Supporting Information for:

Characterization of an amorphous iridium water-oxidation catalyst electrodeposited from organometallic precursors

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Additional SEM Images.

Image S1. Wide view of **BL** on FTO-coated glass. FTO is visible in lower portion of the image.

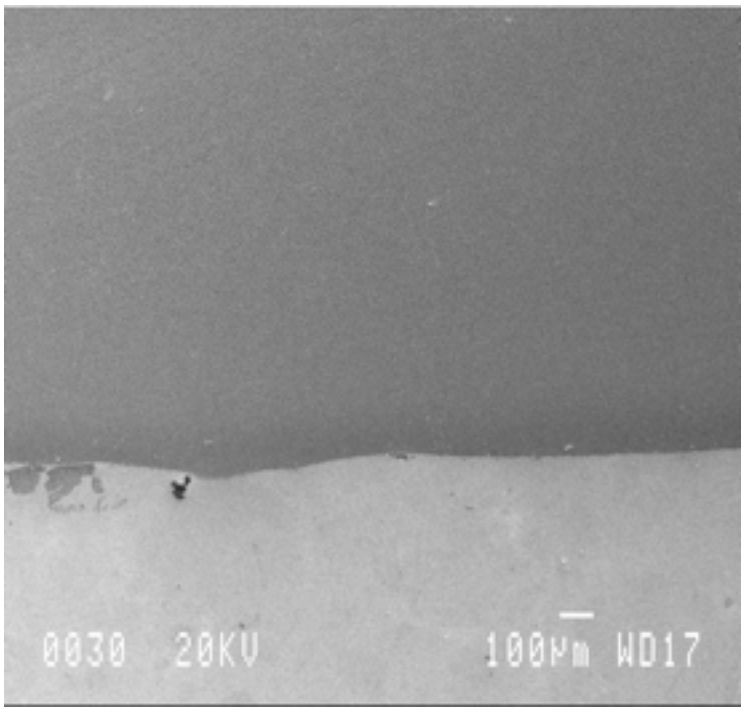


Image S2. Aged sample of **BL**. Cracking is readily apparent.

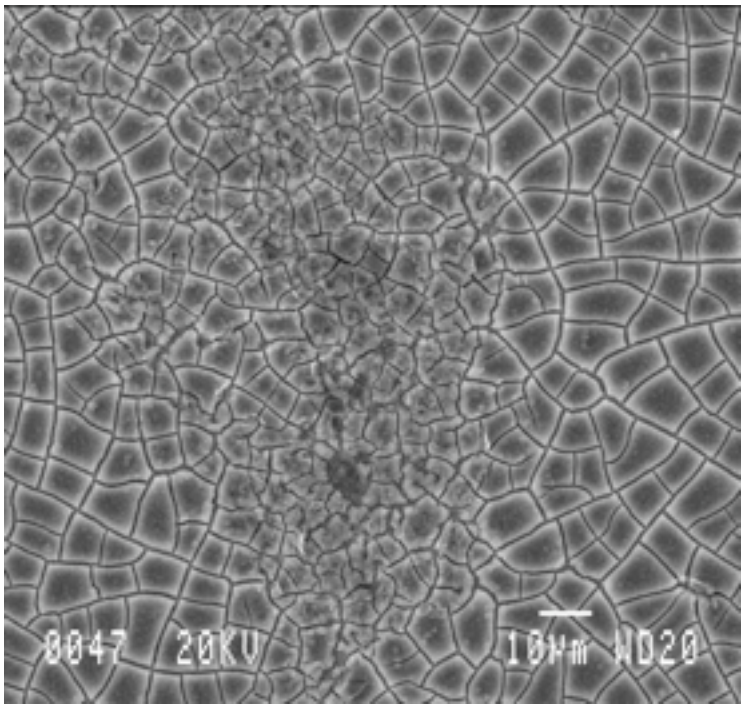


Image S3. Wide view of a fresh **BL**.

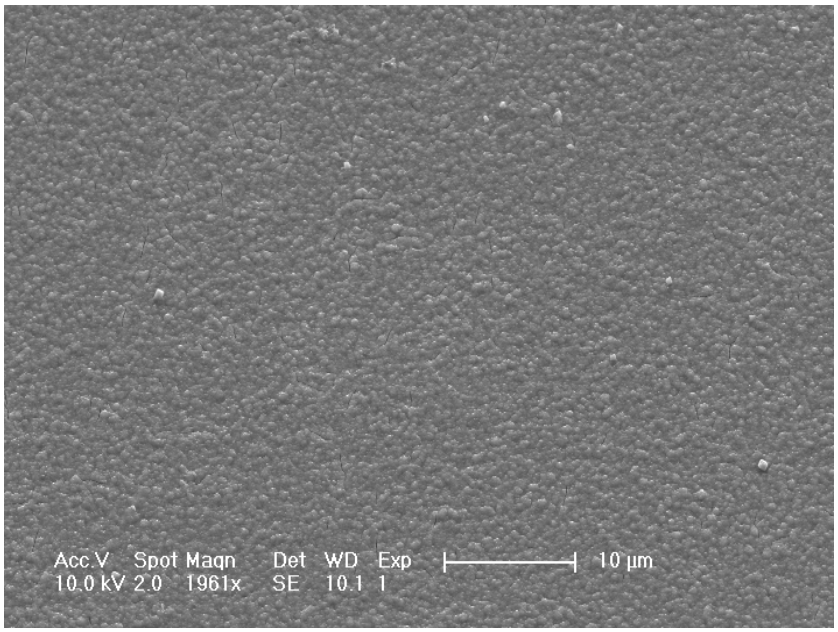


Figure S1. a) Substructure **I** with "structural" water molecules in the first hydration shell of the complex. Ir, O, C and H atoms are shown in green, red, light blue and white sphere, respectively. EXAFS (a) and PDF (b) spectra for substructure **I** with a solvation shell of 3 water molecules. Structures were optimized by DFT with the same level of theory as for substructure **I**.

