | Reference       | ExptNo |
|-------|-----|--------------------|------|-------|-----|-------|----------------------|-----------------|--------|
| Ir+++ | sp  | NaClO <sub>4</sub> | 25°C | 0.10M | U   |       |                      | 1976MPd (17283) | 64     |
|       |     |                    |      |       |     |       | Kout[Ir(en)3+L]=0.28 |                 |        |

for I=0.5 M Kout=-0.03

\*\*\*\*\*
CH2O<sub>2</sub> HL Formic acid CAS 64-18-6 (37)  
Methanoic acid; H.COOH

---

| 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)2Cl <sub>2</sub> +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).

\*\*\*\*\*
C2H4O<sub>2</sub> HL Acetic acid CAS 64-19-7 (36)  
Ethanoic acid; CH<sub>3</sub>.COOH

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| 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)2Cl <sub>2</sub> +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; (CH<sub>3</sub>)<sub>2</sub>SO

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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 (22102) | 67     |
|       |     |        |      |      |     |       | K(IrA+L)=3.8 |                 |        |

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

\*\*\*\*\*
C4H6N<sub>2</sub> L N-Me-Imidazole CAS 616-47-7 (354)  
N-Methyl-1,3-diazole; C<sub>3</sub>H<sub>3</sub>N<sub>2</sub>.CH<sub>3</sub>

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

\*\*\*\*\*
C5H5N L Pyridine CAS 110-86-1 (31)  
Pyridine, Azine;

| Metal  | Mtd | Medium | Temp | Conc            | Cal | Flags    | Lg     | K values | Reference       | ExptNo |
|--|-----|--------|------|-----------------|-----|----------|--------|----------|-----------------|--------|
| Ir+++  | sp  | non-aq | 25°C | 100%            | U   | M        |        |          | 1989KCb (36647) | 69     |
| K(IrA+L)=4.8   |     |        |      |                 |     |          |        |          |                 |        |
| A=octaethylporphyrin(C3H7). Medium: benzene              |     |        |      |                 |     |          |        |          |                 |        |
| 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        |        |          | 1999CEa (37078) | 70     |
| *K(IrL(H2O)3)=-3.86                                      |     |        |      |                 |     |          |        |          |                 |        |
| K(2IrL(OH)=(IrL)2(u-OH)3)=-1.6                           |     |        |      |                 |     |          |        |          |                 |        |
| K(IrL+C1)=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.                      |     |        |      |                 |     |          |        |          |                 |        |
| 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        |        |          | 1989KCb (51179) | 71     |
| K(IrA+L)=1.6   |     |        |      |                 |     |          |        |          |                 |        |
| A=octaethylporphyrin(C3H7). Medium: benzene              |     |        |      |                 |     |          |        |          |                 |        |
| 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        |        |          | 1989KCb (51513) | 72     |
| K(IrA+L)=8.2   |     |        |      |                 |     |          |        |          |                 |        |
| A=octaethylporphyrin(C3H7). Medium: benzene              |     |        |      |                 |     |          |        |          |                 |        |
| 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   |          |        |          | 1975ZFa (55149) | 73     |
| K(Ir(NH3)5+H-1L)=2.4                                     |     |        |      |                 |     |          |        |          |                 |        |
| C18H15P  |     | L      |      |                 | CAS | 603-35-0 | (621)  |          |                 |        |
| Triphenylphosphine; (C6H5)3P                             |     |        |      |                 |     |          |        |          |                 |        |
| Metal  | Mtd | Medium | Temp | Conc            | Cal | Flags    | Lg     | K values | Reference       | ExptNo |

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

A=octaethylporphyrin(C3H7). 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