

## Supporting Information

### **Multiphoton tandem photoredox catalysis of $[\text{Ir}(\text{dFCF}_3\text{ppy})_2(\text{dtbbpy})]^+$ facilitating radical acylation reactions**

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## 1. Materials and Methods

**Materials.** [Ir(dF(CF<sub>3</sub>)ppy)<sub>2</sub>(dtbbpy)]PF<sub>6</sub> (Macklin), [Ir(dF(CF<sub>3</sub>)ppy)<sub>2</sub>(dtbbpy)]PF<sub>6</sub> (Macklin), 4-iodotoluene (Aladdin), 4-iodobenzoylformic acid (Chemzju), (E)-3-(2-isocyanophenyl)acrylonitrile (Chemzju), 3-pentyl-2-ketone (Adamas), 4-Chlorobenzoylformic acid (APINNO), β-(Naphthalen-1-yl)-2-oxoacetic acid (Bidepharm), Phenylglyoxylic acid (Innochem), triethylamine (TEA, Innochem), Pd(Nixantphos)Cl<sub>2</sub> (Chemzju), Acetonitrile (CH<sub>3</sub>CN, Macklin), *N,N*-Dimethylformamide (DMF, Innochem), Disodium Hydrogen Phosphate (Na<sub>2</sub>HPO<sub>4</sub>, Innochem), Monosodium phosphate (NaH<sub>2</sub>PO<sub>4</sub>, Innochem) were used as received. Ultrapure water was obtained by Millipore filtration.

**Laser flash photolysis.** Nanosecond time-resolved transient absorption spectra were measured using a flash photolysis setup Edinburgh LP980 spectrometer (Edinburgh Instruments Ltd.). A Surelite II-10 Q-Switched Nd:YAG laser (Continuum) provides third harmonic laser pulses at 355 nm with a repetition rate of 10 Hz and maximum output of 1.5 W. The laser output was directed to a Horizon I Mid-band Optical Parametric Oscillator (OPO) (Continuum) to produce tunable pump pulses from 192 nm to 2750 nm spectral region. In this work, the sample was excited by a 430 nm laser pulse (1 Hz, 20 mJ/pulse/cm<sup>2</sup>, fwhm ≈ 7 ns). Each measurement was performed in a quartz cuvette with 1 cm path length at room temperature. The analyzing light was from a 150 W pulsed xenon lamp. A monochromator equipped with a photomultiplier for collecting the spectral range from 300 to 700 nm was used to analyze transient absorption spectra. The signals from the photomultiplier were displayed and recorded as a function of time on a 100 MHz (1.25 Gs/s sampling rate) oscilloscope (Tektronix, TDS 3012C), and the data were transferred to a personal computer. Data were analyzed by the online software of the LP980 spectrophotometer. The fitting quality was judged by weighted residuals and reduced  $\chi^2$  value.

**Steady-state Spectral Measurement.** The UV-vis absorption spectra were measured using a UV-vis spectrometer (U-3010, Hitachi). Each measurement was collected from 300 to 700 at a scan speed of 600 nm/min. The spectrum of a blank sample containing the pure solvent was used as the background, which was subtracted from the averaged spectra. Emission spectra were measured on a fluorescence spectrometer (F4600, Hitachi). Quartz cuvettes of 1 × 1 cm were used for all absorption and emission spectral measurements. Fourier transform infrared (FTIR) spectra were recorded using a Bruker Vertex 80 V, with a spectral resolution of 4 cm<sup>-1</sup>. The 2 mm-thick CaF<sub>2</sub> windows (100 μm optical path length) was used for the measurements.

**Computational Methods.** The geometries were fully optimized at the B3LYP/LANL2DZ: 6-31G\*\* level of theory and at the B3LYP/6-31G\*\* level of theory, for Ir species and substrate species, respectively. The harmonic vibrational frequencies analysis was performed to identify the geometry as local minima and to extract zero-point vibrational energy corrections. Bulk solvation effects were simulated by using the polarizable continuum model (PCM). The vertical electronic excitations were calculated using time-dependent (TD)-B3LYP method based on the ground-state geometry optimized at the same level. All the calculations were carried out using the Gaussian 09 program package. GaussView molecular modeling software was used to plot the molecular orbitals and draw the molecular structure.

## 2. Additional experimental and calculational results.

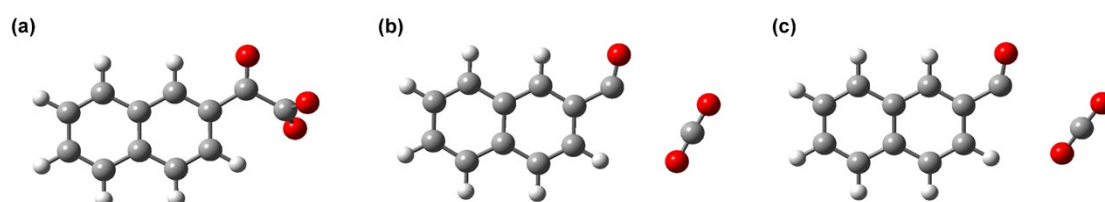
**Fig. S1** (a) Steady-state UV-vis absorption spectra for 150  $\mu\text{M}$  IrIII (black), 10 mM PhCOCOOH (red) and 150  $\mu\text{M}$  IrIII + 10 mM PhCOCOOH (blue) in ACN/phosphate buffer (pH 7, v/v = 1:1); (b) Steady-state emission spectra of IrIII (150  $\mu\text{M}$ ) at different concentrations of PhCOCOOH under deoxygenated conditions in ACN-phosphate buffer (pH 7, v/v = 1:1) following 430 nm excitation; (c) Transient emission kinetics of  $^3\text{IrIII}^*$  at 470 nm at different concentrations of PhCOCOOH; (d) Stern-Volmer plot obtained from the decay lifetime of  $^3\text{IrIII}^*$  with different concentrations of PhCOCOOH.

**Fig. S2** (a) Steady-state UV-vis absorption spectra for 150  $\mu\text{M}$  IrIII (black), 10 mM Cl-PhCOCOOH (red) and 150  $\mu\text{M}$  IrIII with 10 mM Cl-PhCOCOOH (blue) in ACN-phosphate buffer (pH 7, v/v = 1:1); (b) Steady-state emission spectra of IrIII (150  $\mu\text{M}$ ) at different concentrations of Cl-PhCOCOOH under deoxygenated conditions in ACN-phosphate buffer (pH 7, v/v = 1:1) following 430 nm excitation; (c) Transient emission kinetics of  $^3\text{IrIII}^*$  at 470 nm at different concentrations of Cl-PhCOCOOH; (d) Stern-Volmer plot obtained from the decay lifetime of  $^3\text{IrIII}^*$  with different concentrations of Cl-PhCOCOOH.

**Fig. S3** (a) Steady-state UV-vis absorption spectra for 150  $\mu\text{M}$  IrIII (black), 10 mM I-PhCOCOOH (red) and 150  $\mu\text{M}$  IrIII with 10 mM I-PhCOCOOH (blue) in ACN/phosphate buffer (pH 7, v/v = 1:1); (b) Steady-state emission spectra of IrIII (150  $\mu\text{M}$ ) at different concentrations of I-PhCOCOOH under deoxygenated conditions in ACN-phosphate buffer (pH 7, v/v = 1:1) following 430 nm excitation; (c) Transient emission kinetics of  $^3\text{IrIII}^*$  at 470 nm at different concentrations of I-PhCOCOOH; (d) Stern-Volmer plot obtained from the decay lifetime of  $^3\text{IrIII}^*$  with different concentrations of I-PhCOCOOH.

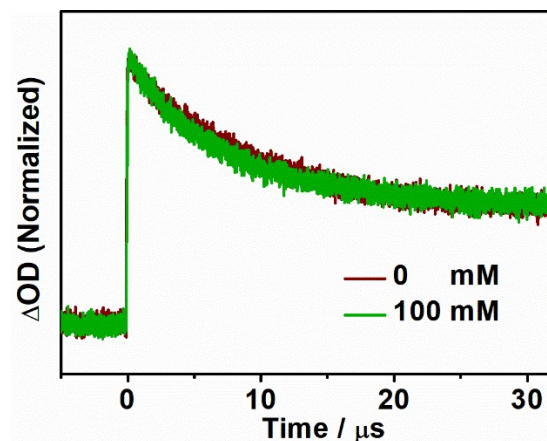
**Fig. S4** Cyclic voltammogram of NaphCOCOOH (a), PhCOCOOH (b), Cl-PhCOCOOH (c), I-PhCOCOOH (d) in DMSO. The anodic peak potentials, vs saturated calomel electrode (SCE), are 0.88 V for NaphCOCOOH, 0.96 V for PhCOCOOH, 1.03 V for Cl-PhCOCOOH and 0.51 V for I-PhCOCOOH, respectively.

**Fig. S5** (a) Steady-state UV-vis absorption spectra for 150  $\mu\text{M}$  IrIII (black), 10 mM 3-pentyl-2-ketone (red) and 150  $\mu\text{M}$  IrIII + 10 mM 3-pentyl-2-ketone (blue) in ACN/phosphate buffer (pH 7, v/v = 1:1); (b) Transient emission kinetics at 470 nm of  $^3\text{IrIII}^*$  with different concentrations of 3-pentyl-2-ketone under deoxygenated conditions in ACN/phosphate buffer (pH 7, v/v = 1:1); (c) Stern-Volmer plot obtained from the decay lifetime of  $^3\text{IrIII}^*$  with different concentrations of 3-pentyl-2-ketone.

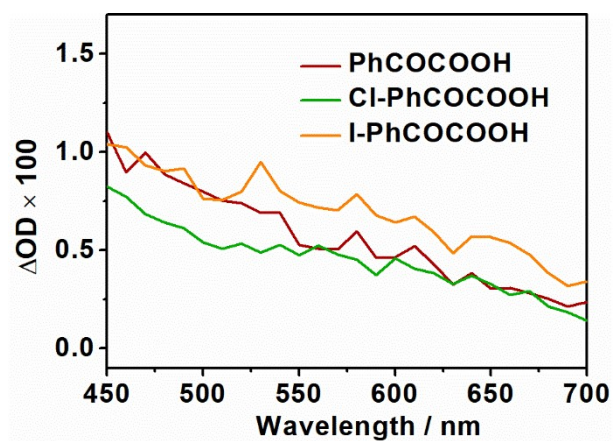


**Fig. S6** (a) The input structure of NaphCOCOO $^{\bullet}$  radical; The optimized structures of NaphCOCOO $^{\bullet}$  radical obtained at the level of B3LYP/6-31G $^{**}$ /PCM/water (b) and B3LYP/6-31G $^{**}$ /PCM/acetonitrile (c).

In comparison with the input structure of NaphCOCOO $^{\bullet}$  radical, the optimized structures reveal that CO $_2$  has been already detached, suggesting the expulsion of CO $_2$  from the NaphCOCOO $^{\bullet}$  radical to yield the acyl radical is a barrier-free process. Consequently, once this open-shell dicarbonyl radical is formed, a rapid detachment of CO $_2$  can be anticipated.



**Fig. S7** Representative decay-traces at 525 nm for IrIII (150  $\mu$ M) + NaphCOCOOH (10 mM) (red) and IrIII (150  $\mu$ M) + NaphCOCOOH (10 mM) + 3-pentyl-2-ketone (100 mM) (green).



**Fig. S8** Transient absorption spectra of IrIII (150  $\mu$ M) +  $\alpha$ -keto acids (10 mM, red: PhCOCOOH; green: Cl-PhCOCOOH; orange: I-PhCOCOOH) at 20  $\mu$ s.



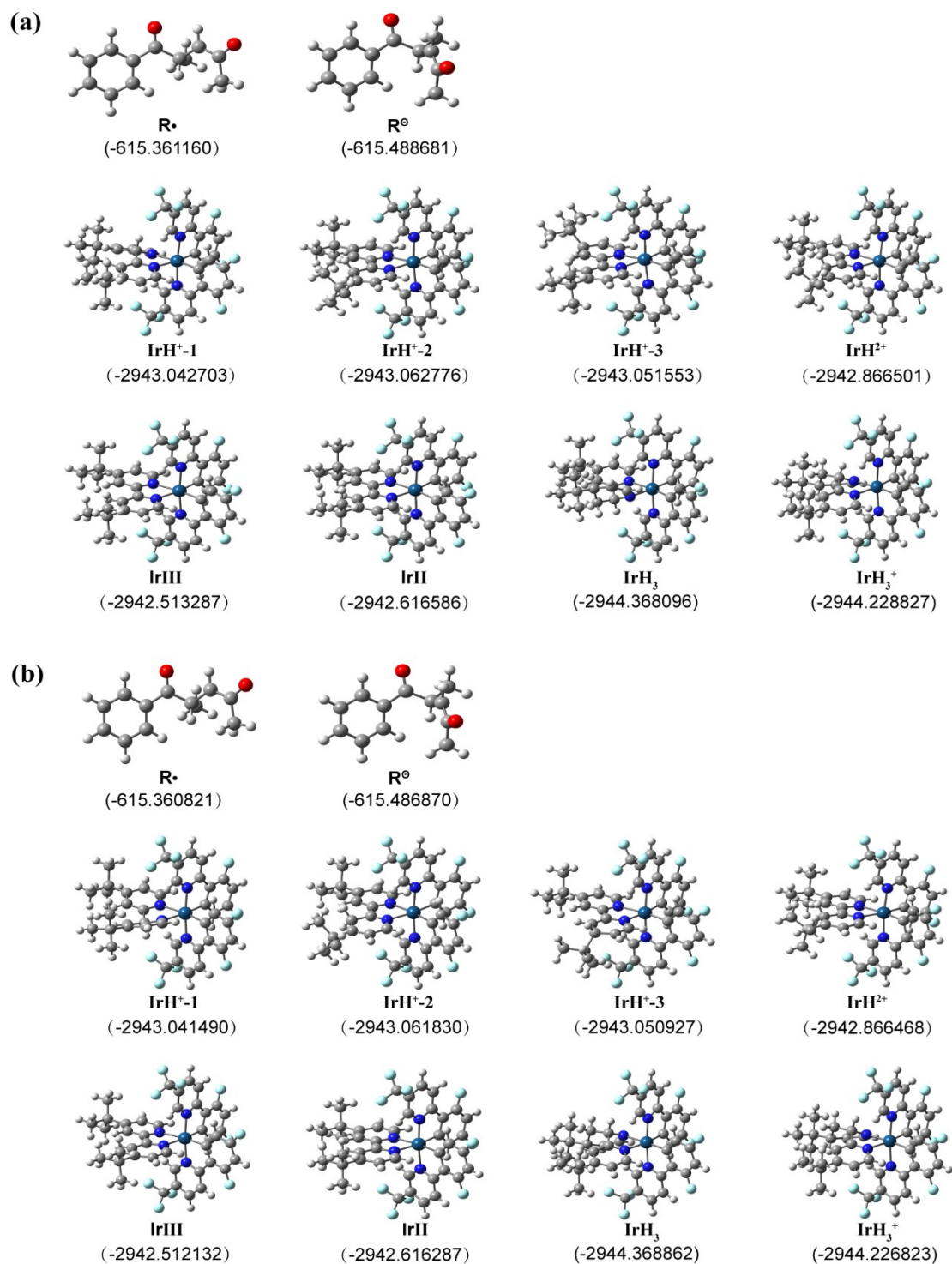
**Fig. S9** Normalized kinetics curves for transient absorptions at (a) 450 nm, (b) 525 nm and (c) 650 nm of **IrIII** (150  $\mu\text{M}$ ) + NaphCOCOOH (10 mM) (red) and **IrIII** (150  $\mu\text{M}$ ) + NaphCOCOOH (10 mM) + 3-penten-2-one (100 mM) (green) under deoxygenated conditions in ACN/phosphate buffer (pH 7, v/v =1:1) at a longer time scale.

