Supporting Information

An Alternative Reaction Pathway for Iridium Catalyzed Water Oxidation Driven by CAN

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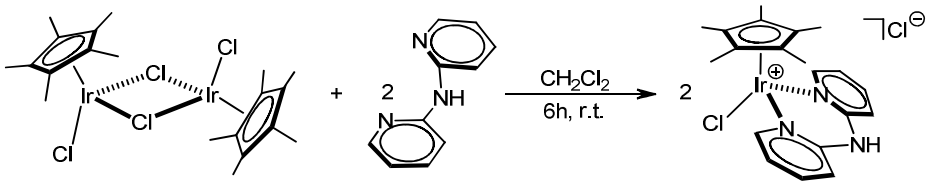
Material and Methods. $[Cp^*IrCl(\mu\text{-}Cl)]_2$,[1] $[Cp^*Ir(bpy)Cl]Cl$ (**1**; bpy = 2,2'-bipyridine),[2] $[Cp^*Ir(bzpy)(NO_3)]NO_3$ (**3**; bzpy = 2-benzoylpyridine)[2] and $[Cp^*Ir(H_2O)_3](NO_3)_2$ (**4**)[3] were prepared according to the literature. IrO_2 (**5**) was purchased from Alfa Aesar (99.99%, metals basis; Ir 84.5%) and used as received. Stock solutions of Ce^{+4} for kinetic measurements were prepared from $(NH_4)_2Ce(NO_3)_6$ (≥ 98.0%, Sigma-Aldrich). Purelab Option-R7 (Elga labwater) was used to purify water (Resistivity = 18 MΩ-cm; TOC < 20 ppb). Acid solutions were prepared from concentrated HNO_3 (Trace Metal Grade, ≥ 65%, Sigma-Aldrich) and distilled, deionized water. Deuterated solvents were used as received. 1D and 2D ^1H, ^{13}C, ^{15}N, ^1H-COSY, ^1H-NOESY, ^{13}C JMOD, ^1H,^{13}C-HMQC, ^1H,^{13}C-HMBC and ^1H,^{15}N-HMBC NMR spectra were measured on a Bruker DRX 400 equipped with a QNP probe and on a Bruker Avance III HD 400 spectrometer equipped with a Smartprobe. Referencing is relative to external TMS (^1H and ^{13}C) and CH_3NO_2 (^{15}N).

X-Ray studies. A single crystal of **2** suitable for X-Ray diffraction (a yellow block with approximate dimensions of 0.25 mm x 0.15 mm x 0.1 mm) was obtained by slow diffusion of n-hexane into a solution of **2** in methylene chloride. Data were collected on a XCALIBUR (Kuma4CCD) diffractometer, using Mo-Kα graphite monochromated radiation (λ = 0.71073 Å), ω and p scans and the frame data were acquired with the CRYSALIS (CCD 171) software. The structure was solved using direct methods and refined against $|F^2|$. The Laue symmetry was determined to 1.696 g cm^{-3} (Z = 4 and FW = 1104) and the investigation of the observed systematic absences are consistent with the orthorombic space group P $2_12_12_1$ (no. 19). The data were collected at room temperature. The lattice parameters founded was: a = 9.263(4), b = 13.429(5) and c = 17.935(7) Å, α = 90(0)°, β = 90(0)°, γ = 90(0)° and V = 2231.0(16) $Å^3$. Data were collected within θ range of 3.16 < θ < 29.36° and in the index ranges $-12 \le h \le 12$, $-18 \le k \le 17$, $-24 \le l \le 23$ with a total of 21899 reflections collected of which 5833 were unique reflections independent. The frames s were processed using the CRYSALISIS (RED 171) software to give the *hkl* file corrected for scan spin, background, and Lorentz and polarization affects. Standard reflections, measured periodically, showed no apparent variation in intensity during data collection and so, no correction for crystal decomposition was necessary. The data were corrected for absorption using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm. The structure was solved by the direct method using the Sir97 program[4] and refined by the full-matrix least-squares method on F^2 using SHELXL-97[5] WinGX[6] version. All non-hydrogen atoms were refined anisotropically. Almost all the hydrogen atoms were added at the calculated positions and refined using a rigid model. The final cycle of full-matrix least-squares refinement against $|F^2|$ was based on 5833 observed reflections [$F_0 > 4\sigma(F_0)$] and 233 variable parameters and converged with unweighted and weighted

agreement factors of R = 0.0581 and R_w= 0.0879, and GOF = 1.045. Attached CIF contains the supplementary crystallographic data for **2**.

Synthesis and characterization of 2. Complex **2** was synthetized by the reaction of $[Cp^*IrCl_2]_2$ with 2.2 equivalents of 2,2'-dipyridylamine in dichloromethane at room temperature (Scheme S1).



Scheme S1. Synthesis of **2**.

After 6 hours, the solution was concentrated under reduced pressure. Yellow crystals were obtained by slow evaporation of the solvent, washed several times with n-hexane and finally dried under vacuum (80% yield). Anal. Calc. for $C_{20}H_{24}Cl_2IrN_3$: C, 46.01; H, 6.44; N, 6.80. (theoretical C, 46.57; H, 6.10; N, 6.52). ^{1}H NMR (400.13 MHz in D_2O, 298K, J values in Hz, δ values in ppm): δ = 8.27 (ddd, H1, $^3J_{H1,H2}$ = 6.00, $^4J_{H1,H3}$ = 1.84, $^5J_{H1,H4}$ = 0.64), δ = 7.14 (ddd, H2, $^3J_{H1,H2}$ = 6.00, $^3J_{H2,H3}$ = 7.32, $^4J_{H2,H4}$ = 1.28), δ = 7.82 (ddd, H3, $^3J_{H2,H3}$ = 7.32, $^3J_{H3,H4}$ = 9, $^4J_{H1,H3}$ = 1.84), δ = 7.2 (ddd, H4 $^3J_{H3,H4}$ = 9, $^4J_{H2,H4}$ = 1.28, $^5J_{H1,H4}$ = 0.64), δ = 5.37 (s, H7) and δ = 1.33 (s, H9). ^{15}N NMR (40.56 MHz in D_2O, 298K, δ values in ppm): δ = 181.48 (s, N6) and 116.36 (s, N7). ^{13}C NMR (100.64 MHz in D_2O, 298K, δ values in ppm): δ = 151.53 (C1), δ = 121.26 (C2), δ = 141.26 (C3), δ = 114.37 (C4), δ = 151.59 (C5), δ = 88.77 (C8) and δ = 7.62 (C9).

Catalytic Studies

Catalytic activity was monitored by means of a multi-technique approach based on detecting both the production of oxygen and the depletion of Ce^{+4}. In particular, differential manometry and oximetry were employed to follow the kinetics of formation of molecular oxygen in the gas phase and in solution, respectively. Instead, the depletion of CAN was followed by means of UV-Vis.

Differential Manometry

Experiments were performed by dissolving 13.7 – 27.4 mg of CAN (25 – 50 μmol) in 4 – 4.5 mL of acidic water (HNO_3, pH 1) into a working cell. The same amount of water was transferred into a second identical reference cell. Both cells were equipped with a side arm for the connection to the manometer and with a septum to seal the system, which was kept at a constant temperature (T = 25°C) and allowed to equilibrate under stirring for at least 20 min. When a steady baseline was achieved, a water solution of the catalyst (C) and water were injected in the working and reference cell, respectively, to reach a final volume of 5 mL in each reactor and measured started. The

concentration of the stock solution of C was adjusted, depending on the final [C] desired, in order to have a maximum injection volume of 1 mL.

Clark Electrode

39-40.6 mL of an aqueous solution of CAN were transferred into a reactor, which was subsequently sealed. The system was thermostated at 25°C under stirring for at least 20 min. As soon as a stable baseline was obtained, 0.4 – 2 mL of a solution of C was injected into the reactor to reach the final volume of 41 ml and the measurement started. The concentrations of CAN used were 10 mM and 5 mM, while the catalyst concentration was changed between 1 μM and 125 μM.

UV-Vis

UV-Vis experiments were performed by transferring 100 – 500 μL of a solution of catalyst into a cuvette and adding acidic water (HNO_3, pH 1) to reach a final volume of 2 mL. The system was allowed to equilibrate under stirring for 20 min at 25 °C and, after the background correction, 1 mL of a solution of CAN was injected (final volume = 3 mL). The disappearance of CAN was followed at λ = 340, 410 or 420 nm depending on its concentration (1, 5 or 10 mM, respectively), whereas the concentration of the stock solution of C was adjusted depending on the desired final concentration.

Multiple addition experiments with differential manometer

250 μL of a solution 1.25 mM of catalyst were injected into the working cell containing 13.7 mg (25 μmol) of CAN dissolved in 4.75 mL of acidic water. After the evolution of O_2 went to completion, 250 μL of a solution of CAN (0.102 M) were injected. The same procedure was repeated two more times.

Multiple addition experiments with UV-Vis

125 μL of a solution 1.25 mM of catalyst were injected into a cuvette containing 6.85 mg (12.5 μmol) of CAN dissolved in 2.5 mL of acidic water. After about 7 minutes, under the assumption that all O_2 was evolved, 125 μL of a solution of CAN (0.102 M) were injected. The same procedure was repeated two more times.

Dynamic light scattering

The hydrodynamic size distribution of nanoparticles was measured by dynamic light scattering (DLS) using a NICOMP 380 ZLS equipped with a 55 mW He-Ne Coherent Innova 70-3 Laser source at 654.0 nm and APD detector (Particle Sizing System, Inc, Santa Barbara, CA, USA). All determinations were performed at 20°C upon proper dilution when required.

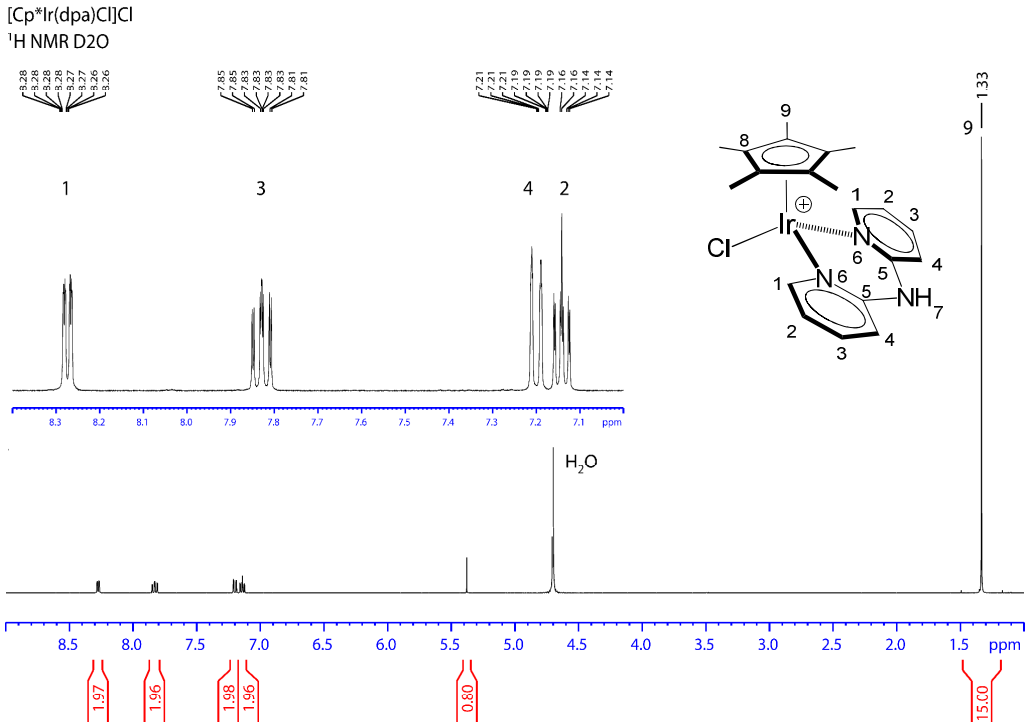


Figure S1. ^{1}H NMR spectrum of **2** in D_2O.

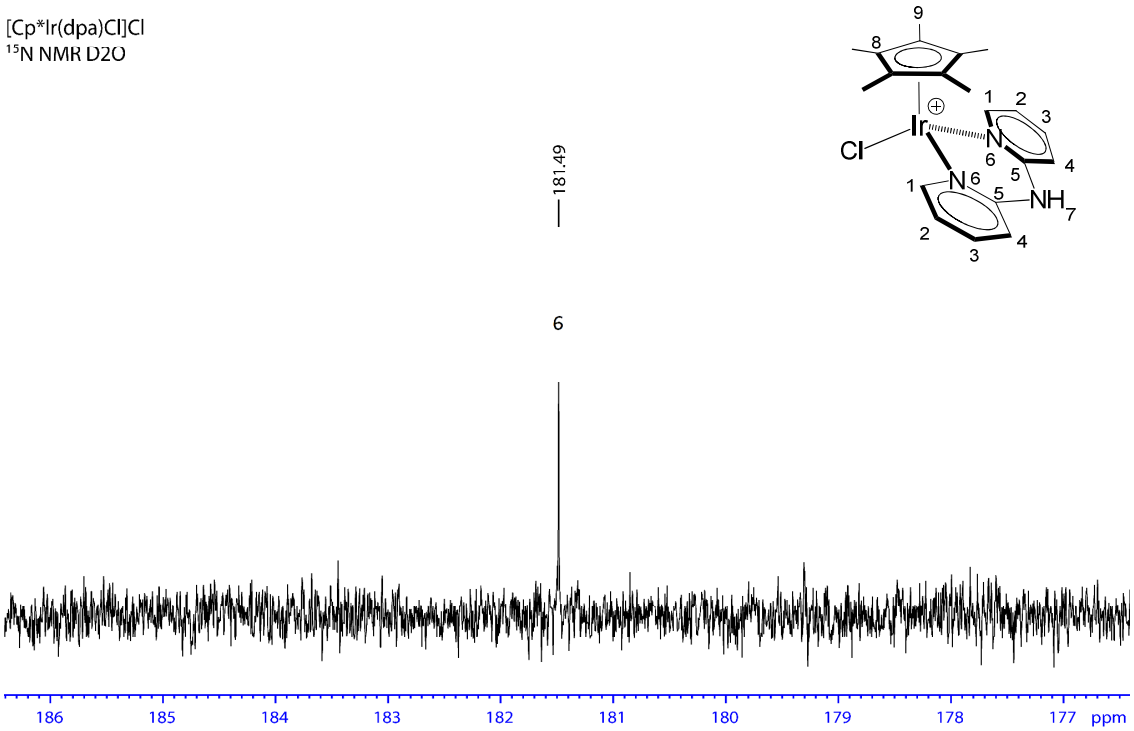


Figure S2. ^{15}N NMR spectrum of **2** in D_2O.

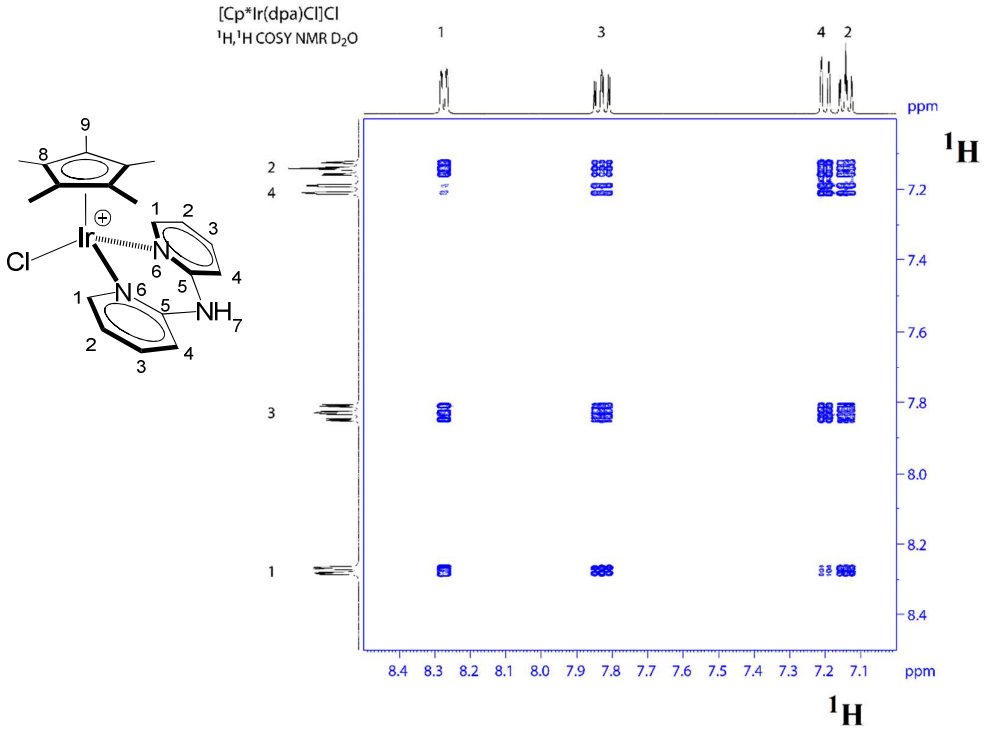


Figure S3. ^{1}H,^{1}H COSY NMR spectrum of **2** in D_2O.

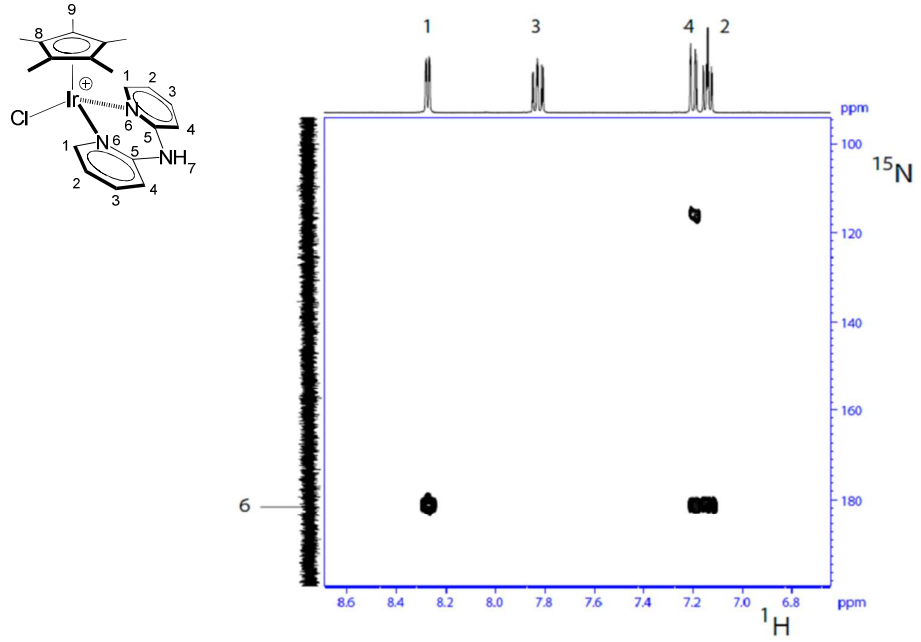


Figure S4. ^{1}H, ^{15}N HMBC NMR spectrum of **2** in D_2O.

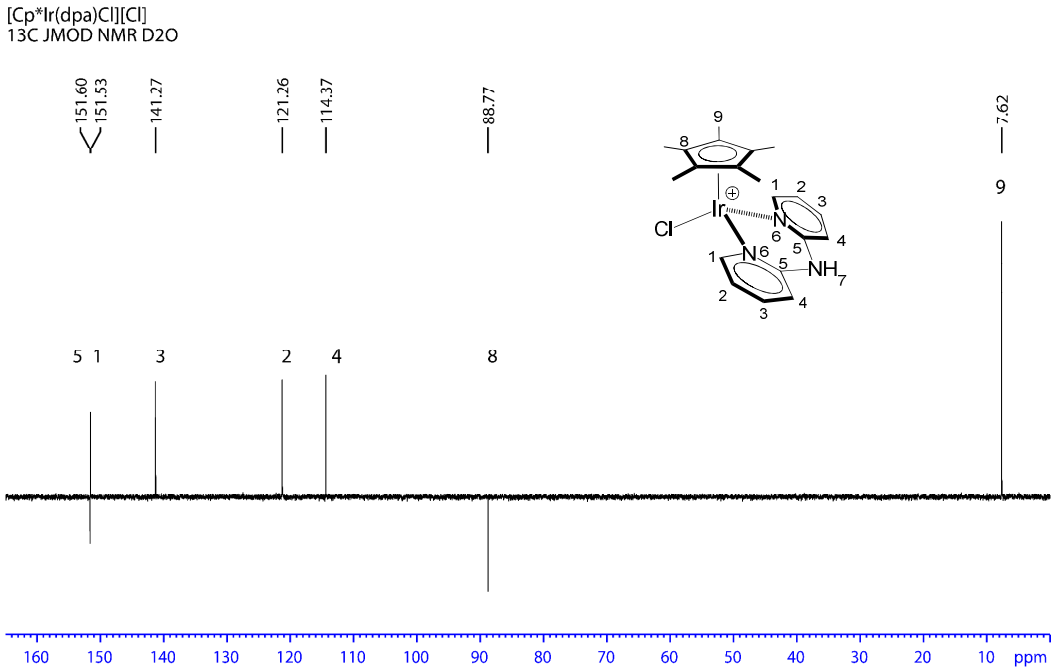


Figure S5. ^{13}C JMOD NMR spectrum of **2** in D_2O.

Table S1. Summary of catalytic results obtained for **2** at different R values.

Entry	Technique	[Cat] (μM)	[CAN] (mM)	R	TOF (min^{-1})	
					TOF_i	TOF_{LT}
WOC **1**						
1	Manometry	500	10	20	0.3	-
2	Manometry	250	10	40	2.1	-
3	Manometry	125	10	80	3.5	-
4[7]	Manometry	29.8	3.56	120	2.9	-
5[7]	Manometry	40	27.7	692	6.2	-
6	Manometry	5	5	1000	-	4.6
7	Manometry	5	10	2000	-	6.1
8	Manometry	5	20	4000	-	7.3
9	Manometry	5	40	8000	-	6.6
WOC **2**						
10	Manometry	500	10	20	-	0.3
11	Manometry	250	10	40	-	1.2
12	Manometry	167	10	60	-	4.1
13	Manometry	125	10	80	-	5
14	Manometry	62.5	10	160	-	14.3
15	Manometry	31.2	10	320	-	30.7
16	Manometry	15.6	10	640	-	37.7
17	Manometry	2.5	10	4000	-	11.7
18	Manometry	1	10	10000	-	6.1
19	Manometry	5	5	1000	9.1	25.0
20	Manometry	5	10	2000	8.5	24.7
21	Manometry	5	20	4000	9.7	18.0
22	Manometry	5	25	5000	8.7	10.1
23	Manometry	5	30	6000	-	5.7
24	Manometry	5	40	8000	-	4.5
25	Clark Electrode	1	10	10000	7.6	-
26	Clark Electrode	2.5	10	4000	9.0	-
27	Clark Electrode	5	10	2000	4.2	-
28	UV-Vis	0.5	1	2000	-	5
29	UV-Vis	1	1	1000	-	7.2

30	UV-Vis	2	1	500	-	9.5
31	UV-Vis	5	1	200	-	9.3
32	UV-Vis	5	10	2000	-	27.7
33	UV-Vis	125	10	80	-	19.7

Table S2. Kinetic data for WO experiments with **1**, **2**, **3**, **4** and **5** ([CAN] = 5 mM for **1**, **2**, **3** and **4**; [CAN] = 10 mM for **5**).