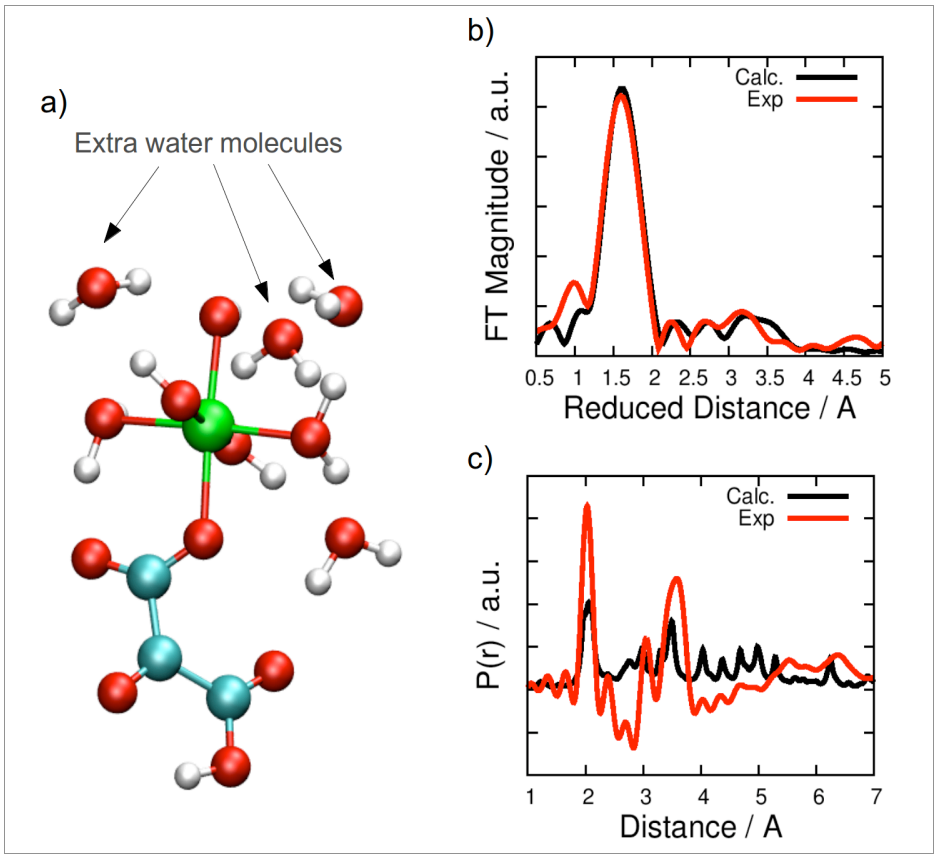


Figure S2: EXAFS (a) and PDF (c) for the DFT optimized structure of compound **I**. EXAFS (b) and PDF (d) for the Monte Carlo refined structure of substructure **I**. The RMSD between the DFT optimized structure and the MC refined model is 0.013 Å.

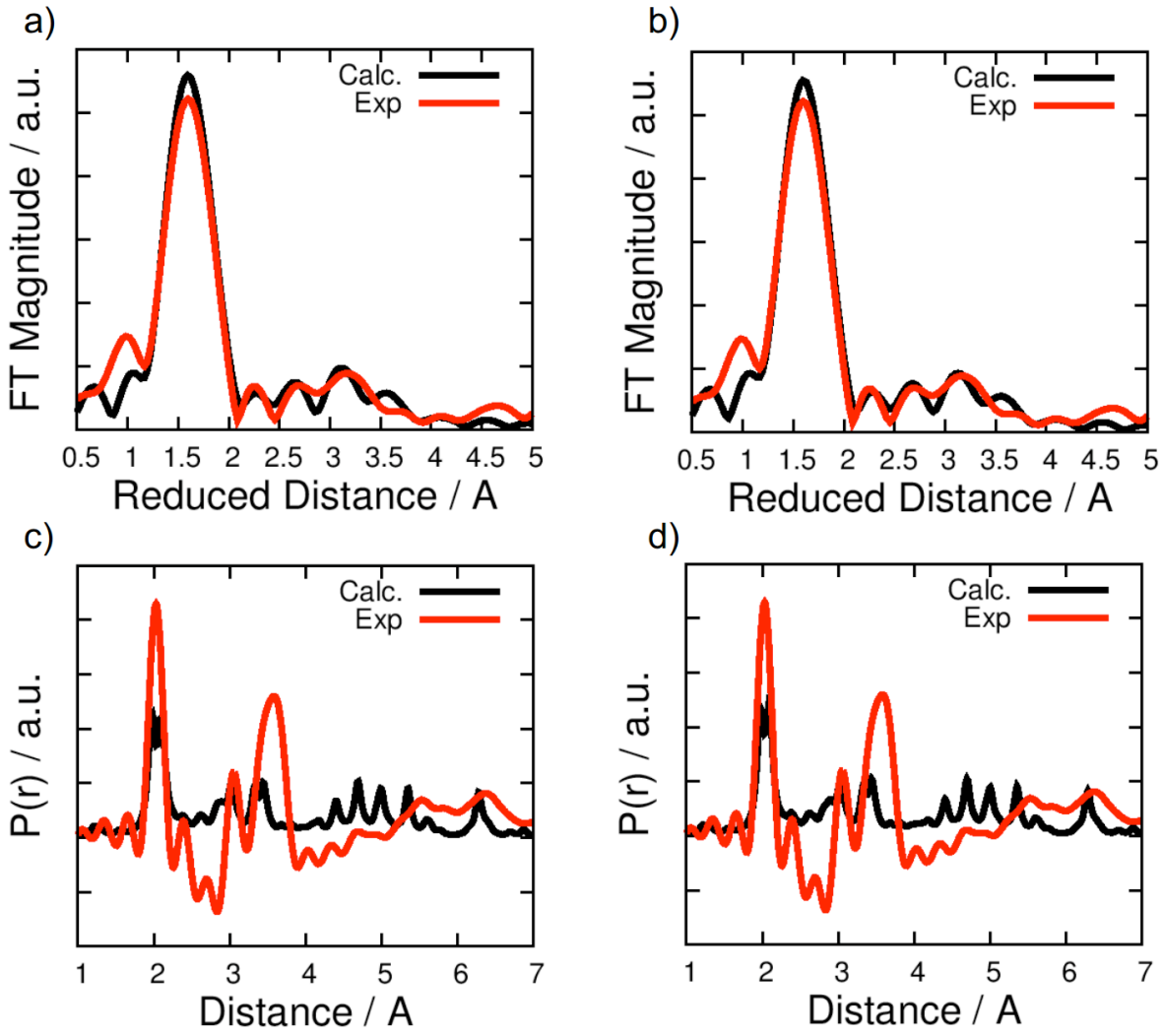
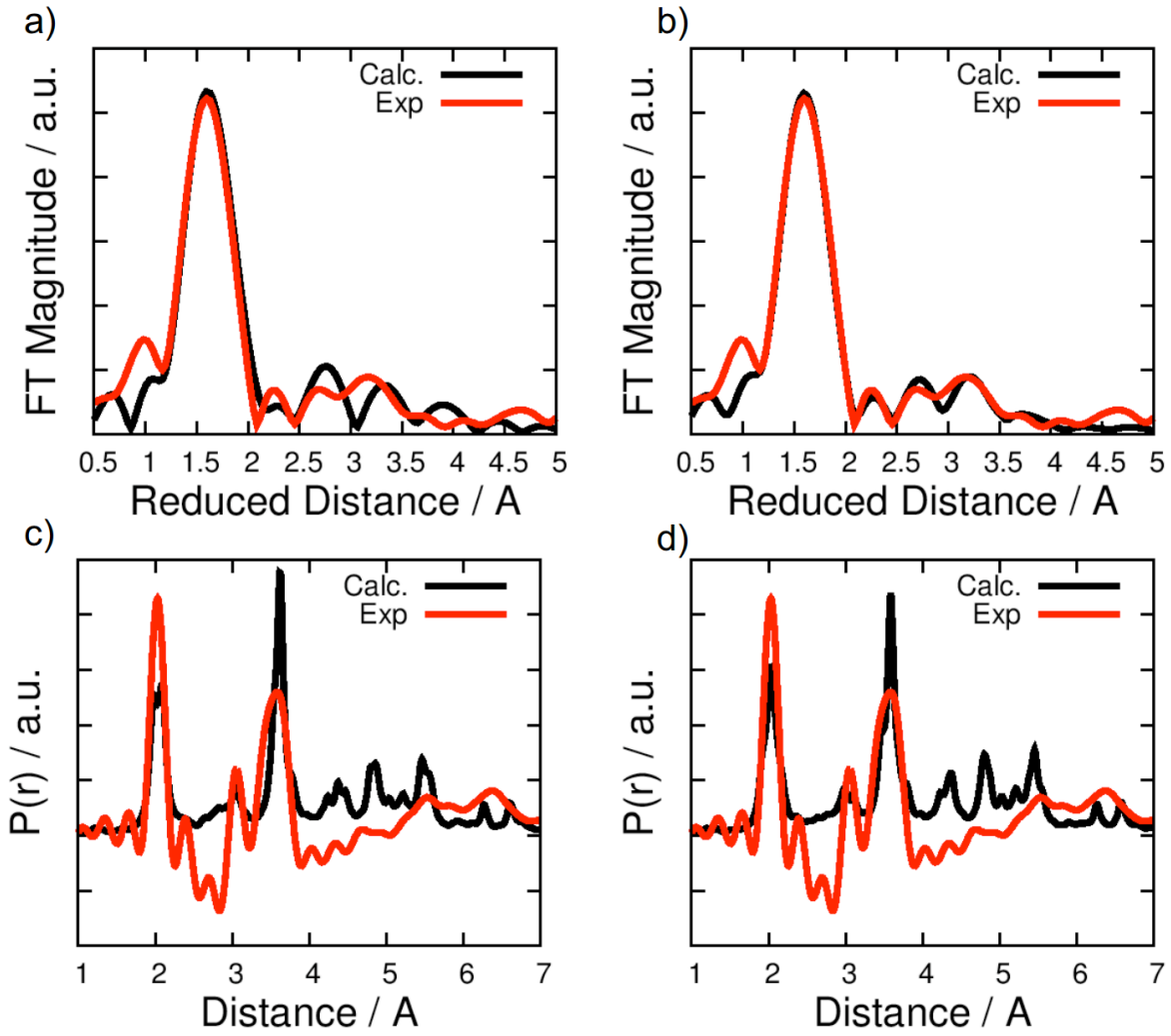