**Fig. S10** Steady-state emission spectra of **IrIII** (150  $\mu$ M) +  $\alpha$ -keto acids (10 mM, a: PhCOCOOH; d: Cl-PhCOCOOH; g:I-PhCOCOOH) + 3-pentyl-2-ketone (100 mM) under deoxygenated conditions in ACN/phosphate buffer (pH 7, v/v = 1:1) under continuous illumination by 430 nm laser (20 mJ); Species analysis of **IrIII** +  $\alpha$ -keto acids (b: PhCOCOOH; e: Cl-PhCOCOOH; h: I-PhCOCOOH) + 3-pentyl-2-ketone; Steady-state emission spectra of **IrIII** +  $\alpha$ -keto acids (c: PhCOCOOH; f: Cl-PhCOCOOH; i: I-PhCOCOOH) + 3-pentyl-2-ketone before (black) and after (red) continuous illumination by 430 nm laser (20 mJ).

**Fig. S11** Steady-state emission spectra of S1 (a) and S2 (d) under deoxygenated conditions in DMA following 430 nm excitation; (S1: IrIII (150  $\mu$ M) + PhCOCOOH (40 mM) + 4-Iodotoluene (20 mM) + Ni (2 mM) with 40 mM Li<sub>2</sub>CO<sub>3</sub>, S2: IrIII (150  $\mu$ M) + PhCOCOOH (200 mM) + 2-alkenylarylisocyanides (100 mM) with 160 mM Na<sub>2</sub>HPO<sub>4</sub>); Species analysis of S1 (b) and S2 (e); Steady-state emission spectra of S1 (c) and S2 (f) before (black) and after (red) continuous illumination by 430 nm laser (20 mJ).

**Fig. S12** (a) Decay-traces at 525 nm for **IrIII** (150  $\mu$ M) + NaphCOCOOH (10 mM) + 3-pentyl-2-ketone (100 mM) under deoxygenated conditions in ACN/phosphate buffer (v/v = 1:1) at different pH following 430 nm excitation; (b) Normalized kinetics curves for transient absorptions at 525 nm for **IrIII** (150  $\mu$ M) at different concentrations of NaphCOCOOH under deoxygenated conditions in ACN/phosphate buffer (pH 7, v/v = 1:1) following 430 nm excitation.

As depicted in Fig. S12a, as the pH value increases, the decay kinetics at 530 nm gradually slows down, accompanied by an increase in absorption intensity after the decay. Such a tendency is consistent with the expectation that at a higher pH, the protonation of **IrII** into **IrH<sup>+</sup>** would be prohibited, leading to a higher proportion of **IrII** exhibiting stronger absorption at 530 nm in the equilibrium between **IrII** and **IrH<sup>+</sup>**. These findings demonstrate the observed decay of **IrII** corresponds to its protonation, thereby reinforcing the proposed identification of this new Ir species as **IrH<sup>+</sup>**.

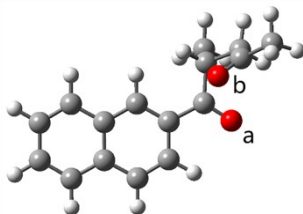


**Fig. S13** The structures of reactant and related intermediates of IrIII photocatalytic radical acylation reactions optimized at the level of B3LYP/6-31G\*\*/PCM/water (a) and B3LYP/6-31G\*\*/PCM/acetonitrile (b). The parentheses indicate Gibbs Free Energy (G) (in Hartree) calculated with Zero-Point Energy (ZPE) correction. Note that among the three possible structures of IrH<sup>+</sup> (IrH<sup>+</sup>-1, IrH<sup>+</sup>-2, and IrH<sup>+</sup>-3), IrH<sup>+</sup>-2 is shown to be the most stable. Therefore, the Gibbs Free Energy (G) for IrH<sup>+</sup> used in this work is based on the structure of IrH<sup>+</sup>-2.

**Table S1.** Oxidation potential of  $\alpha$ -keto acids and the calculated  $\Delta G_0$ .

Donor ( $\alpha$ -keto acids) $E(D^{*+}/D)$ vs SCE / V		Acceptor (IrIII) $E(A^{*+}/A)$ vs SCE / V	$\Delta G_0$ [ $E(D^{*+}/D) - E(A^{*+}/A)$ ]
NaphCOCOOH	0.88	1.21	-0.33
PhCOCOOH	0.96		-0.25
Cl-PhCOCOOH	1.03		-0.18
I-PhCOCOOH	0.51		-0.70

**Table S2.** B3LYP/6-31G\*\* calculated IR frequencies and IR intensities for relevant species in  $D_2O$  with the solvent effect simulated by PCM model, as well as the observed IR frequencies for these species. Note:  $C=O^a$  indicates the carbonyl group of NaphCOCOOH;  $C=O^b$  belongs to 3-Penten-2-keone; The values in parentheses are scaled by a factor of 0.96, which is usually adopted for B3LYP method.

Species	$\nu_{\text{calc}}/\text{cm}^{-1}$ (PCM = $D_2O$ )	Intensity/ $\text{km mol}^{-1}$	$\nu_{\text{exp}}/\text{cm}^{-1}$
<b>Final 1,4-addition product</b>			
	$C=O^b$ 1774 (1703)	226	1672
	$C=O^a$ 1729 (1660)	451	1643

**Table S3.** B3LYP/6-31G\*\* calculated Gibbs Free Energy difference [ $\Delta G = \sum G(\text{product}) - \sum G(\text{reactant})$ ] in H<sub>2</sub>O and in ACN, respectively.

Reactions	$\Delta G$ (kJ/mol)	
	H <sub>2</sub> O	ACN
$\text{IrII} + \text{R} \begin{array}{c} \text{O} \\ \parallel \\ \text{C} \\   \\ \text{C} \cdot \\   \\ \text{C} \\ \parallel \\ \text{O} \end{array} \longrightarrow \text{IrIII} + \text{R} \begin{array}{c} \text{O} \\ \parallel \\ \text{C} \\   \\ \text{C}^- \\   \\ \text{C} \\ \parallel \\ \text{O} \end{array}$	-63.59	-57.51
$\text{IrH}_3^+ + \text{IrII} \longrightarrow \text{IrH}_3 + \text{IrIII}$	-99.46	-99.46
$\text{IrH}_3^* + \text{R} \begin{array}{c} \text{O} \\ \parallel \\ \text{C} \\   \\ \text{C} \cdot \\   \\ \text{C} \\ \parallel \\ \text{O} \end{array} \longrightarrow \text{IrH}_3^+ + \text{R} \begin{array}{c} \text{O} \\ \parallel \\ \text{C} \\   \\ \text{C}^- \\   \\ \text{C} \\ \parallel \\ \text{O} \end{array}$	-186.19	-175.08
$\text{IrH}_3 + \text{R} \begin{array}{c} \text{O} \\ \parallel \\ \text{C} \\   \\ \text{C} \cdot \\   \\ \text{C} \\ \parallel \\ \text{O} \end{array} \longrightarrow \text{IrH}_3^+ + \text{R} \begin{array}{c} \text{O} \\ \parallel \\ \text{C} \\   \\ \text{C}^- \\   \\ \text{C} \\ \parallel \\ \text{O} \end{array}$	41.96	308.42
$\text{IrH}^+ + \text{R} \begin{array}{c} \text{O} \\ \parallel \\ \text{C} \\   \\ \text{C} \cdot \\   \\ \text{C} \\ \parallel \\ \text{O} \end{array} \longrightarrow \text{IrH}^{2+} + \text{R} \begin{array}{c} \text{O} \\ \parallel \\ \text{C} \\   \\ \text{C}^- \\   \\ \text{C} \\ \parallel \\ \text{O} \end{array}$	128.55	180.51

#### 4. Optimized Cartesian Coordinates

##### 1,4-addition product (in D<sub>2</sub>O)

C	2.10784600	-0.63364000	0.89010300
H	1.64702600	-1.43858500	0.31250900
C	3.70207200	-0.31324000	-1.07555200
C	5.11026100	-0.30813100	-1.62989600
H	5.57602500	-1.28714300	-1.46881400
H	5.09407300	-0.08532200	-2.69759800
H	5.72811800	0.42770000	-1.10438700
C	2.03351300	-0.99049300	2.39046600
H	2.56388100	-1.92746600	2.58418900
H	2.49383800	-0.20426200	2.99730400
H	0.99820400	-1.11272300	2.72151900
O	2.72547700	-0.18602800	-1.79996500
C	-0.80285200	1.88244600	0.19890200
C	-2.14820700	1.93164900	-0.06259300
C	-2.91607100	0.73761300	-0.17374600
C	-2.25390300	-0.52250200	-0.00736200
C	-0.85979400	-0.53974500	0.25871800
H	-4.81106800	1.70587300	-0.56879900
H	-0.21651500	2.78989500	0.28688400
H	-2.64828100	2.88819800	-0.18803800
C	-4.30996300	0.75020300	-0.44211700
C	-3.01185500	-1.72094300	-0.11544500
H	-0.38280600	-1.50632700	0.38121700
C	-4.36332900	-1.67533300	-0.37596000
C	-5.01707300	-0.42885600	-0.54069100
H	-2.50587900	-2.67415400	0.01112900
H	-4.93413200	-2.59522700	-0.45684400
H	-6.08302000	-0.40687300	-0.74631700
C	-0.13214200	0.63430400	0.36298500
C	1.33574700	0.66811500	0.65415500
O	1.91224500	1.74674100	0.76658900
C	3.55972100	-0.48633500	0.42751300
H	4.15309500	-1.35508800	0.73839200
H	4.02184100	0.38514300	0.90777500

##### R\* (in H<sub>2</sub>O)

C	2.29215900	-0.57980100	-0.02307600
C	1.02750200	-0.00785300	0.52471900
C	-3.05310700	1.63329000	-0.02917400
C	-1.76884300	1.11672100	0.14215800
C	-1.52661500	-0.25618500	-0.03303000



C	-2.59839200	-1.09714900	-0.38338800
C	-3.87712100	-0.57983700	-0.55919600
C	-4.10727900	0.78857800	-0.38155600
H	-3.22884700	2.69506200	0.11136800
H	-0.96742900	1.79279400	0.41712000
H	-2.40273300	-2.15558700	-0.51421800
H	-4.69551800	-1.23836900	-0.83323900
H	-5.10533900	1.19400600	-0.51743900
C	-0.18004400	-0.88475500	0.13990900
O	-0.03627600	-2.09575100	0.02135800
C	3.42278600	0.16843500	-0.50794600
O	4.43543400	-0.44368000	-0.90000400
C	3.37556700	1.68588900	-0.54835100
H	4.34024000	2.06335000	-0.88991900
H	3.15308500	2.10724000	0.43759500
H	2.59491700	2.03459000	-1.23380300
H	2.39027900	-1.66115700	-0.03809800
H	0.88747400	1.00856400	0.15108000
C	1.08407400	0.05594000	2.08385500
H	1.22488200	-0.94574200	2.49806700
H	0.15626700	0.47324700	2.48527800
H	1.91533800	0.68780700	2.40583000

R<sup>⊖</sup> (in H<sub>2</sub>O)

C	1.96018400	0.10704300	0.51501600
C	1.38326500	0.94593200	-0.60513500
C	-2.44173700	-1.36509100	-0.95359400
C	-1.26955600	-0.60927900	-0.92185700
C	-1.14231300	0.48152400	-0.04494500
C	-2.23080100	0.79675200	0.78686300
C	-3.39853600	0.03768700	0.76331200
C	-3.50910500	-1.04881000	-0.10903500
H	-2.52187700	-2.20286800	-1.64036600
H	-0.45668200	-0.87653100	-1.58653300
H	-2.13554900	1.65090600	1.44877300
H	-4.22416100	0.29335900	1.42161100
H	-4.41907600	-1.64127900	-0.13341200
C	0.06087700	1.39198500	-0.00032100
O	-0.02391900	2.45902900	0.62047600
C	2.24174300	-1.25847900	0.54417900
O	2.67550700	-1.87782700	1.57278100
C	2.05186400	-2.12355400	-0.71275400
H	2.92449500	-2.77792700	-0.81602400