	C	R	UV-Vis		DM
			k_1^{obs}	TOF	k_2^{obs}
	μM		mM min^{-1}	min^{-1}	min^{-1}
WOC **1**					
1	62.5	80	0.64	10.2	0.10
2	31.25	160	0.31	9.9	0.05
3	15.66	320	0.10	6.4	0.05
WOC **2**					
4	62.50	80	1.09	17.4	0.55
5	31.25	160	0.64	20.5	0.73
6	15.66	320	0.26	16.6	0.48
WOC **3**					
7	62.5	80	2.48	39.68	0.38
8	31.25	160	1.00	31.25	0.41
WOC **4**					
9	500	10	17.84	35.68	0.33
10	250	20	13.02	52.08	0.38
11	125	40	6.66	53.28	0.44
12	62.5	80	4.15	66.4	0.45
WOC **5**					
13	2000	5	5.36	2.68	1.49
14	1000	10	2.25	2.25	1.45
15	500	20	1.38	2.76	0.66
16	250	40	0.27	1.08	0.38

Table S3. Kinetic data for the multiple addition experiments with **2** and **4** ([CAN] = 5 mM).

	C	R	TOF	
			UV-Vis	DM
	μM		min^{-1}	min^{-1}
WOC **2**				
1	62.5	80	10.0	5.6
2	59.5	80	13.7	11.8
3	56.8	80	11.9	5.7
4	54.3	80	8.1	3.1
WOC **4**				
5	62.5	80	69.9	2.9
6	59.5	80	129.3	9.3
7	56.8	80	102.5	6.2
8	54.3	80	92.3	3.1

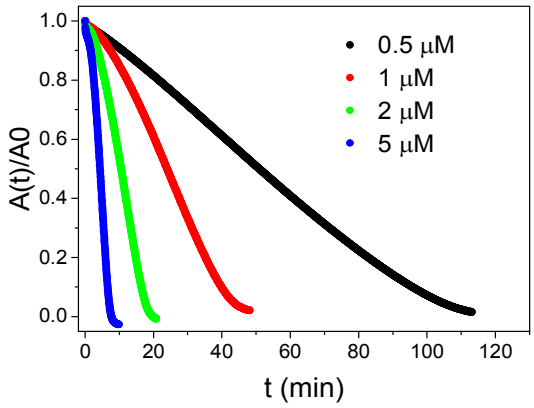


Figure S6. Selected trends of $A(t)/A_0$ *vs* t for different concentrations of **2** ([CAN] = 1 mM).

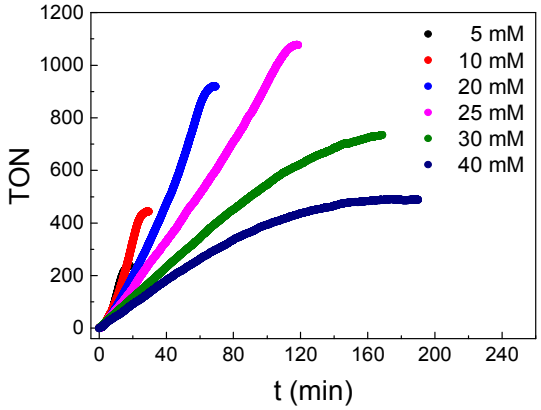


Figure S7. TON *vs* t trends obtained by means of differential manometer ([**2**] = 5 μM).

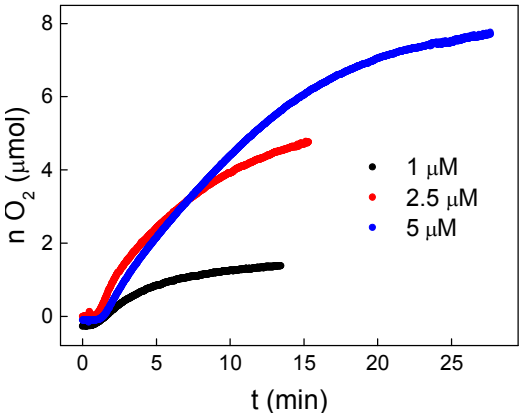


Figure S8. Selected trends of O_2 production collected by means Clark electrode ([CAN] = 10 mM).

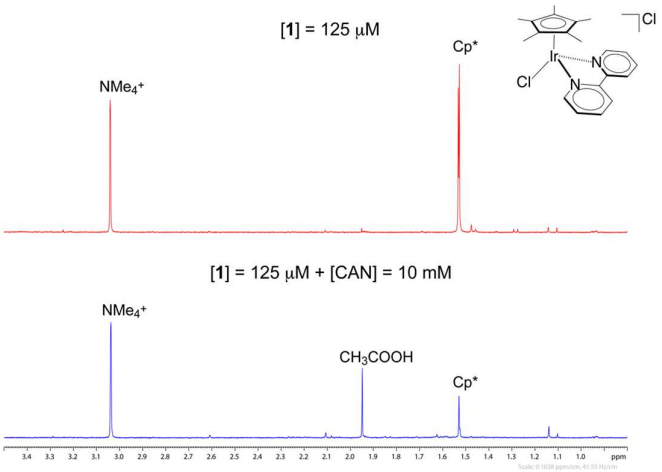


Figure S9. ^{1}H NMR spectra of **1** in DNO_3/D_2O (0.1 M) before (top) and after (bottom) ca 20 min from the addition of CAN (R = 80). Using NMe_4^+ as internal standard for integration, it was found that 25% of CH_3COOH formed and 31% of the initial Cp* resonance was still present.

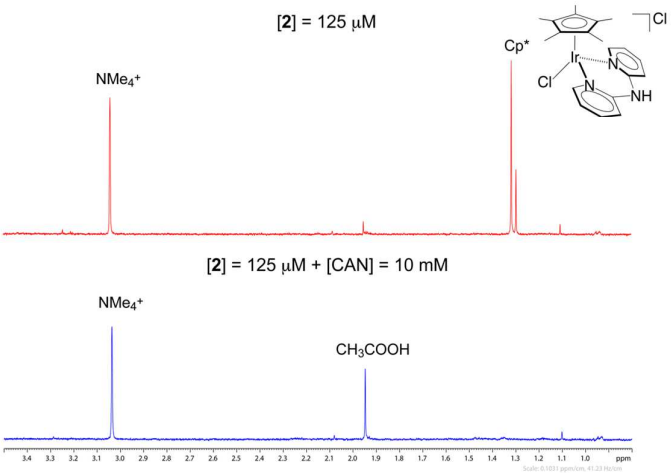


Figure S10. ^{1}H NMR spectra of **2** in DNO_3/D_2O (0.1 M) before (top) and after (bottom) ca 20 min from the addition of CAN (R = 80). Using NMe_4^+ as internal standard for integration, it was found that 41% of CH_3COOH formed, whereas the Cp* resonance completely disappeared.

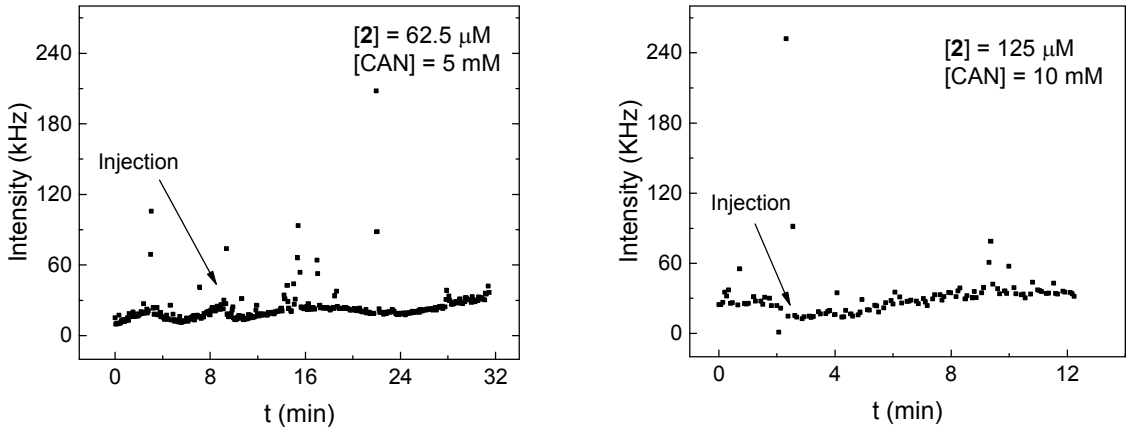


Figure S11. Light scattering intensity *vs* time trend for the reaction of **2** with 80 equivalents of CAN in acidic water (pH 1 by HNO_3) at room temperature.

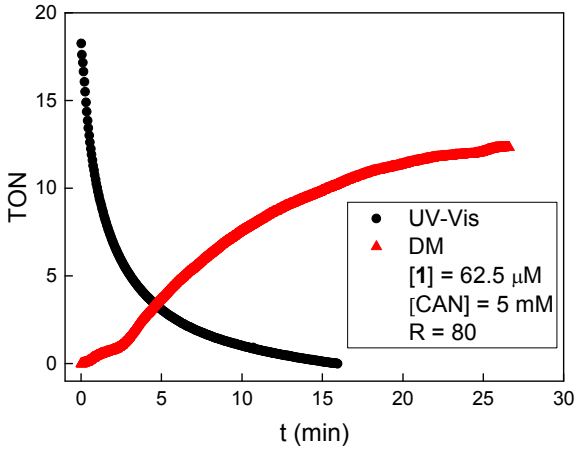


Figure S12. Comparison between the kinetics collected by means of UV-Vis and Differential Manometer for **1**, R = 80.

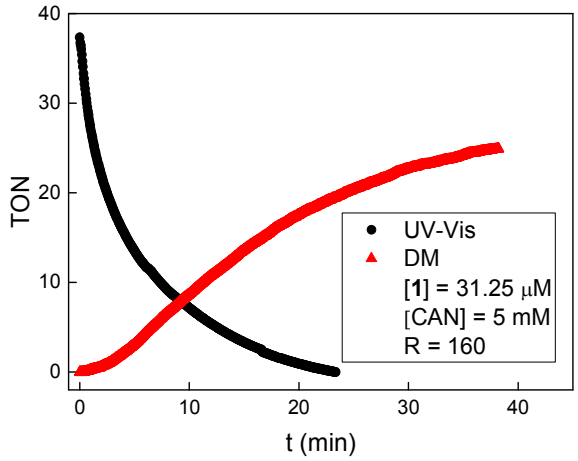


Figure S13. Comparison between the kinetics collected by means of UV-Vis and Differential Manometer for **1**, R = 160.

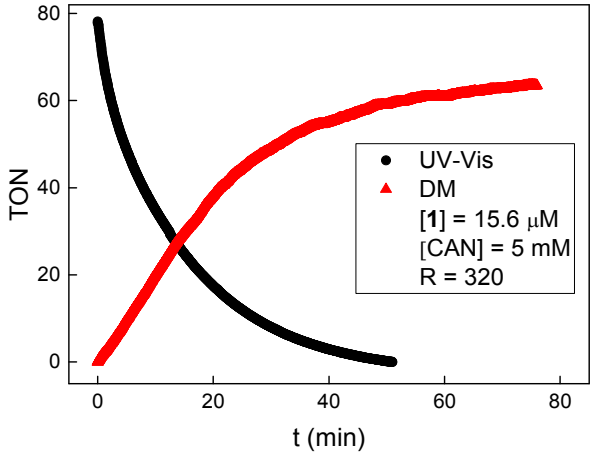


Figure S14. Comparison between the kinetics collected by means of UV-Vis and Differential Manometer for **1,** R = 320.

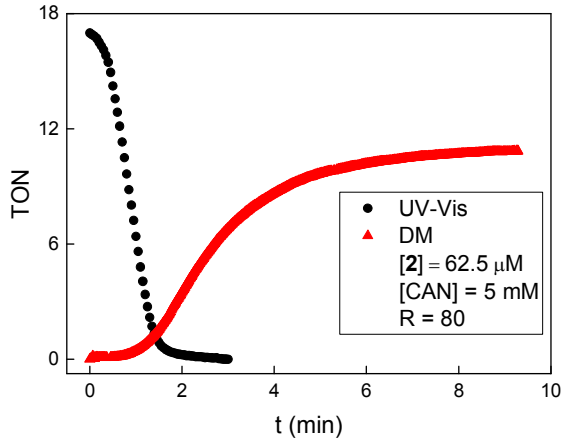


Figure S15. Comparison between the kinetics collected by means of UV-Vis and Differential Manometer for **2**, R = 80.

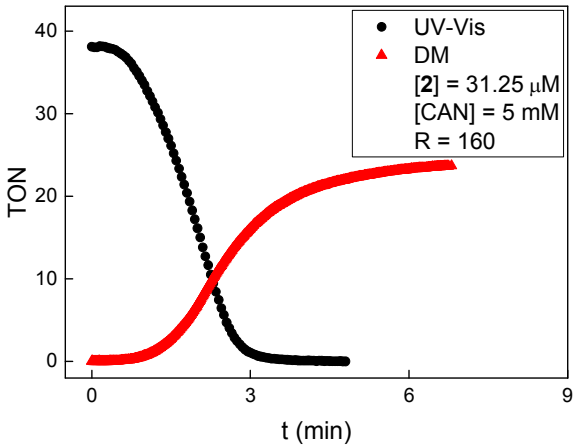


Figure S16. Comparison between the kinetics collected by means of UV-Vis and Differential Manometer for **2**, R = 160.

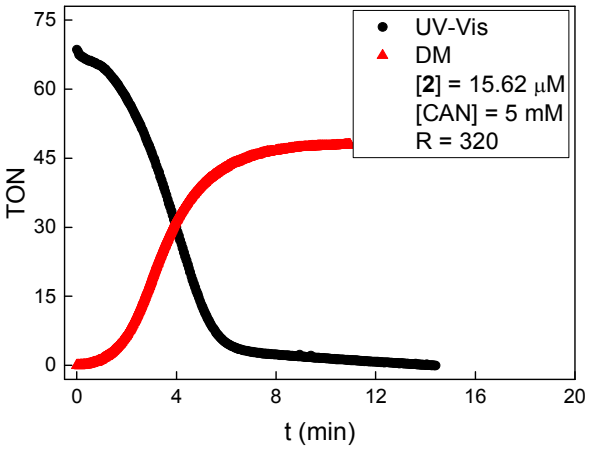


Figure S17. Comparison between the kinetics collected by means of UV-Vis and Differential Manometer for **2**, R = 320.

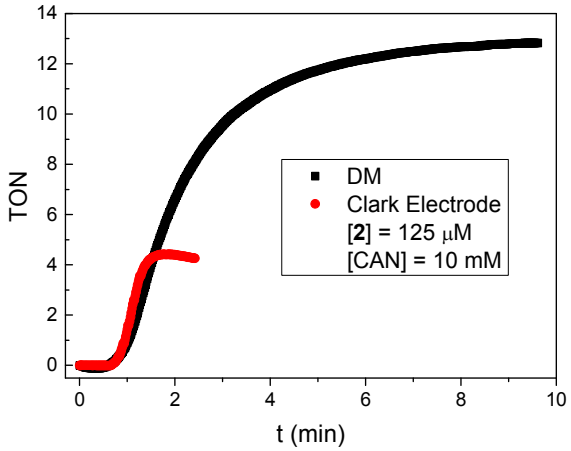


Figure S18. TON *vs* t trends obtained for **2** by means of Differential Manometer (black) and Clark Electrode (red).

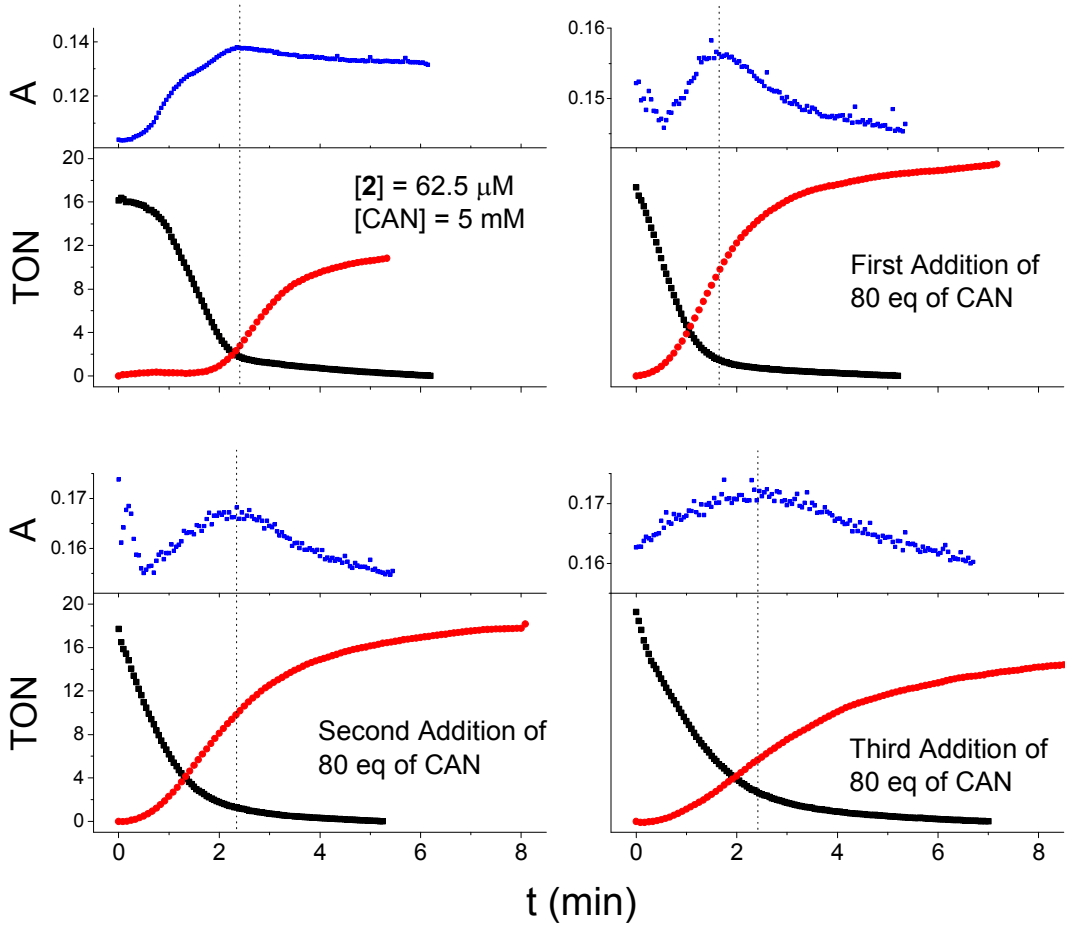


Figure S19. Multiple addition experiment performed using **2**. $[\mathbf{2}]_0$ = 62.5μM, [CAN] = 5 mM. 160 equivalents of CAN were added for each injection. The top trace in blue refers to the variation of intensity of the UV-Vis band at 575 nm.

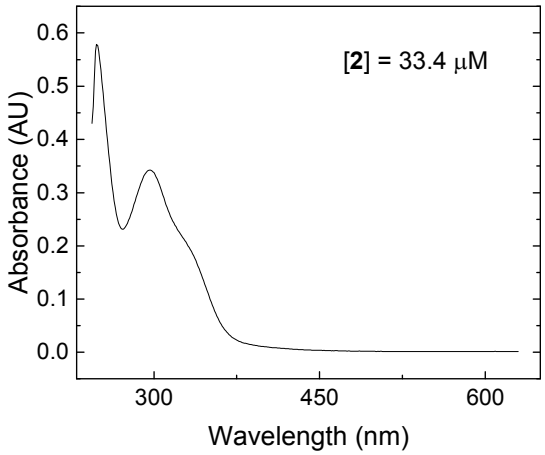


Figure S20. UV-Vis spectrum of **2** recorded in H_2O (pH = 1, HNO_3). [**2**] = 33.4 μM.

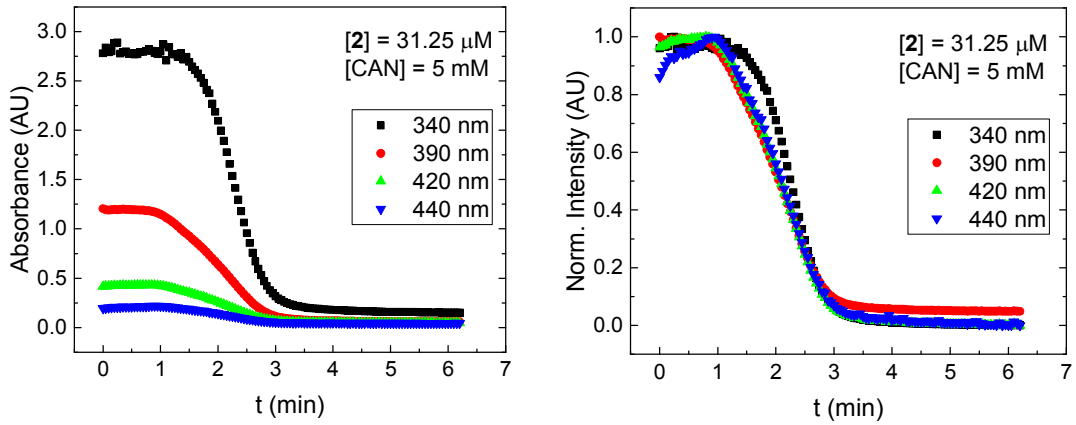


Figure S21. Depletion of CAN followed at several wavelengths ([**2**] = 31.25 μM and [CAN] = 5mM). Left panel shows the trend of absorbance vs time; in the right panel absorbance was normalized.