Figure S3. EXAFS (a) and PDF (c) for the DFT optimized structure of compound **II**. EXAFS (b) and PDF (d) for the Monte Carlo refined structure of substructure **II**. The RMSD between the DFT optimized structure and the MC refined model is 0.058 Å.



Cartesian Coordinates from the DFT Model of substructure I (in Å)

Ir	2.25545	4.71439	0.87549
C	1.67269	-0.25254	0.83424
C	1.14754	0.62924	-0.34178
C	1.61736	2.08601	-0.47006
O	1.66535	2.67621	0.65536
O	1.85979	2.52339	-1.59590
O	0.35345	5.17847	0.66860
O	2.80937	6.51247	1.41407
O	1.88185	4.51616	2.91583
O	4.12984	4.03813	0.86858
O	2.80274	4.91416	-1.13989
O	0.37595	0.11976	-1.11611
O	2.47052	0.09469	1.66723
O	1.15229	-1.47265	0.79737
O	3.35114	2.34836	3.12934
H	3.31127	6.95951	0.72240
H	2.41345	3.73578	3.22755
H	3.75424	4.71275	-1.04970
H	2.40388	4.09086	-1.55272
H	0.55066	-1.51915	0.02982
H	4.31728	3.46268	1.62218
H	0.21212	5.68876	-0.13985
H	2.21781	5.34067	3.29966
H	2.95952	1.70719	2.50618
H	3.71182	1.85049	3.86868

Cartesian Coordinates from the DFT MC refined Model of substructure I (in Å)

Ir	2.25917	4.72064	0.87599
C	1.67269	-0.25254	0.83424
C	1.14754	0.62924	-0.34178
C	1.61736	2.08601	-0.47006
O	1.68089	2.70361	0.68224
O	1.85979	2.52339	-1.59590
O	0.35375	5.17845	0.66858
O	2.81901	6.52684	1.41157
O	1.87729	4.52202	2.91527
O	4.13524	4.03054	0.87168

O	2.79637	4.92686	-1.14136
O	0.37595	0.11976	-1.11611
O	2.47052	0.09469	1.66723
O	1.15229	-1.47265	0.79737
O	3.35321	2.35348	3.12964

Cartesian Coordinates from the DFT Model of substructure II (in Å)

Ir	2.63549	4.44528	1.43108
C	-0.05399	-0.02274	-0.28577
C	0.14486	0.89043	0.95044
C	0.55502	2.34838	0.71213
O	1.71139	2.62854	1.08207
O	-0.36264	3.03210	0.18681
Ir	-0.41388	5.00311	-0.44626
O	0.99632	5.68431	0.95986
O	3.67632	6.25391	1.69759
O	1.68565	4.39278	3.18885
O	4.19330	3.42019	1.99895
O	3.36960	4.91394	-0.35891
O	1.07054	4.90541	-1.81266
O	-1.71989	5.34184	0.98241
O	-0.55456	6.89861	-1.33154
O	-1.71446	4.60558	-1.86561
O	-0.03366	0.43307	2.04890
O	0.14103	0.33429	-1.41810
O	-0.43469	-1.24588	0.04735
O	-0.07266	2.62693	-3.05847
H	4.01550	6.23258	0.76436
H	2.25779	4.73903	3.88465
H	2.66385	4.87942	-1.03964
H	0.93459	4.11650	-2.36513
H	-2.16971	4.52318	1.23278
H	0.49872	5.72965	1.79162
H	-1.33178	6.75722	-1.90475
H	-0.50549	-1.29525	1.01913
H	4.01270	2.48071	1.85739
H	-1.47141	3.77059	-2.30041
H	0.22800	6.80964	-1.91505
H	-0.06609	2.40348	-3.99370

H	0.05972	1.81079	-2.55144
H	2.98582	6.93618	1.70879

Cartesian Coordinates from the DFT MC refined Model of substructure II (in Å)

Ir	2.59654	4.39504	1.38555
C	-0.05399	-0.02274	-0.28577
C	0.14486	0.89043	0.95044
C	0.59773	2.29286	0.67449
O	1.67204	2.61195	0.97078
O	-0.42640	3.02311	0.25960
Ir	-0.37403	4.99234	-0.45403
O	0.99416	5.69251	0.92951
O	3.64709	6.31368	1.67305
O	1.68636	4.39187	3.19794
O	4.08024	3.43719	1.94275
O	3.43844	4.84989	-0.32650
O	1.00831	4.99002	-1.77539
O	-1.74041	5.34207	1.00068
O	-0.51680	6.83792	-1.28104
O	-1.68043	4.60343	-1.91491
O	-0.03366	0.43307	2.04890
O	0.14103	0.33429	-1.41810
O	-0.43469	-1.24588	0.04735
O	-0.08507	2.64540	-2.97657