H	1.92631200	-1.56869900	-1.64701600
H	1.17886300	-2.77823800	-0.59116900
H	2.12237200	0.64591900	1.44973900
H	1.19921500	0.32202100	-1.48337600
C	2.25394400	2.13876800	-1.02550900
H	2.44938300	2.79095800	-0.16985000
H	1.77144800	2.74428000	-1.80355400
H	3.21357900	1.78161000	-1.41220200

IrH<sup>+</sup>-1 (in H<sub>2</sub>O)

Ir	-0.78228900	-0.28171800	0.01031200
C	-2.13378200	-0.76833400	-1.41906300
C	-1.88058400	-2.01108900	-2.07422500
C	-3.25175100	-0.02058500	-1.81144800
C	-2.75935400	-2.43470000	-3.08607700
C	-4.08162900	-0.49386700	-2.82052600
C	-3.86412900	-1.69981700	-3.47973600
H	-3.49803100	0.92748300	-1.34854900
F	-2.54950400	-3.60780000	-3.72892400
F	-5.15160900	0.24224000	-3.18358300
H	-4.52316300	-2.05279800	-4.26261300
N	0.00453400	-2.10015000	-0.63538200
C	1.13674800	-2.64273300	-0.15581100
C	-0.69288400	-2.73403100	-1.63251800
C	1.63803000	-3.84864500	-0.62230200
C	-0.22219000	-3.96036600	-2.13359500
C	0.93967300	-4.52066700	-1.62978800
H	1.64998900	-2.08692800	0.61561700
H	1.30627900	-5.46323900	-2.02124000
N	0.73459100	0.68947100	-1.27351200
C	1.80260400	1.21905700	-0.63728600
C	0.74449100	0.64458200	-2.62063200
C	2.90022600	1.70538800	-1.34345600
C	1.80235300	1.12150600	-3.37641000
C	2.92964600	1.66849200	-2.74379200
H	-0.13002800	0.20937800	-3.08962200
H	3.73868300	2.11124000	-0.79746200
H	1.73595300	1.05421800	-4.45593400
N	0.82676600	0.21829900	1.37594000
C	1.10374300	-0.32418000	2.54259400
C	1.67248200	1.31684300	0.88998300
C	2.23634700	-0.00976800	3.31879700
C	2.95105700	1.52861500	1.64771500
C	3.21329000	0.91056200	2.84199800

H	2.35747200	-0.52216300	4.26501900
H	3.62413100	2.27885200	1.25509200
N	-1.76416600	1.44558500	0.61034800
C	-2.66252100	1.29645300	1.63560900
C	-1.56961700	2.65159800	0.04886200
C	-3.35504300	2.42240000	2.11378300
C	-2.23877200	3.78640900	0.48270400
C	-3.14426000	3.66640300	1.54160600
H	-3.67583200	4.53532500	1.91359900
C	-2.00431900	-1.05114300	1.42049100
C	-2.79703000	-0.07917000	2.10269400
C	-2.10236300	-2.39298000	1.80891000
C	-3.63797800	-0.50519500	3.14411300
C	-2.95576000	-2.74942900	2.84730600
C	-3.73776900	-1.82884500	3.53765600
H	-1.52645700	-3.17257500	1.32401800
H	-4.39579000	-2.12621500	4.34413200
H	-0.86081500	2.69336500	-0.76707600
H	0.41159300	-1.08601800	2.89197200
C	4.48558900	1.16141600	3.66478400
C	4.11387200	2.19166000	-3.56673000
C	5.25137600	2.72728700	-2.67783800
H	4.92457900	3.56777000	-2.05692600
H	5.65941600	1.95034600	-2.02301000
H	6.06775500	3.08536600	-3.31170300
C	3.61831600	3.33991900	-4.47967300
H	4.45114300	3.71721800	-5.08178200
H	2.83355400	3.00877400	-5.16587900
H	3.22324200	4.17104200	-3.88666800
C	4.66935000	1.03940700	-4.43878400
H	5.51295300	1.40238700	-5.03459100
H	5.02366100	0.21070100	-3.81739800
H	3.91707000	0.64850500	-5.12988000
C	5.23861500	-0.17816000	3.84924600
H	6.14431900	-0.01535700	4.44244100
H	4.63086100	-0.92384400	4.37024800
H	5.53557900	-0.59831600	2.88287100
C	5.43125300	2.16419600	2.97952300
H	6.32575700	2.29836600	3.59492900
H	5.75662400	1.80998700	1.99587600
H	4.96548000	3.14748800	2.85687900
C	4.08491400	1.72502900	5.04915500
H	3.55520700	2.67764800	4.94705600
H	3.44000100	1.03595400	5.60248700

H	4.98213800	1.89660600	5.65276900
H	-0.77047200	-4.45818500	-2.91806800
H	-4.05416600	2.30971100	2.92787900
C	2.88422700	-4.43497500	-0.02188300
F	2.59628000	-5.37874800	0.90361600
F	3.64907000	-5.03032900	-0.96191600
F	3.63848900	-3.49688400	0.58971700
C	-2.02425800	5.10334000	-0.20869400
F	-0.85135600	5.13557700	-0.87629500
F	-3.00119000	5.35746200	-1.10898600
F	-2.02663700	6.12696100	0.67125900
F	-3.03559800	-4.04565200	3.20863000
F	-4.39871200	0.38943500	3.81734800
H	1.06918200	2.23607200	1.04837900

IrH<sup>+</sup>-2 (in H<sub>2</sub>O)

Ir	-0.82274200	-0.07911800	-0.00556500
C	-2.27094500	-0.36520300	1.37210500
C	-2.73371800	0.83247700	1.99690200
C	-2.81686900	-1.58956800	1.77817700
C	-3.71556600	0.73612300	2.99729500
C	-3.78557800	-1.61641200	2.77467200
C	-4.25815400	-0.47002800	3.40602300
H	-2.50459200	-2.52929500	1.33809000
F	-4.17495400	1.85030800	3.61392500
F	-4.29808700	-2.80469700	3.15313700
H	-5.01383500	-0.51175200	4.17998900
N	-1.17859200	1.88940700	0.55292400
C	-0.53679100	2.94499800	0.02404500
C	-2.12218800	2.07267500	1.53098600
C	-0.78855300	4.24538200	0.43497700
C	-2.40706800	3.37403200	1.97965600
C	-1.74275000	4.46031100	1.43435400
H	0.19286300	2.72960800	-0.74393400
H	-1.95800100	5.46393800	1.78440400
N	0.88604600	-0.08351500	1.36563300
C	2.10061000	0.15636800	0.78811000
C	0.83203700	-0.26033300	2.69419500
C	3.26930100	0.20902000	1.56738000
C	1.95708300	-0.21666900	3.50810600
C	3.22522600	0.02331800	2.95121500
H	-0.15155200	-0.44625400	3.10997200
H	4.21174700	0.40137500	1.07565200
H	1.82705700	-0.37133600	4.57258000

N	0.92817000	0.33201800	-1.28378600
C	0.87746800	0.50446900	-2.61603300
C	2.11380900	0.35363400	-0.64984000
C	2.03217600	0.68279700	-3.42238900
C	3.40871800	0.60708300	-1.37842700
C	3.28338800	0.71584500	-2.87961100
H	1.87478500	0.77953200	-4.48903900
H	3.86301700	1.53084200	-0.98324500
N	-0.66950000	-2.07161000	-0.57628100
C	-1.48788400	-2.46426200	-1.60410700
C	0.17573800	-2.95061800	-0.01066400
C	-1.42830200	-3.79059300	-2.06625400
C	0.26430300	-4.26866000	-0.43232600
C	-0.55445700	-4.69332800	-1.48373200
H	-0.50514600	-5.71510200	-1.84407700
C	-2.22381200	-0.13452100	-1.46151800
C	-2.35397600	-1.40225900	-2.10546500
C	-3.02714700	0.92649600	-1.89860900
C	-3.27943800	-1.53513400	-3.15427900
C	-3.92306800	0.72983700	-2.94291700
C	-4.07463600	-0.49063500	-3.59371600
H	-2.97238800	1.90918700	-1.44528100
H	-4.77876700	-0.62452200	-4.40493600
H	0.79005100	-2.57795300	0.79685100
H	-0.10908900	0.48643200	-3.06194400
C	4.56410200	0.84765700	-3.70001100
C	4.47294800	0.07288500	3.84229900
C	5.75374900	0.36319900	3.03826700
H	5.95357700	-0.41298100	2.29237500
H	5.70592700	1.33081500	2.52805200
H	6.60909500	0.39246000	3.71954300
C	4.63460000	-1.29320700	4.55297400
H	5.51668900	-1.26920500	5.20095500
H	3.76918800	-1.53556500	5.17649300
H	4.76766600	-2.10135200	3.82655500
C	4.29009700	1.18813800	4.90046600
H	5.16991200	1.22694900	5.55068900
H	4.17470500	2.16714800	4.42442300
H	3.41551400	1.01257800	5.53328900
C	4.26802200	1.15366500	-5.18066900
H	5.21089700	1.26354500	-5.72424100
H	3.70534200	0.34682300	-5.66019500
H	3.70449600	2.08503400	-5.29634300
C	5.44808600	1.98494100	-3.12956400

H	6.33986200	2.09915500	-3.75334700
H	4.91302600	2.94027700	-3.12637900
H	5.78686400	1.77625500	-2.11082800
C	5.34707000	-0.49067800	-3.62345800
H	5.63995800	-0.74139800	-2.59966100
H	4.75230100	-1.31776800	-4.02343300
H	6.26311800	-0.41085200	-4.21757100
H	-3.14595700	3.52006000	2.75220700
H	-2.06736000	-4.09899300	-2.87906800
C	-0.08046600	5.39908800	-0.21653600
F	-0.86287600	6.00676500	-1.13774700
F	0.26013700	6.34129200	0.68884600
F	1.04667800	5.00797400	-0.84800700
C	1.19302000	-5.22874100	0.25534600
F	2.12088700	-4.59041900	0.99920400
F	0.52222300	-6.06260000	1.08268500
F	1.84445800	-6.00609500	-0.63660900
F	-4.68605200	1.76408100	-3.35070800
F	-3.42758500	-2.72132600	-3.78991800
H	4.13273800	-0.17879900	-1.11733500

IrH<sup>+</sup>-3 (in H<sub>2</sub>O)

Ir	0.68919900	-0.35056300	-0.05871600
C	1.87227200	-0.86134100	-1.62218300
C	2.85527900	0.11822600	-1.95762000
C	1.79844700	-2.03001600	-2.39047000
C	3.70760900	-0.12619100	-3.04774600
C	2.67123900	-2.21125200	-3.45712500
C	3.63909200	-1.27742800	-3.81348900
H	1.07458700	-2.80870700	-2.17985400
F	4.64945500	0.78141500	-3.39718500
F	2.58354100	-3.34219800	-4.18582600
H	4.30995700	-1.43709900	-4.64793100
N	1.93678200	1.31125300	-0.12337100
C	1.84972600	2.34626800	0.72952300
C	2.87959100	1.31294500	-1.11924700
C	2.68968600	3.44664400	0.64545400
C	3.74877200	2.41057400	-1.24350700
C	3.65684800	3.47667900	-0.36393700
H	1.08550200	2.28094300	1.49165000
H	4.32499500	4.32515100	-0.46285200
N	-0.79395600	0.82198400	-1.17733200
C	-1.75231100	1.43448800	-0.44056700
C	-0.77731900	1.01660200	-2.51013200

C	-2.70668500	2.25789000	-1.04790100
C	-1.69999000	1.81801700	-3.16049000
C	-2.70502300	2.47280600	-2.42856200
H	0.00547700	0.50346200	-3.05554900
H	-3.45263400	2.73844200	-0.43220100
H	-1.62266000	1.92608000	-4.23587700
N	-0.64665800	0.41448800	1.46132600
C	-0.52577200	0.17611200	2.80110700
C	-1.71703300	1.17439500	1.02235300
C	-1.41958700	0.61664000	3.73287900
C	-2.66520700	1.64826400	1.88993500
C	-2.64608900	1.37662200	3.35716500
H	-1.22385100	0.40347600	4.77710500
H	-3.47756500	2.25290900	1.50962200
N	-0.38190100	-2.12980200	-0.03541700
C	0.14808900	-3.13747800	0.72884800
C	-1.53197700	-2.31799200	-0.70370000
C	-0.52478500	-4.36909900	0.80671900
C	-2.22739900	-3.51704800	-0.65632100
C	-1.71025200	-4.56173500	0.11606200
H	-2.23142000	-5.51058100	0.18113000
C	1.87810700	-1.45639000	1.14653000
C	1.39807800	-2.77887700	1.39088900
C	3.07071300	-1.05018500	1.75799900
C	2.13886800	-3.62034000	2.23779100
C	3.75571900	-1.93121600	2.58700200
C	3.31679300	-3.22540800	2.84846300
H	3.48355800	-0.05979600	1.60603700
H	3.86524700	-3.89681200	3.49673400
H	-1.89381800	-1.48061700	-1.28383500
H	0.35125500	-0.39046400	3.09075100
C	-4.00295400	0.70880800	3.89391000
C	-3.72695800	3.37071200	-3.13740300
C	-4.74501500	3.98399100	-2.15863700
H	-5.32905700	3.21602900	-1.64092000
H	-4.26098500	4.61714500	-1.40793100
H	-5.44744600	4.61232400	-2.71386400
C	-4.49448300	2.52741200	-4.18480400
H	-5.22393000	3.15864600	-4.70216600
H	-3.82638200	2.10293900	-4.93976300
H	-5.03528300	1.70380200	-3.70771700
C	-2.97227000	4.51985200	-3.84967300
H	-3.68817500	5.16228900	-4.37236500
H	-2.42461500	5.13613000	-3.12939400