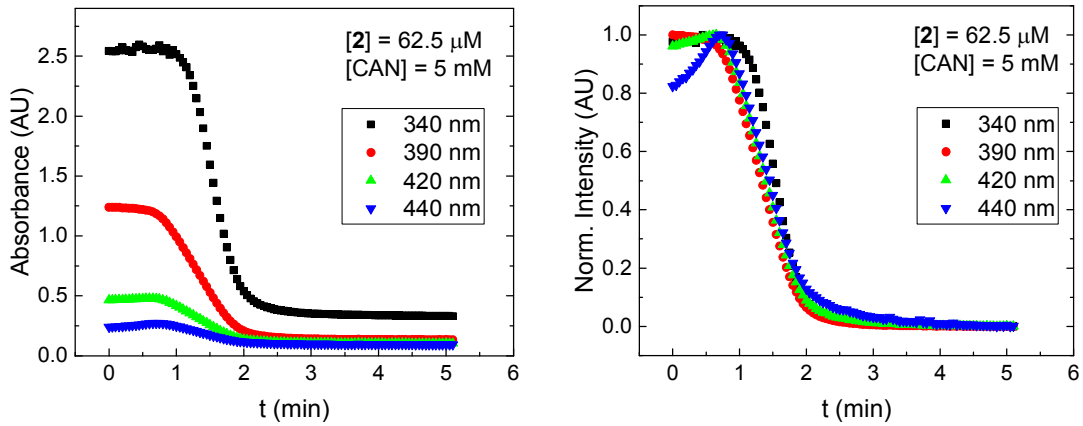


Figure S22. Depletion of CAN followed at several wavelengths ([**2**] = 62.5 μM and [CAN] = 5mM). Left panel shows the trend of absorbance *vs* time; in the right panel absorbance was normalized.

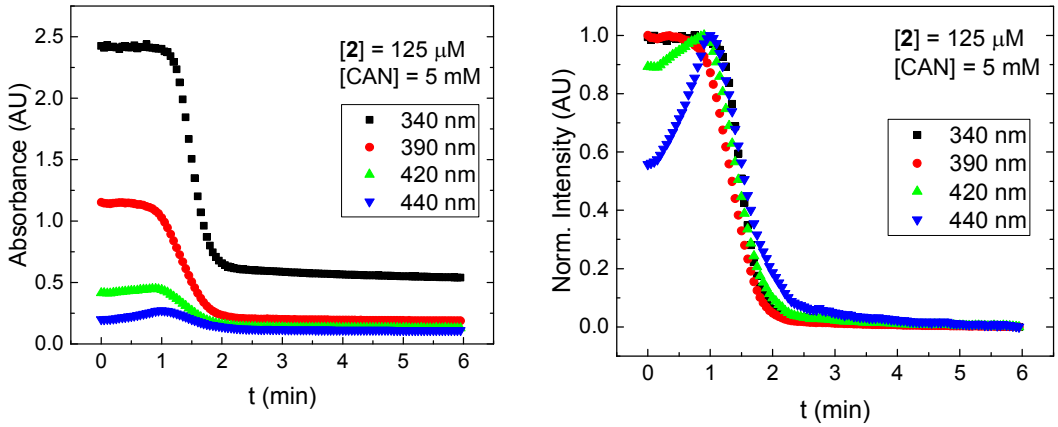


Figure S23. Depletion of CAN followed at several wavelengths ([**2**] = 125 μM and [CAN] = 5mM). Left panel shows the trend of absorbance *vs* time; in the right panel absorbance was normalized.

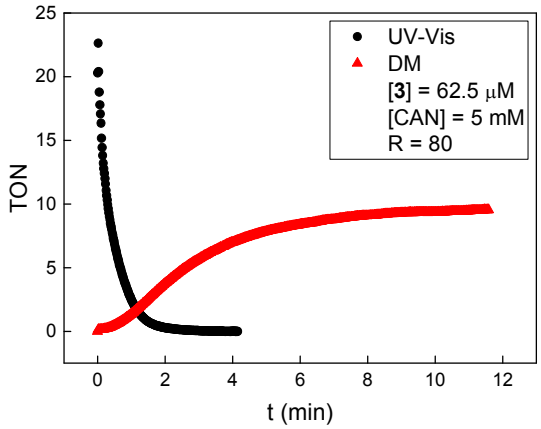


Figure S24. Comparison between the kinetics collected by means of UV-Vis and Differential Manometer for **3**, R = 80.

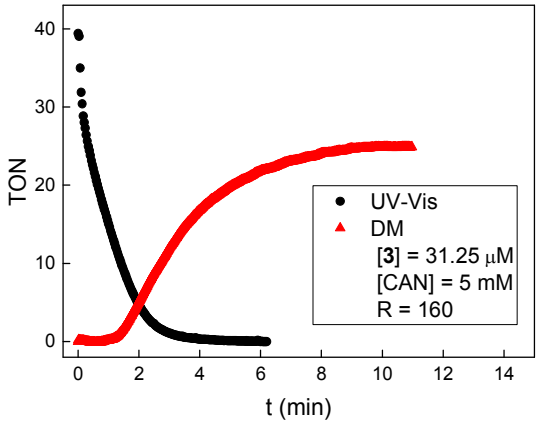


Figure S25. Comparison between the kinetics collected by means of UV-Vis and Differential Manometer for **3**, R = 160.

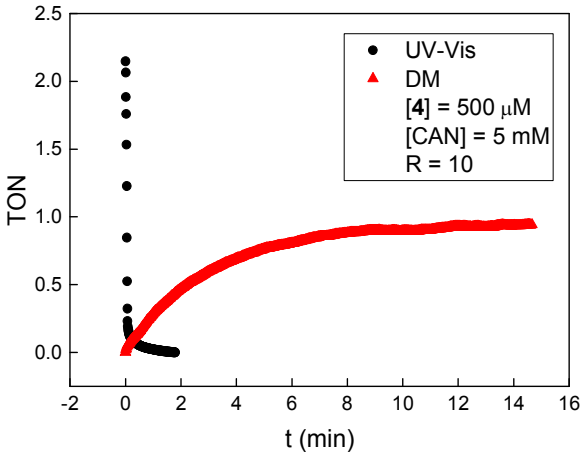


Figure S26. Comparison between the kinetics collected by means of UV-Vis and Differential Manometer for **4**, R = 10.

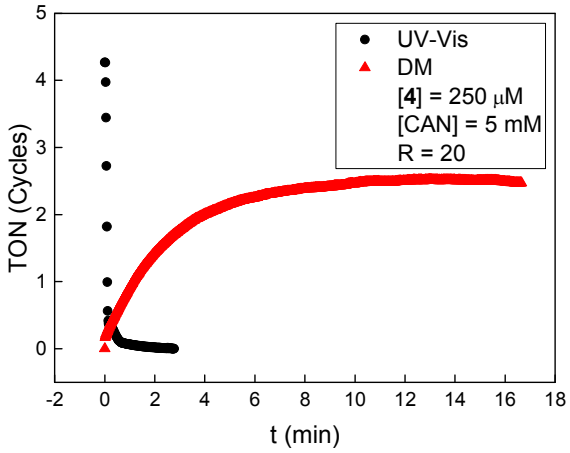


Figure S27. Comparison between the kinetics collected by means of UV-Vis and Differential Manometer for **4**, R = 20.

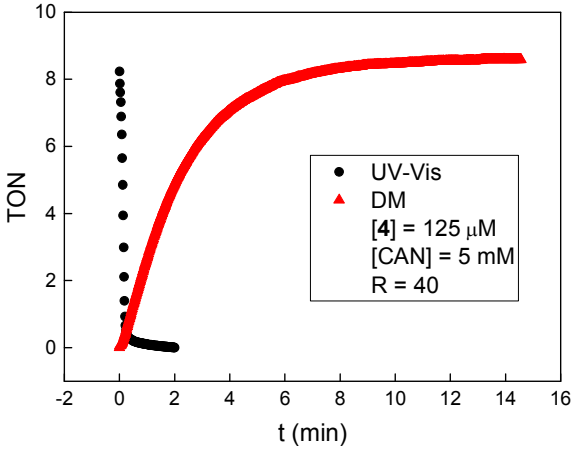


Figure S28. Comparison between the kinetics collected by means of UV-Vis and Differential Manometer for **4**, R = 40.

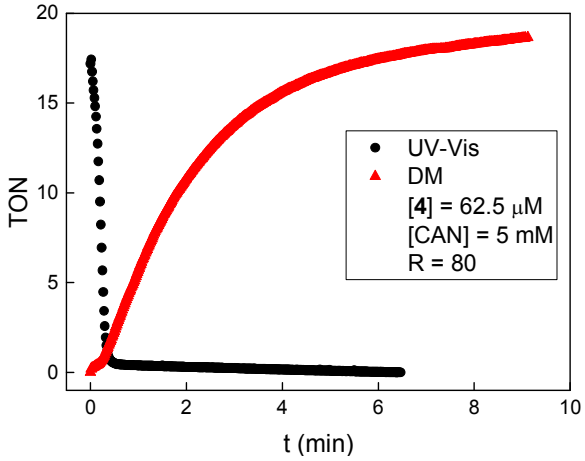


Figure S29. Comparison between the kinetics collected by means of UV-Vis and Differential Manometer for **4**, R = 80.

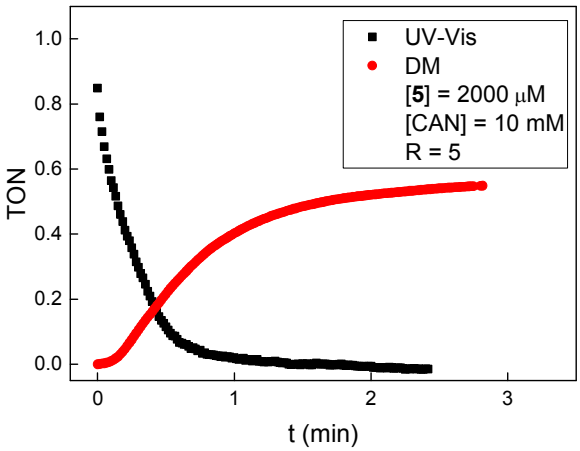


Figure S30. Comparison between the kinetics collected by means of UV-Vis and Differential Manometer for **5**, R = 5.

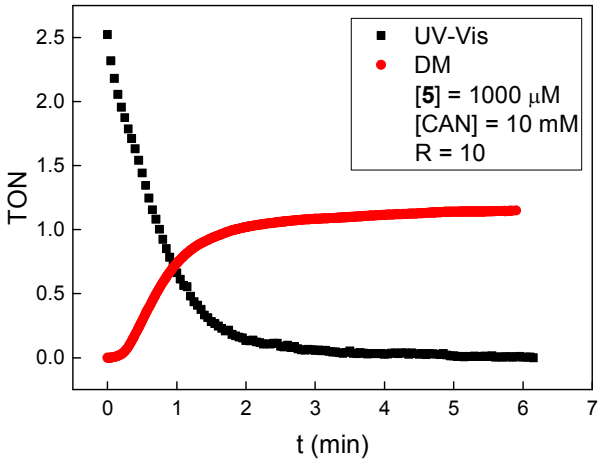


Figure S31. Comparison between the kinetics collected by means of UV-Vis and Differential Manometer for **5**, R = 10.

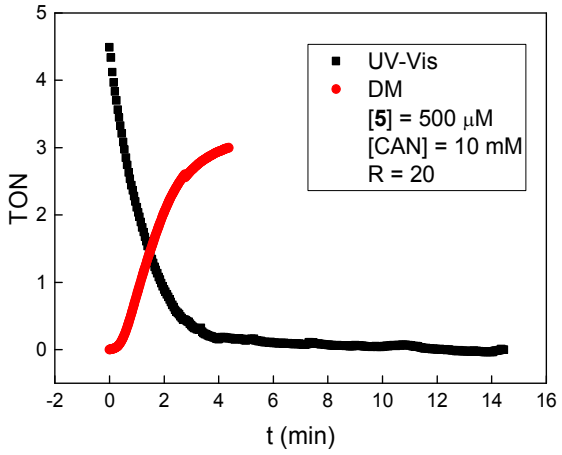


Figure S32. Comparison between the kinetics collected by means of UV-Vis and Differential Manometer for **5**, R = 20.

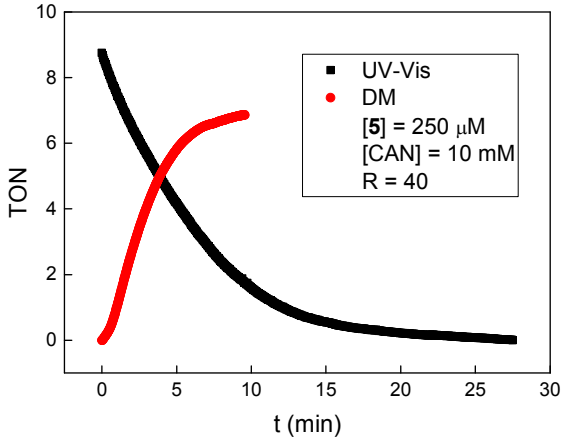


Figure S33. Comparison between the kinetics collected by means of UV-Vis and Differential Manometer for **5**, R = 40.

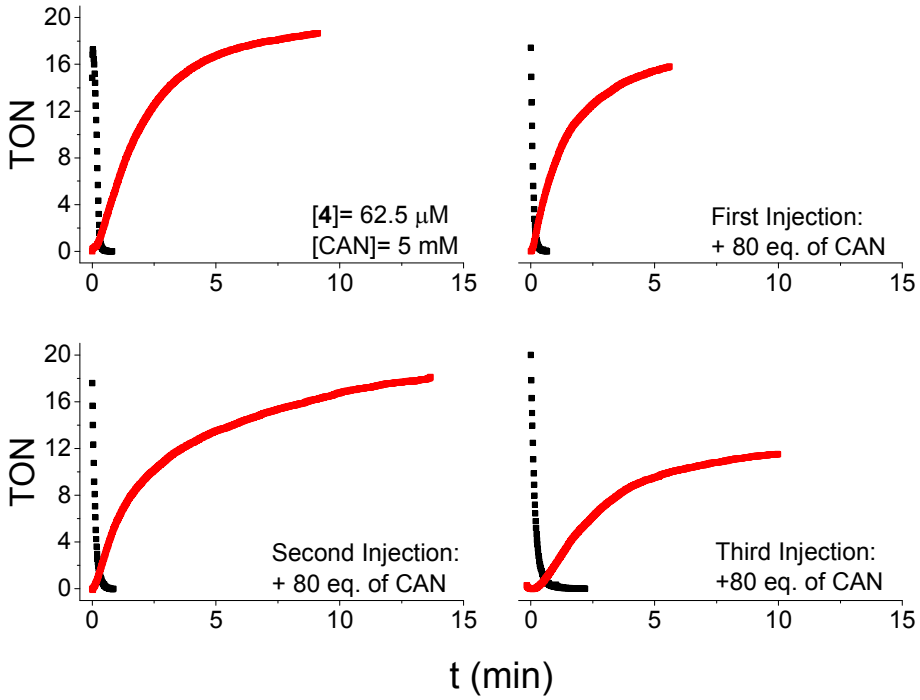


Figure S34. Multiple addition experiment performed using **4**. $[\mathbf{4}]_0$ = 62.5 μM, [CAN]= 5 mM. 80 equivalents of CAN were added in each injection.

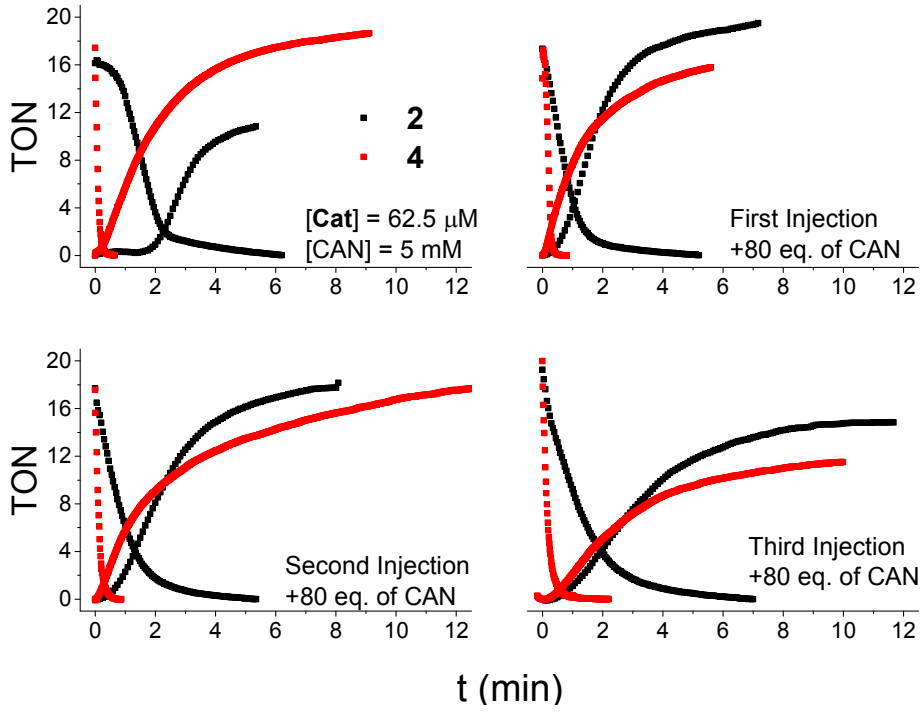


Figure S35. Comparison of multiple addition experiment for **2** and **4** performed under exactly the same experimental conditions ($[\text{Cat}]_0$ = 62.5 μM, [CAN] = 5 mM. 80 equivalents of CAN were added in each injection.

Kinetic Treatment

The kinetic model adopted consists of two consecutive, irreversible reactions:

$4\ Ce^{4+} + 2\ H_2O \rightarrow X$

$X \rightarrow O_2$

Initial conditions for t = 0 are:

$$[Ce^{4+}] = [Ce^{4+}]_0 \qquad \text{(S1)}$$

$$[X] = 0 \qquad \text{(S2)}$$

$$[O_2] = 0 \qquad \text{(S3)}$$

While at all time:

$$[Ce^{4+}]_0 = [Ce^{4+}] + 4[X] + 4\,[O_2]. \qquad \text{(S4)}$$

The kinetic law for CAN depletion was found to be zero order with respect to cerium, thus the differential rate equations for the concentrations of $[Ce^{4+}]$, [X] and $[O_2]$ can be expressed as:

$$-\frac{1}{4}\frac{d[Ce^{4+}]}{dt} = k_1^{obs} \qquad \text{with } k_1^{obs} = k_1[Ir]^n \qquad \text{(S5)}$$

$$\frac{d[X]}{dt} = k_1^{obs} - k_2^{obs}[X] \qquad \text{(S6)}$$

$$\frac{d[O_2]}{dt} = k_2^{obs}[X] \qquad \text{(S7)}$$

Integrating S5 and S6, S8 and [X] are obtained, respectively. Substituting [X] in S4 affords S9:

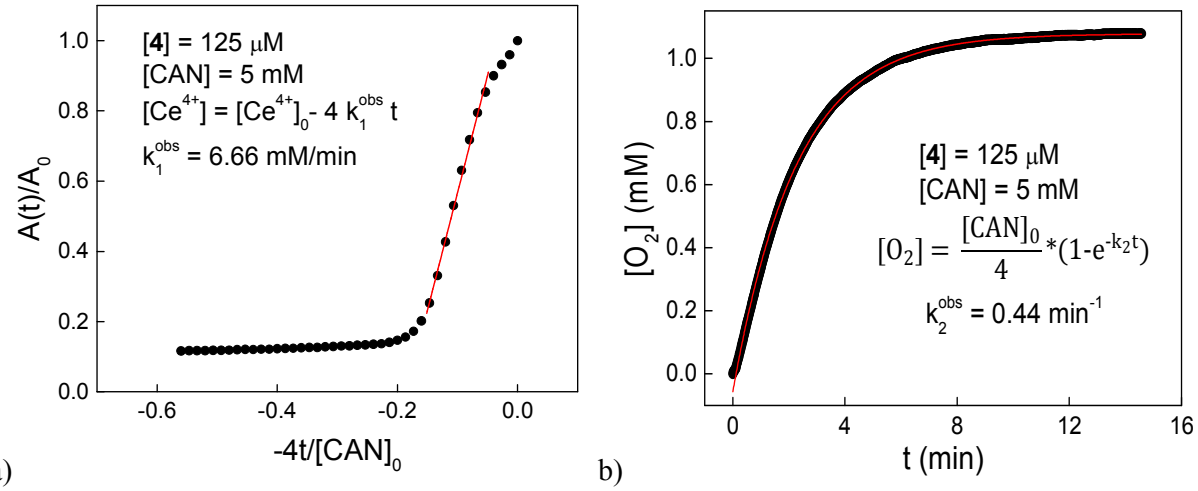
$$[Ce^{4+}] = [Ce^{4+}]_0 - 4k_1^{obs}t \qquad \text{(S8)}$$

$$[O_2] = k_1^{obs}t - \frac{k_1^{obs}t}{k_2^{obs}t}\left(1 - e^{-k_2^{obs}t}\right) \qquad \text{(S9)}$$

Because $k_1^{obs}\,t >> k_2^{obs}\,t$, S9 can be written as:

$$[O_2] = \frac{[Ce^{4+}]_0}{4}\,(1 - e^{-k_2^{obs}t}) \qquad \text{(S10)}$$

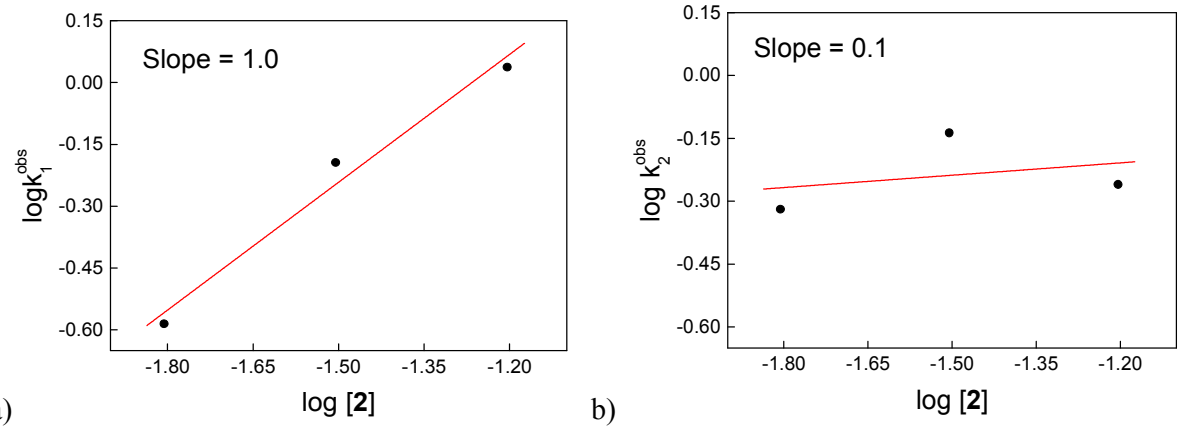
An example of fitting for both cerium depletion and oxygen evolution, using equations S8 and S10, respectively, are reported for catalyst **4** in Figure S36.



a) b)

Figure S36. a) Linear fit related to CAN depletion and b) exponential function fit for O_2 evolution.

The reaction orders with respect to the catalyst are reported in Figure S37**,** which shows log k^{obs} *vs* log [**2**] for both k_1^{obs} and k_2^{obs}.



a) b)

Figure S37. a) log k_1^{obs} *vs* log[**2**] plot and b) log k_2^{obs} vs log[**2**].