Cartesian Coordinates from the DFT Model of substructure I with solvation shell (in Å)

Ir	2.25545	4.71439	0.87549
C	1.67269	-0.25254	0.83424
C	1.14754	0.62924	-0.34178
C	1.61736	2.08601	-0.47006
O	1.66535	2.67621	0.65536
O	1.85979	2.52339	-1.59590
O	0.35345	5.17847	0.66860
O	2.80937	6.51247	1.41407
O	1.88185	4.51616	2.91583
O	4.12984	4.03813	0.86858
O	2.80274	4.91416	-1.13989
O	0.37595	0.11976	-1.11611

O	2.47052	0.09469	1.66723
O	1.15229	-1.47265	0.79737
O	3.35114	2.34836	3.12934
H	3.31127	6.95951	0.72240
H	2.41345	3.73578	3.22755
H	3.75424	4.71275	-1.04970
H	2.40388	4.09086	-1.55272
H	0.55066	-1.51915	0.02982
H	4.31728	3.46268	1.62218
H	0.21212	5.68876	-0.13985
H	2.21781	5.34067	3.29966
H	2.95952	1.70719	2.50618
H	3.71182	1.85049	3.86868
O	2.93158	7.02952	3.65496
H	2.90605	6.88951	2.70557
H	3.19930	7.93297	3.83856
O	0.61886	6.40315	-1.78386
H	1.44491	5.96916	-1.55829
H	0.69998	7.34947	-1.64422
O	-0.61370	4.74392	2.98279
H	0.22206	4.61398	3.43690
H	-0.44746	4.92420	2.05464

Cartesian Coordinates from the DFT MC refined Model of substructure I with solvation shell (in Å)

Ir	2.23652	4.61460	0.80641
C	1.82515	-0.34639	0.99580
C	1.11630	0.48698	-0.11385
C	1.56214	1.93409	-0.35948
O	1.63473	2.61841	0.73235
O	1.77048	2.29853	-1.51627
O	0.37530	5.23930	0.77066
O	2.84936	6.55440	0.96008
O	2.04183	4.33268	2.81354
O	4.12819	4.09715	0.71567
O	2.52953	4.77886	-1.29842
O	0.23597	-0.04537	-0.74226
O	2.75053	0.03771	1.66438
O	1.30834	-1.56242	1.10256

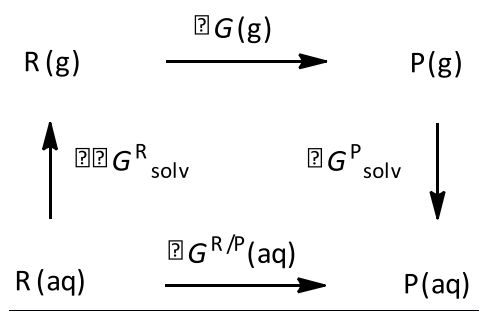
O	3.83331	2.35240	2.88666
O	2.05081	6.71290	3.57788
O	0.97884	7.30253	-0.91996
O	-0.56475	6.35593	3.06226

Computational Details

Absolute redox potentials due to the reduction of R to form P under aqueous conditions were computed as follows:

$$E_{\text{calc}}^{\text{abs}}\left[\text{V}\right] = -\frac{\Delta G^{\text{R/P}}\left(\text{aq}\right)}{nF}, \tag{1}$$

where F is the Faraday constant and n is the number of moles of electrons involved in the redox reaction. Aqueous changes in the free energy $\Delta G^{\text{R/P}}(\text{aq})$ were found using the thermodynamic cycle:



and

$$\Delta G^{\text{R/P}}\left(\text{aq}\right) = \Delta G^{\text{R/P}}\left(\text{g}\right) + \Delta G_{\text{solv}}^{\text{P}} - \Delta G_{\text{solv}}^{\text{R}}, \tag{2}$$

where $\Delta G(\text{g}) = \Delta H(\text{g}) - T\Delta S(\text{g})$ is the free energy state transition in the gas phase. The solvation free energies ΔG_{solv} were calculated using the standard self-consistent reaction field approach based on gas-phase geometries with a dielectric constant of 80.37 and a solvent radius of 1.40 Å for water as the solvating medium, as implemented in Jaguar, version 7.7 [1]. More details of the computational methods employed are described elsewhere [2].

Atomic coordinates in Å (below and following pages) of the minimum energy structures of precursor **2** and states formed upon its electrochemical oxidation (Scheme 1 in the main text) obtained by DFT at the UB3LYP/LACVP/6-311G* level of theory. Structures of lowest and next-highest spin multiplicity were investigated for the lowest free energy ΔG(aq) configuration.

$[(Cp^*Ir)_2(OH)_3]^{2+}$

(Multiplicity = 2)

Ir	-1.065989	-0.884446	0.658010
Ir	-3.234397	-1.623037	2.832305
O	-1.218181	-0.732116	2.667778
O	-3.072203	-0.384384	1.029782
O	-2.093277	-2.643422	1.224683
C	-0.141569	-1.925787	-1.134571
C	0.907300	-1.556542	-0.199948
C	0.888172	-0.124113	-0.069515
C	-0.812219	-0.736157	-1.578303
C	-0.189944	0.390135	-0.914994
C	-0.485512	1.829943	-1.174989
C	-0.424481	-3.321628	-1.573765
C	-1.897307	-0.650366	-2.602054
C	1.899310	-2.496931	0.400423
C	1.864143	0.710558	0.691911
H	-1.523425	1.990871	-1.466255
H	-0.262593	2.462622	-0.316092
H	0.139068	2.177839	-2.006211
H	-2.599597	0.154501	-2.387048
H	-1.455163	-0.449068	-3.583575
H	-2.463121	-1.577488	-2.684467
H	-1.397676	-3.420998	-2.052203
H	0.330235	-3.616696	-2.311914
H	-0.362946	-4.030029	-0.747261
H	1.457683	-3.467424	0.626705
H	2.714376	-2.667397	-0.311844
H	2.345075	-2.101724	1.312471
H	2.316613	0.166812	1.520567
H	2.676290	1.009364	0.019432
H	1.413905	1.623390	1.081682
C	-3.577837	-2.740827	4.666888
C	-3.869967	-1.336685	4.904703
C	-4.492245	-3.210556	3.651053
C	-4.928246	-0.939266	4.017445
C	-5.311161	-2.101449	3.223883
C	-4.582056	-4.615318	3.153998
H	-3.608898	-5.106001	3.134336
H	-5.225297	-5.192198	3.827600
H	-5.021297	-4.676025	2.158599
C	-6.446303	-2.154590	2.252577
H	-6.325174	-2.952739	1.520556
H	-7.381304	-2.343586	2.790666
H	-6.564393	-1.215964	1.711072