H	-2.25804200	4.14616700	-4.58924000
C	-3.92469700	0.58606300	5.42737000
H	-4.88098000	0.21980600	5.81469500
H	-3.15349400	-0.11892300	5.75018300
H	-3.72342100	1.55503100	5.89761400
C	-5.19304900	1.61854200	3.53488300
H	-6.10546600	1.22578700	3.99501700
H	-5.04588700	2.63908500	3.90542200
H	-5.37167200	1.66640400	2.45679000
C	-4.19578100	-0.68083500	3.26363000
H	-4.26577200	-0.61936600	2.17257500
H	-3.36916700	-1.35327900	3.51497900
H	-5.12124800	-1.13495700	3.63285900
H	4.48729600	2.41667300	-2.02993000
H	-0.11246500	-5.16217200	1.41093400
C	2.58691000	4.55777900	1.65178200
F	3.52378600	4.43969200	2.62035300
F	2.77188800	5.76392400	1.07391300
F	1.38365600	4.57418200	2.26346800
C	-3.48516700	-3.69356500	-1.45933400
F	-4.06052100	-2.50931100	-1.75866600
F	-3.24423100	-4.32545900	-2.63099100
F	-4.39395200	-4.43699400	-0.79335900
F	4.90095100	-1.52139400	3.16840700
F	1.71237900	-4.87935600	2.49412100
H	-2.62537100	2.35179300	3.87918200

IrH<sup>2+</sup> (in H<sub>2</sub>O)

Ir	0.80371100	-0.09450500	0.00349600
C	2.23874000	-0.41229700	-1.37575800
C	2.75927600	0.77391300	-1.97173200
C	2.71990400	-1.65398100	-1.80399200
C	3.73707200	0.64937400	-2.97355600
C	3.68845800	-1.70805000	-2.80093100
C	4.21855500	-0.57394000	-3.40663500
H	2.36109100	-2.58600400	-1.38537800
F	4.25080300	1.75103800	-3.56493700
F	4.13884300	-2.91144300	-3.20231100
H	4.97259000	-0.63724400	-4.18071600
N	1.25328300	1.87517400	-0.50903900
C	0.67199200	2.95386700	0.04447700
C	2.21053700	2.03144800	-1.47861400
C	0.99980100	4.24765100	-0.33001100
C	2.56872400	3.32508900	-1.89480900



C	1.96643600	4.43333900	-1.32305800
H	-0.07236600	2.76988200	0.80553100
H	2.23993500	5.43152400	-1.64680900
N	-0.93040600	0.02009000	-1.35073200
C	-2.14201700	0.28743200	-0.77940300
C	-0.88072800	-0.10838300	-2.67956500
C	-3.30586200	0.41951500	-1.54685500
C	-2.00883500	0.01720900	-3.49290300
C	-3.26777700	0.28918100	-2.94124000
H	0.09164800	-0.32255000	-3.10673400
H	-4.24531600	0.62797800	-1.05542500
H	-1.87783800	-0.10315900	-4.56187000
N	-0.96514500	0.32296700	1.28952100
C	-0.93249800	0.40107100	2.64856600
C	-2.14173000	0.42054800	0.67174200
C	-2.03943400	0.55663700	3.47701200
C	-3.39171800	0.68720600	1.43673200
C	-3.30300700	0.68556600	2.92152900
H	-1.87627600	0.57839900	4.54560600
H	-3.74939100	1.69191000	1.14398800
N	0.59974600	-2.10498200	0.51313800
C	1.42509900	-2.55215800	1.51274700
C	-0.26229100	-2.94848600	-0.08240400
C	1.35566700	-3.89701100	1.91518700
C	-0.36118300	-4.28231400	0.28086100
C	0.46504400	-4.76237400	1.30243400
H	0.41023300	-5.79921500	1.61596600
C	2.20527100	-0.23268600	1.45288000
C	2.30943700	-1.52399000	2.05065600
C	3.02207100	0.80010400	1.92540200
C	3.22994100	-1.70834300	3.09654800
C	3.91270800	0.55182200	2.96489800
C	4.04141100	-0.69259900	3.57224400
H	2.98603800	1.79815200	1.50634200
H	4.74081900	-0.86629200	4.37999100
H	-0.88006200	-2.53723800	-0.86796300
H	0.05915100	0.32666700	3.08247300
C	-4.56293700	0.79669400	3.74339900
C	-4.50841400	0.42465200	-3.83026500
C	-5.77382100	0.74803300	-3.01504500
H	-6.01471100	-0.04477900	-2.29937600
H	-5.68202900	1.69457400	-2.47204300
H	-6.62413100	0.84261700	-3.69580000
C	-4.72702300	-0.91250200	-4.58089200

H	-5.60627400	-0.82733400	-5.22663000
H	-3.87335100	-1.17339000	-5.21290000
H	-4.89767300	-1.73528800	-3.87956400
C	-4.26831000	1.56360600	-4.85160200
H	-5.14474500	1.66153300	-5.49927000
H	-4.10933200	2.52082000	-4.34541000
H	-3.40297000	1.36719300	-5.49081700
C	-4.28915000	1.38314100	5.14490900
H	-5.23901200	1.47343200	5.67762000
H	-3.64121300	0.74157100	5.74729300
H	-3.84000000	2.37836900	5.08170600
C	-5.64722500	1.63938200	3.03452100
H	-6.52807300	1.68798700	3.67882500
H	-5.30444800	2.66383300	2.85725100
H	-5.96655900	1.20427000	2.08436500
C	-5.08096000	-0.67374800	3.90091200
H	-5.33408200	-1.12253500	2.93678100
H	-4.34577900	-1.30671200	4.40367900
H	-5.98740400	-0.64090300	4.51203500
H	3.31723700	3.44770000	-2.66198100
H	2.00190900	-4.24977900	2.70382100
C	0.36009700	5.42297300	0.35517100
F	1.17888800	5.95760400	1.28829100
F	0.07181000	6.40521800	-0.52377300
F	-0.78567200	5.07795700	0.98023100
C	-1.31264600	-5.20155200	-0.43330700
F	-2.19774100	-4.52116300	-1.19138900
F	-0.65601700	-6.05542200	-1.24893700
F	-2.01279000	-5.95526300	0.44104500
F	4.68959700	1.55791800	3.40777700
F	3.35344700	-2.91597700	3.69111500
H	-4.19829400	0.02371600	1.10050900

IrIII (in H<sub>2</sub>O)

Ir	0.00000000	0.00000000	0.80565000
C	-0.09440000	1.41623800	2.24319300
C	-1.41715300	1.86193500	2.54376300
C	0.98256700	2.00052600	2.92197300
C	-1.58707000	2.87136100	3.50620900
C	0.74669900	2.99634500	3.86262000
C	-0.52797400	3.45563400	4.17947900
H	2.00702800	1.70021800	2.73554000
F	-2.82650300	3.32031400	3.81458500
F	1.79632600	3.54797100	4.50436700

H	-0.69113800	4.23186700	4.91613700
N	-2.05770300	0.26516800	0.91141600
C	-2.94163900	-0.42198000	0.16809400
C	-2.49313000	1.21450600	1.80035200
C	-4.30886900	-0.20566700	0.25549600
C	-3.87013100	1.47082100	1.91689300
C	-4.77893900	0.76365500	1.14703400
H	-2.53241200	-1.15906200	-0.50853200
H	-5.84105200	0.96491600	1.23353900
N	0.00000000	1.33805100	-0.93904100
C	-0.02804600	0.74129100	-2.15697900
C	-0.04204400	2.68150900	-0.87885800
C	-0.10875200	1.50030900	-3.32863000
C	-0.11596700	3.48088100	-2.00867100
C	-0.15794500	2.89737200	-3.28502800
H	-0.01256900	3.11502400	0.11362500
H	-0.14245600	0.99290900	-4.28138400
H	-0.14516100	4.55604100	-1.87675400
N	0.00000000	-1.33805100	-0.93904100
C	0.04204400	-2.68150900	-0.87885800
C	0.02804600	-0.74129100	-2.15697900
C	0.11596700	-3.48088100	-2.00867100
C	0.10875200	-1.50030900	-3.32863000
C	0.15794500	-2.89737200	-3.28502800
H	0.14516100	-4.55604100	-1.87675400
H	0.14245600	-0.99290900	-4.28138400
N	2.05770300	-0.26516800	0.91141600
C	2.49313000	-1.21450600	1.80035200
C	2.94163900	0.42198000	0.16809400
C	3.87013100	-1.47082100	1.91689300
C	4.30886900	0.20566700	0.25549600
C	4.77893900	-0.76365500	1.14703400
H	5.84105200	-0.96491600	1.23353900
C	0.09440000	-1.41623800	2.24319300
C	1.41715300	-1.86193500	2.54376300
C	-0.98256700	-2.00052600	2.92197300
C	1.58707000	-2.87136100	3.50620900
C	-0.74669900	-2.99634500	3.86262000
C	0.52797400	-3.45563400	4.17947900
H	-2.00702800	-1.70021800	2.73554000
H	0.69113800	-4.23186700	4.91613700
H	2.53241200	1.15906200	-0.50853200
H	0.01256900	-3.11502400	0.11362500
C	0.25842200	-3.77098700	-4.54173900

C	-0.25842200	3.77098700	-4.54173900
C	-0.29426200	2.93459500	-5.83395800
H	0.61451100	2.33721700	-5.96068200
H	-1.15854200	2.26297400	-5.86284800
H	-0.36992200	3.60433100	-6.69545700
C	0.96807400	4.71438600	-4.59610000
H	0.90560500	5.34877300	-5.48609800
H	1.01954100	5.37066900	-3.72259800
H	1.90110800	4.14435100	-4.64930400
C	-1.55586800	4.61233300	-4.46118000
H	-1.63904900	5.24679200	-5.34938200
H	-2.44030600	3.96868600	-4.41845700
H	-1.56724500	5.26468400	-3.58331600
C	-0.96807400	-4.71438600	-4.59610000
H	-0.90560500	-5.34877300	-5.48609800
H	-1.01954100	-5.37066900	-3.72259800
H	-1.90110800	-4.14435100	-4.64930400
C	0.29426200	-2.93459500	-5.83395800
H	0.36992200	-3.60433100	-6.69545700
H	-0.61451100	-2.33721700	-5.96068200
H	1.15854200	-2.26297400	-5.86284800
C	1.55586800	-4.61233300	-4.46118000
H	2.44030600	-3.96868600	-4.41845700
H	1.56724500	-5.26468400	-3.58331600
H	1.63904900	-5.24679200	-5.34938200
H	-4.21341100	2.22337700	2.60966100
H	4.21341100	-2.22337700	2.60966100
C	-5.26095500	-1.03399700	-0.56008000
F	-5.78285500	-2.05032900	0.16425900
F	-6.30051800	-0.29514900	-1.00284000
F	-4.65754500	-1.58265600	-1.63605300
C	5.26095500	1.03399700	-0.56008000
F	4.65754500	1.58265600	-1.63605300
F	5.78285500	2.05032900	0.16425900
F	6.30051800	0.29514900	-1.00284000
F	-1.79632600	-3.54797100	4.50436700
F	2.82650300	-3.32031400	3.81458500

IrII (in H<sub>2</sub>O)

Ir	0.00000000	0.00000000	0.81859500
C	0.22534200	1.41082900	2.25446700
C	-0.96605100	2.14497500	2.54839900
C	1.39816700	1.74010900	2.95082000
C	-0.91467900	3.16483100	3.51307400

C	1.38310100	2.76052700	3.89273200
C	0.24116800	3.49588400	4.19931700
H	2.33084400	1.21651100	2.77200600
F	-2.02602500	3.88204700	3.81343800
F	2.52414000	3.06287500	4.54935600
H	0.24933400	4.28767400	4.93747400
N	-1.93380100	0.73298200	0.90770500
C	-2.93657300	0.27230900	0.14169000
C	-2.15378700	1.75635200	1.79421400
C	-4.21990300	0.79551000	0.21007900
C	-3.43981300	2.31604700	1.89599200
C	-4.47358900	1.83773100	1.10757900
H	-2.68303000	-0.53022400	-0.53774900
H	-5.46426300	2.27268100	1.18167200
N	0.35641900	1.29517000	-0.88892100
C	0.18719400	0.68899200	-2.13080300
C	0.69212000	2.60148600	-0.84651200
C	0.40243200	1.46262000	-3.31163300
C	0.89674100	3.38001600	-1.96588500
C	0.75401500	2.79489700	-3.26402600
H	0.80310100	3.02146700	0.14812500
H	0.28232000	0.97283500	-4.26831500
H	1.16707700	4.42137800	-1.83856600
N	-0.35641900	-1.29517000	-0.88892100
C	-0.69212000	-2.60148600	-0.84651200
C	-0.18719400	-0.68899200	-2.13080300
C	-0.89674100	-3.38001600	-1.96588500
C	-0.40243200	-1.46262000	-3.31163300
C	-0.75401500	-2.79489700	-3.26402600
H	-1.16707700	-4.42137800	-1.83856600
H	-0.28232000	-0.97283500	-4.26831500
N	1.93380100	-0.73298200	0.90770500
C	2.15378700	-1.75635200	1.79421400
C	2.93657300	-0.27230900	0.14169000
C	3.43981300	-2.31604700	1.89599200
C	4.21990300	-0.79551000	0.21007900
C	4.47358900	-1.83773100	1.10757900
H	5.46426300	-2.27268100	1.18167200
C	-0.22534200	-1.41082900	2.25446700
C	0.96605100	-2.14497500	2.54839900
C	-1.39816700	-1.74010900	2.95082000
C	0.91467900	-3.16483100	3.51307400
C	-1.38310100	-2.76052700	3.89273200
C	-0.24116800	-3.49588400	4.19931700