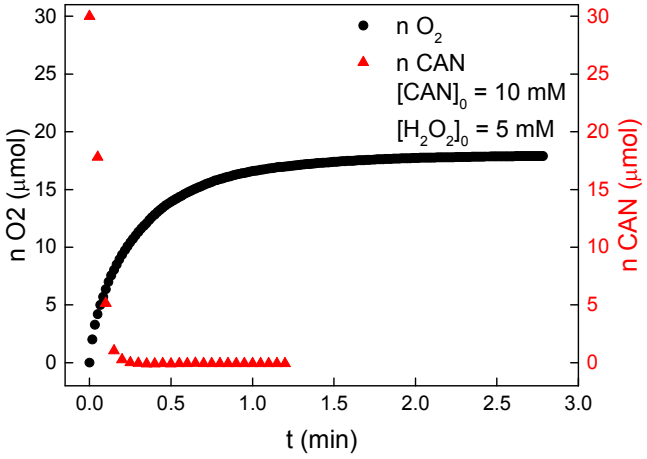


Figure S38. Time course of the reaction between CAN and H_2O_2. The black trend represents the depletion of Ce(IV) followed by means of UV-Vis, whereas the red trend is the production of oxygen monitored using differential manometer. The CAN/O_2 ratio indicates that the reaction proceeds through the oxidation of H_2O_2

Table S4. Summary of kinetic results for H_2O_2 oxidation promoted by CAN.

[CAN] mM	[H_2O_2] mM	k_{CAN} mM/min	k_{O2} mM/min
10	5	99.5	73.0

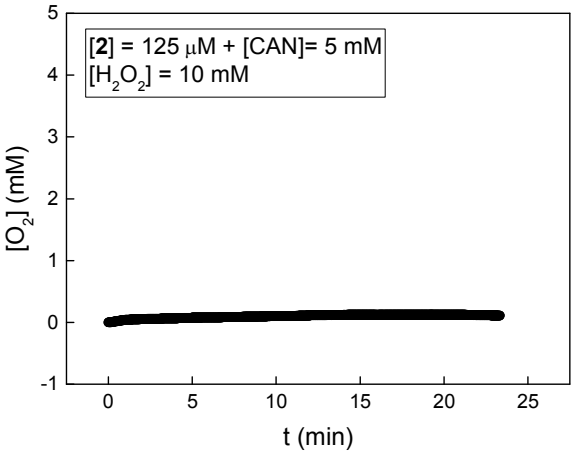


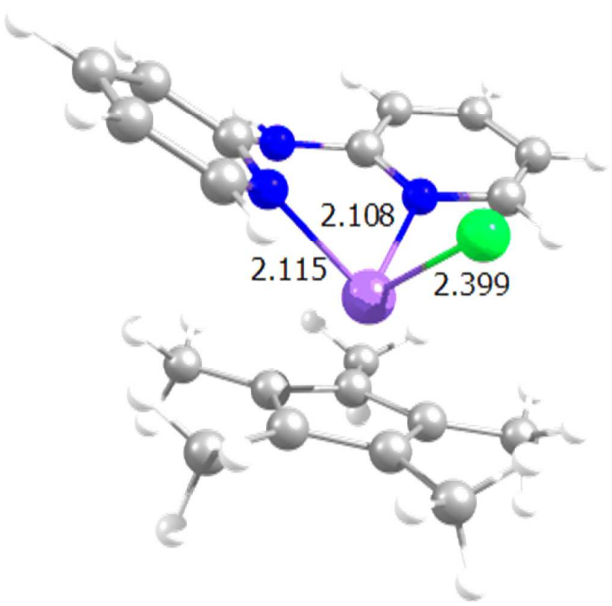
Figure S39. Time course of the reaction between **2** and H_2O_2. **2** was allowed to react with a solution of CAN (5mM) before injection.

Computational Details

All the DFT static calculations were performed with the Gaussian09 set of programs.[8] The electronic configuration of the molecular systems was described with the standard split-valence basis set with a polarization function of Ahlrichs and co-workers for H, C, N, and Cl (SVP keyword in Gaussian09).[9] For Ir we used the small-core, quasi-relativistic Stuttgart/Dresden effective core potential, with an associated valence basis set contracted (standard SDD keywords in Gaussian09).[10] The geometry optimizations were performed without symmetry constraints, and the characterization of the located stationary points was performed by analytical frequency calculations. The BP86 functional was employed in geometry optimizations and frequency calculations, including the D3 dispersion correction of Grimme.[11] Gibbs energies, ΔG, were built through single point energy calculations on the BP86-d3/SVP geometries using the M06 functional[12] and the triple-ζ valence plus polarization on main group atoms (TZVP keyword in Gaussian).[13] Solvent effects were included with the PCM model using H_2O as solvent.[14] To these M06/TZVP electronic energies in solvent, zero point energy and thermal and entropic corrections were included from the gas phase frequency calculations at the BP86-d3/SVP level of theory.

Table S5. Coordinate data sets and absolute energy (in a.u.), 3D structure for DFT optimized complexes with selected distances (in Å).

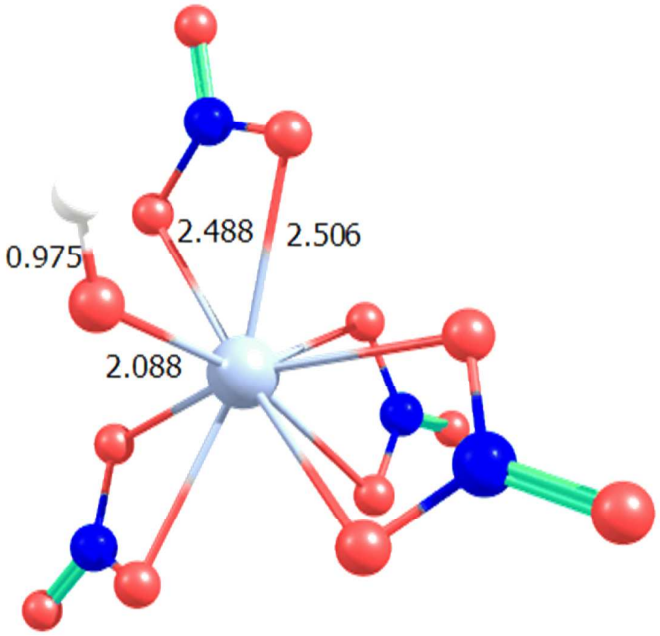
[Cp*Ir(dpa)Cl]$^{+1}$



Zero-point correction= 0.390163 (Hartree/Particle)
Thermal correction to Energy= 0.416521
Thermal correction to Enthalpy= 0.417465
Thermal correction to Gibbs Free Energy= 0.333756
Sum of electronic and zero-point Energies= -1504.395280
Sum of electronic and thermal Energies= -1504.368922
Sum of electronic and thermal Enthalpies= -1504.367977
Sum of electronic and thermal Free Energies= -1504.451687

C	-0.315515	1.851171	3.081742
C	0.536685	0.691161	3.327870
C	-1.679365	1.396348	2.903867
C	-0.333578	-0.490261	3.361084
C	-1.692444	-0.066001	3.089331
C	0.123803	-1.891650	3.627220
H	0.182661	-2.073487	4.721427
H	-0.572069	-2.635585	3.194319
H	1.130903	-2.073732	3.202759
C	2.001485	0.733986	3.644451
H	2.163541	0.930168	4.726374
H	2.499404	-0.224660	3.400599
H	2.506933	1.538034	3.075099
C	0.170966	3.263450	3.016346
H	0.414699	3.616260	4.041130
H	1.082673	3.338172	2.392040
H	-0.587483	3.941574	2.584597
C	-2.888099	2.255379	2.684390
H	-3.348024	2.532323	3.657304
H	-2.628904	3.191447	2.153638
H	-3.658790	1.727750	2.089029
C	-2.914719	-0.931959	3.047958
H	-3.437453	-0.917180	4.028247
H	-3.630848	-0.575468	2.281283
H	-2.658429	-1.982484	2.811797
C	2.017378	-1.060803	0.446711
C	0.030712	-2.245672	0.047149
C	2.803623	-2.173912	0.147760
H	2.447636	-0.081397	0.702194
C	0.765484	-3.412206	-0.263752
C	2.161031	-3.379013	-0.194388
H	3.899205	-2.091930	0.178260
H	0.236601	-4.324603	-0.579149
H	2.744920	-4.280879	-0.433181
C	-2.600934	1.098279	-0.602538
C	-2.190600	-1.207222	-0.456889
C	-3.759725	0.898580	-1.353483
H	-2.220421	2.099812	-0.353801
C	-3.355843	-1.483195	-1.207276
C	-4.154661	-0.421590	-1.641885
H	-4.336652	1.764485	-1.707500
H	-3.609558	-2.523340	-1.463014
H	-5.065034	-0.622276	-2.226936
N	-1.858999	0.064938	-0.121369
N	0.657765	-1.109759	0.444141
N	-1.366225	-2.260030	-0.041217
H	-1.747720	-3.182556	-0.260553
Cl	0.639888	1.959500	-0.136125
Ir	-0.421628	0.437189	1.384507

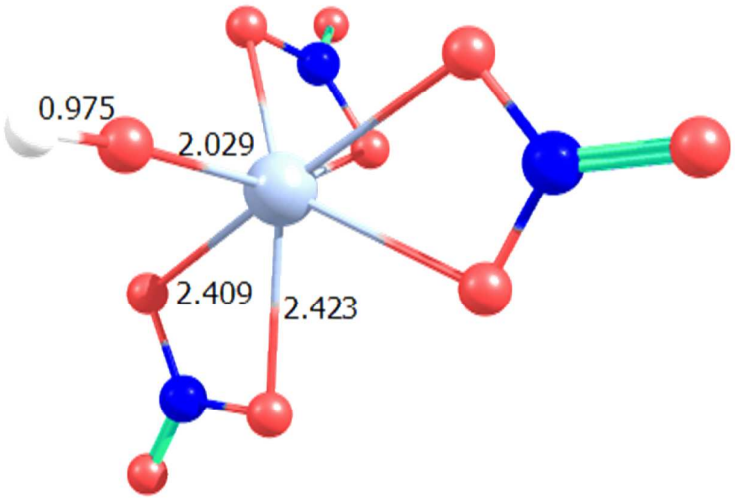
$[Ce^{IV}(NO_3)_4OH]^{-1}$



Ce	-1.208993	0.529062	-0.129153
N	-0.054520	1.393737	2.425309
N	0.512066	-0.265664	-2.348369
N	-1.197338	3.200462	-1.360116
N	-4.110075	0.388261	-0.435105
O	-1.322371	1.394896	2.200719
O	0.419281	1.765869	3.487905
O	0.915813	0.474058	-1.363079
O	1.249879	-0.567287	-3.271363
O	-3.313302	-0.298680	-1.174763
O	-5.320809	0.363856	-0.573241
O	-0.708134	2.989519	-0.189889
O	-1.193803	4.300738	-1.884794
O	-0.707687	-0.655513	-2.277590
O	0.680261	0.964467	1.458354
O	-1.696881	2.162219	-1.948533
O	-3.535577	1.108536	0.473595
O	-0.958479	-1.321187	0.805261
H	-0.281769	-1.610817	1.445064

Zero-point correction= 0.073029 (Hartree/Particle)
Thermal correction to Energy= 0.094198
Thermal correction to Enthalpy= 0.095143
Thermal correction to Gibbs Free Energy= 0.018497
Sum of electronic and zero-point Energies= -1671.844713
Sum of electronic and thermal Energies= -1671.823544
Sum of electronic and thermal Enthalpies= -1671.822600
Sum of electronic and thermal Free Energies= -1671.899245

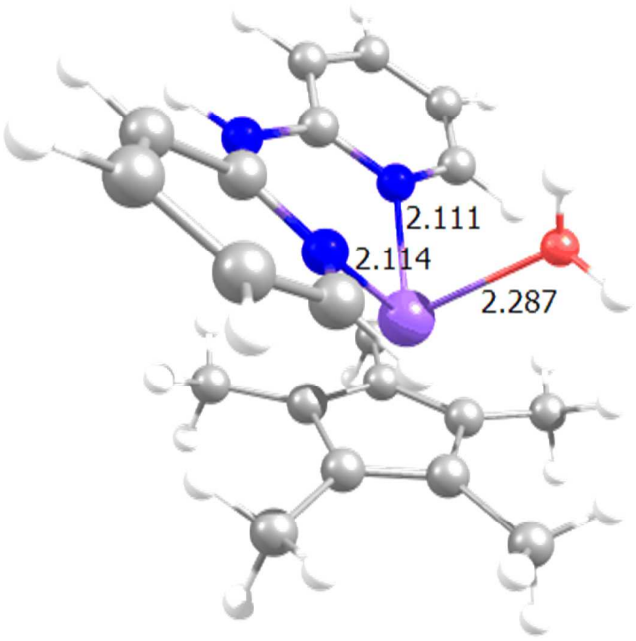
$[Ce^{IV}(NO_3)_3OH]^{+o}$



Ce	-1.023692	0.348389	-0.013076
N	-0.138372	1.745807	2.328517
N	0.513269	-0.152888	-2.380663
N	-3.282511	1.850210	-0.937012
O	-1.372606	1.370369	2.139926
O	0.221211	2.335123	3.314746
O	1.028263	0.353783	-1.301559
O	1.148116	-0.364538	-3.381378
O	-3.390524	0.647249	-0.464570
O	-4.218629	2.495645	-1.329870
O	-0.760434	-0.413254	-2.283142
O	0.660687	1.425340	1.356407
O	-2.057959	2.306327	-0.950218
O	-1.080557	-1.535744	0.736456
H	-0.987341	-2.434025	1.104794

Zero-point correction= 0.056813 (Hartree/Particle)
Thermal correction to Energy= 0.073762
Thermal correction to Enthalpy= 0.074706
Thermal correction to Gibbs Free Energy= 0.005420
Sum of electronic and zero-point Energies= -1391.580450
Sum of electronic and thermal Energies= -1391.563500
Sum of electronic and thermal Enthalpies= -1391.562556
Sum of electronic and thermal Free Energies= -1391.631842

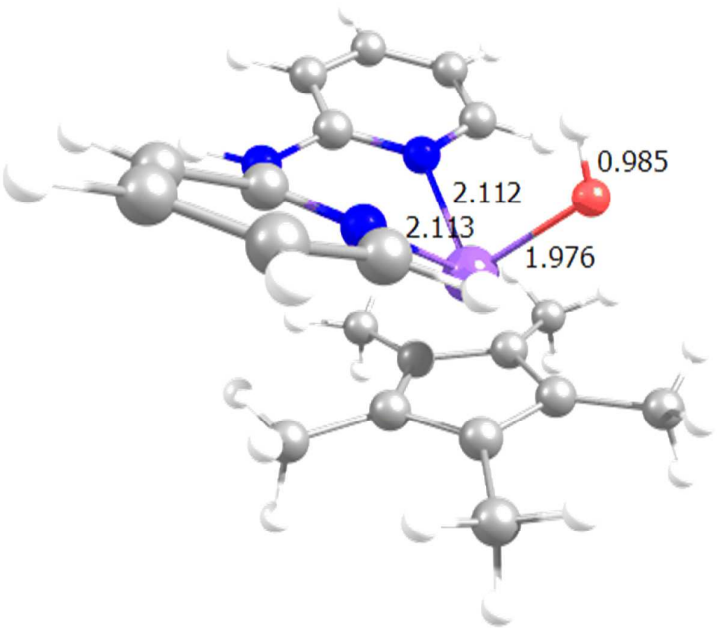
[Cp*Ir(dpa)OH$_2$]$^{+2}$



Zero-point correction= 0.413495 (Hartree/Particle)
Thermal correction to Energy= 0.440824
Thermal correction to Enthalpy= 0.441768
Thermal correction to Gibbs Free Energy= 0.357426
Sum of electronic and zero-point Energies= -1120.291106
Sum of electronic and thermal Energies= -1120.263777
Sum of electronic and thermal Enthalpies= -1120.262833
Sum of electronic and thermal Free Energies= -1120.347175

C	0.157007	1.804881	2.743629
C	0.819114	0.544978	2.970861
C	-1.262135	1.646346	3.135982
C	-0.184330	-0.428111	3.430535
C	-1.456678	0.296464	3.594739
C	0.086206	-1.833154	3.869455
H	0.363468	-1.846419	4.945981
H	-0.806258	-2.475932	3.745763
H	0.922584	-2.283922	3.302213
C	2.269280	0.244648	2.771117
H	2.787460	0.302281	3.752737
H	2.425427	-0.776739	2.373409
H	2.758357	0.966378	2.091199
C	0.787404	3.087844	2.300037
H	0.978836	3.735818	3.182823
H	1.757181	2.922200	1.794130
H	0.130150	3.656230	1.613213
C	-2.275489	2.747423	3.137638
H	-2.187131	3.328815	4.081582
H	-2.112613	3.464033	2.308584
H	-3.312584	2.364881	3.082690
C	-2.707228	-0.290700	4.166020
H	-2.634629	-0.283259	5.275194
H	-3.609215	0.286054	3.889332
H	-2.849512	-1.342992	3.852669
C	1.471163	0.170514	-0.493949
C	0.488968	-1.948187	-0.211421
C	2.526818	-0.354008	-1.232866
H	1.381519	1.247889	-0.293303
C	1.547388	-2.547996	-0.935983
C	2.574366	-1.748844	-1.439453
H	3.298884	0.315939	-1.637343
H	1.539313	-3.633913	-1.117116
H	3.398373	-2.205454	-2.008997
C	-3.556117	-0.840131	0.988078
C	-1.889690	-2.417542	0.477817
C	-4.573351	-1.777901	0.847507
H	-3.771285	0.204407	1.256603
C	-2.875842	-3.425995	0.341698
C	-4.219781	-3.107505	0.533555
H	-5.621340	-1.476330	0.986555
H	-2.575269	-4.447828	0.063029
H	-4.991903	-3.884245	0.422560
N	-2.231887	-1.147899	0.833440
N	0.482924	-0.610969	0.037896
N	-0.554562	-2.746998	0.254078
H	-0.404627	-3.746368	0.092323
Ir	-0.783366	0.242045	1.495077
O	-1.417469	1.497113	-0.308932
H	-1.768644	1.015077	-1.087517
H	-2.028041	2.247703	-0.159051

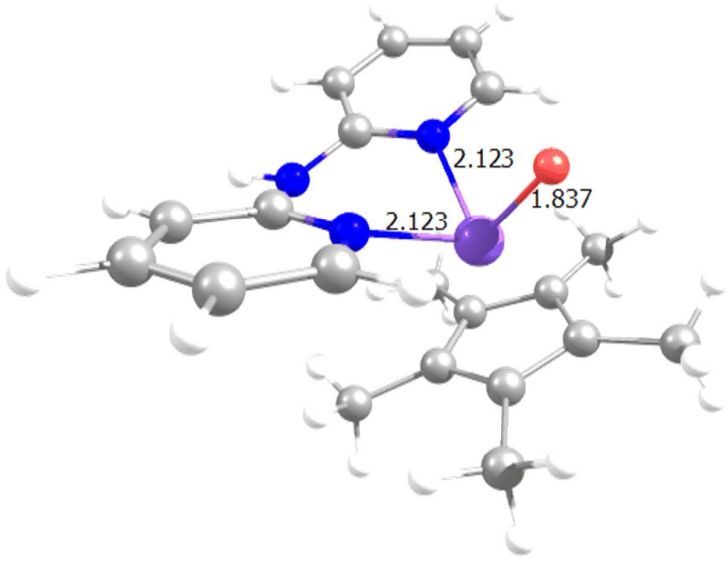
[Cp*Ir(dpa)OH]$^{+2}$



Zero-point correction= 0.401988 (Hartree/Particle)
Thermal correction to Energy= 0.428481
Thermal correction to Enthalpy= 0.429425
Thermal correction to Gibbs Free Energy= 0.345766
Sum of electronic and zero-point Energies= -1119.657380
Sum of electronic and thermal Energies= -1119.630887
Sum of electronic and thermal Enthalpies= -1119.629943
Sum of electronic and thermal Free Energies= -1119.713601

C	-0.236140	1.976742	2.816350
C	0.885237	1.040586	2.827431
C	-1.431204	1.242922	3.225116
C	0.377394	-0.266740	3.272030
C	-1.032672	-0.143688	3.514148
C	1.215328	-1.491840	3.452747
H	1.726346	-1.446881	4.438770
H	0.607865	-2.415556	3.429899
H	2.003444	-1.566566	2.678179
C	2.320182	1.378774	2.584427
H	2.792807	1.674235	3.547497
H	2.891213	0.513896	2.195153
H	2.433882	2.229356	1.885939
C	-0.164194	3.431469	2.488478
H	0.055938	4.005248	3.414742
H	0.635293	3.646695	1.754856
H	-1.118268	3.806128	2.072742
C	-2.787282	1.823520	3.462639
H	-2.857505	2.163407	4.519852
H	-2.982042	2.702429	2.819336
H	-3.591301	1.078362	3.307931
C	-1.957240	-1.214048	3.999254
H	-2.102678	-1.106535	5.095921
H	-2.956143	-1.136748	3.527077
H	-1.553819	-2.226125	3.810626
C	1.670370	-0.538687	-0.358348
C	0.194505	-2.305577	0.151889
C	2.604587	-1.409318	-0.912897
H	1.832893	0.548641	-0.327075
C	1.109184	-3.241045	-0.384482
C	2.323709	-2.791579	-0.906962
H	3.535325	-1.010008	-1.341021
H	0.846859	-4.309998	-0.406636
H	3.041615	-3.512173	-1.328363
C	-3.483256	-0.065499	0.519785
C	-2.258989	-2.080247	0.569496
C	-4.686056	-0.739899	0.327891
H	-3.431470	1.031976	0.571107
C	-3.449135	-2.822407	0.390404
C	-4.667981	-2.149534	0.281877
H	-5.619518	-0.169476	0.217116
H	-3.402071	-3.919700	0.314869
H	-5.599797	-2.718671	0.140352
N	-2.295315	-0.724751	0.665449
N	0.499208	-0.981331	0.188961
N	-1.031391	-2.741325	0.661456
H	-1.120794	-3.760993	0.686485
Ir	-0.628574	0.383270	1.341481
O	-0.768731	1.645213	-0.172242
H	-0.955396	1.216175	-1.039478