C	-5.592405	0.398137	3.974438
H	-5.983218	0.629937	2.983294
H	-6.442216	0.404184	4.665721
H	-4.921548	1.201807	4.278281
C	-3.219529	-0.472366	5.933952
H	-3.197969	0.576042	5.637089
H	-3.786105	-0.537324	6.869197
H	-2.199748	-0.788432	6.153135
C	-2.617410	-3.587830	5.439420
H	-1.782455	-3.007767	5.832636
H	-3.128845	-4.041180	6.295095
H	-2.211174	-4.398452	4.834285
H	-0.478391	-0.911824	3.258069
H	-3.231151	0.560229	1.146820
H	-2.723627	-2.889563	0.533849

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

(Multiplicity = 3)

Ir	-1.291679	-0.983617	0.485808
Ir	-3.105140	-1.587215	2.836995
O	-1.029356	-0.874410	2.610454
O	-3.061359	-0.127220	1.202369
O	-2.365202	-2.501477	1.278052
C	-0.087686	-1.985977	-1.065242
C	0.762279	-1.577125	0.018245
C	0.750219	-0.108875	0.064182
C	-0.647062	-0.779378	-1.663817
C	-0.109692	0.371655	-0.969873
C	-0.355870	1.798493	-1.336165
C	-0.300186	-3.383329	-1.547002
C	-1.550759	-0.735248	-2.846704
C	1.618074	-2.459262	0.865575
C	1.576452	0.716784	0.990089
H	-1.361666	1.957108	-1.725303
H	-0.201284	2.475099	-0.496324
H	0.344981	2.095064	-2.124195
H	-2.202347	0.138347	-2.840471
H	-0.937860	-0.675137	-3.755445
H	-2.166499	-1.629842	-2.933867
H	-1.274274	-3.512936	-2.017336
H	0.463596	-3.626990	-2.293242
H	-0.217575	-4.108198	-0.738432
H	1.252277	-3.484831	0.880261
H	2.637496	-2.475279	0.465702
H	1.668537	-2.103326	1.894462
H	1.696678	0.241588	1.964043
H	2.580721	0.828061	0.564901
H	1.173863	1.719710	1.130168
C	-3.369427	-2.739017	4.686476
C	-3.692499	-1.362214	5.059501
C	-4.334395	-3.169811	3.695951

C	-4.783207	-0.930761	4.267321
C	-5.171520	-2.030477	3.380792
C	-4.469484	-4.545014	3.131931
H	-3.521462	-5.081338	3.128974
H	-5.172882	-5.116726	3.746975
H	-4.854908	-4.532978	2.113156
C	-6.354434	-2.029278	2.468778
H	-6.258014	-2.769748	1.675842
H	-7.256489	-2.272216	3.041316
H	-6.512743	-1.055645	2.005200
C	-5.474643	0.391009	4.333985
H	-5.840298	0.713724	3.358811
H	-6.348773	0.305798	4.989208
H	-4.839061	1.174950	4.744528
C	-2.994062	-0.586395	6.126584
H	-3.123974	0.489403	6.013773
H	-3.410700	-0.863027	7.101639
H	-1.926603	-0.806579	6.163738
C	-2.354041	-3.601240	5.361983
H	-1.476483	-3.034062	5.672363
H	-2.794074	-4.044387	6.262399
H	-2.022484	-4.418151	4.722215
H	-0.919630	0.044140	2.892106
H	-3.143485	0.823229	1.339221

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

(Multiplicity = 4)

Ir	-1.132274	-1.054190	0.740062
Ir	-3.032116	-1.563169	2.786231
O	-0.938762	-0.967149	2.908376
O	-2.770124	-0.057163	1.436545
O	-1.963696	-2.721978	1.522058
C	-0.302746	-1.962396	-1.127505
C	0.786089	-1.517066	-0.293680
C	0.680123	-0.067154	-0.165343
C	-1.102877	-0.807695	-1.481264
C	-0.471807	0.365619	-0.901527
C	-0.935420	1.771056	-1.093648
C	-0.541693	-3.362476	-1.582779
C	-2.273673	-0.797290	-2.406115
C	1.906019	-2.356763	0.226623
C	1.665607	0.803050	0.538787
H	-2.022955	1.846804	-1.095602
H	-0.547721	2.444131	-0.330615
H	-0.580143	2.134004	-2.064595
H	-2.965419	0.013971	-2.180711
H	-1.919859	-0.649749	-3.432892
H	-2.823918	-1.737340	-2.384021
H	-1.592779	-3.552842	-1.795932
H	0.018418	-3.533616	-2.508890
H	-0.201756	-4.095452	-0.852238

H	1.607145	-3.393990	0.372402
H	2.730053	-2.348018	-0.495858
H	2.296042	-1.980095	1.171863
H	2.091496	0.315448	1.415776
H	2.495412	1.020195	-0.143679
H	1.237082	1.757185	0.843045
C	-3.716635	-2.717535	4.564182
C	-3.964473	-1.302485	4.822587
C	-4.520408	-3.101600	3.430578
C	-4.898897	-0.824823	3.845495
C	-5.229934	-1.928761	2.960982
C	-4.634223	-4.475669	2.862028
H	-3.714979	-5.047425	2.982776
H	-5.430152	-5.012444	3.390353
H	-4.893860	-4.463354	1.804226
C	-6.242768	-1.891615	1.865965
H	-6.045508	-2.638486	1.097733
H	-7.233027	-2.106164	2.283822
H	-6.295619	-0.912229	1.390998
C	-5.479692	0.546975	3.757806
H	-5.609021	0.871377	2.725089
H	-6.470025	0.545450	4.226841
H	-4.873231	1.288511	4.275390
C	-3.403790	-0.532181	5.970028
H	-3.394902	0.541625	5.787473
H	-4.029726	-0.708341	6.852539
H	-2.393324	-0.851911	6.225298
C	-2.891641	-3.625349	5.415838
H	-2.033698	-3.112900	5.850536
H	-3.504560	-4.000070	6.243493
H	-2.525579	-4.487934	4.860567
H	-0.869678	-0.047295	3.198536

$[(Cp^*Ir)_2(O)_3]^{2+}$

(Multiplicity = 1)

Ir	-1.424252	-1.337390	0.439910
Ir	-2.679016	-1.186205	3.085279
O	-1.543161	-0.096484	3.857720
O	-3.084680	-0.608362	1.215654
O	-1.776509	-2.558204	1.961534
C	-0.380518	-2.170250	-1.320392
C	0.628106	-1.791242	-0.379332
C	0.504161	-0.368691	-0.150634
C	-1.115396	-0.956705	-1.714345
C	-0.553711	0.147001	-1.002082
C	-0.941701	1.583946	-1.135168
C	-0.587735	-3.525000	-1.907166
C	-2.173850	-0.898234	-2.763857
C	1.648285	-2.690897	0.240227
C	1.369044	0.446014	0.744037
H	-1.978133	1.700659	-1.449641