H	-2.33084400	-1.21651100	2.77200600
H	-0.24933400	-4.28767400	4.93747400
H	2.68303000	0.53022400	-0.53774900
H	-0.80310100	-3.02146700	0.14812500
C	-0.99338800	-3.64997000	-4.51580800
C	0.99338800	3.64997000	-4.51580800
C	0.80100500	2.85354800	-5.81958600
H	1.49987900	2.01347200	-5.89058000
H	-0.21704200	2.46032200	-5.90946500
H	0.98055800	3.50698700	-6.67935300
C	2.44115200	4.19782500	-4.48959200
H	2.62373800	4.82482000	-5.36937400
H	2.63051500	4.80674600	-3.60071100
H	3.16892600	3.37940300	-4.49893600
C	0.00000000	4.83747500	-4.51988000
H	0.17180900	5.46994700	-5.39782300
H	-1.03504400	4.48116100	-4.55535600
H	0.11054600	5.46383200	-3.62980800
C	-2.44115200	-4.19782500	-4.48959200
H	-2.62373800	-4.82482000	-5.36937400
H	-2.63051500	-4.80674600	-3.60071100
H	-3.16892600	-3.37940300	-4.49893600
C	-0.80100500	-2.85354800	-5.81958600
H	-0.98055800	-3.50698700	-6.67935300
H	-1.49987900	-2.01347200	-5.89058000
H	0.21704200	-2.46032200	-5.90946500
C	0.00000000	-4.83747500	-4.51988000
H	1.03504400	-4.48116100	-4.55535600
H	-0.11054600	-5.46383200	-3.62980800
H	-0.17180900	-5.46994700	-5.39782300
H	-3.61414700	3.12297300	2.59079800
H	3.61414700	-3.12297300	2.59079800
C	-5.31963700	0.21517900	-0.63090600
F	-6.06280900	-0.67857600	0.06373800
F	-6.16879500	1.17280500	-1.06392500
F	-4.84043900	-0.42972700	-1.71636700
C	5.31963700	-0.21517900	-0.63090600
F	4.84043900	0.42972700	-1.71636700
F	6.06280900	0.67857600	0.06373800
F	6.16879500	-1.17280500	-1.06392500
F	-2.52414000	-3.06287500	4.54935600
F	2.02602500	-3.88204700	3.81343800

IrH<sub>3</sub> (in H<sub>2</sub>O)

Ir	0.83463600	-0.31808900	-0.03737200
C	2.06576300	-0.84166100	1.49965400
C	1.68561600	-2.03043100	2.19468000
C	3.22643700	-0.17110000	1.92072300
C	2.48792400	-2.48538500	3.25561400
C	3.97278000	-0.66756500	2.97993400
C	3.63299500	-1.82814100	3.67072200
H	3.56830000	0.73529500	1.43315800
F	2.16262700	-3.61608600	3.93205200
F	5.08688500	-0.00671200	3.36585500
H	4.23022100	-2.20420900	4.49153800
N	-0.16181100	-2.00726200	0.69552400
C	-1.35036200	-2.44187100	0.24231700
C	0.44471500	-2.65373600	1.74631200
C	-1.98962600	-3.55403200	0.77564600
C	-0.16290400	-3.79100200	2.30707000
C	-1.37698900	-4.24751300	1.82205000
H	-1.79328000	-1.87830700	-0.57096600
H	-1.84951300	-5.11969000	2.26022100
N	-0.65079000	0.84928700	1.11633400
C	-1.59602900	1.47556500	0.37542400
C	-0.77581600	0.83486700	2.45740400
C	-2.68594600	2.09482200	0.99131400
C	-1.83711000	1.43204300	3.11723900
C	-2.84108600	2.08446800	2.38274300
H	0.00782500	0.32151800	3.00358500
H	-3.42006300	2.58501200	0.36739600
H	-1.87171800	1.37676700	4.19919400
N	-0.60008700	0.29874100	-1.54780300
C	-1.32896200	-0.57537300	-2.31184900
C	-1.29886400	1.51701700	-1.12746400
C	-2.63264300	-0.47047800	-2.68623900
C	-2.48504600	1.89054400	-2.03955500
C	-3.46681000	0.72081400	-2.26645500
H	-3.04726000	-1.23088900	-3.33953800
H	-2.98178100	2.78078500	-1.64374600
N	2.00139600	1.25656600	-0.68349000
C	2.90332900	0.96851600	-1.67674200
C	1.92629300	2.50154500	-0.18246700
C	3.71948200	1.99363700	-2.18888200
C	2.72031100	3.53944400	-0.64878800
C	3.62989500	3.27821400	-1.67983300
H	4.25634700	4.06960000	-2.07638900
C	2.01774700	-1.28284100	-1.34196500

C	2.91526500	-0.43628800	-2.06411900
C	2.00606100	-2.65425900	-1.64219100
C	3.73599000	-1.00439700	-3.05231100
C	2.84496400	-3.15268200	-2.62934500
C	3.72355800	-2.35423000	-3.35827100
H	1.34737600	-3.34331800	-1.12548900
H	4.36853800	-2.76333300	-4.12536800
H	1.20440500	2.65531300	0.60890000
H	-0.75475000	-1.44187000	-2.64535300
C	-4.64606900	1.05548900	-3.24530300
C	-4.03194200	2.73555600	3.10001100
C	-5.00041900	3.42392800	2.12007000
H	-4.51081400	4.22604300	1.55814000
H	-5.43236400	2.71592900	1.40516300
H	-5.82726900	3.87038100	2.68063700
C	-3.50602600	3.79721100	4.09620900
H	-4.34741100	4.26643800	4.61650400
H	-2.84931400	3.35950900	4.85365600
H	-2.94783800	4.58230900	3.57584900
C	-4.80842800	1.64202600	3.87332000
H	-5.65840400	2.09050100	4.39832100
H	-5.19520200	0.87829000	3.19067900
H	-4.17999400	1.14479300	4.61789900
C	-5.62499900	-0.13834300	-3.27601300
H	-6.48939400	0.09044600	-3.91001500
H	-5.15916000	-1.04517900	-3.67279100
H	-5.99923300	-0.36610200	-2.27074300
C	-5.42662300	2.28666900	-2.73894800
H	-6.32359400	2.44766400	-3.34783200
H	-5.75127400	2.15015700	-1.70013100
H	-4.83137700	3.20375000	-2.78834200
C	-4.14652900	1.32978100	-4.67761200
H	-3.50695700	2.21763200	-4.72233800
H	-3.57273200	0.48321000	-5.06742200
H	-4.99406900	1.50259800	-5.35098900
H	0.31897600	-4.29950800	3.12756100
H	4.41921500	1.76878700	-2.97917800
C	-3.29078000	-4.02196300	0.19148800
F	-3.10221700	-4.93446100	-0.79222700
F	-4.06909700	-4.61284200	1.12507200
F	-3.99870100	-3.00605700	-0.34820600
C	2.63324700	4.89931700	-0.01987500
F	1.44624800	5.09899400	0.59328700
F	3.59548700	5.08125200	0.91562200



F	2.79178500	5.87987300	-0.93560300
F	2.81582100	-4.47480300	-2.90705900
F	4.59217100	-0.22688000	-3.76133400
H	-0.58452100	2.35352300	-1.21850300
H	-2.05499800	2.18370700	-3.00323000
H	-3.95811000	0.51441000	-1.29782900

IrH<sub>3</sub><sup>+</sup> (in H<sub>2</sub>O)

Ir	0.80344100	-0.31124200	-0.02480300
C	2.09300900	-0.81158700	1.46126100
C	1.75109800	-1.99918900	2.17393800
C	3.25302800	-0.11898600	1.83271100
C	2.59056800	-2.42908700	3.21637400
C	4.04030500	-0.59471400	2.87413800
C	3.73783800	-1.74997800	3.58772600
H	3.56699800	0.78725000	1.32945500
F	2.29876000	-3.55264900	3.91312900
F	5.15257400	0.08727900	3.21448300
H	4.36450400	-2.10695700	4.39497700
N	-0.12942300	-2.03037400	0.72391100
C	-1.30128600	-2.51406500	0.27906600
C	0.51856200	-2.65853900	1.75830300
C	-1.89025900	-3.65206200	0.80942300
C	-0.03875900	-3.81925000	2.32274100
C	-1.23975000	-4.32070500	1.84956900
H	-1.77991100	-1.96933800	-0.52057700
H	-1.67240000	-5.21191200	2.29054800
N	-0.66827000	0.84392900	1.17414700
C	-1.65282300	1.44760300	0.46650800
C	-0.75079500	0.83435400	2.51776900
C	-2.73789000	2.04454100	1.10261000
C	-1.80477500	1.41486200	3.20472200
C	-2.84589700	2.03906100	2.50072000
H	0.05938500	0.34128500	3.04264400
H	-3.50245800	2.51669300	0.50280700
H	-1.80312000	1.36755500	4.28729400
N	-0.74124400	0.23320400	-1.42856000
C	-1.26292000	-0.51103700	-2.40474800
C	-1.40837500	1.49401600	-1.04440600
C	-2.54101900	-0.34112400	-2.92571000
C	-2.57176900	1.90424600	-1.96530800
C	-3.45839200	0.72070800	-2.40085500
H	-2.87294500	-1.04851500	-3.67727000
H	-3.15420100	2.69031600	-1.48448600

N	1.94541600	1.28435500	-0.69152600
C	2.84380200	1.00110500	-1.68833600
C	1.86323300	2.52695000	-0.18415400
C	3.65049400	2.03144300	-2.20116800
C	2.64846500	3.56986200	-0.65294000
C	3.55399700	3.31459200	-1.68762900
H	4.17494700	4.10981300	-2.08503800
C	1.97245200	-1.26174000	-1.36740800
C	2.85732500	-0.40250700	-2.08542600
C	1.95205700	-2.62557800	-1.68239400
C	3.66660200	-0.95651800	-3.09091000
C	2.77991300	-3.11149100	-2.68868900
C	3.64899200	-2.30284400	-3.41413900
H	1.30248900	-3.32256800	-1.16567600
H	4.28501000	-2.70085200	-4.19444300
H	1.14995200	2.67364300	0.61642600
H	-0.65378500	-1.34973700	-2.73368500
C	-4.63020200	1.08715700	-3.37669100
C	-4.02664400	2.66992400	3.25026200
C	-5.04684100	3.31698800	2.29559100
H	-4.59984900	4.12528900	1.70780600
H	-5.48405100	2.58720100	1.60626800
H	-5.86534300	3.74777300	2.87960300
C	-3.49024100	3.76017400	4.20984000
H	-4.32444200	4.21347100	4.75476500
H	-2.79364600	3.35193200	4.94771600
H	-2.97509800	4.55192400	3.65653600
C	-4.74372600	1.56750800	4.06761400
H	-5.58499100	2.00333000	4.61617700
H	-5.13531800	0.78331200	3.41159000
H	-4.07597300	1.09917500	4.79638800
C	-5.52485500	-0.15514000	-3.57343100
H	-6.37301500	0.09187500	-4.22028300
H	-4.99265300	-0.98756200	-4.04400700
H	-5.92491800	-0.50928000	-2.61667600
C	-5.49532300	2.20227400	-2.75403100
H	-6.38488800	2.37197700	-3.36937600
H	-5.83387100	1.92922500	-1.74775600
H	-4.96054300	3.15444900	-2.68752800
C	-4.09986000	1.55723200	-4.74633000
H	-3.49736300	2.46719700	-4.66212700
H	-3.48655400	0.78956400	-5.23045400
H	-4.93725500	1.78129700	-5.41539400
H	0.47346400	-4.31286200	3.13370300

H	4.34887300	1.81386500	-2.99442300
C	-3.17863600	-4.17020200	0.23568800
F	-2.96271300	-5.14189800	-0.68036800
F	-3.96494200	-4.70335900	1.19440100
F	-3.88236200	-3.19547900	-0.38036800
C	2.55753200	4.92971800	-0.01963000
F	1.37670200	5.11461000	0.60781100
F	3.53042100	5.11461500	0.90169300
F	2.69504500	5.90978600	-0.93732600
F	2.74474800	-4.42667000	-2.98173200
F	4.51229000	-0.17064000	-3.79731000
H	-0.63451800	2.26484200	-1.17159900
H	-2.12726300	2.35696900	-2.85648600
H	-3.93960500	0.30798100	-1.49657100

R\* (in ACN)

C	2.29214700	-0.57996200	-0.02298300
C	1.02753100	-0.00739800	0.52442200
C	-3.05352400	1.63288200	-0.02871800
C	-1.76931200	1.11639700	0.14311300
C	-1.52673000	-0.25635100	-0.03259300
C	-2.59810300	-1.09731900	-0.38399200
C	-3.87677900	-0.58008000	-0.56040400
C	-4.10729900	0.78817200	-0.38223000
H	-3.22957200	2.69455200	0.11231600
H	-0.96810100	1.79235600	0.41905600
H	-2.40204900	-2.15564800	-0.51514400
H	-4.69488400	-1.23860800	-0.83534800
H	-5.10534700	1.19350500	-0.51856800
C	-0.18012400	-0.88486900	0.14096600
O	-0.03642300	-2.09586800	0.02380200
C	3.42284400	0.16788600	-0.50824800
O	4.43573600	-0.44424500	-0.89920700
C	3.37527300	1.68544700	-0.55035700
H	4.34008600	2.06260400	-0.89182100
H	3.15224000	2.10793800	0.43500000
H	2.59502600	2.03329300	-1.23674000
H	2.39012500	-1.66132700	-0.03716000
H	0.88722300	1.00851100	0.14934300
C	1.08450700	0.05847000	2.08340600
H	1.22550900	-0.94269500	2.49877900
H	0.15677100	0.47608700	2.48472900
H	1.91587900	0.69068800	2.40449900