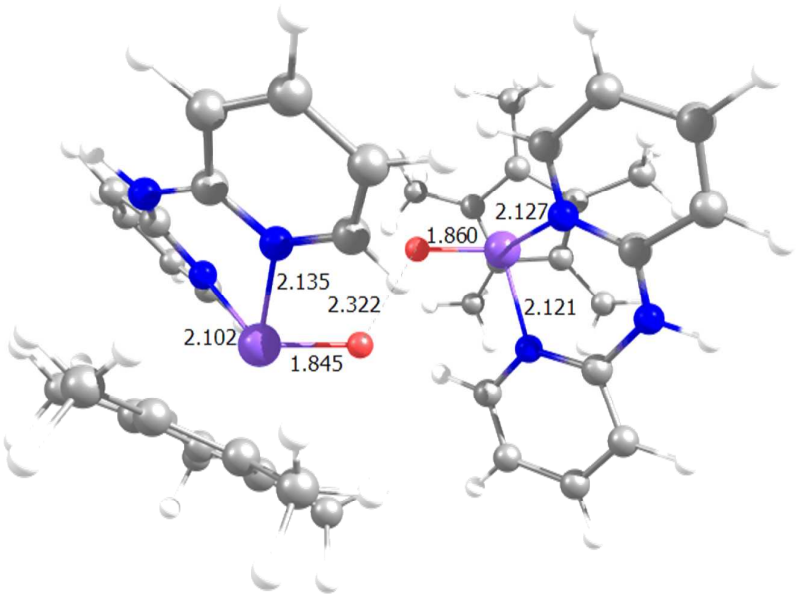
[Cp*Ir(dpa)O]$^{+2}$



Zero-point correction= 0.391162 (Hartree/Particle)
Thermal correction to Energy= 0.417192
Thermal correction to Enthalpy= 0.418136
Thermal correction to Gibbs Free Energy= 0.335422
Sum of electronic and zero-point Energies= -1119.015149
Sum of electronic and thermal Energies= -1118.989119
Sum of electronic and thermal Enthalpies= -1118.988175
Sum of electronic and thermal Free Energies= -1119.070888

C	0.013457	1.927459	2.758921
C	0.841007	0.734306	2.864678
C	-1.349034	1.559112	3.141851
C	0.003509	-0.370394	3.340196
C	-1.331379	0.146686	3.528287
C	0.480092	-1.750910	3.678825
H	0.841127	-1.778351	4.729582
H	-0.329063	-2.499564	3.584804
H	1.322148	-2.064571	3.032313
C	2.313874	0.660083	2.634120
H	2.834397	0.827277	3.602977
H	2.625925	-0.333319	2.259749
H	2.668792	1.436485	1.931119
C	0.463929	3.301491	2.385330
H	0.615504	3.896290	3.312755
H	1.420148	3.293548	1.830317
H	-0.293802	3.826859	1.772217
C	-2.499551	2.507024	3.257138
H	-2.430409	3.051219	4.224776
H	-2.488436	3.263141	2.448779
H	-3.475202	1.986068	3.240443
C	-2.502517	-0.622349	4.041640
H	-2.496653	-0.578657	5.153185
H	-3.464737	-0.197000	3.700428
H	-2.458804	-1.689994	3.753401
C	1.538445	-0.099376	-0.552524
C	0.430325	-2.094373	-0.025652
C	2.551163	-0.772977	-1.207298
H	1.508320	0.997755	-0.494702
C	1.447008	-2.838799	-0.652954
C	2.514504	-2.175562	-1.235585
H	3.358933	-0.205894	-1.691790
H	1.368716	-3.935606	-0.704114
H	3.309275	-2.748314	-1.737778
C	-3.544770	-0.566293	0.732206
C	-1.991039	-2.317148	0.584703
C	-4.614645	-1.433891	0.612106
H	-3.680025	0.521556	0.814956
C	-3.039847	-3.253137	0.485406
C	-4.353585	-2.810154	0.509362
H	-5.639930	-1.037192	0.595740
H	-2.807311	-4.321480	0.357261
H	-5.178974	-3.533392	0.421959
N	-2.259891	-1.003471	0.750912
N	0.516742	-0.749104	0.056336
N	-0.671111	-2.754578	0.513000
H	-0.583241	-3.774873	0.488958
Ir	-0.761715	0.378721	1.314256
O	-1.205630	1.551927	-0.038129

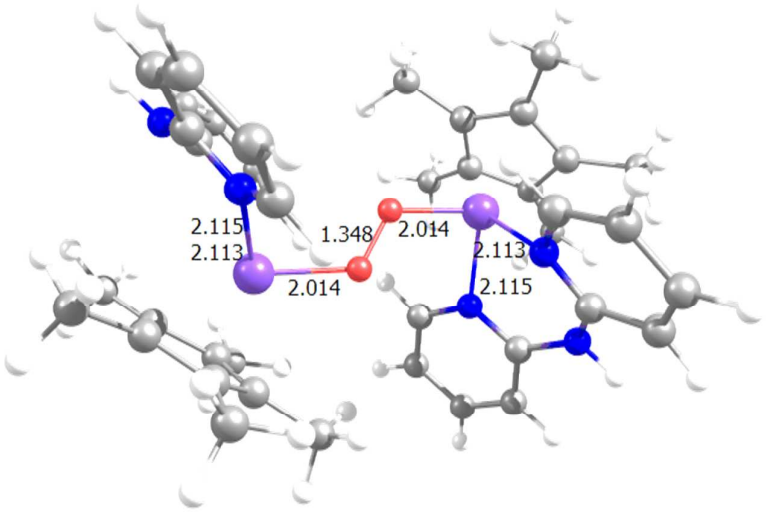
[Cp*Ir(dpa)O···O[Cp*Ir(dpa)]$^{+4}$



Zero-point correction= 0.782386 (Hartree/Particle)
Thermal correction to Energy= 0.835501
Thermal correction to Enthalpy= 0.836446
Thermal correction to Gibbs Free Energy= 0.693165
Sum of electronic and zero-point Energies= -2237.812545
Sum of electronic and thermal Energies= -2237.759430
Sum of electronic and thermal Enthalpies= -2237.758485
Sum of electronic and thermal Free Energies= -2237.901766

C	-0.422262	2.063533	2.940164
C	0.852416	1.371659	2.754971
C	-1.373864	1.112445	3.502639
C	0.680226	-0.014036	3.211110
C	-0.677330	-0.173769	3.664094
C	1.754490	-1.050685	3.238273
H	2.335180	-0.944407	4.181533
H	1.343835	-2.077328	3.218998
H	2.468948	-0.932863	2.400873
C	2.143592	1.993656	2.339759
H	2.675971	2.359055	3.247671
H	2.819270	1.267903	1.847346
H	1.994391	2.865607	1.675082
C	-0.673086	3.514862	2.692307
H	-0.398335	4.091836	3.602753
H	-0.061499	3.899530	1.854203
H	-1.739372	3.716173	2.477601
C	-2.748097	1.419179	3.997048
H	-2.684903	1.723776	5.066660
H	-3.217125	2.256343	3.446253
H	-3.414428	0.536203	3.957652
C	-1.277701	-1.405498	4.256580
H	-1.207179	-1.342710	5.365431
H	-2.350873	-1.508962	4.004877
H	-0.744028	-2.322388	3.944692
C	1.488130	-0.081240	-0.484940
C	0.439419	-2.083654	0.174122
C	2.519114	-0.763622	-1.123553
H	1.450352	1.017206	-0.446559
C	1.464679	-2.837489	-0.449359
C	2.514306	-2.176122	-1.087476
H	3.325992	-0.205747	-1.620846
H	1.422183	-3.938005	-0.432541
H	3.322763	-2.754560	-1.562262
C	-3.513871	-0.612909	1.225849
C	-1.924714	-2.336362	0.988614
C	-4.566209	-1.519065	1.311915
H	-3.671185	0.473931	1.285899
C	-2.951081	-3.309244	1.079599
C	-4.272848	-2.900376	1.256934
H	-5.596926	-1.157175	1.439004
H	-2.699444	-4.378856	1.002995
H	-5.075143	-3.650442	1.342527
N	-2.213715	-1.011467	1.092504
N	0.478625	-0.724826	0.172215
N	-0.606300	-2.748312	0.811217
H	-0.483462	-3.764925	0.852786
Ir	-0.719940	0.431942	1.472256
O	-1.390406	1.660373	0.009891
C	-2.290346	0.670342	-4.242153
C	-1.358558	1.693960	-4.712758
C	-3.615266	1.273026	-4.153484
C	-2.120268	2.933571	-4.915981
C	-3.495463	2.678219	-4.573408
C	-1.556189	4.213988	-5.437613
H	-1.540604	4.175660	-6.549574
H	-2.168046	5.088215	-5.147253
H	-0.513622	4.377089	-5.102639
C	0.070889	1.484071	-5.085983
H	0.123281	1.190330	-6.159381
H	0.671595	2.408074	-4.981184
H	0.542334	0.671445	-4.501360
C	-1.958421	-0.764163	-3.991490
H	-2.053482	-1.331751	-4.943312
H	-0.919870	-0.886376	-3.629557
H	-2.647783	-1.222278	-3.257599
C	-4.896084	0.563183	-3.865880
H	-5.322402	0.188607	-4.824371
H	-4.752664	-0.313976	-3.206917
H	-5.655928	1.234312	-3.421604
C	-4.631065	3.641442	-4.677166
H	-5.136372	3.497267	-5.658187
H	-5.393258	3.474189	-3.891767
H	-4.292255	4.693052	-4.633592
C	0.456997	3.541577	-2.209367
C	-1.278449	5.127349	-2.078736
C	1.438682	4.526840	-2.166543
H	0.705214	2.473718	-2.295890
C	-0.328628	6.178311	-2.040946
C	1.032600	5.878479	-2.099066
H	2.502066	4.249295	-2.208340
H	-0.670519	7.222093	-1.958142
H	1.777034	6.690390	-2.084220
C	-4.623410	2.575463	-0.982911
C	-3.682451	4.671822	-1.504073
C	-5.763949	3.159651	-0.440966
H	-4.487785	1.484786	-1.023204
C	-4.822518	5.326504	-0.975028
C	-5.872272	4.568612	-0.456288
H	-6.564979	2.528253	-0.029674
H	-4.868674	6.427006	-0.970940
H	-6.768165	5.069086	-0.055682
N	-3.611193	3.313860	-1.528279
N	-0.877198	3.833116	-2.189577
N	-2.636651	5.432078	-2.021181
H	-2.834770	6.437104	-2.052697
Ir	-2.213033	2.289531	-2.734596
O	-1.658347	1.056705	-1.229440

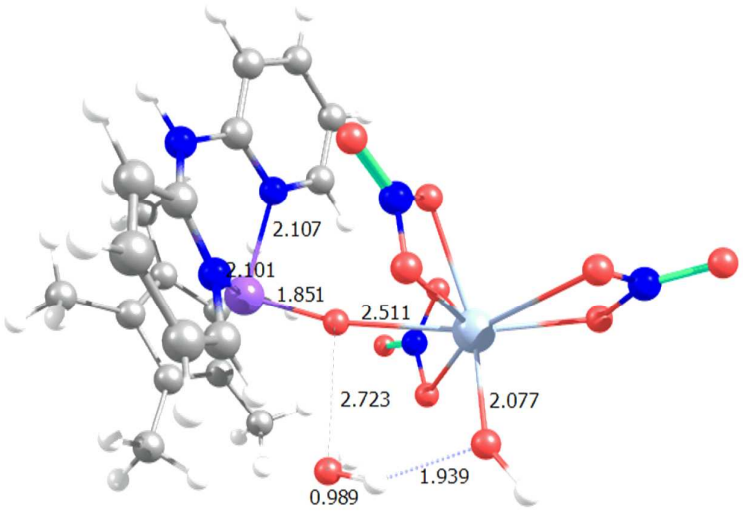
[Cp*Ir(dpa)OO[Cp*Ir(dpa)]$^{+4}$



Zero-point correction= 0.783751 (Hartree/Particle)
Thermal correction to Energy= 0.837185
Thermal correction to Enthalpy= 0.838130
Thermal correction to Gibbs Free Energy= 0.695018
Sum of electronic and zero-point Energies= -2237.852011
Sum of electronic and thermal Energies= -2237.798577
Sum of electronic and thermal Enthalpies= -2237.797633
Sum of electronic and thermal Free Energies= -2237.940744

C	-0.217716	1.931607	2.761275
C	0.972275	1.171457	2.386005
C	-1.103951	1.053524	3.512529
C	0.822571	-0.184870	2.930948
C	-0.446303	-0.256946	3.614809
C	1.841439	-1.271380	2.830102
H	2.576007	-1.154083	3.657776
H	1.391475	-2.276555	2.930413
H	2.409038	-1.223421	1.880807
C	2.198672	1.717165	1.728757
H	2.898700	2.088645	2.510367
H	2.743037	0.945139	1.151570
H	1.963059	2.570838	1.064779
C	-0.453000	3.376860	2.468086
H	0.034807	3.991435	3.256355
H	-0.017841	3.670823	1.492998
H	-1.530509	3.626258	2.466992
C	-2.361474	1.447541	4.215271
H	-2.106321	1.791000	5.243192
H	-2.883568	2.282792	3.711197
H	-3.061736	0.598071	4.328293
C	-0.989963	-1.435022	4.352998
H	-0.725155	-1.337510	5.429537
H	-2.094080	-1.490582	4.294133
H	-0.560424	-2.388705	3.994173
C	0.978213	-0.396963	-0.888682
C	-0.011317	-2.332341	0.008984
C	1.835521	-1.136091	-1.697591
H	1.000419	0.702063	-0.872105
C	0.839877	-3.144554	-0.782983
C	1.774826	-2.546198	-1.627349
H	2.560996	-0.625316	-2.347522
H	0.749765	-4.241219	-0.733808
H	2.448916	-3.171081	-2.234484
C	-3.646826	-0.676981	1.737017
C	-2.189469	-2.465470	1.258064
C	-4.691806	-1.540267	2.049572
H	-3.762088	0.415295	1.788917
C	-3.209437	-3.395427	1.574140
C	-4.459746	-2.932452	1.985260
H	-5.668523	-1.134315	2.351283
H	-3.012417	-4.475488	1.484992
H	-5.255714	-3.648889	2.243634
N	-2.406924	-1.125726	1.369204
N	0.088185	-0.976521	-0.032393
N	-0.943851	-2.936476	0.846066
H	-0.856256	-3.956661	0.891816
Ir	-0.809740	0.256439	1.432409
O	-1.506081	1.535297	0.041022
C	-1.883954	0.900194	-4.241616
C	-0.918576	1.979527	-4.435198
C	-3.223032	1.447239	-4.411668
C	-1.674861	3.200510	-4.747616
C	-3.080739	2.874627	-4.730747
C	-1.074115	4.526937	-5.077407
H	-0.841496	4.557009	-6.165206
H	-1.767222	5.362498	-4.866380
H	-0.124694	4.700687	-4.535401
C	0.568548	1.838169	-4.484664
H	0.881234	1.612480	-5.528751
H	1.087212	2.770277	-4.188476
H	0.922967	1.005822	-3.846773
C	-1.548981	-0.529343	-3.969747
H	-1.404055	-1.058448	-4.937306
H	-0.611876	-0.625732	-3.388102
H	-2.361647	-1.044798	-3.424292
C	-4.501508	0.675951	-4.444995
H	-4.689390	0.335380	-5.488266
H	-4.466498	-0.227454	-3.807034
H	-5.371046	1.294075	-4.150625
C	-4.209673	3.803034	-5.033942
H	-4.482507	3.696956	-6.107685
H	-5.115658	3.564444	-4.444008
H	-3.938226	4.861984	-4.867173
C	0.242681	3.708503	-1.463113
C	-1.523796	5.249789	-1.649620
C	1.153510	4.701219	-1.115822
H	0.542115	2.655199	-1.561081
C	-0.645324	6.310052	-1.309962
C	0.698810	6.037872	-1.056231
H	2.206248	4.445007	-0.926865
H	-1.032366	7.338770	-1.238193
H	1.389781	6.858423	-0.805747
C	-4.960939	2.583948	-1.524613
C	-3.981142	4.720516	-1.689635
C	-6.212599	3.119856	-1.239889
H	-4.795331	1.498571	-1.584532
C	-5.231080	5.326837	-1.415505
C	-6.353386	4.525259	-1.204634
H	-7.068301	2.452470	-1.060501
H	-5.307153	6.424384	-1.361701
H	-7.332000	4.988559	-1.001473
N	-3.864434	3.366081	-1.769736
N	-1.064588	3.973431	-1.749587
N	-2.864225	5.528402	-1.896962
H	-3.080636	6.530146	-1.912185
Ir	-2.194452	2.448657	-2.682898
O	-1.778850	1.132582	-1.215894

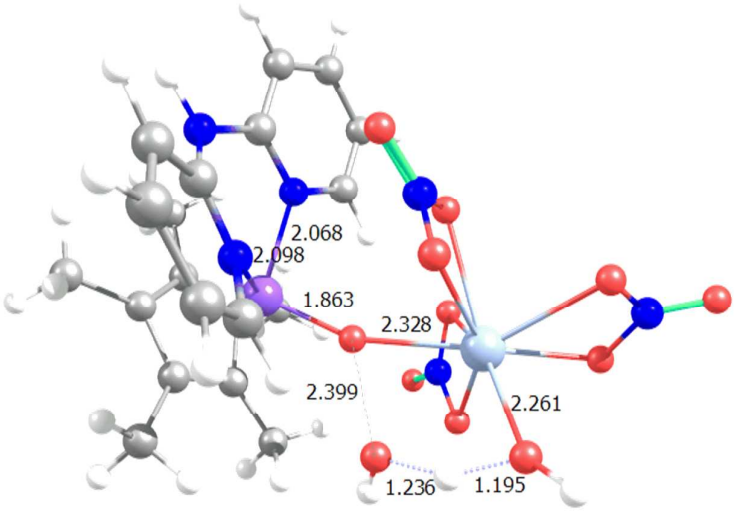
[Cp*Ir(dpa)O-Ce^{IV}(NO$_3$)$_3$OH]$^{+2}$+OH$_2$



Zero-point correction= 0.475181 (Hartree/Particle)
Thermal correction to Energy= 0.521338
Thermal correction to Enthalpy= 0.522282
Thermal correction to Gibbs Free Energy= 0.393436
Sum of electronic and zero-point Energies= -2587.024617
Sum of electronic and thermal Energies= -2586.978461
Sum of electronic and thermal Enthalpies= -2586.977517
Sum of electronic and thermal Free Energies= -2587.106363

C	-1.047059	1.565066	3.321479
C	0.283408	1.926795	2.852967
C	-1.098841	0.094392	3.426514
C	1.011814	0.691685	2.568747
C	0.152199	-0.434492	2.971620
C	2.440452	0.586345	2.145644
H	3.086251	0.576800	3.051927
H	2.639115	-0.351988	1.592892
H	2.747751	1.441576	1.515684
C	0.834102	3.308447	2.754096
H	1.514997	3.465780	3.620383
H	1.439749	3.460724	1.839187
H	0.039225	4.073647	2.810909
C	-2.104437	2.518593	3.773094
H	-3.101475	2.040754	3.806813
H	-1.867034	2.868358	4.801971
H	-2.154977	3.402926	3.107660
C	-2.266729	-0.679809	3.946293
H	-2.241226	-0.674284	5.057570
H	-3.228506	-0.225898	3.638195
H	-2.247887	-1.733646	3.612739
C	0.553747	-1.872898	2.910813
H	1.168017	-2.118637	3.803992
H	-0.321411	-2.548505	2.906153
H	1.173147	-2.086932	2.018197
C	0.819554	-0.739075	-0.796422
C	-1.092444	-1.948591	-0.107851
C	1.312311	-1.828502	-1.506084
H	1.324578	0.238549	-0.805441
C	-0.629502	-3.093511	-0.794603
C	0.582339	-3.035576	-1.483695
H	2.246805	-1.726309	-2.075812
H	-1.246093	-4.005090	-0.811780
H	0.944833	-3.919844	-2.030261
C	-3.684136	1.368922	0.926365
C	-3.246496	-0.949290	0.696354
C	-5.058233	1.157583	0.896326
H	-3.228021	2.371101	0.989947
C	-4.632932	-1.222469	0.682707
C	-5.537764	-0.166209	0.794440
H	-5.741945	2.016996	0.942836
H	-4.984193	-2.256506	0.545965
H	-6.619759	-0.368542	0.772916
N	-2.806324	0.324859	0.866201
N	-0.339464	-0.816601	-0.077890
N	-2.327016	-1.985930	0.543170
H	-2.768439	-2.908811	0.505875
Ir	-0.786160	0.762880	1.242557
O	-0.792142	1.990127	-0.142707
Ce	-0.991266	3.163196	-2.353664
N	1.555397	3.187706	-0.932500
N	-2.217165	0.533394	-2.274419
N	-1.039652	3.587393	-5.159604
O	0.687492	4.145847	-0.827623
O	2.477482	3.063537	-0.147860
O	-1.005695	0.703664	-2.677621
O	-2.702242	-0.572748	-2.117374
O	-0.084240	3.993443	-4.349549
O	-1.026603	3.785105	-6.337266
O	-2.867037	1.615744	-2.007347
O	1.343165	2.359084	-1.890117
O	-1.986202	2.954189	-4.532376
O	-1.830660	4.263100	0.937988
H	-0.875998	4.411520	0.768205
O	-2.206968	4.759560	-1.815895
H	-2.229882	4.649334	0.119573
H	-2.683211	5.558413	-2.123540

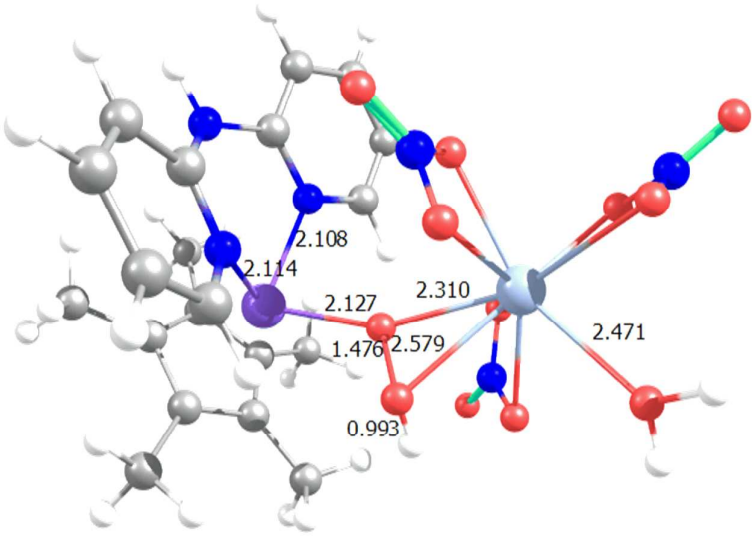
[Cp*Ir(dpa)O-Ce^{IV}(NO$_3$)$_3$OH]$^{+2}$···OH$_2$