H	-0.804803	2.136359	-0.205798
H	-0.311562	2.059177	-1.894666
H	-2.837861	-0.045044	-2.631123
H	-1.698190	-0.796362	-3.746005
H	-2.778717	-1.804529	-2.789113
H	-1.631131	-3.706032	-2.164761
H	-0.005247	-3.605053	-2.832434
H	-0.253321	-4.318621	-1.240135
H	1.296837	-3.719412	0.314749
H	2.550394	-2.695710	-0.381002
H	1.940442	-2.359283	1.236300
H	1.744036	-0.127324	1.591265
H	2.240078	0.789632	0.172090
H	0.858378	1.332328	1.119128
C	-3.526927	-2.679728	4.586776
C	-3.936306	-1.335234	4.945345
C	-4.238694	-3.058549	3.356793
C	-4.784223	-0.848256	3.873133
C	-4.993841	-1.953544	2.923695
C	-4.096162	-4.383151	2.703483
H	-3.083039	-4.487954	2.298272
H	-4.246492	-5.187305	3.428577
H	-4.805348	-4.519248	1.889464
C	-5.842326	-1.841220	1.710816
H	-5.945929	-2.791647	1.191198
H	-6.841476	-1.484528	1.976315
H	-5.405983	-1.115398	1.015977
C	-5.505310	0.451857	3.828860
H	-5.651303	0.798371	2.805774
H	-6.500120	0.315612	4.272695
H	-4.998280	1.230630	4.396717
C	-3.607254	-0.616895	6.210304
H	-3.596096	0.464500	6.080206
H	-4.374635	-0.854615	6.955913
H	-2.644015	-0.919776	6.618891
C	-2.707064	-3.610024	5.408045
H	-2.030475	-3.086880	6.082294
H	-3.379594	-4.220486	6.024571
H	-2.128000	-4.293347	4.786470

$[(Cp^*Ir)_2(OH)_3]^+$

(Multiplicity = 1)

Ir	-1.095283	-1.031603	0.555346
Ir	-3.213861	-1.599303	2.833154
O	-1.143673	-1.071356	2.694606
O	-3.051540	-0.324742	1.107440
O	-2.287837	-2.678140	1.231019
C	-0.022589	-1.894549	-1.140372
C	0.915656	-1.488604	-0.121349
C	0.785255	-0.048276	0.040435
C	-0.763877	-0.736892	-1.575351

C	-0.246345	0.411891	-0.842836
C	-0.668679	1.831119	-1.058470
C	-0.189550	-3.291172	-1.648336
C	-1.774909	-0.680184	-2.678105
C	1.931310	-2.359496	0.549606
C	1.634427	0.797115	0.936281
H	-1.730824	1.905393	-1.295355
H	-0.472478	2.454742	-0.185759
H	-0.116173	2.262233	-1.900144
H	-2.546703	0.064119	-2.478860
H	-1.292940	-0.414209	-3.624985
H	-2.273842	-1.638826	-2.822381
H	-1.171466	-3.449949	-2.094420
H	0.559342	-3.494607	-2.421049
H	-0.056633	-4.027022	-0.854927
H	1.592114	-3.393316	0.617122
H	2.872193	-2.352603	-0.011227
H	2.145333	-2.019626	1.563301
H	1.902989	0.270331	1.852839
H	2.567118	1.060657	0.426420
H	1.139079	1.728432	1.212762
C	-3.547369	-2.682343	4.683988
C	-3.756129	-1.261775	4.921601
C	-4.527408	-3.105508	3.712648
C	-4.826849	-0.817313	4.077707
C	-5.306084	-1.960215	3.310841
C	-4.692995	-4.504609	3.211094
H	-3.734864	-5.017379	3.124044
H	-5.315070	-5.075634	3.908307
H	-5.180932	-4.535123	2.236763
C	-6.487232	-1.956308	2.390965
H	-6.442190	-2.771126	1.667886
H	-7.415513	-2.072786	2.960445
H	-6.557637	-1.023831	1.829876
C	-5.424911	0.553874	4.042450
H	-5.780170	0.814331	3.044565
H	-6.285440	0.604065	4.718185
H	-4.715925	1.319216	4.359658
C	-3.010504	-0.439131	5.924416
H	-3.023126	0.622546	5.675849
H	-3.468968	-0.550021	6.912755
H	-1.970147	-0.754950	6.011733
C	-2.582358	-3.562849	5.414551
H	-1.665919	-3.029950	5.669656
H	-3.027167	-3.928888	6.346155
H	-2.299621	-4.430226	4.817760
H	-0.949726	-0.213883	3.085826
H	-3.099785	0.617559	1.297803
H	-2.956073	-2.871133	0.563428

$[(Cp^*Ir)_2(OH)_2(O)]^+$

(Multiplicity = 2)

Ir	-1.093240	-1.057638	0.558821
Ir	-3.203803	-1.626182	2.828811
O	-1.107543	-0.974779	2.751382
O	-3.021642	-0.219918	1.163444
O	-2.256415	-2.463533	1.313453
C	-0.031204	-1.883591	-1.165529
C	0.916451	-1.477607	-0.155867
C	0.780492	-0.035790	0.021745
C	-0.795973	-0.725543	-1.565472
C	-0.267596	0.425993	-0.841369
C	-0.701615	1.842377	-1.043714
C	-0.199596	-3.269520	-1.700430
C	-1.845515	-0.674995	-2.630880
C	1.953928	-2.340619	0.490805
C	1.650066	0.806862	0.901479
H	-1.770031	1.910296	-1.251252
H	-0.484367	2.466203	-0.176053
H	-0.173505	2.276253	-1.899473
H	-2.609496	0.069379	-2.406198
H	-1.395312	-0.413668	-3.594735
H	-2.347299	-1.635273	-2.748193
H	-1.223304	-3.458591	-2.022600
H	0.454902	-3.410494	-2.567292
H	0.062984	-4.024159	-0.959519
H	1.636839	-3.382157	0.540276
H	2.888625	-2.302780	-0.079046
H	2.170230	-2.014817	1.508653
H	1.927564	0.281057	1.815599
H	2.576353	1.061860	0.375642
H	1.165826	1.742691	1.181810
C	-3.579523	-2.673950	4.696970
C	-3.783938	-1.246304	4.917699
C	-4.546239	-3.106484	3.717807
C	-4.838723	-0.805129	4.052100
C	-5.300600	-1.954500	3.281526
C	-4.729476	-4.507305	3.228151
H	-3.799631	-5.074218	3.265675
H	-5.461586	-5.024060	3.857874
H	-5.096023	-4.533874	2.202147
C	-6.445829	-1.951880	2.318232
H	-6.368590	-2.766696	1.598607
H	-7.393457	-2.069062	2.854898
H	-6.493840	-1.019862	1.754819
C	-5.430799	0.566377	3.989568
H	-5.754647	0.819126	2.979320
H	-6.310215	0.623345	4.639623
H	-4.729108	1.331941	4.322246
C	-3.057993	-0.422224	5.934759
H	-3.072212	0.639795	5.688283