R<sup>⊖</sup> (in ACN)

C	1.96079800	0.10479500	0.51485800
C	1.38597900	0.94471300	-0.60540000
C	-2.44376300	-1.35861200	-0.95729800
C	-1.27027900	-0.60487400	-0.92485000
C	-1.13953300	0.48260500	-0.04438800
C	-2.22619100	0.79675300	0.79019000
C	-3.39512200	0.03961300	0.76610300
C	-3.50913400	-1.04366500	-0.10979200
H	-2.52638700	-2.19387100	-1.64688900
H	-0.45891900	-0.87110000	-1.59179900
H	-2.12827800	1.64868200	1.45457100
H	-4.21912000	0.29427500	1.42688800
H	-4.42009900	-1.63464300	-0.13453800
C	0.06452100	1.39208400	0.00011400
O	-0.01938300	2.45910200	0.62115200
C	2.23694000	-1.26214900	0.54437400
O	2.66884000	-1.88308500	1.57220100
C	2.04206100	-2.12647800	-0.71259400
H	2.90864300	-2.78924000	-0.81278200
H	1.92445200	-1.57099800	-1.64761400
H	1.16225300	-2.77234100	-0.59295700
H	2.12473100	0.64349200	1.44928100
H	1.20117700	0.32113800	-1.48375400
C	2.25830400	2.13642800	-1.02520700
H	2.45258700	2.78893000	-0.16953700
H	1.77747800	2.74197200	-1.80433200
H	3.21834100	1.77827600	-1.41002100

IrH<sup>+</sup>-1 (in ACN)

Ir	-0.78254000	-0.28066600	0.01024100
C	-2.13469100	-0.76625800	-1.41887200
C	-1.88350700	-2.01008900	-2.07276500
C	-3.25124100	-0.01699400	-1.81209500
C	-2.76287600	-2.43324700	-3.08435500
C	-4.08189900	-0.48988900	-2.82080500
C	-3.86628900	-1.69684600	-3.47883100
H	-3.49632000	0.93175200	-1.34995200
F	-2.55469900	-3.60720300	-3.72600800
F	-5.15037200	0.24762700	-3.18461900
H	-4.52592400	-2.04949600	-4.26134800
N	0.00161600	-2.10057200	-0.63412500
C	1.13325100	-2.64422100	-0.15444300

C	-0.69719900	-2.73458200	-1.63023900
C	1.63251000	-3.85155000	-0.61937400
C	-0.22875500	-3.96257700	-2.12952500
C	0.93238700	-4.52405600	-1.62537500
H	1.64776000	-2.08793400	0.61583800
H	1.29726000	-5.46788800	-2.01544200
N	0.73625600	0.68715900	-1.27417500
C	1.80504400	1.21576400	-0.63839600
C	0.74618300	0.64100200	-2.62125800
C	2.90311900	1.70044300	-1.34506300
C	1.80467400	1.11586400	-3.37746800
C	2.93256400	1.66230200	-2.74541300
H	-0.12894300	0.20649300	-3.08980400
H	3.74212400	2.10589800	-0.79958600
H	1.73836100	1.04755100	-4.45693600
N	0.82718800	0.21832600	1.37579400
C	1.10200400	-0.32236300	2.54385400
C	1.67521700	1.31469600	0.88887700
C	2.23434600	-0.00848200	3.32062500
C	2.95420500	1.52434600	1.64664600
C	3.21392200	0.90848400	2.84264400
H	2.35351400	-0.51891200	4.26815400
H	3.63008400	2.27143700	1.25284700
N	-1.76214700	1.44833100	0.60923700
C	-2.66123300	1.30088000	1.63412000
C	-1.56553300	2.65388000	0.04741500
C	-3.35225500	2.42820700	2.11149300
C	-2.23277500	3.78999300	0.48064200
C	-3.13909500	3.67168700	1.53912300
H	-3.66948500	4.54161900	1.91049400
C	-2.00625900	-1.04766100	1.42032400
C	-2.79791500	-0.07424000	2.10169100
C	-2.10646600	-2.38912400	1.80919500
C	-3.64027500	-0.49863300	3.14269800
C	-2.96114700	-2.74399300	2.84716200
C	-3.74221900	-1.82195300	3.53665700
H	-1.53182700	-3.16993400	1.32476400
H	-4.40133600	-2.11810200	4.34268400
H	-0.85678200	2.69400600	-0.76861800
H	0.40795300	-1.08217000	2.89393100
C	4.48613800	1.15805500	3.66595200
C	4.11733700	2.18335800	-3.56885900
C	5.25529300	2.71887600	-2.68049200
H	4.92926000	3.56036000	-2.06051700

H	5.66275000	1.94226200	-2.02489400
H	6.07202600	3.07561600	-3.31460200
C	3.62306400	3.33105000	-4.48322900
H	4.45634300	3.70667600	-5.08571300
H	2.83803400	3.00001400	-5.16917400
H	3.22888700	4.16340600	-3.89137000
C	4.67162900	1.02947400	-4.43953100
H	5.51555800	1.39085600	-5.03579600
H	5.02513800	0.20108900	-3.81726300
H	3.91895600	0.63858100	-5.13020100
C	5.23621600	-0.18278700	3.85320600
H	6.14175000	-0.02094600	4.44687400
H	4.62657800	-0.92643400	4.37491700
H	5.53319700	-0.60509200	2.88777000
C	5.43442700	2.15767700	2.97974200
H	6.32862700	2.29122000	3.59566900
H	5.76014100	1.80096100	1.99712100
H	4.97085400	3.14173900	2.85487900
C	4.08556000	1.72497800	5.04901500
H	3.55773100	2.67842200	4.94490200
H	3.43906900	1.03818400	5.60332100
H	4.98269300	1.89600800	5.65286100
H	-0.77838100	-4.46066300	-2.91289600
H	-4.05214300	2.31678900	2.92512400
C	2.87834900	-4.43856500	-0.01872900
F	2.58974600	-5.37923100	0.90946300
F	3.64126600	-5.03719200	-0.95803000
F	3.63451000	-3.49972800	0.58971800
C	-2.01544100	5.10651400	-0.21083400
F	-0.84283300	5.13533100	-0.87941200
F	-2.99231100	5.36336200	-1.11007000
F	-2.01392300	6.12974000	0.66944600
F	-3.04298600	-4.03977700	3.20884200
F	-4.39995900	0.39746200	3.81499500
H	1.07348200	2.23513500	1.04658700

IrH<sup>+</sup>-2 (in ACN)

Ir	-0.82294500	-0.07766700	-0.00564000
C	-2.27186300	-0.35790800	1.37247800
C	-2.73213700	0.84194800	1.99489800
C	-2.82028000	-1.58027200	1.78084800
C	-3.71443700	0.74961500	2.99528600
C	-3.78936300	-1.60322300	2.77716000
C	-4.25961300	-0.45458800	3.40618300

H	-2.51007000	-2.52146600	1.34251800
F	-4.17126700	1.86596200	3.60969700
F	-4.30424000	-2.78956400	3.15774000
H	-5.01566200	-0.49324000	4.17994600
N	-1.17442100	1.89271600	0.54931100
C	-0.53013800	2.94596200	0.01879300
C	-2.11800300	2.07986300	1.52670000
C	-0.77904000	4.24768900	0.42712500
C	-2.40045600	3.38282600	1.97246500
C	-1.73351800	4.46661500	1.42542100
H	0.19930000	2.72756100	-0.74855100
H	-1.94682200	5.47143400	1.77325200
N	0.88591500	-0.08312500	1.36579400
C	2.10112400	0.15319500	0.78814600
C	0.83112400	-0.25683700	2.69474100
C	3.26957900	0.20582300	1.56781600
C	1.95594400	-0.21323700	3.50898600
C	3.22473300	0.02357400	2.95212700
H	-0.15300300	-0.44014800	3.11045800
H	4.21258400	0.39551800	1.07608900
H	1.82534500	-0.36539200	4.57375100
N	0.92958000	0.32673100	-1.28452200
C	0.87961700	0.49645800	-2.61715100
C	2.11514400	0.34699800	-0.65033300
C	2.03486900	0.67075800	-3.42360700
C	3.41082800	0.59606000	-1.37922000
C	3.28611900	0.70235000	-2.88071400
H	1.87794700	0.76592900	-4.49047000
H	3.86729900	1.51955300	-0.98579600
N	-0.67456900	-2.07153100	-0.57280500
C	-1.49492900	-2.46434600	-1.59906200
C	0.16947900	-2.95129400	-0.00652300
C	-1.43889200	-3.79187000	-2.05845300
C	0.25491900	-4.27028700	-0.42577800
C	-0.56625900	-4.69529100	-1.47523900
H	-0.51962700	-5.71794300	-1.83347600
C	-2.22473200	-0.13249500	-1.46094100
C	-2.35859800	-1.40129800	-2.10201900
C	-3.02558100	0.92956200	-1.89978000
C	-3.28530600	-1.53418000	-3.14980600
C	-3.92295200	0.73290000	-2.94291800
C	-4.07812700	-0.48863400	-3.59089500
H	-2.96846800	1.91301500	-1.44844600
H	-4.78341500	-0.62251500	-4.40110500

H	0.78550400	-2.57834100	0.79957500
H	-0.10694000	0.47972100	-3.06317500
C	4.56716700	0.83046800	-3.70119500
C	4.47210800	0.07322000	3.84369500
C	5.75340500	0.36312200	3.04028900
H	5.95410400	-0.41362800	2.29522300
H	5.70600000	1.33044700	2.52944500
H	6.60824800	0.39294300	3.72213500
C	4.63302600	-1.29288700	4.55454400
H	5.51477200	-1.26911900	5.20295300
H	3.76722900	-1.53493500	5.17763900
H	4.76624500	-2.10116500	3.82829000
C	4.28919900	1.18868600	4.90162800
H	5.16906200	1.22767100	5.55171500
H	4.17371600	2.16765100	4.42550100
H	3.41480600	1.01326300	5.53473000
C	4.27180200	1.13488200	-5.18234400
H	5.21492500	1.24217000	-5.72594400
H	3.70774800	0.32841100	-5.66085400
H	3.71012900	2.06717200	-5.29949800
C	5.45325700	1.96695500	-3.13243400
H	6.34518200	2.07866500	-3.75641000
H	4.92006300	2.92333200	-3.13070700
H	5.79186700	1.75916800	-2.11345000
C	5.34753400	-0.50925600	-3.62261500
H	5.64029000	-0.75895800	-2.59851300
H	4.75117500	-1.33587500	-4.02119900
H	6.26360000	-0.43225500	-4.21703200
H	-3.13962200	3.53194000	2.74418400
H	-2.07976400	-4.10046400	-2.86977600
C	-0.06730600	5.39830100	-0.22609500
F	-0.84580800	6.00396100	-1.15162900
F	0.27230800	6.34258900	0.67728800
F	1.06117000	5.00286300	-0.85285700
C	1.18319600	-5.23077800	0.26209300
F	2.11363100	-4.59218600	1.00275500
F	0.51268500	-6.06157300	1.09238300
F	1.83159000	-6.01070700	-0.62967700
F	-4.68342700	1.76809900	-3.35226700
F	-3.43681200	-2.72137700	-3.78260500
H	4.13318500	-0.19083800	-1.11640400
IrH <sup>+</sup> -3 (in ACN)			
Ir	0.68711200	-0.35328100	-0.05932600



C	1.86764200	-0.86543200	-1.62427400
C	2.85682900	0.10939900	-1.95546600
C	1.78695100	-2.03046700	-2.39722500
C	3.70795900	-0.13578400	-3.04641900
C	2.65899600	-2.21282400	-3.46438100
C	3.63255200	-1.28343000	-3.81680500
H	1.05866900	-2.80586100	-2.18978200
F	4.65516000	0.76761800	-3.39196900
F	2.56453800	-3.34013800	-4.19746400
H	4.30269900	-1.44394800	-4.65165600
N	1.94578900	1.30034800	-0.11623700
C	1.86548800	2.33214900	0.74124700
C	2.88872400	1.30020100	-1.11199800
C	2.71231500	3.42752900	0.66200200
C	3.76508200	2.39278300	-1.23128700
C	3.67984600	3.45564700	-0.34720400
H	1.10090500	2.26816200	1.50311500
H	4.35342000	4.30026700	-0.44235700
N	-0.78822400	0.83361100	-1.17372000
C	-1.74416800	1.44759100	-0.43501700
C	-0.76792200	1.03626200	-2.50527600
C	-2.69152700	2.28157400	-1.03897600
C	-1.68422700	1.84750600	-3.15245100
C	-2.68610700	2.50476800	-2.41834900
H	0.01264000	0.52142800	-3.05233900
H	-3.43462900	2.76436300	-0.42153800
H	-1.60433200	1.96156600	-4.22704300
N	-0.64562500	0.41332000	1.46322500
C	-0.52726500	0.16859100	2.80208200
C	-1.71340800	1.17814100	1.02633400
C	-1.42151100	0.60678900	3.73457400
C	-2.66317900	1.64801800	1.89435400
C	-2.64664400	1.36976400	3.36048000
H	-1.22758100	0.38876200	4.77813200
H	-3.47480000	2.25452300	1.51534100
N	-0.39512300	-2.12593900	-0.04469200
C	0.12838100	-3.14039500	0.71516200
C	-1.54562300	-2.30421900	-0.71494700
C	-0.55193300	-4.36839300	0.78651200
C	-2.24817800	-3.49936300	-0.67402400
C	-1.73783200	-4.55076800	0.09381700
H	-2.26465100	-5.49683000	0.15373000
C	1.86792400	-1.47158700	1.14217200
C	1.37975400	-2.79226900	1.38000400