Zero-point correction= 0.470873 (Hartree/Particle)
Thermal correction to Energy= 0.515990
Thermal correction to Enthalpy= 0.516935
Thermal correction to Gibbs Free Energy= 0.391232
Sum of electronic and zero-point Energies= -2587.015344
Sum of electronic and thermal Energies= -2586.970226
Sum of electronic and thermal Enthalpies= -2586.969282
Sum of electronic and thermal Free Energies= -2587.094984

C	-0.970175	1.468808	3.335829
C	0.332654	1.891098	2.795950
C	-0.967904	0.001122	3.442491
C	1.089523	0.689284	2.497907
C	0.282016	-0.468342	2.926944
C	2.494181	0.635835	1.995896
H	3.192225	0.744665	2.855946
H	2.723914	-0.331596	1.510475
H	2.710202	1.456241	1.284064
C	0.811332	3.296849	2.661795
H	1.331149	3.586825	3.601273
H	1.532791	3.420405	1.831929
H	-0.027435	4.001781	2.515287
C	-2.047849	2.376762	3.830849
H	-3.043309	1.894626	3.796641
H	-1.842907	2.642059	4.892149
H	-2.090281	3.318226	3.250817
C	-2.076604	-0.815362	4.024577
H	-2.013069	-0.790572	5.133941
H	-3.069318	-0.413196	3.742748
H	-2.022863	-1.871799	3.704367
C	0.728690	-1.889385	2.833992
H	1.403760	-2.112498	3.689021
H	-0.119484	-2.596903	2.879951
H	1.305650	-2.080451	1.907976
C	0.737402	-0.795078	-0.696786
C	-1.203040	-1.965738	0.006604
C	1.176779	-1.883161	-1.441406
H	1.264300	0.172058	-0.701829
C	-0.790668	-3.104268	-0.719994
C	0.408711	-3.067147	-1.431645
H	2.099677	-1.794271	-2.031947
H	-1.437667	-3.994150	-0.744064
H	0.733456	-3.948975	-2.005426
C	-3.686419	1.437643	0.822904
C	-3.309136	-0.895466	0.769979
C	-5.067630	1.254730	0.796869
H	-3.220714	2.441114	0.808921
C	-4.697493	-1.138598	0.753790
C	-5.580756	-0.055935	0.781986
H	-5.726653	2.134269	0.785021
H	-5.069150	-2.172096	0.683590
H	-6.666997	-0.234379	0.765823
N	-2.833477	0.373433	0.845642
N	-0.412293	-0.858455	0.041126
N	-2.405890	-1.964115	0.707049
H	-2.866611	-2.878329	0.719631
Ir	-0.814133	0.762385	1.260772
O	-0.821973	2.152821	0.020955
Ce	-1.066531	3.218776	-2.033984
N	1.598520	3.299345	-0.874675
N	-2.260113	0.580423	-2.185261
N	-0.594985	3.758506	-4.781976
O	0.818814	4.318765	-0.910139
O	2.600237	3.261522	-0.182220
O	-1.010820	0.775965	-2.426658
O	-2.731634	-0.537046	-2.055159
O	0.148989	4.216712	-3.807958
O	-0.396619	4.003351	-5.935439
O	-2.964343	1.648796	-2.040950
O	1.220130	2.288794	-1.587671
O	-1.574944	3.008542	-4.358140
O	-2.202964	4.110239	0.144595
H	-1.523959	4.630867	0.621992
O	-2.555899	4.919951	-2.023772
H	-2.589018	4.746850	-0.842145
H	-3.194755	5.494111	-2.487293

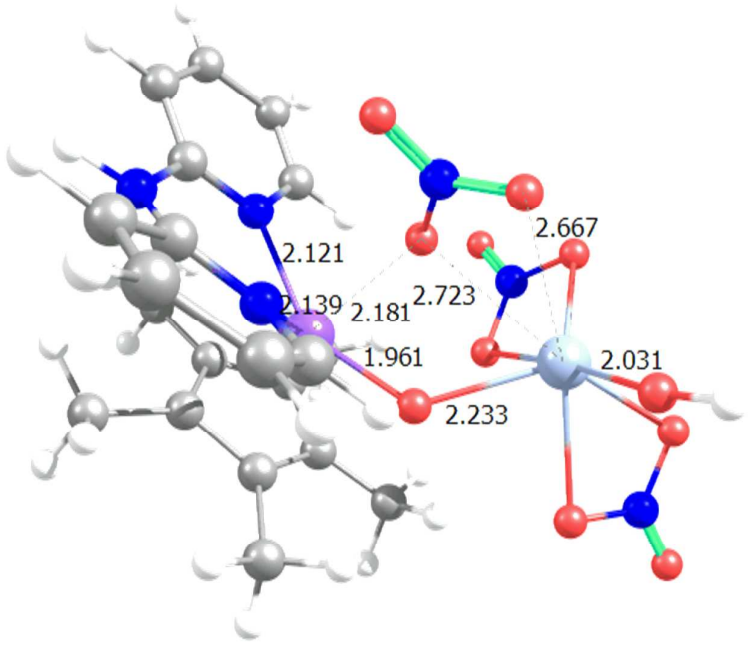
[Cp*Ir(dpa)OOH-Ce^{IV}(NO$_3$)$_3$OH$_2$]$^{+2}$



Zero-point correction= 0.477872 (Hartree/Particle)
Thermal correction to Energy= 0.523326
Thermal correction to Enthalpy= 0.524271
Thermal correction to Gibbs Free Energy= 0.397783
Sum of electronic and zero-point Energies= -2587.025184
Sum of electronic and thermal Energies= -2586.979730
Sum of electronic and thermal Enthalpies= -2586.978786
Sum of electronic and thermal Free Energies= -2587.105274

C	-1.070033	1.396360	3.582178
C	0.181153	1.888079	3.034299
C	-1.005718	-0.073484	3.560215
C	1.018295	0.757083	2.651689
C	0.279767	-0.459468	2.998415
C	2.427981	0.826212	2.149534
H	3.131226	0.916526	3.005549
H	2.707986	-0.086344	1.589409
H	2.591831	1.700855	1.491201
C	0.570858	3.324586	2.892123
H	1.210512	3.610530	3.755655
H	1.173797	3.508277	1.981274
H	-0.308272	3.997104	2.907914
C	-2.165493	2.213502	4.195559
H	-3.148812	1.713786	4.103370
H	-1.967673	2.361451	5.279000
H	-2.244219	3.215092	3.730697
C	-2.061249	-0.994959	4.083340
H	-1.923940	-1.139513	5.176676
H	-3.076015	-0.580966	3.925599
H	-2.010518	-1.989250	3.601027
C	0.778504	-1.857603	2.818476
H	1.377096	-2.152503	3.707117
H	-0.053221	-2.579895	2.716148
H	1.433413	-1.946824	1.930443
C	0.739249	-0.499349	-0.756765
C	-1.191996	-1.760302	-0.306860
C	1.193641	-1.421804	-1.693908
H	1.299629	0.421156	-0.542498
C	-0.783931	-2.738426	-1.244006
C	0.415807	-2.572295	-1.935454
H	2.137593	-1.236955	-2.225826
H	-1.428581	-3.609580	-1.435848
H	0.736111	-3.324887	-2.672016
C	-3.824266	1.262874	1.285884
C	-3.319722	-0.970591	0.760333
C	-5.188984	0.998004	1.342158
H	-3.419171	2.272074	1.438572
C	-4.689358	-1.314010	0.832996
C	-5.626452	-0.326773	1.135681
H	-5.896557	1.814183	1.544969
H	-5.006129	-2.345103	0.614363
H	-6.696507	-0.579973	1.184617
N	-2.898410	0.290984	1.040054
N	-0.423485	-0.666939	-0.062421
N	-2.388748	-1.940770	0.390289
H	-2.811536	-2.858045	0.227550
Ir	-0.871032	0.658196	1.514653
O	-0.852938	2.140111	-0.010676
Ce	-0.857448	2.910923	-2.188505
N	1.630598	3.480352	-0.825147
N	-2.736563	0.757772	-2.120919
N	-0.790583	2.679569	-5.016221
O	0.671005	4.358034	-0.861906
O	2.550582	3.554660	-0.044672
O	-1.507828	0.630507	-2.531128
O	-3.473671	-0.190512	-1.985382
O	0.236393	2.469165	-4.232168
O	-0.763683	2.523542	-6.199899
O	-3.077824	1.968484	-1.845117
O	1.490986	2.508995	-1.663580
O	-1.849136	3.078666	-4.360005
O	-1.620554	3.377286	0.230646
H	-0.903913	3.977320	0.566212
O	-1.267204	5.295521	-2.692022
H	-0.760573	6.064302	-2.358327
H	-1.782466	5.599598	-3.468471

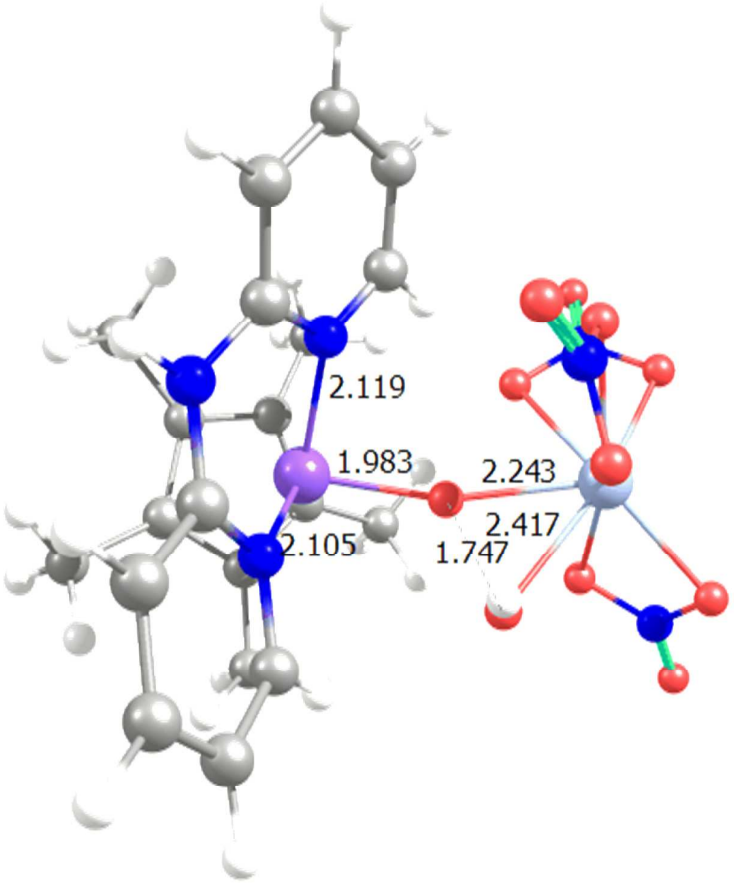
[Cp*Ir(dpa)O-Ce^{IV}(NO$_3$)$_3$OH]$^{+2}$



Zero-point correction= 0.451472 (Hartree/Particle)
Thermal correction to Energy= 0.493981
Thermal correction to Enthalpy= 0.494926
Thermal correction to Gibbs Free Energy= 0.376270
Sum of electronic and zero-point Energies= -2510.655410
Sum of electronic and thermal Energies= -2510.612901
Sum of electronic and thermal Enthalpies= -2510.611957
Sum of electronic and thermal Free Energies= -2510.730612

C	-0.862464	1.567452	2.697910
C	0.320026	2.029211	1.948422
C	-0.778713	0.121580	2.821597
C	1.071066	0.873236	1.534713
C	0.448388	-0.292019	2.155889
C	2.367384	0.896965	0.799874
H	3.140645	1.376173	1.439933
H	2.725834	-0.115514	0.539979
H	2.285156	1.501809	-0.125371
C	0.673167	3.443447	1.753070
H	-0.178878	4.013099	1.318685
H	0.859233	3.899475	2.751943
H	1.555337	3.580983	1.106030
C	-1.857125	2.476799	3.325751
H	-2.757041	1.939999	3.677520
H	-1.391758	2.986425	4.197487
H	-2.157264	3.256898	2.595944
C	-1.653202	-0.730115	3.683949
H	-1.267851	-0.700880	4.726698
H	-2.693423	-0.354057	3.704294
H	-1.665212	-1.784211	3.353390
C	1.031651	-1.654736	2.211586
H	1.705927	-1.682985	3.099853
H	0.269529	-2.442115	2.359020
H	1.653632	-1.894975	1.329502
C	0.282499	-1.339164	-0.924733
C	-1.562748	-2.348487	0.139932
C	0.660070	-2.534530	-1.521562
H	0.820571	-0.402175	-1.130486
C	-1.209792	-3.602441	-0.417326
C	-0.091400	-3.697304	-1.242253
H	1.525017	-2.549748	-2.200022
H	-1.850840	-4.477510	-0.229971
H	0.179785	-4.663837	-1.694498
C	-4.208362	1.080500	0.865153
C	-3.632795	-1.195162	0.986629
C	-5.548640	0.812179	1.126829
H	-3.814531	2.096904	0.708574
C	-4.977466	-1.524967	1.275767
C	-5.942118	-0.520522	1.349022
H	-6.266605	1.643886	1.162498
H	-5.254859	-2.581617	1.413208
H	-6.990976	-0.775719	1.565098
N	-3.258662	0.101554	0.806287
N	-0.784421	-1.260150	-0.070390
N	-2.710481	-2.240790	0.910670
H	-3.136278	-3.148272	1.118699
Ir	-1.201084	0.674980	0.691308
O	-1.931660	2.464306	0.360033
Ce	-1.715652	3.564182	-1.570987
N	-2.457697	0.534198	-2.073573
N	0.805192	2.359675	-2.321409
N	-0.537139	6.094410	-0.944266
O	-1.268062	0.879608	-1.479485
O	-2.838616	-0.615866	-2.033891
O	-0.610034	5.620688	-2.147840
O	-0.007759	7.131611	-0.660519
O	0.641615	2.862525	-1.133760
O	1.692028	1.559478	-2.554759
O	-3.038077	1.493677	-2.607901
O	-0.061132	2.728283	-3.190158
O	-1.097564	5.312171	-0.050977
O	-3.566152	4.360688	-1.826798
H	-4.358685	4.819741	-2.170009

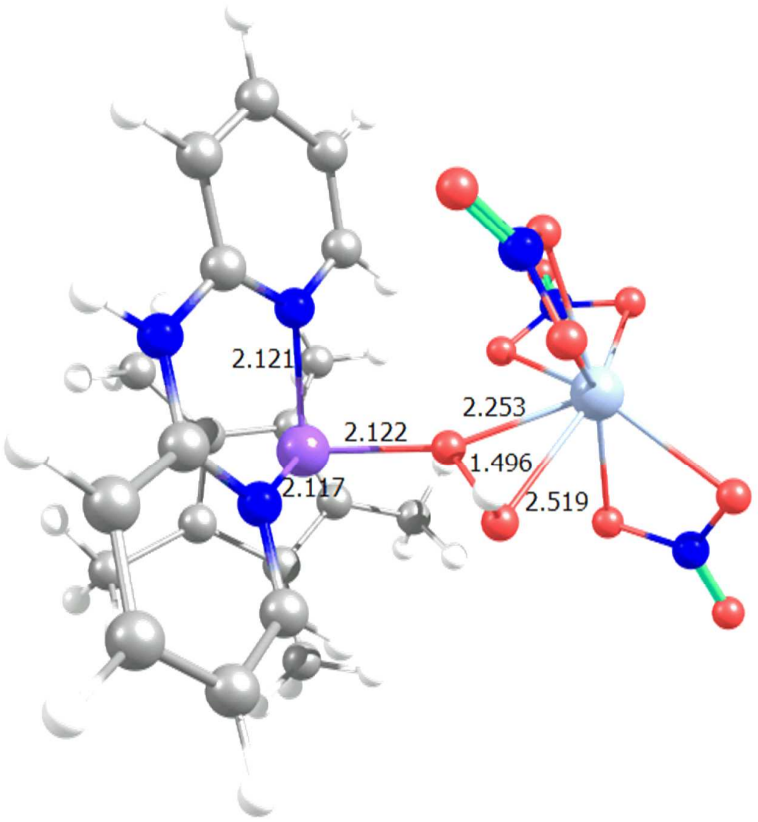
[Cp*Ir(dpa)O···(OH)Ce^{IV}(NO$_3$)$_3$]$^{+2}$



Zero-point correction= 0.452188 (Hartree/Particle)
Thermal correction to Energy= 0.494387
Thermal correction to Enthalpy= 0.495331
Thermal correction to Gibbs Free Energy= 0.375127
Sum of electronic and zero-point Energies= -2510.631697
Sum of electronic and thermal Energies= -2510.589498
Sum of electronic and thermal Enthalpies= -2510.588554
Sum of electronic and thermal Free Energies= -2510.708758

C	-0.966162	1.682471	3.151819
C	0.148922	1.994682	2.260546
C	-0.923871	0.247039	3.418623
C	0.849813	0.762954	1.946014
C	0.165176	-0.331494	2.658352
C	2.131495	0.642272	1.184190
H	2.982112	0.816680	1.878611
H	2.262749	-0.368014	0.752615
H	2.197300	1.387450	0.369406
C	0.501468	3.363252	1.784975
H	-0.398998	3.957606	1.537201
H	1.044662	3.896801	2.595195
H	1.148722	3.332518	0.890968
C	-1.860088	2.687709	3.808039
H	-2.802526	2.235599	4.170788
H	-1.343687	3.122948	4.691376
H	-2.104271	3.524644	3.125336
C	-1.864234	-0.492283	4.314353
H	-1.489012	-0.432452	5.359311
H	-2.879370	-0.050240	4.303698
H	-1.938704	-1.562933	4.046844
C	0.602417	-1.762250	2.663018
H	1.419925	-1.900680	3.403081
H	-0.222855	-2.445261	2.938791
H	0.995495	-2.068360	1.674029
C	0.098264	-0.702767	-1.144695
C	-1.618670	-2.055360	-0.285929
C	0.538088	-1.708588	-1.999561
H	0.574741	0.285902	-1.126666
C	-1.213837	-3.120542	-1.122485
C	-0.126014	-2.949163	-1.978925
H	1.382064	-1.513464	-2.675651
H	-1.776504	-4.066580	-1.109721
H	0.189902	-3.770847	-2.639565
C	-4.160537	0.846452	1.783887
C	-3.621496	-1.335725	1.074903
C	-5.467684	0.486799	2.090129
H	-3.798334	1.876698	1.903457
C	-4.936729	-1.767130	1.384739
C	-5.857477	-0.857590	1.900120
H	-6.167647	1.243438	2.472274
H	-5.223904	-2.812885	1.195303
H	-6.880978	-1.185361	2.138836
N	-3.242610	-0.049180	1.303948
N	-0.948913	-0.872189	-0.284379
N	-2.718295	-2.249316	0.551892
H	-3.085916	-3.203673	0.513029
Ir	-1.239624	0.591203	1.219835
O	-1.569236	1.889411	-0.242169
Ce	-1.385486	3.113706	-2.112352
N	-2.183189	0.518592	-3.050648
N	1.451453	2.902956	-2.423248
N	-1.679516	5.849282	-1.424934
O	-0.996028	0.989764	-3.260417
O	-2.449264	-0.657373	-3.101669
O	-2.212246	5.284132	-2.482714
O	-1.841312	6.994563	-1.134241
O	0.812130	2.482949	-1.352950
O	2.631779	2.764897	-2.569100
O	-3.056115	1.428020	-2.730345
O	0.668257	3.470204	-3.284943
O	-0.957016	5.012942	-0.724891
O	-3.067537	2.771797	-0.410040
H	-3.626797	2.043883	-0.784119

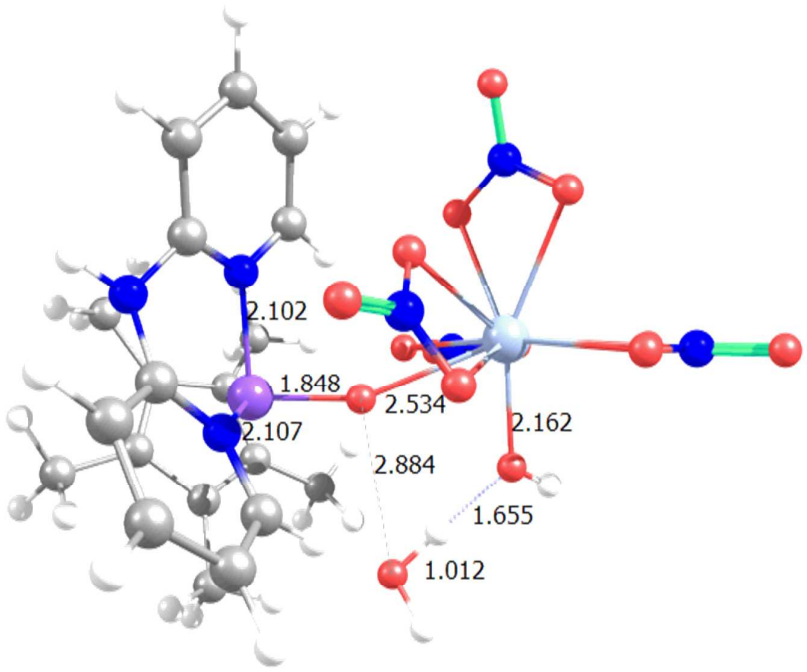
[Cp*Ir(dpa)OOH-Ce^{IV}(NO$_3$)$_3$]$^{+2}$



Zero-point correction= 0.453474 (Hartree/Particle)
Thermal correction to Energy= 0.496126
Thermal correction to Enthalpy= 0.497070
Thermal correction to Gibbs Free Energy= 0.375529
Sum of electronic and zero-point Energies= -2510.632533
Sum of electronic and thermal Energies= -2510.589881
Sum of electronic and thermal Enthalpies= -2510.588936
Sum of electronic and thermal Free Energies= -2510.710478