H	-3.531755	-0.537569	6.915259
H	-2.017670	-0.733117	6.036145
C	-2.630242	-3.545632	5.457624
H	-1.708498	-3.017307	5.703290
H	-3.087311	-3.877049	6.395971
H	-2.356978	-4.434178	4.888677
H	-0.971088	-0.085444	3.098126
H	-2.973841	0.703428	1.440820

$[(Cp^*Ir)_2(OH)(O)_2]^+$

(Multiplicity = 3)

Ir	-1.109589	-1.042890	0.653340
Ir	-3.116717	-1.581064	2.813839
O	-1.024814	-0.979561	2.826185
O	-2.894830	-0.272929	1.265859
O	-2.178924	-2.605475	1.349836
C	-0.166540	-1.933277	-1.135377
C	0.874950	-1.498038	-0.245338
C	0.758584	-0.053158	-0.109974
C	-0.954424	-0.780765	-1.512289
C	-0.351317	0.389333	-0.891002
C	-0.807940	1.799100	-1.095677
C	-0.396980	-3.335815	-1.598081
C	-2.081036	-0.757854	-2.497378
C	1.973179	-2.340656	0.324856
C	1.696611	0.807213	0.675916
H	-1.895989	1.869548	-1.117159
H	-0.446384	2.464428	-0.312079
H	-0.432293	2.178349	-2.051769
H	-2.796416	0.032883	-2.270780
H	-1.695100	-0.579064	-3.506674
H	-2.624126	-1.702637	-2.513032
H	-1.447457	-3.520205	-1.821265
H	0.176923	-3.521503	-2.512035
H	-0.082745	-4.065176	-0.852021
H	1.674519	-3.384616	0.417730
H	2.854972	-2.303813	-0.323773
H	2.275643	-1.995524	1.314057
H	2.030627	0.312511	1.588774
H	2.588072	1.024452	0.077994
H	1.246517	1.760918	0.951296
C	-3.667887	-2.712957	4.648616
C	-3.903084	-1.298377	4.900809
C	-4.526341	-3.106782	3.565326
C	-4.878145	-0.826402	3.971318
C	-5.252349	-1.940781	3.112718
C	-4.652911	-4.485160	3.001061
H	-3.723982	-5.047264	3.092774
H	-5.432368	-5.034038	3.539836
H	-4.927115	-4.466439	1.946660
C	-6.322987	-1.911490	2.067179

H	-6.161770	-2.670491	1.301834
H	-7.300346	-2.101469	2.523540
H	-6.371825	-0.942846	1.569439
C	-5.467534	0.546516	3.898557
H	-5.617074	0.865006	2.866303
H	-6.443749	0.560508	4.394505
H	-4.837935	1.288727	4.388486
C	-3.260860	-0.510750	5.998451
H	-3.276110	0.560623	5.798751
H	-3.798957	-0.678303	6.937501
H	-2.225074	-0.811990	6.159777
C	-2.799443	-3.611638	5.472891
H	-1.898200	-3.101312	5.814120
H	-3.342874	-3.954675	6.359824
H	-2.486777	-4.494040	4.914962
H	-0.970356	-0.056785	3.103576

$[(Cp^*Ir)_2(O)_3]^+$

(Multiplicity = 2)

Ir	-1.156640	-1.069237	0.634979
Ir	-3.131401	-1.594784	2.764673
O	-1.175252	-0.982312	2.684203
O	-3.019537	-0.349839	1.132119
O	-2.289640	-2.664292	1.234207
C	-0.055585	-1.880553	-1.134047
C	0.893941	-1.472253	-0.126907
C	0.741714	-0.040625	0.062352
C	-0.816380	-0.729724	-1.539245
C	-0.309396	0.415677	-0.798028
C	-0.770813	1.827434	-0.976044
C	-0.210508	-3.267109	-1.670491
C	-1.844930	-0.677745	-2.625494
C	1.954422	-2.328073	0.492803
C	1.581189	0.799852	0.970592
H	-1.844757	1.880651	-1.156082
H	-0.547785	2.442172	-0.104587
H	-0.267169	2.276639	-1.838582
H	-2.608739	0.073099	-2.422104
H	-1.371931	-0.420025	-3.579161
H	-2.347921	-1.636020	-2.754301
H	-1.225606	-3.457889	-2.017571
H	0.465134	-3.409374	-2.520720
H	0.034615	-4.021056	-0.922621
H	1.647279	-3.371905	0.557047
H	2.869240	-2.288002	-0.108223
H	2.205916	-1.993400	1.499362
H	1.822592	0.275443	1.895501
H	2.524779	1.051781	0.475085
H	1.086021	1.733245	1.235969
C	-3.554828	-2.657565	4.673005
C	-3.743002	-1.233195	4.883308

C	-4.520402	-3.082401	3.688855
C	-4.793523	-0.787407	4.016485
C	-5.274774	-1.934823	3.262108
C	-4.706626	-4.483474	3.202124
H	-3.774101	-5.047213	3.222794
H	-5.424699	-5.003625	3.844982
H	-5.091423	-4.511826	2.183119
C	-6.438449	-1.932646	2.320598
H	-6.374164	-2.742728	1.594282
H	-7.373223	-2.058985	2.877101
H	-6.507354	-0.995807	1.767268
C	-5.362737	0.593601	3.937129
H	-5.659491	0.849077	2.919596
H	-6.253552	0.664761	4.570211
H	-4.653193	1.347291	4.277075
C	-2.992122	-0.405083	5.876574
H	-3.020389	0.655205	5.627991
H	-3.435177	-0.526811	6.870637
H	-1.945856	-0.704978	5.941517
C	-2.636586	-3.543116	5.456501
H	-1.723114	-3.022963	5.745292
H	-3.130764	-3.879706	6.374181
H	-2.349177	-4.430293	4.892249

$[(Cp^*Ir)_2(OH)_2(O)]^0$

(Multiplicity = 1)

Ir	-1.110793	-0.994326	0.614000
Ir	-3.164906	-1.545123	2.828215
O	-1.104867	-0.837835	2.786309
O	-3.021199	-0.116766	1.189619
O	-2.251594	-2.470971	1.316568
C	-0.191474	-2.029543	-1.037898
C	0.828819	-1.596479	-0.111251
C	0.823458	-0.135346	-0.099708
C	-0.876961	-0.857775	-1.527862
C	-0.212805	0.315309	-0.963168
C	-0.555168	1.735101	-1.296225
C	-0.506412	-3.449398	-1.390788
C	-1.969838	-0.825028	-2.551504
C	1.827381	-2.468821	0.585672
C	1.790071	0.714040	0.667010
H	-1.630996	1.866973	-1.424798
H	-0.229458	2.425800	-0.516498
H	-0.072624	2.044042	-2.231234
H	-2.670802	-0.011931	-2.356468
H	-1.561253	-0.683918	-3.559497
H	-2.544481	-1.751554	-2.549365
H	-1.551132	-3.563786	-1.679528
H	0.119385	-3.787964	-2.224591
H	-0.336775	-4.112619	-0.542398
H	1.431782	-3.471619	0.749570