C	3.06187600	-1.07505600	1.75712800
C	2.11463300	-3.64198800	2.22387800
C	3.74075900	-1.96383400	2.58299300
C	3.29399000	-3.25667700	2.83783600
H	3.48080000	-0.08647200	1.61006700
H	3.83783900	-3.93423000	3.48357800
H	-1.90207000	-1.46186900	-1.29128600
H	0.34809000	-0.40132000	3.09031300
C	-4.00496500	0.70138500	3.89289700
C	-3.70062300	3.41389300	-3.12356200
C	-4.71622900	4.02815000	-2.14291100
H	-5.30647000	3.26106300	-1.63094500
H	-4.22939100	4.65366400	-1.38761600
H	-5.41345400	4.66449100	-2.69553600
C	-4.47207400	2.58196600	-4.17716900
H	-5.19605000	3.22125700	-4.69225700
H	-3.80563700	2.15702400	-4.93332300
H	-5.01961600	1.75955200	-3.70575700
C	-2.93692400	4.56208900	-3.82767000
H	-3.64754800	5.21224900	-4.34799000
H	-2.38657800	5.17059500	-3.10284700
H	-2.22378200	4.18802900	-4.56808400
C	-3.92795000	0.57126500	5.42580500
H	-4.88542000	0.20585700	5.81090400
H	-3.15891900	-0.13735700	5.74580100
H	-3.72433500	1.53745200	5.90075100
C	-5.19327900	1.61480100	3.53742500
H	-6.10685400	1.22092600	3.99422800
H	-5.04510700	2.63303900	3.91384500
H	-5.37074000	1.66895100	2.45941700
C	-4.19942600	-0.68492900	3.25588700
H	-4.26933600	-0.61816900	2.16512200
H	-3.37377500	-1.35970200	3.50417000
H	-5.12548700	-1.13966700	3.62277000
H	4.50385300	2.39730500	-2.01749200
H	-0.14478900	-5.16673800	1.38731400
C	2.61631200	4.53543500	1.67264100
F	3.55565800	4.41081400	2.63771200
F	2.80321300	5.74288600	1.09831400
F	1.41476400	4.55337100	2.28786600
C	-3.50585100	-3.66424100	-1.47978800
F	-4.07660700	-2.47490800	-1.76833800
F	-3.26583300	-4.28543800	-2.65716400
F	-4.41767800	-4.41052000	-0.82159000

F	4.88729900	-1.56326100	3.16775600
F	1.68036300	-4.89953400	2.47381400
H	-2.62580200	2.34262400	3.88669300

IrH<sup>2+</sup> (in ACN)

Ir	0.80371400	-0.09473800	0.00349700
C	2.23867700	-0.41275400	-1.37578400
C	2.75934200	0.77337900	-1.97177200
C	2.71964300	-1.65451500	-1.80403700
C	3.73706300	0.64871000	-2.97365500
C	3.68817200	-1.70871300	-2.80099000
C	4.21838300	-0.57466500	-3.40672500
H	2.36069600	-2.58647800	-1.38541500
F	4.25086500	1.75030800	-3.56510400
F	4.13842900	-2.91215300	-3.20237100
H	4.97238800	-0.63806600	-4.18082900
N	1.25380000	1.87489400	-0.50878700
C	0.67290500	2.95367300	0.04495100
C	2.21091200	2.03100100	-1.47851700
C	1.00097700	4.24740500	-0.32948200
C	2.56931800	3.32459000	-1.89471000
C	1.96742900	4.43294300	-1.32274000
H	-0.07141600	2.76981200	0.80607100
H	2.24106400	5.43109300	-1.64649000
N	-0.93033300	0.02038600	-1.35072100
C	-2.14188400	0.28805400	-0.77942500
C	-0.88059400	-0.10796000	-2.67955000
C	-3.30562000	0.42056100	-1.54693600
C	-2.00862700	0.01794700	-3.49295300
C	-3.26750700	0.29025000	-2.94133800
H	0.09177200	-0.32231300	-3.10666600
H	-4.24502400	0.62934200	-1.05553800
H	-1.87757400	-0.10239700	-4.56191400
N	-0.96500900	0.32315300	1.28949200
C	-0.93232800	0.40140800	2.64857600
C	-2.14157900	0.42104100	0.67175000
C	-2.03922700	0.55743900	3.47697400
C	-3.39150100	0.68810400	1.43669200
C	-3.30282300	0.68645900	2.92150000
H	-1.87611600	0.57928000	4.54557000
H	-3.74871300	1.69298200	1.14397700
N	0.59909800	-2.10520600	0.51291500
C	1.42451700	-2.55281000	1.51228900
C	-0.26345600	-2.94831400	-0.08244500

C	1.35469400	-3.89768500	1.91458900
C	-0.36277000	-4.28213100	0.28072000
C	0.46356600	-4.76263900	1.30199600
H	0.40841500	-5.79948900	1.61543700
C	2.20529400	-0.23351700	1.45279100
C	2.30923700	-1.52499000	2.05024200
C	3.02235800	0.79898500	1.92548100
C	3.22982100	-1.70979000	3.09600200
C	3.91301900	0.55028200	2.96485100
C	4.04151900	-0.69431600	3.57187700
H	2.98655600	1.79711400	1.50660100
H	4.74097800	-0.86834700	4.37950700
H	-0.88131200	-2.53675400	-0.86777000
H	0.05930500	0.32676600	3.08247600
C	-4.56268500	0.79765500	3.74340400
C	-4.50807400	0.42607100	-3.83040000
C	-5.77348300	0.74930200	-3.01513300
H	-6.01440200	-0.04367700	-2.29965600
H	-5.68168000	1.69570900	-2.47190800
H	-6.62378300	0.84406700	-3.69587600
C	-4.72676800	-0.91080100	-4.58147800
H	-5.60594000	-0.82529000	-5.22728200
H	-3.87307300	-1.17161600	-5.21348400
H	-4.89763500	-1.73380900	-3.88046000
C	-4.26778300	1.56534200	-4.85136600
H	-5.14413700	1.66350000	-5.49910700
H	-4.10881700	2.52238900	-4.34485500
H	-3.40237200	1.36905200	-5.49052100
C	-4.28877900	1.38341400	5.14517000
H	-5.23866700	1.47416100	5.67775300
H	-3.64138600	0.74113500	5.74738800
H	-3.83896100	2.37836800	5.08245000
C	-5.64670800	1.64095800	3.03481900
H	-6.52759000	1.68946700	3.67909100
H	-5.30360400	2.66539900	2.85811700
H	-5.96608400	1.20641500	2.08441100
C	-5.08111700	-0.67270800	3.90041600
H	-5.33445500	-1.12110200	2.93617000
H	-4.34599100	-1.30601700	4.40284600
H	-5.98745600	-0.63983600	4.51168300
H	3.31766400	3.44703800	-2.66207500
H	2.00098200	-4.25082200	2.70301800
C	0.36167000	5.42283400	0.35587100
F	1.18105300	5.95763300	1.28837600

F	0.07281400	6.40491700	-0.52307700
F	-0.78371300	5.07791200	0.98168300
C	-1.31479100	-5.20092300	-0.43328000
F	-2.19994800	-4.52010000	-1.19089800
F	-0.65872200	-6.05484200	-1.24932400
F	-2.01484500	-5.95457400	0.44118500
F	4.69014500	1.55610600	3.40792700
F	3.35319000	-2.91758500	3.69026800
H	-4.19840200	0.02510100	1.10027700

IrIII (in ACN)

Ir	0.00000000	0.00000000	0.80573000
C	-0.09410700	1.41583600	2.24368400
C	-1.41679700	1.86162800	2.54439600
C	0.98288500	1.99945700	2.92282900
C	-1.58663400	2.87035400	3.50766300
C	0.74716200	2.99464400	3.86427000
C	-0.52747600	3.45392400	4.18136000
H	2.00731200	1.69883000	2.73673500
F	-2.82600700	3.31918800	3.81609800
F	1.79674700	3.54550100	4.50628700
H	-0.69050700	4.22948700	4.91874400
N	-2.05756000	0.26570800	0.91139100
C	-2.94158200	-0.42085300	0.16762100
C	-2.49280200	1.21486100	1.80065900
C	-4.30874500	-0.20412400	0.25461100
C	-3.86983200	1.47159300	1.91684600
C	-4.77866400	0.76507300	1.14644200
H	-2.53233200	-1.15792000	-0.50902000
H	-5.84075500	0.96661100	1.23270300
N	0.00000000	1.33804700	-0.93927700
C	-0.02810400	0.74131900	-2.15724000
C	-0.04226800	2.68150300	-0.87909000
C	-0.10935800	1.50037400	-3.32886200
C	-0.11665200	3.48090600	-2.00887200
C	-0.15899200	2.89747400	-3.28528500
H	-0.01270500	3.11491700	0.11346400
H	-0.14324400	0.99300600	-4.28165000
H	-0.14608000	4.55606500	-1.87695400
N	0.00000000	-1.33804700	-0.93927700
C	0.04226800	-2.68150300	-0.87909000
C	0.02810400	-0.74131900	-2.15724000
C	0.11665200	-3.48090600	-2.00887200
C	0.10935800	-1.50037400	-3.32886200

C	0.15899200	-2.89747400	-3.28528500
H	0.14608000	-4.55606500	-1.87695400
H	0.14324400	-0.99300600	-4.28165000
N	2.05756000	-0.26570800	0.91139100
C	2.49280200	-1.21486100	1.80065900
C	2.94158200	0.42085300	0.16762100
C	3.86983200	-1.47159300	1.91684600
C	4.30874500	0.20412400	0.25461100
C	4.77866400	-0.76507300	1.14644200
H	5.84075500	-0.96661100	1.23270300
C	0.09410700	-1.41583600	2.24368400
C	1.41679700	-1.86162800	2.54439600
C	-0.98288500	-1.99945700	2.92282900
C	1.58663400	-2.87035400	3.50766300
C	-0.74716200	-2.99464400	3.86427000
C	0.52747600	-3.45392400	4.18136000
H	-2.00731200	-1.69883000	2.73673500
H	0.69050700	-4.22948700	4.91874400
H	2.53233200	1.15792000	-0.50902000
H	0.01270500	-3.11491700	0.11346400
C	0.26022700	-3.77113400	-4.54190700
C	-0.26022700	3.77113400	-4.54190700
C	-0.29854600	2.93473000	-5.83403300
H	0.60992100	2.33726900	-5.96256500
H	-1.16308000	2.26338000	-5.86139300
H	-0.37559500	3.60439800	-6.69541600
C	0.96718300	4.71327800	-4.59775900
H	0.90437100	5.34766200	-5.48769200
H	1.02031000	5.36958100	-3.72439500
H	1.89960500	4.14236700	-4.65202300
C	-1.55675600	4.61374600	-4.45981300
H	-1.64044600	5.24812500	-5.34796800
H	-2.44180600	3.97103800	-4.41593000
H	-1.56643300	5.26633200	-3.58212900
C	-0.96718300	-4.71327800	-4.59775900
H	-0.90437100	-5.34766200	-5.48769200
H	-1.02031000	-5.36958100	-3.72439500
H	-1.89960500	-4.14236700	-4.65202300
C	0.29854600	-2.93473000	-5.83403300
H	0.37559500	-3.60439800	-6.69541600
H	-0.60992100	-2.33726900	-5.96256500
H	1.16308000	-2.26338000	-5.86139300
C	1.55675600	-4.61374600	-4.45981300
H	2.44180600	-3.97103800	-4.41593000

H	1.56643300	-5.26633200	-3.58212900
H	1.64044600	-5.24812500	-5.34796800
H	-4.21296800	2.22392900	2.60993800
H	4.21296800	-2.22392900	2.60993800
C	-5.26085300	-1.03202100	-0.56151200
F	-5.78280500	-2.04854000	0.16218700
F	-6.29994200	-0.29275100	-1.00431000
F	-4.65686100	-1.58018500	-1.63758500
C	5.26085300	1.03202100	-0.56151200
F	4.65686100	1.58018500	-1.63758500
F	5.78280500	2.04854000	0.16218700
F	6.29994200	0.29275100	-1.00431000
F	-1.79674700	-3.54550100	4.50628700
F	2.82600700	-3.31918800	3.81609800

IrII (in ACN)

Ir	0.00000000	0.00000000	0.81832800
C	0.22527200	1.41058900	2.25444600
C	-0.96620100	2.14439300	2.54880700
C	1.39814200	1.73991900	2.95064500
C	-0.91492100	3.16383600	3.51390000
C	1.38304300	2.75993600	3.89298500
C	0.24095700	3.49489400	4.20003800
H	2.33086200	1.21649600	2.77154800
F	-2.02644600	3.88066500	3.81469000
F	2.52407900	3.06234300	4.54945500
H	0.24905800	4.28634500	4.93855200
N	-1.93374600	0.73295800	0.90755200
C	-2.93640100	0.27257300	0.14116300
C	-2.15384800	1.75585000	1.79457000
C	-4.21982500	0.79547400	0.20984700
C	-3.44003200	2.31520900	1.89669300
C	-4.47367300	1.83710900	1.10803300
H	-2.68265500	-0.52944800	-0.53881400
H	-5.46447900	2.27176700	1.18235600
N	0.35614400	1.29526000	-0.88906400
C	0.18721300	0.68901300	-2.13090200
C	0.69125700	2.60170700	-0.84663200
C	0.40282500	1.46254900	-3.31171300
C	0.89576600	3.38023400	-1.96597700
C	0.75388800	2.79492300	-3.26410200
H	0.80185100	3.02173200	0.14803600
H	0.28356900	0.97244500	-4.26832500
H	1.16551600	4.42176200	-1.83877300