C	-0.952465	1.674462	3.153806
C	0.169044	1.990841	2.274573
C	-0.912166	0.235385	3.406384
C	0.887178	0.770104	1.963619
C	0.203248	-0.330022	2.659778
C	2.181398	0.665186	1.218546
H	3.022978	0.852681	1.920107
H	2.330427	-0.344117	0.790333
H	2.248507	1.408035	0.401829
C	0.508019	3.361921	1.794495
H	-0.398115	3.942911	1.534923
H	1.031906	3.907577	2.609619
H	1.169788	3.337060	0.911131
C	-1.843589	2.677481	3.820853
H	-2.780933	2.221603	4.191854
H	-1.321619	3.114543	4.699545
H	-2.100011	3.514366	3.142133
C	-1.848335	-0.518146	4.295574
H	-1.463988	-0.488833	5.338163
H	-2.860518	-0.069628	4.302224
H	-1.934287	-1.580595	3.999262
C	0.648206	-1.758047	2.663457
H	1.458509	-1.892840	3.412251
H	-0.175261	-2.446935	2.929887
H	1.053813	-2.059030	1.677845
C	0.141394	-0.727846	-1.107184
C	-1.648713	-2.029400	-0.328710
C	0.574386	-1.732969	-1.965291
H	0.649764	0.243586	-1.056678
C	-1.249558	-3.098725	-1.165675
C	-0.130343	-2.952549	-1.983523
H	1.444996	-1.557605	-2.612447
H	-1.841404	-4.026727	-1.183353
H	0.180732	-3.775493	-2.644836
C	-4.146214	0.881058	1.820048
C	-3.655021	-1.276296	1.026111
C	-5.451741	0.530920	2.145054
H	-3.768016	1.899689	1.976508
C	-4.971147	-1.699626	1.347042
C	-5.868602	-0.798003	1.913487
H	-6.129198	1.283277	2.573378
H	-5.276554	-2.734770	1.129496
H	-6.891765	-1.119605	2.161339
N	-3.247647	-0.003820	1.285684
N	-0.938654	-0.870294	-0.281587
N	-2.786380	-2.197254	0.457367
H	-3.187102	-3.135934	0.384634
Ir	-1.207813	0.562820	1.258196
O	-1.643802	1.945195	-0.291859
Ce	-1.313863	3.102880	-2.196414
N	-2.155159	0.497312	-3.064654
N	1.513838	2.850073	-2.397736
N	-1.844310	5.779737	-1.437918
O	-0.969988	0.956052	-3.305919
O	-2.441801	-0.671055	-3.114671
O	-2.315809	5.201690	-2.519565
O	-2.100267	6.898965	-1.119139
O	0.834401	2.467082	-1.339771
O	2.694234	2.694478	-2.507047
O	-3.008835	1.422436	-2.717173
O	0.760511	3.406630	-3.299349
O	-1.066450	4.981361	-0.750827
O	-2.972014	2.630199	-0.360368
H	-3.535728	1.927446	-0.784368

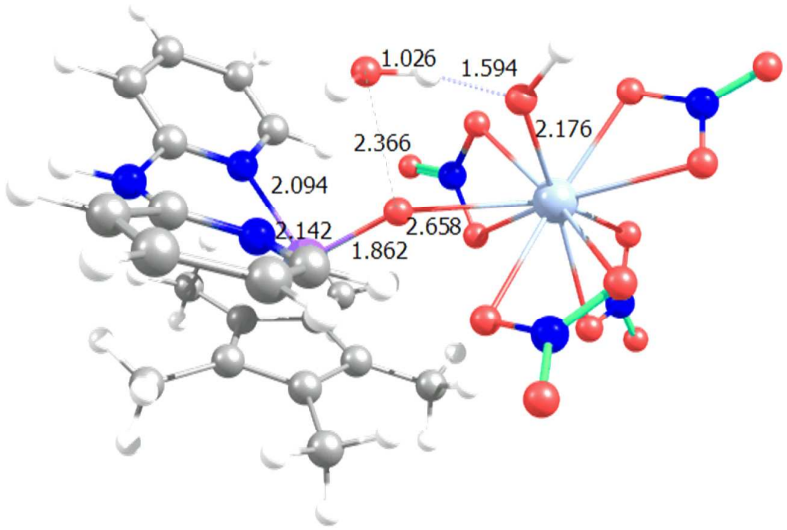
[Cp*Ir(dpa)O-Ce^{IV}(NO$_3$)$_4$OH]$^{+1}$+OH$_2$



Zero-point correction= 0.491400 (Hartree/Particle)
Thermal correction to Energy= 0.541418
Thermal correction to Enthalpy= 0.542362
Thermal correction to Gibbs Free Energy= 0.406297
Sum of electronic and zero-point Energies= -2867.462742
Sum of electronic and thermal Energies= -2867.412724
Sum of electronic and thermal Enthalpies= -2867.411780
Sum of electronic and thermal Free Energies= -2867.547845

C	-0.180650	-0.203979	3.127387
C	0.937290	0.504351	2.511561
C	-0.050324	-1.631828	2.789202
C	1.708969	-0.459744	1.739213
C	1.095512	-1.784817	1.945714
C	3.001891	-0.204848	1.034364
H	3.841152	-0.357125	1.747891
H	3.153181	-0.907441	0.192199
H	3.054330	0.827970	0.642594
C	1.219845	1.960876	2.670224
H	1.649273	2.129480	3.681962
H	1.939962	2.319850	1.914033
H	0.281902	2.547412	2.591347
C	-1.175500	0.395678	4.066605
H	-2.085535	-0.228328	4.151989
H	-0.723557	0.477727	5.079225
H	-1.465820	1.406595	3.717574
C	-0.978021	-2.708671	3.260923
H	-0.706623	-3.014026	4.293815
H	-2.027274	-2.354493	3.283644
H	-0.928755	-3.604499	2.614118
C	1.612199	-3.056643	1.350718
H	2.463782	-3.430399	1.958356
H	0.837113	-3.845161	1.324868
H	1.985640	-2.897866	0.320317
C	0.815142	-0.934061	-1.754593
C	-0.922216	-2.448277	-1.241574
C	1.031773	-1.521813	-2.997780
H	1.364443	-0.036490	-1.436392
C	-0.732063	-3.100810	-2.476683
C	0.249249	-2.633932	-3.356401
H	1.756556	-1.063019	-3.684644
H	-1.390923	-3.936846	-2.755233
H	0.378568	-3.115837	-4.337464
C	-3.317060	0.001751	1.338786
C	-2.829157	-2.078536	0.323047
C	-4.657665	-0.345871	1.491184
H	-2.915968	0.998606	1.623098
C	-4.166466	-2.496616	0.489226
C	-5.080609	-1.626514	1.085709
H	-5.359262	0.385927	1.915047
H	-4.484414	-3.474946	0.098713
H	-6.131496	-1.932974	1.201229
N	-2.421915	-0.880904	0.811719
N	-0.131148	-1.401965	-0.894209
N	-1.915639	-2.890387	-0.354679
H	-2.327745	-3.780032	-0.645998
Ir	-0.381100	-0.366212	0.917768
O	-0.797839	1.185365	0.004960
Ce	-0.674261	2.848230	-1.903232
N	2.090359	3.146432	-0.742536
N	-2.616277	0.544762	-2.009196
N	0.517528	1.680802	-4.308928
N	-1.819911	5.081666	-3.276944
O	1.535825	4.030499	-1.464032
O	3.206102	3.266389	-0.254114
O	-1.468450	0.507844	-2.590418
O	-3.330680	-0.452920	-1.945147
O	-2.483109	4.001446	-3.003379
O	-2.289539	6.006623	-3.890399
O	1.074250	1.607689	-3.135068
O	0.890576	0.989350	-5.235290
O	-2.940413	1.658909	-1.477419
O	1.389836	2.077768	-0.517472
O	-0.453475	2.510833	-4.384778
O	-0.603760	5.078261	-2.820301
O	-1.100500	3.949631	-0.092307
H	-0.802981	4.873447	0.030599
O	-2.023199	2.742874	2.099925
H	-2.660663	3.394358	2.448496
H	-1.682161	3.180936	1.253562

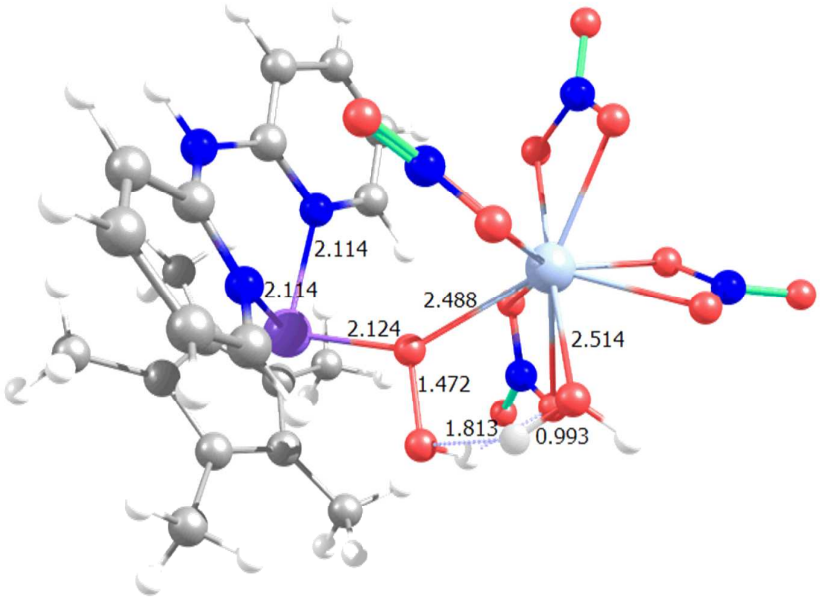
[Cp*Ir(dpa)O-Ce^{IV}(NO$_3$)$_4$OH]$^{+1}$···OH$_2$



Zero-point correction= 0.490823 (Hartree/Particle)
Thermal correction to Energy= 0.539974
Thermal correction to Enthalpy= 0.540918
Thermal correction to Gibbs Free Energy= 0.407130
Sum of electronic and zero-point Energies= -2867.431735
Sum of electronic and thermal Energies= -2867.382584
Sum of electronic and thermal Enthalpies= -2867.381640
Sum of electronic and thermal Free Energies= -2867.515428

C	-0.062022	-0.256810	2.933522
C	1.213271	0.356115	2.557054
C	-0.037510	-1.666706	2.503316
C	1.964698	-0.616577	1.794522
C	1.192079	-1.868277	1.795305
C	3.373816	-0.469422	1.328394
H	4.055151	-0.774268	2.153732
H	3.591269	-1.111141	0.454351
H	3.596362	0.573884	1.043676
C	1.679396	1.689342	3.017458
H	1.952261	1.593905	4.092531
H	2.559034	2.042937	2.456095
H	0.889193	2.458051	2.939079
C	-1.104138	0.384052	3.793069
H	-2.073633	-0.145486	3.731441
H	-0.768796	0.351948	4.852910
H	-1.259275	1.443177	3.509990
C	-1.079598	-2.689567	2.836103
H	-0.895217	-3.099548	3.852067
H	-2.095156	-2.247937	2.837216
H	-1.069561	-3.531815	2.119536
C	1.659889	-3.146218	1.173646
H	2.344414	-3.664913	1.878548
H	0.820692	-3.831643	0.949418
H	2.227789	-2.963468	0.240816
C	1.126768	-1.260410	-1.793164
C	-0.842909	-2.443856	-1.252576
C	1.345209	-2.047877	-2.921064
H	1.807459	-0.428098	-1.541630
C	-0.658870	-3.286492	-2.370733
C	0.448236	-3.095108	-3.201261
H	2.209769	-1.829800	-3.563418
H	-1.407296	-4.061919	-2.594110
H	0.595448	-3.744139	-4.078130
C	-2.927321	0.607137	0.944114
C	-2.754166	-1.588795	0.111583
C	-4.301402	0.474638	1.145483
H	-2.366803	1.522898	1.192290
C	-4.139824	-1.789131	0.295136
C	-4.913798	-0.752353	0.828473
H	-4.866516	1.323075	1.556470
H	-4.599515	-2.743415	-0.004650
H	-5.994261	-0.898283	0.980145
N	-2.170181	-0.418701	0.466934
N	0.071149	-1.480190	-0.958280
N	-1.967153	-2.605249	-0.440960
H	-2.495381	-3.456395	-0.646657
Ir	-0.051887	-0.260906	0.740256
O	-0.309817	1.397837	-0.064587
	0.279663	3.981302	-0.266050
N	-1.833416	3.897035	1.888887
N	2.361806	2.001480	-1.020758
N	2.305867	5.160775	1.452409
N	0.406252	6.362905	-1.864999
O	-1.671027	4.896173	1.137373
O	-2.719954	3.790165	2.723283
O	2.331308	2.461304	0.173718
O	3.087206	1.048840	-1.326302
O	0.964072	5.263405	-2.240815
O	0.508743	7.404239	-2.465605
O	1.238920	4.561373	1.904482
O	3.201709	5.516453	2.181869
O	1.581590	2.548554	-1.863834
O	-0.983428	2.910219	1.716151
O	2.319058	5.316264	0.176902
O	-0.296143	6.249803	-0.771310
O	-1.308440	3.472683	-1.663933
H	-1.691346	4.091534	-2.316256
O	-0.965017	0.980581	-2.299038
H	-1.786774	0.727503	-1.831236
H	-1.026967	2.000930	-2.207993

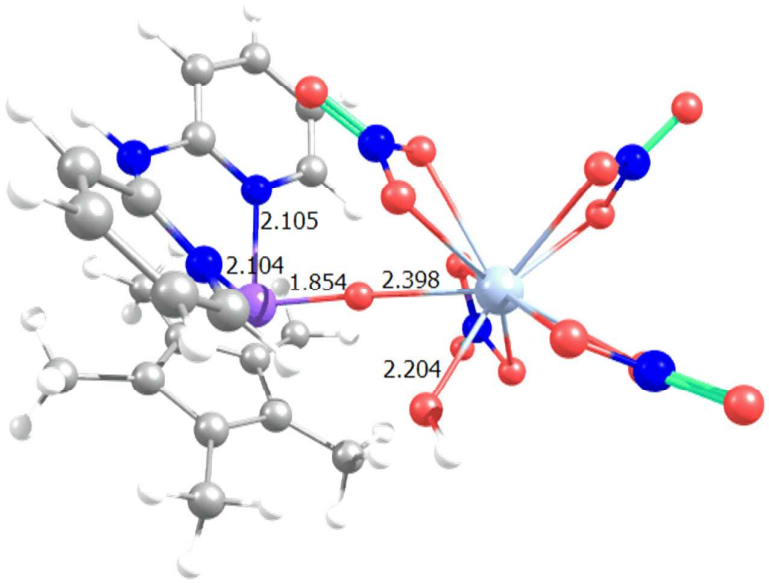
[Cp*Ir(dpa)OOH-Ce^{IV}(NO$_3$)$_4$OH$_2$]$^{+1}$



Zero-point correction= 0.495996 (Hartree/Particle)
Thermal correction to Energy= 0.544339
Thermal correction to Enthalpy= 0.545283
Thermal correction to Gibbs Free Energy= 0.414665
Sum of electronic and zero-point Energies= -2867.470357
Sum of electronic and thermal Energies= -2867.422013
Sum of electronic and thermal Enthalpies= -2867.421069
Sum of electronic and thermal Free Energies= -2867.551688

C	-1.175536	1.519586	3.386742
C	0.048736	2.068425	2.833243
C	-1.029481	0.053776	3.398550
C	0.926172	0.980495	2.439348
C	0.259842	-0.273290	2.821604
C	2.320409	1.123320	1.907197
H	3.032813	1.299616	2.742086
H	2.649469	0.208715	1.378023
H	2.404427	1.976157	1.205297
C	0.390417	3.519355	2.739660
H	1.027222	3.780390	3.613337
H	0.977274	3.756260	1.831881
H	-0.509253	4.159044	2.772706
C	-2.310520	2.300870	3.975479
H	-3.255394	1.724310	3.950840
H	-2.101272	2.558677	5.035890
H	-2.472537	3.244194	3.419163
C	-2.031329	-0.912426	3.951295
H	-1.889196	-1.022118	5.047578
H	-3.067537	-0.561187	3.779069
H	-1.926641	-1.913077	3.490533
C	0.836304	-1.646056	2.659184
H	1.470421	-1.896423	3.535955
H	0.042900	-2.413634	2.580004
H	1.470990	-1.714001	1.754358
C	0.760404	-0.457986	-0.831481
C	-1.068637	-1.818214	-0.295057
C	1.311130	-1.427598	-1.666803
H	1.227581	0.529066	-0.720444
C	-0.560166	-2.847539	-1.117383
C	0.639002	-2.653946	-1.805173
H	2.235837	-1.202957	-2.214808
H	-1.130658	-3.781842	-1.231515
H	1.031862	-3.443923	-2.462805
C	-3.961093	1.063202	1.131160
C	-3.275328	-1.141406	0.712072
C	-5.300201	0.690386	1.205521
H	-3.637706	2.107441	1.238816
C	-4.611738	-1.594684	0.813023
C	-5.626232	-0.674115	1.068174
H	-6.072198	1.455814	1.364885
H	-4.841883	-2.656268	0.637541
H	-6.671981	-1.011077	1.128992
N	-2.962429	0.157639	0.935134
N	-0.398684	-0.646073	-0.145083
N	-2.267213	-2.044355	0.389955
H	-2.613970	-2.998142	0.269075
Ir	-0.972245	0.742580	1.341594
O	-1.447777	2.203778	-0.125138
Ce	-1.235567	2.528141	-2.582714
N	1.090225	3.531921	-0.983524
N	-3.345276	0.528957	-2.140687
N	-0.584590	0.590678	-4.594512
N	-0.384704	4.445893	-4.566367
O	0.036956	4.273588	-1.181751
O	1.975662	3.870764	-0.216814
O	-2.091446	0.219008	-2.110863
O	-4.219089	-0.291166	-1.926822
O	-1.569316	4.428494	-4.013142
O	-0.073875	5.246899	-5.409000
O	0.160814	0.770412	-3.556724
O	-0.375101	-0.262510	-5.420789
O	-3.587102	1.762744	-2.388353
O	1.104232	2.429531	-1.620760
O	-1.593505	1.410703	-4.667810
O	0.402708	3.531370	-4.115899
O	-1.756230	3.463983	0.570494
H	-0.989459	4.021961	0.243395
O	-2.840780	4.264831	-1.729761
H	-2.604621	5.175450	-1.998290
H	-2.759619	4.212649	-0.741293

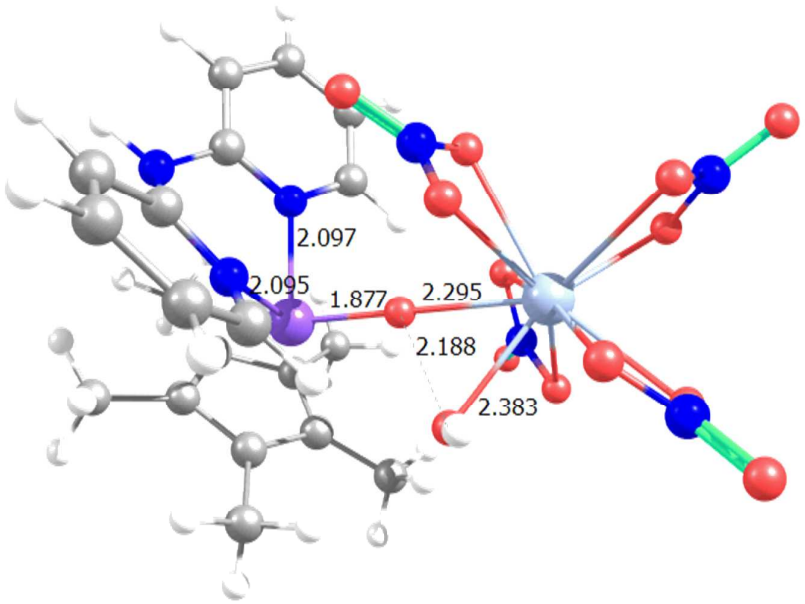
[Cp*Ir(dpa)O-Ce^{IV}(NO$_3$)$_4$(OH)]$^{+1}$



Zero-point correction= 0.465513 (Hartree/Particle)
Thermal correction to Energy= 0.513590
Thermal correction to Enthalpy= 0.514534
Thermal correction to Gibbs Free Energy= 0.380442
Sum of electronic and zero-point Energies= -2791.082385
Sum of electronic and thermal Energies= -2791.034308
Sum of electronic and thermal Enthalpies= -2791.033364
Sum of electronic and thermal Free Energies= -2791.167456

C	-1.108883	0.932229	3.807253
C	0.179117	1.303365	3.242275
C	-1.087600	-0.520531	4.067339
C	0.953909	0.083460	3.043646
C	0.169723	-1.033801	3.602707
C	2.346473	-0.004063	2.501608
H	3.081049	0.152298	3.321102
H	2.546230	-0.999483	2.060091
H	2.532927	0.766309	1.727092
C	0.566269	2.697194	2.877068
H	0.638947	3.304553	3.804218
H	1.537323	2.742105	2.351976
C	-2.190872	1.901207	4.169245
H	-3.177448	1.406377	4.248711
H	-1.966467	2.371801	5.150787
H	-2.256213	2.703918	3.407238
C	-2.202671	-1.291030	4.703984
H	-2.147689	-1.192268	5.809049
H	-3.190781	-0.905891	4.384065
H	-2.153202	-2.367148	4.452992
C	0.633185	-2.456913	3.639811
H	-0.203545	-3.159289	3.811358
H	1.139789	-2.740140	2.695960
H	1.367996	-2.589297	4.462333
C	0.533703	-1.506101	-0.349632
C	-1.313887	-2.739870	0.451836
C	0.931584	-2.555798	-1.174377
H	1.043066	-0.528993	-0.349711
C	-0.947390	-3.843679	-0.345462
C	0.190847	-3.752893	-1.150986
H	1.800316	-2.423589	-1.834114
H	-1.583473	-4.741338	-0.361090
H	0.478379	-4.602188	-1.789395
C	-3.803046	0.600888	1.417831
C	-3.407440	-1.727209	1.328580
C	-5.182763	0.410299	1.376059
H	-3.331410	1.600900	1.394931
C	-4.793424	-1.982497	1.305538
C	-5.683199	-0.904804	1.346594
H	-5.848591	1.283797	1.346216
H	-5.157806	-3.016189	1.208904
H	-6.767670	-1.090492	1.314993
N	-2.946406	-0.457111	1.451612
N	-0.537722	-1.627380	0.483610
N	-2.484846	-2.776285	1.222356
H	-2.930891	-3.696671	1.221346
Ir	-0.916615	-0.075247	1.853945
O	-0.884072	1.142133	0.455477
Ce	-1.279323	2.789136	-1.242635
N	1.574777	2.648501	-0.307070
N	-2.416644	0.062655	-1.616099
N	-0.868959	2.841265	-4.107851
N	-2.842342	5.156929	-1.951028
O	0.823378	3.689385	-0.265222
O	2.650010	2.603954	0.285571
O	-1.217370	0.306746	-1.993658
O	-2.847709	-1.084683	-1.516545
O	-3.435811	4.107500	-1.509153
O	-3.435734	6.120006	-2.383958
O	0.098921	2.953223	-3.257363
O	-0.694325	2.855081	-5.303347
O	-3.128069	1.082096	-1.296520
O	1.121306	1.650771	-0.964858
O	-2.037967	2.708382	-3.569818
O	-1.546270	5.112107	-1.897946
O	-2.076132	3.329305	0.740030
H	-2.773187	4.016620	0.778445
H	-0.206197	3.162850	2.226390