H	2.748358	-2.562446	-0.002678
H	2.094006	-2.064435	1.563390
H	2.018916	0.277367	1.640689
H	2.735874	0.816095	0.121669
H	1.401049	1.719036	0.839094
C	-3.520468	-2.761452	4.573853
C	-3.865468	-1.390645	4.944214
C	-4.412503	-3.164297	3.511308
C	-4.912889	-0.946673	4.090870
C	-5.240162	-2.032592	3.168823
C	-4.438649	-4.508240	2.853053
H	-3.442506	-4.949811	2.820035
H	-5.101707	-5.191527	3.395987
H	-4.789015	-4.438329	1.823355
C	-6.346810	-2.008370	2.159672
H	-6.176406	-2.735663	1.365421
H	-7.311654	-2.239689	2.627184
H	-6.429227	-1.028939	1.685866
C	-5.613653	0.376443	4.136708
H	-5.877904	0.723183	3.136025
H	-6.542316	0.306541	4.715697
H	-4.996322	1.147858	4.600336
C	-3.235286	-0.628031	6.068850
H	-3.354848	0.449877	5.947099
H	-3.689431	-0.903427	7.028122
H	-2.166231	-0.835445	6.141071
C	-2.535080	-3.634537	5.288359
H	-1.663863	-3.064790	5.615313
H	-2.986966	-4.097127	6.174339
H	-2.172069	-4.434129	4.641849
H	-1.051322	0.085661	3.063291
H	-2.903938	0.781357	1.524456

$[(Cp^*Ir)_2(OH)(O)_2]^0$

(Multiplicity = 2)

Ir	-1.086000	-1.069367	0.665049
Ir	-3.097355	-1.606364	2.828271
O	-0.944702	-1.166066	2.856919
O	-2.747607	-0.185445	1.422951
O	-2.247494	-2.583930	1.292126
C	-0.178730	-1.905662	-1.153669
C	0.899270	-1.430660	-0.340759
C	0.711601	-0.001249	-0.151802
C	-1.050725	-0.782772	-1.462126
C	-0.462538	0.402403	-0.857013
C	-1.031631	1.783254	-0.965537
C	-0.383008	-3.308704	-1.635562
C	-2.234689	-0.798080	-2.379567
C	2.065471	-2.226674	0.158575
C	1.647569	0.888583	0.607550
H	-2.105453	1.776194	-0.770133

H	-0.575135	2.466175	-0.248394
H	-0.868472	2.193907	-1.968315
H	-2.979414	-0.062785	-2.071619
H	-1.939451	-0.569916	-3.411022
H	-2.723859	-1.773151	-2.380588
H	-1.440913	-3.574267	-1.639295
H	-0.000493	-3.426520	-2.655987
H	0.129101	-4.031068	-0.999248
H	1.816830	-3.284071	0.256513
H	2.917870	-2.147272	-0.527286
H	2.396352	-1.881151	1.139301
H	2.045718	0.387847	1.491790
H	2.498808	1.177854	-0.019727
H	1.156125	1.803573	0.940155
C	-3.783972	-2.696639	4.679762
C	-3.948615	-1.266032	4.877194
C	-4.571174	-3.070238	3.543984
C	-4.844393	-0.766704	3.883255
C	-5.217779	-1.877307	3.020126
C	-4.732564	-4.450673	2.986417
H	-3.891077	-5.091825	3.250439
H	-5.646800	-4.917928	3.369908
H	-4.794687	-4.431772	1.897705
C	-6.223056	-1.820332	1.910976
H	-6.053739	-2.612418	1.180281
H	-7.244186	-1.931780	2.295748
H	-6.165424	-0.870427	1.377617
C	-5.327495	0.640774	3.715232
H	-5.252370	0.954816	2.672612
H	-6.374295	0.733000	4.026103
H	-4.741500	1.342832	4.309275
C	-3.320720	-0.481639	5.988516
H	-3.261298	0.581117	5.750983
H	-3.904888	-0.583948	6.910485
H	-2.308118	-0.829388	6.200188
C	-2.998683	-3.611144	5.568831
H	-2.092842	-3.129140	5.940127
H	-3.592201	-3.918944	6.438453
H	-2.689948	-4.515057	5.042410
H	-0.915328	-0.236079	3.116173

$[(Cp^*Ir)_2(O)_3]^0$

(Multiplicity = 3)

Ir	-1.123439	-1.060895	0.604563
Ir	-3.162404	-1.605850	2.796109
O	-1.142073	-1.169274	2.672317
O	-2.956316	-0.365303	1.187106
O	-2.134029	-2.695203	1.369927
C	-0.054619	-1.860040	-1.156818
C	0.894854	-1.453197	-0.149541
C	0.726139	-0.022230	0.051188

C	-0.811183	-0.709403	-1.569502
C	-0.322457	0.430916	-0.818376
C	-0.803137	1.839779	-0.981749
C	-0.215817	-3.253032	-1.681845
C	-1.851275	-0.660687	-2.646251
C	1.944980	-2.310885	0.487519
C	1.556650	0.822901	0.966938
H	-1.880769	1.875006	-1.148269
H	-0.591894	2.441415	-0.097240
H	-0.314739	2.319601	-1.837934
H	-2.625938	0.073266	-2.419306
H	-1.403734	-0.386163	-3.609077
H	-2.344916	-1.624893	-2.773462
H	-1.222590	-3.424227	-2.063670
H	0.490740	-3.439046	-2.498807
H	-0.033664	-3.994277	-0.903199
H	1.639417	-3.357450	0.520181
H	2.890290	-2.255450	-0.065656
H	2.140300	-2.001038	1.515275
H	1.795444	0.290824	1.888744
H	2.500810	1.102639	0.485187
H	1.039277	1.741267	1.246374
C	-3.586498	-2.652345	4.673546
C	-3.758105	-1.221274	4.870909
C	-4.556475	-3.069149	3.690672
C	-4.815650	-0.774348	4.008735
C	-5.313028	-1.920362	3.272363
C	-4.738925	-4.470308	3.195021
H	-3.787638	-5.001003	3.146462
H	-5.405378	-5.029594	3.861493
H	-5.172045	-4.489168	2.194671
C	-6.470998	-1.909388	2.322370
H	-6.405838	-2.722753	1.598614
H	-7.419522	-2.018896	2.861810
H	-6.515759	-0.976224	1.758910
C	-5.365095	0.615431	3.913547
H	-5.645801	0.862177	2.888545
H	-6.256848	0.724178	4.541900
H	-4.635989	1.358485	4.237952
C	-2.994832	-0.390488	5.855686
H	-3.001318	0.665092	5.582086
H	-3.430499	-0.480455	6.857631
H	-1.951956	-0.704860	5.914199
C	-2.653608	-3.538500	5.440862
H	-1.715764	-3.027756	5.664541
H	-3.099560	-3.854296	6.391672
H	-2.402908	-4.437363	4.876082

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[1] *Jaguar, version 7.7* (Schrodinger, LLC, New York, NY, 2010).

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