N	-0.35614400	-1.29526000	-0.88906400
C	-0.69125700	-2.60170700	-0.84663200
C	-0.18721300	-0.68901300	-2.13090200
C	-0.89576600	-3.38023400	-1.96597700
C	-0.40282500	-1.46254900	-3.31171300
C	-0.75388800	-2.79492300	-3.26410200
H	-1.16551600	-4.42176200	-1.83877300
H	-0.28356900	-0.97244500	-4.26832500
N	1.93374600	-0.73295800	0.90755200
C	2.15384800	-1.75585000	1.79457000
C	2.93640100	-0.27257300	0.14116300
C	3.44003200	-2.31520900	1.89669300
C	4.21982500	-0.79547400	0.20984700
C	4.47367300	-1.83710900	1.10803300
H	5.46447900	-2.27176700	1.18235600
C	-0.22527200	-1.41058900	2.25444600
C	0.96620100	-2.14439300	2.54880700
C	-1.39814200	-1.73991900	2.95064500
C	0.91492100	-3.16383600	3.51390000
C	-1.38304300	-2.75993600	3.89298500
C	-0.24095700	-3.49489400	4.20003800
H	-2.33086200	-1.21649600	2.77154800
H	-0.24905800	-4.28634500	4.93855200
H	2.68265500	0.52944800	-0.53881400
H	-0.80185100	-3.02173200	0.14803600
C	-0.99365000	-3.64997700	-4.51582100
C	0.99365000	3.64997700	-4.51582100
C	0.80196400	2.85343800	-5.81963500
H	1.50108800	2.01354400	-5.89029700
H	-0.21597000	2.45998900	-5.90983400
H	0.98166400	3.50682000	-6.67942000
C	2.44130000	4.19808300	-4.48904200
H	2.62414800	4.82519900	-5.36869800
H	2.63022200	4.80694300	-3.60002800
H	3.16920800	3.37980100	-4.49807500
C	0.00000000	4.83724300	-4.52043400
H	0.17207900	5.46976200	-5.39830000
H	-1.03493300	4.48069300	-4.55634000
H	0.10990800	5.46363600	-3.63031100
C	-2.44130000	-4.19808300	-4.48904200
H	-2.62414800	-4.82519900	-5.36869800
H	-2.63022200	-4.80694300	-3.60002800
H	-3.16920800	-3.37980100	-4.49807500
C	-0.80196400	-2.85343800	-5.81963500



H	-0.98166400	-3.50682000	-6.67942000
H	-1.50108800	-2.01354400	-5.89029700
H	0.21597000	-2.45998900	-5.90983400
C	0.00000000	-4.83724300	-4.52043400
H	1.03493300	-4.48069300	-4.55634000
H	-0.10990800	-5.46363600	-3.63031100
H	-0.17207900	-5.46976200	-5.39830000
H	-3.61443600	3.12167500	2.59203200
H	3.61443600	-3.12167500	2.59203200
C	-5.31968900	0.21572600	-0.63140600
F	-6.06494900	-0.67569400	0.06400100
F	-6.16690500	1.17423900	-1.06636700
F	-4.84064000	-0.43140300	-1.71545800
C	5.31968900	-0.21572600	-0.63140600
F	4.84064000	0.43140300	-1.71545800
F	6.06494900	0.67569400	0.06400100
F	6.16690500	-1.17423900	-1.06636700
F	-2.52407900	-3.06234300	4.54945500
F	2.02644600	-3.88066500	3.81469000

IrH<sub>3</sub> (in ACN)

Ir	0.83598300	-0.31420400	-0.03381000
C	2.07214000	-0.82578500	1.50350900
C	1.70146300	-2.01633800	2.20069100
C	3.22777800	-0.14579500	1.92306900
C	2.50756200	-2.46334700	3.26200400
C	3.97843400	-0.63474000	2.98276800
C	3.64773100	-1.79668500	3.67564900
H	3.56262400	0.76229900	1.43383300
F	2.19049900	-3.59504600	3.94078400
F	5.08744000	0.03537400	3.36723200
H	4.24806500	-2.16674000	4.49692700
N	-0.14988500	-2.00537100	0.70647000
C	-1.33641900	-2.44685100	0.25733000
C	0.46482400	-2.64976200	1.75460100
C	-1.96508000	-3.56709800	0.78828400
C	-0.13145800	-3.79379800	2.31243200
C	-1.34321600	-4.25997400	1.82838100
H	-1.78672700	-1.88337500	-0.55237800
H	-1.80621400	-5.13904100	2.26221500
N	-0.65279100	0.85212000	1.11712300
C	-1.60325300	1.46901200	0.37501600
C	-0.77356900	0.84599900	2.45863100
C	-2.69435400	2.08685500	0.99026100

C	-1.83559100	1.44256200	3.11787700
C	-2.84507700	2.08513300	2.38217700
H	0.01442600	0.34002900	3.00547600
H	-3.43287700	2.56918400	0.36538900
H	-1.86642000	1.39459400	4.20032000
N	-0.60598200	0.28611300	-1.54339400
C	-1.32899500	-0.59452500	-2.30522600
C	-1.31028900	1.50286400	-1.12889200
C	-2.63369300	-0.49902500	-2.67900500
C	-2.50046700	1.86482100	-2.04027400
C	-3.47501300	0.68773200	-2.26054400
H	-3.04345800	-1.26278800	-3.33145100
H	-3.00215900	2.75359100	-1.64733000
N	1.99297900	1.26289600	-0.69119700
C	2.89336600	0.97419100	-1.68573900
C	1.91166300	2.51050400	-0.19789400
C	3.70118700	2.00128100	-2.20714300
C	2.69712500	3.55061600	-0.67376000
C	3.60485600	3.28852800	-1.70623700
H	4.22452400	4.08151000	-2.11020000
C	2.02145200	-1.28001200	-1.33559400
C	2.91257200	-0.43268900	-2.06462100
C	2.01699200	-2.65316600	-1.62758900
C	3.73455600	-1.00199900	-3.05107500
C	2.85670000	-3.15272700	-2.61346200
C	3.72923700	-2.35364000	-3.34891700
H	1.36351800	-3.34308000	-1.10549800
H	4.37501700	-2.76366700	-4.11483700
H	1.19139400	2.66446200	0.59493300
H	-0.74915900	-1.45804900	-2.63657700
C	-4.65935400	1.01159900	-3.23678900
C	-4.03666300	2.73575600	3.09871400
C	-5.01309500	3.41006800	2.11695400
H	-4.53062700	4.21070200	1.54681900
H	-5.44325000	2.69356200	1.40947400
H	-5.84058700	3.85588100	2.67705600
C	-3.51225900	3.80915600	4.08308900
H	-4.35382400	4.27842600	4.60308600
H	-2.84968600	3.38181000	4.84132000
H	-2.96083700	4.59261800	3.55314900
C	-4.80376400	1.64490900	3.88503800
H	-5.65367200	2.09336300	4.41015700
H	-5.18968900	0.87326400	3.21085900
H	-4.16931000	1.15740700	4.63093500

C	-5.62980100	-0.18924600	-3.26182900
H	-6.49740600	0.03171900	-3.89421500
H	-5.15845600	-1.09370700	-3.65741900
H	-5.99970500	-0.41714900	-2.25500900
C	-5.44722100	2.23840300	-2.73118100
H	-6.34680300	2.39185400	-3.33814000
H	-5.76837100	2.10186500	-1.69126300
H	-4.85848100	3.15949300	-2.78404200
C	-4.16573800	1.28593700	-4.67113200
H	-3.53269100	2.17824900	-4.71985400
H	-3.58683200	0.44264500	-5.06041000
H	-5.01637900	1.45092300	-5.34257200
H	0.35746300	-4.30168400	3.12916200
H	4.39947700	1.77578600	-2.99853400
C	-3.26553800	-4.03003800	0.19783700
F	-3.07591100	-4.76259800	-0.92571900
F	-3.95825400	-4.80472800	1.06007100
F	-4.05896800	-2.99112400	-0.14683900
C	2.60276000	4.91399500	-0.05358700
F	1.41361500	5.11183200	0.55623200
F	3.56228300	5.10632200	0.88258800
F	2.75825800	5.88946800	-0.97515400
F	2.83461900	-4.47656700	-2.88309700
F	4.58508300	-0.22389400	-3.76627100
H	-0.60083300	2.34293600	-1.22661500
H	-2.07416500	2.15641200	-3.00605800
H	-3.96175200	0.48068300	-1.28972100

IrH<sub>3</sub><sup>+</sup> (in ACN)

Ir	0.80394000	-0.31055600	-0.02502500
C	2.09424500	-0.80733800	1.46159600
C	1.75430900	-1.99479000	2.17544000
C	3.25307400	-0.11253400	1.83231800
C	2.59445500	-2.42230600	3.21839600
C	4.04122800	-0.58595100	2.87421000
C	3.74054400	-1.74093900	3.58904200
H	3.56597200	0.79343500	1.32794900
F	2.30414800	-3.54544900	3.91629500
F	5.15220200	0.09812600	3.21370900
H	4.36787700	-2.09608200	4.39658000
N	-0.12577200	-2.03088300	0.72506100
C	-1.29659400	-2.51733900	0.28046200
C	0.52323100	-2.65682800	1.76021200
C	-1.88383000	-3.65564100	0.81199200

C	-0.03211900	-3.81811400	2.32561400
C	-1.23220900	-4.32209800	1.85291100
H	-1.77587100	-1.97452400	-0.52011100
H	-1.66342000	-5.21361100	2.29469200
N	-0.67047400	0.84340400	1.17258400
C	-1.65457200	1.44669600	0.46400400
C	-0.75410400	0.83423200	2.51614100
C	-2.73964700	2.04483600	1.09911000
C	-1.80855300	1.41510900	3.20210000
C	-2.84861600	2.04011200	2.49721400
H	0.05566700	0.34119600	3.04171600
H	-3.50355000	2.51743900	0.49865000
H	-1.80805100	1.36779400	4.28466500
N	-0.74143400	0.23043400	-1.42946700
C	-1.26231200	-0.51533700	-2.40505500
C	-1.40991100	1.49110000	-1.04696600
C	-2.54091000	-0.34787600	-2.92551100
C	-2.57423200	1.89828400	-1.96797800
C	-3.45969200	0.71256500	-2.40017200
H	-2.87203500	-1.05570700	-3.67699900
H	-3.15705300	2.68486700	-1.48843000
N	1.94312300	1.28658200	-0.69281500
C	2.84273000	1.00390800	-1.68873700
C	1.85835900	2.52955900	-0.18674800
C	3.64798200	2.03529600	-2.20193600
C	2.64202400	3.57345500	-0.65590600
C	3.54883900	3.31873600	-1.68967800
H	4.16880400	4.11468900	-2.08719700
C	1.97537900	-1.26015700	-1.36612300
C	2.85900300	-0.39993100	-2.08446400
C	1.95790600	-2.62429000	-1.67957000
C	3.67011900	-0.95341600	-3.08882100
C	2.78744600	-3.10972100	-2.68479300
C	3.65532500	-2.30008100	-3.41059000
H	1.30992200	-3.32219000	-1.16211600
H	4.29273300	-2.69772000	-4.18993900
H	1.14425100	2.67563900	0.61322100
H	-0.65165200	-1.35300600	-2.73386500
C	-4.63463200	1.07538400	-3.37342800
C	-4.02990800	2.67121200	3.24565700
C	-5.04354100	3.32800500	2.29060500
H	-4.59036000	4.13685100	1.70829700
H	-5.48229300	2.60398600	1.59621600
H	-5.86194500	3.76009300	2.87374000

C	-3.49409800	3.75351500	4.21446200
H	-4.32938800	4.20728100	4.75723000
H	-2.80369900	3.33812000	4.95415000
H	-2.97230500	4.54627200	3.66890700
C	-4.75421100	1.56603500	4.05293100
H	-5.59615400	2.00114400	4.60098300
H	-5.14591100	0.78748900	3.39026400
H	-4.09079100	1.09075900	4.78118000
C	-5.52486800	-0.17013300	-3.56994300
H	-6.37600000	0.07485500	-4.21359900
H	-4.99094700	-0.99941300	-4.04410700
H	-5.92067500	-0.52799000	-2.61279100
C	-5.50277300	2.18617300	-2.74729200
H	-6.39459500	2.35316500	-3.36002300
H	-5.83768600	1.91019500	-1.74052300
H	-4.97177700	3.14047300	-2.68077000
C	-4.10872600	1.54909700	-4.74347400
H	-3.51024900	2.46172800	-4.65955700
H	-3.49280100	0.78457500	-5.22927300
H	-4.94821400	1.76987800	-5.41094300
H	0.48112400	-4.31008900	3.13692900
H	4.34741900	1.81807200	-2.99436600
C	-3.17148000	-4.17618800	0.23865900
F	-2.95417800	-5.14675200	-0.67800100
F	-3.95625500	-4.71091600	1.19751000
F	-3.87711700	-3.20209000	-0.37662800
C	2.54823500	4.93374400	-0.02376100
F	1.36623700	5.11671800	0.60230700
F	3.51968700	5.12089400	0.89831200
F	2.68466500	5.91310400	-0.94220600
F	2.75501700	-4.42510600	-2.97630700
F	4.51456400	-0.16653300	-3.79541400
H	-0.63685300	2.26256900	-1.17555300
H	-2.13097900	2.34949700	-2.86054500
H	-3.93814000	0.30011000	-1.49423700