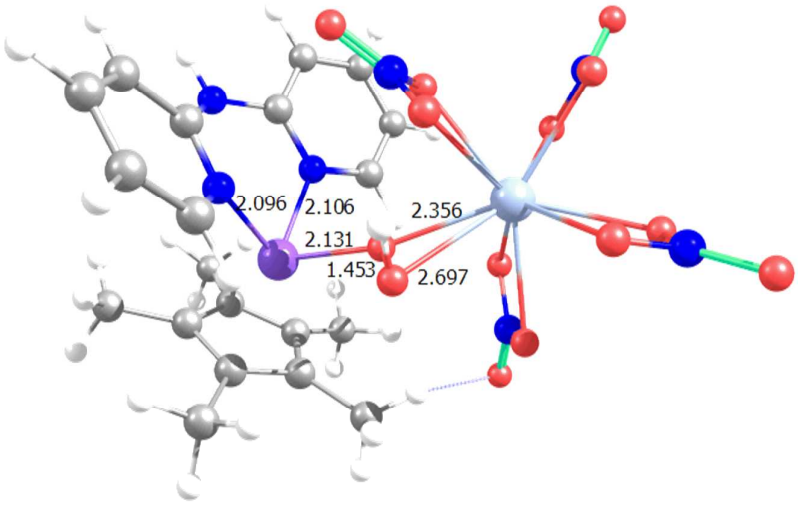
[Cp*Ir(dpa)O···(OH)Ce^{IV}(NO$_3$)$_4$]$^{+1}$



Zero-point correction= 0.467508 (Hartree/Particle)
Thermal correction to Energy= 0.513868
Thermal correction to Enthalpy= 0.514812
Thermal correction to Gibbs Free Energy= 0.387008
Sum of electronic and zero-point Energies= -2791.078466
Sum of electronic and thermal Energies= -2791.032106
Sum of electronic and thermal Enthalpies= -2791.031162
Sum of electronic and thermal Free Energies= -2791.158966

C	-1.108442	1.031667	3.781637
C	0.181123	1.360412	3.168350
C	-1.121839	-0.410261	4.069192
C	0.911677	0.116762	2.987450
C	0.099416	-0.968756	3.570147
C	2.294291	-0.034345	2.437838
H	3.035917	0.078666	3.258391
H	2.445360	-1.036214	1.991118
H	2.519064	0.730830	1.669327
C	0.625324	2.743819	2.831054
H	0.753031	3.319169	3.772705
H	1.585511	2.757184	2.284965
C	-2.149260	2.038965	4.158543
H	-3.134102	1.568083	4.339448
H	-1.846585	2.561921	5.091772
H	-2.252956	2.797492	3.356438
C	-2.244887	-1.135315	4.741604
H	-2.208252	-0.952670	5.836669
H	-3.228324	-0.775978	4.378912
H	-2.189847	-2.226724	4.573219
C	0.516450	-2.405902	3.610885
H	-0.339176	-3.078431	3.806694
H	0.991433	-2.714140	2.658497
H	1.266135	-2.556304	4.416615
C	0.496325	-1.430073	-0.296859
C	-1.305923	-2.700747	0.546373
C	0.931173	-2.492803	-1.085675
H	0.976687	-0.438701	-0.331383
C	-0.900710	-3.815635	-0.215325
C	0.233911	-3.713568	-1.024260
H	1.796774	-2.349552	-1.747228
H	-1.504091	-4.735512	-0.195842
H	0.553156	-4.573886	-1.632092
C	-3.892757	0.574572	1.430087
C	-3.422402	-1.732363	1.379164
C	-5.266086	0.346773	1.373553
H	-3.445852	1.581655	1.435699
C	-4.799414	-2.030355	1.338208
C	-5.725009	-0.982963	1.347280
H	-5.957176	1.200208	1.339082
H	-5.127899	-3.077373	1.257903
H	-6.802409	-1.203505	1.303350
N	-3.000676	-0.447831	1.472747
N	-0.575208	-1.557605	0.536539
N	-2.466790	-2.754911	1.326828
H	-2.882949	-3.688844	1.355185
Ir	-0.994286	0.037080	1.831861
O	-1.100651	1.251381	0.404156
Ce	-1.230903	2.735682	-1.340966
N	1.552718	2.552868	-0.328466
N	-2.477150	0.073041	-1.668868
N	-0.768949	3.035682	-4.158276
N	-2.798467	5.158270	-1.611822
O	0.833419	3.609728	-0.265403
O	2.642065	2.467483	0.227636
O	-1.275541	0.290015	-2.067171
O	-2.900398	-1.067119	-1.483781
O	-3.367461	4.011537	-1.405744
O	-3.416357	6.184717	-1.748190
O	0.183481	3.047094	-3.274540
O	-0.570665	3.175503	-5.338276
O	-3.185665	1.109958	-1.424994
O	1.050714	1.567802	-0.985644
O	-1.949931	2.855938	-3.652773
O	-1.500686	5.107261	-1.655322
O	-2.079446	3.157697	0.845539
H	-3.004502	3.364586	0.561681
H	-0.135857	3.261605	2.212758

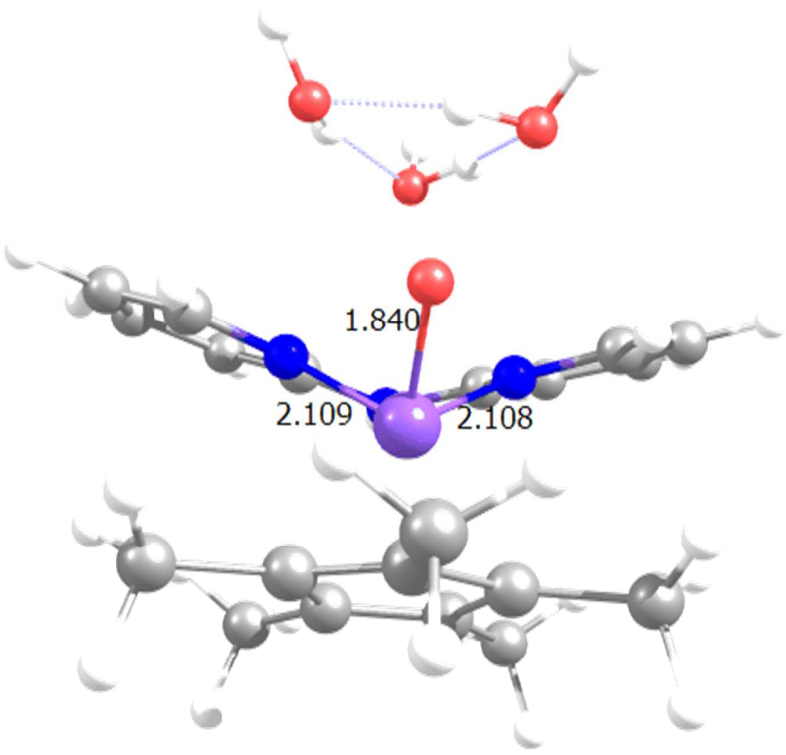
[Cp*Ir(dpa)OOH-Ce^{IV}(NO$_3$)$_4$]$^{+1}$



Zero-point correction= 0.470615 (Hartree/Particle)
Thermal correction to Energy= 0.516130
Thermal correction to Enthalpy= 0.517074
Thermal correction to Gibbs Free Energy= 0.391577
Sum of electronic and zero-point Energies= -2791.099396
Sum of electronic and thermal Energies= -2791.053880
Sum of electronic and thermal Enthalpies= -2791.052936
Sum of electronic and thermal Free Energies= -2791.178433

C	-1.318735	1.237359	4.074706
C	-0.069554	1.641122	3.448690
C	-1.294219	-0.225390	4.204994
C	0.718454	0.454748	3.157169
C	-0.047844	-0.705438	3.639206
C	2.115006	0.414146	2.615999
H	2.844383	0.509215	3.449146
H	2.323937	-0.543881	2.102191
H	2.312510	1.238785	1.904888
C	0.292553	3.059155	3.144667
H	0.423927	3.613858	4.098089
H	1.226993	3.144166	2.563298
C	-2.343255	2.171342	4.644306
H	-3.334308	1.688857	4.745179
H	-2.032099	2.504484	5.658042
H	-2.453975	3.077432	4.016886
C	-2.368302	-1.055515	4.837062
H	-2.231864	-1.077927	5.939320
H	-3.373599	-0.637442	4.631932
H	-2.346801	-2.098649	4.468512
C	0.413468	-2.128480	3.577959
H	-0.438148	-2.834343	3.605683
H	0.994052	-2.323584	2.655364
H	1.073301	-2.350247	4.443758
C	0.410874	-0.855869	-0.167435
C	-1.500202	-2.138468	0.275826
C	0.856181	-1.749747	-1.136914
H	0.957084	0.074162	0.040086
C	-1.105615	-3.086439	-0.694677
C	0.081935	-2.894564	-1.400969
H	1.783173	-1.531946	-1.685143
H	-1.755356	-3.949120	-0.905534
H	0.389324	-3.619714	-2.169581
C	-4.181100	0.771127	2.057319
C	-3.629254	-1.406324	1.386843
C	-5.537632	0.471913	2.127277
H	-3.799773	1.774520	2.290308
C	-4.991549	-1.785222	1.461838
C	-5.948378	-0.845303	1.836297
H	-6.256304	1.255906	2.403762
H	-5.284027	-2.810440	1.189094
H	-7.011017	-1.127545	1.882333
N	-3.233314	-0.150618	1.719548
N	-0.736009	-1.050426	0.542253
N	-2.688954	-2.348172	0.982154
H	-3.108295	-3.257964	0.778991
Ir	-1.204793	0.300011	2.091489
O	-1.277296	1.701761	0.507789
Ce	-1.003719	2.637644	-1.651655
N	1.453085	3.027969	-0.136936
N	-2.888773	0.356754	-1.536717
N	-0.812395	1.908928	-4.401375
N	-1.781266	5.234706	-2.535018
O	0.524207	3.911830	-0.179642
O	2.426008	3.127630	0.589417
O	-1.682553	0.239899	-1.952390
O	-3.601537	-0.611312	-1.322186
O	-2.520149	4.482139	-1.766882
O	-2.135286	6.312990	-2.930606
O	0.179565	1.853017	-3.551727
O	-0.698272	1.589877	-5.555828
O	-3.299132	1.566107	-1.340282
O	1.274988	2.003066	-0.907948
O	-1.917497	2.331268	-3.880874
O	-0.631914	4.708731	-2.825487
O	-2.184949	2.838323	0.684959
H	-3.020360	2.469589	0.275790
H	-0.513518	3.560128	2.572225

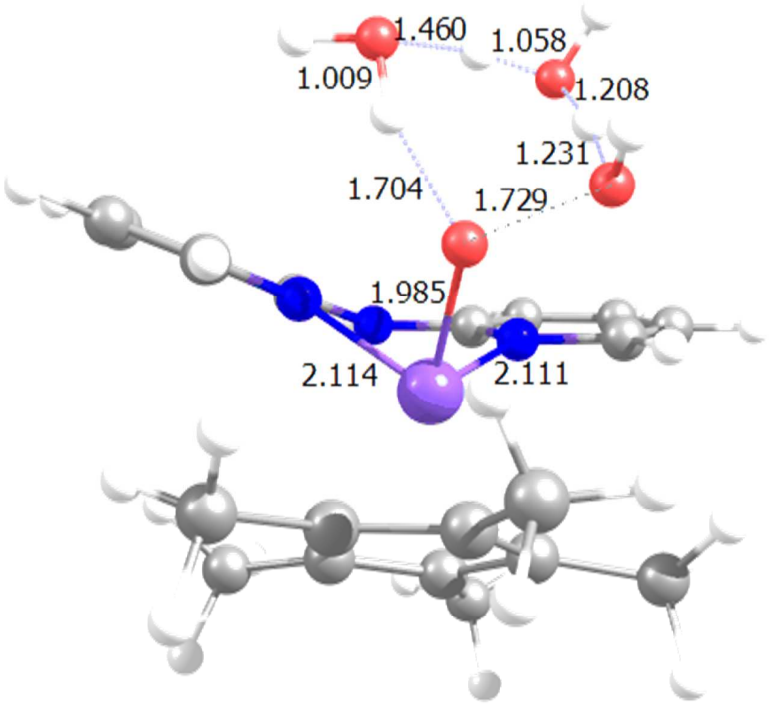
Rh-V-VITZVPd



Zero-point correction= 0.464730 (Hartree/Particle)
Thermal correction to Energy= 0.498579
Thermal correction to Enthalpy= 0.499523
Thermal correction to Gibbs Free Energy= 0.400361
Sum of electronic and zero-point Energies= -1348.118600
Sum of electronic and thermal Energies= -1348.084751
Sum of electronic and thermal Enthalpies= -1348.083807
Sum of electronic and thermal Free Energies= -1348.182969

C	-0.219969	2.048120	3.024104
C	0.903305	1.125017	3.127317
C	-1.423178	1.334134	3.430887
C	0.396286	-0.134930	3.707917
C	-1.013857	-0.008056	3.891902
C	1.249890	-1.319248	4.031829
H	1.774598	-1.144338	4.995869
H	0.653482	-2.244612	4.134126
H	2.028497	-1.483815	3.261154
C	2.344919	1.448572	2.895671
H	2.799169	1.807055	3.845373
H	2.919840	0.559538	2.572224
H	2.472808	2.247683	2.141291
C	-0.150634	3.471061	2.576669
H	0.026546	4.118867	3.462592
H	0.676963	3.638788	1.862229
H	-1.092599	3.798930	2.098528
C	-2.796378	1.910545	3.566982
H	-2.923769	2.319843	4.593158
H	-2.970032	2.737647	2.852994
H	-3.581397	1.143942	3.420021
C	-1.950107	-1.032656	4.448444
H	-2.160661	-0.800748	5.514850
H	-2.921212	-1.030621	3.915517
H	-1.524147	-2.051989	4.401473
C	-3.384021	-0.295536	0.849816
C	-2.108464	-2.253213	1.182738
C	-4.567262	-1.021843	0.755994
H	-3.353836	0.795102	0.728885
C	-3.276579	-3.043545	1.101949
C	-4.511004	-2.422754	0.903546
H	-5.514235	-0.497820	0.564004
H	-3.199314	-4.139080	1.173109
H	-5.427055	-3.030243	0.840797
C	1.818782	-0.755704	0.149626
C	0.355903	-2.471705	0.845265
C	2.785046	-1.672119	-0.251928
H	1.947670	0.327395	0.024422
C	1.301252	-3.449892	0.462744
C	2.524879	-3.046874	-0.073074
H	3.722764	-1.314931	-0.700675
H	1.053587	-4.516976	0.568432
H	3.268024	-3.801444	-0.373880
N	0.647200	-1.150548	0.725155
N	-2.187298	-0.899052	1.102702
N	-0.870634	-2.864052	1.379672
H	-0.942315	-3.875934	1.512299
Ir	-0.553069	0.321294	1.640020
O	-0.643533	1.384254	0.141356
O	0.192126	-0.129243	-2.148408
H	0.552769	0.216315	-2.988017
H	-0.729828	0.261310	-2.075345
O	-2.472643	0.052428	-1.816897
H	-2.304787	-0.932786	-1.818747
H	-3.030346	0.224455	-2.600335
O	-1.193066	-2.329750	-1.632996
H	-1.260562	-2.998621	-2.341223
H	-0.488948	-1.684764	-1.951624

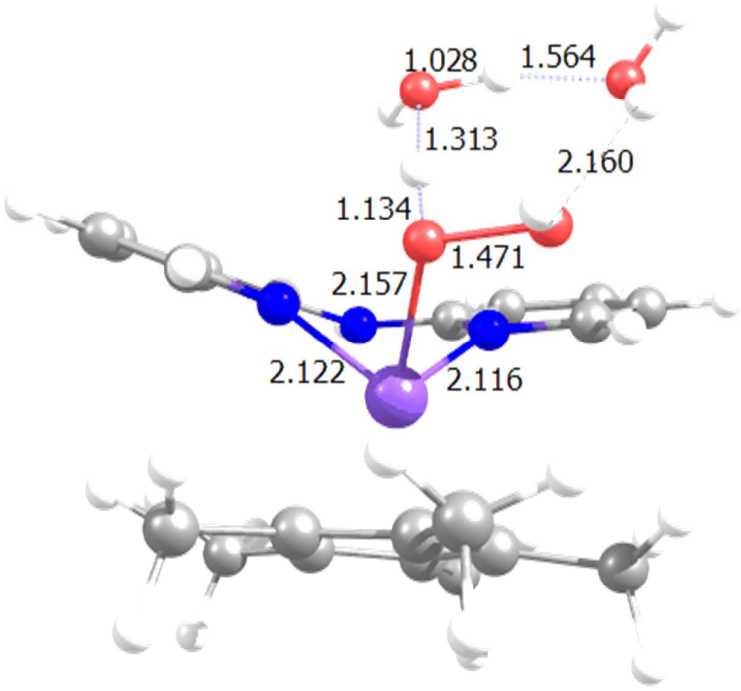
Rh-VTZVP+



Zero-point correction= 0.462291 (Hartree/Particle)
Thermal correction to Energy= 0.494163
Thermal correction to Enthalpy= 0.495108
Thermal correction to Gibbs Free Energy= 0.399638
Sum of electronic and zero-point Energies= -1348.101740
Sum of electronic and thermal Energies= -1348.069867
Sum of electronic and thermal Enthalpies= -1348.068923
Sum of electronic and thermal Free Energies= -1348.164392

C	-0.199136	1.946461	2.708622
C	0.913404	1.014662	2.784401
C	-1.405860	1.254652	3.139708
C	0.394920	-0.253965	3.323523
C	-1.019338	-0.105503	3.542913
C	1.227071	-1.465246	3.606920
H	1.751506	-1.338389	4.578575
H	0.614083	-2.383606	3.672556
H	2.004326	-1.615976	2.831919
C	2.358764	1.336280	2.561588
H	2.800988	1.724040	3.504789
H	2.942070	0.442105	2.270007
H	2.495249	2.114904	1.786774
C	-0.150198	3.366718	2.250932
H	-0.321758	4.044035	3.114230
H	0.824766	3.624024	1.798542
H	-0.944463	3.560891	1.501814
C	-2.749485	1.887322	3.338495
H	-2.780697	2.392074	4.328434
H	-2.957399	2.656210	2.569041
H	-3.567560	1.141988	3.327466
C	-1.953691	-1.129737	4.104100
H	-2.105111	-0.937467	5.188176
H	-2.949452	-1.082452	3.620734
H	-1.557485	-2.156742	3.996118
C	1.837757	-0.575870	-0.210428
C	0.357123	-2.376472	0.065852
C	2.820966	-1.393185	-0.759462
H	1.979543	0.506747	-0.100447
C	1.316845	-3.264034	-0.477859
C	2.558304	-2.772891	-0.881240
H	3.777050	-0.956184	-1.081090
H	1.071029	-4.331382	-0.589052
H	3.311899	-3.456448	-1.301519
C	-3.473804	-0.374488	0.740470
C	-2.126778	-2.285638	0.527534
C	-4.647583	-1.112785	0.616741
H	-3.491629	0.715752	0.877675
C	-3.283154	-3.096957	0.400956
C	-4.547085	-2.511498	0.456326
H	-5.621326	-0.603347	0.653698
H	-3.172644	-4.181383	0.246074
H	-5.449327	-3.135069	0.362116
N	-2.231814	-0.946065	0.724653
N	0.633272	-1.054833	0.220597
N	-0.875694	-2.890469	0.464169
H	-0.923632	-3.910843	0.404812
Ir	-0.593879	0.230972	1.359300
O	-1.069551	1.446289	-0.136537
O	0.197930	1.747759	-1.272500
H	-0.135877	2.623670	-1.570497
H	0.024781	0.882798	-2.131307
O	-0.274914	-0.060108	-2.823678
H	-1.323867	0.022236	-2.708796
H	-0.056018	0.087348	-3.766837
H	-2.207828	0.919586	-1.290653
O	-2.567667	0.556557	-2.161026
H	-3.384154	0.057325	-1.971171

Rh-V-VITZVP+



Zero-point correction= 0.464136 (Hartree/Particle)
Thermal correction to Energy= 0.497459
Thermal correction to Enthalpy= 0.498404
Thermal correction to Gibbs Free Energy= 0.399524
Sum of electronic and zero-point Energies= -1348.113596
Sum of electronic and thermal Energies= -1348.080273
Sum of electronic and thermal Enthalpies= -1348.079329
Sum of electronic and thermal Free Energies= -1348.178209

C	-0.363119	1.925476	2.674999
C	0.811404	1.096172	2.889735
C	-1.520758	1.276943	3.271135
C	0.380756	-0.081198	3.659576
C	-1.047331	0.034065	3.893110
C	1.282411	-1.170493	4.148883
H	1.766931	-0.857588	5.098636
H	0.726516	-2.106502	4.345935
H	2.088094	-1.388376	3.420721
C	2.225146	1.448582	2.541733
H	2.679100	2.044196	3.362909
H	2.851815	0.546782	2.403541
H	2.281740	2.057493	1.618823
C	-0.378050	3.235185	1.956012
H	-0.200349	4.053432	2.687491
H	0.422659	3.291955	1.194656
H	-1.355481	3.430050	1.474523
C	-2.902358	1.846074	3.382359
H	-2.974653	2.488847	4.286151
H	-3.162575	2.473694	2.508149
H	-3.667626	1.052555	3.481640
C	-1.903074	-0.928991	4.654075
H	-2.010856	-0.580874	5.703737
H	-2.920215	-1.000561	4.221701
H	-1.459794	-1.942330	4.678401
C	-3.516696	-0.877501	1.164014
C	-2.116354	-2.731662	1.529697
C	-4.666615	-1.658796	1.237706
H	-3.560523	0.203479	0.966663
C	-3.245742	-3.580104	1.629559
C	-4.525332	-3.038230	1.496648
H	-5.653605	-1.196024	1.095665
H	-3.106536	-4.659846	1.793802
H	-5.409445	-3.689706	1.572627
C	1.721776	-1.122191	0.231754
C	0.362390	-2.847190	1.066598
C	2.741604	-2.009933	-0.100922
H	1.799617	-0.043994	0.036861
C	1.360610	-3.801168	0.758764
C	2.561165	-3.377716	0.184278
H	3.658962	-1.635462	-0.576277
H	1.179870	-4.868099	0.961639
H	3.344966	-4.112264	-0.056238
N	0.563456	-1.522057	0.831543
N	-2.263634	-1.392610	1.340484
N	-0.838183	-3.280231	1.636261
H	-0.840152	-4.275655	1.872859
Ir	-0.662614	-0.060367	1.747283
O	-1.136898	0.648708	-0.233438
O	-0.034152	1.347815	-0.912041
H	-0.457379	2.223287	-1.065863
H	0.823834	0.246037	-2.560179
O	0.839761	-0.705228	-2.806843
H	-0.597923	-1.124780	-2.356218
H	1.092829	-0.734014	-3.752011
O	-1.484468	-1.162094	-1.837259
H	-1.571818	-2.066246	-1.480380
H	-1.333594	-0.218871	-0.937109

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