Supporting Information for

Reduction of Systematic Uncertainty in DFT Redox Potentials of Transition-Metal Complexes

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List of Tables

Table 1: Calculated free energies G_g and enthalpies H_g in the gas phase and solvation free energies ΔG_{solv} in MeCN, DMSO, and DCM at the L1 [UB3LYP/LACVP/6-31G] level of theory.

Complex	G_g (kcal/mol)	H_g (kcal/mol)	ΔG_{solv} (kcal/mol) MeCN	DMSO	DCM
$[FeCp_2]^0$	-320203.96	-320177.72	-4.19	-4.12	-3.57
$[FeCp_2]^+$	-320039.50	-320012.22	-49.39	-49.59	-44.88
$[Ru(bpy)_3]^{2+}$	-990807.97	-990752.93	-124.55	-	-
$[Ru(bpy)_3]^{3+}$	-990532.69	-990477.39	-272.51	-	-
$[Ru(bpy)_3]^{2+} + 2BF_4^-$	-1523680.59	-1523606.76	-	-	-35.93
$[Ru(bpy)_3]^{3+} + 2BF_4^-$	-1523520.39	-1523447.17	-	-	-67.23
$[Ir(acac)_3]^0$	-715258.39	-715206.00	-16.74	-	-13.81
$[Ir(acac)_3]^+$	-715096.68	-715044.03	-54.31	-	-38.90
$[CoCp_2]^0$	-333778.57	-333750.47	-4.26	-	-3.60
$[CoCp_2]^+$	-333643.48	-333617.20	-49.30	-	-44.85
$[NiCp_2]^0$	-348986.55	-348957.57	-3.86	-	-3.26
$[NiCp_2]^+$	-348833.96	-348804.24	-48.82	-	-44.32
$[RuCp_2]^0$	-301673.82	-301646.93	-	-	-3.46
$[RuCp_2]^+$	-301507.78	-301482.01	-	-	-43.47
$[OsCp_2]^0$	-299883.81	-299856.69	-	-	-3.73
$[OsCp_2]^+$	-299722.15	-299692.55	-	-	-43.63
$[FeCp^*_2]^0$	-566703.11	-566655.06	-2.29	-2.31	-1.95
$[FeCp^*_2]^+$	-566563.70	-566514.08	-37.99	-38.22	-34.61
$[CoCp^*_2]^0$	-580279.17	-580225.89	-2.35	-	-1.99
$[CoCp^*_2]^+$	-580168.81	-580120.37	-37.98	-	-34.61
$[NiCp^*_2]^0$	-595484.60	-595429.70	-	-	-2.18
$[NiCp^*_2]^+$	-595360.94	-595306.70	-	-	-34.43
$[RuCp^*_2]^0$	-548172.85	-548123.94	-	-	-1.99
$[RuCp^*_2]^+$	-548029.04	-547979.67	-	-	-34.41
$[OsCp^*_2]^0$	-546385.24	-546336.57	-	-	-1.89
$[OsCp^*_2]^+$	-546238.59	-546190.71	-	-	-34.39
$[Fe(bpy)_3]^{2+}$	-1009344.97	-1009290.53	-126.11	-	-
$[Fe(bpy)_3]^{3+}$	-1009072.72	-1009018.70	-275.47	-	-
$[Co(bpy)_3]^{2+}$	-1022921.83	-1022863.31	-123.76	-	-
$[Co(bpy)_3]^{3+}$	-1022652.45	-1022599.13	-276.50	-	-
$[Os(bpy)_3]^{2+}$	-989031.99	-988977.00	-124.82	-	-

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Table 1 – Continued

Complex	G_g (kcal/mol)	H_g (kcal/mol)	ΔG_{solv} (kcal/mol) MeCN	DMSO	DCM
$[Os(bpy)_3]^{3+}$	-988764.86	-988709.56	-272.51	-	-
$[Ir(bpy)_3]^{2+}$	-997570.31	-997514.90	-125.52	-	-
$[Ir(bpy)_3]^{3+}$	-997343.11	-997288.73	-272.91	-	-

Table 2: Calculated changes in free energy ΔG and absolute redox potentials E^{abs} in MeCN, DMSO, and DCM at the L1 [UB3LYP/LACVP/6-31G] level of theory.

Couple	ΔG (kcal/mol) MeCN	DMSO	DCM	E^{abs} (V) MeCN	DMSO	DCM
$[FeCp_2]^{0/+}$	-119.26	-118.98	-123.14	5.172	5.160	5.340
$[Ru(bpy)_3]^{2+/3+}$	-127.32	-	-	5.521	-	-
$[Ru(bpy)_3]^{2+/3+} + 2BF_4^-$	-	-	-128.89	-	-	5.589
$[Ir(acac)_3]^{0/+}$	-124.14	-	-136.61	5.383	-	5.924
$[CoCp_2]^{0/+}$	-90.05	-	-93.84	3.905	-	4.069
$[NiCp_2]^{0/+}$	-107.62	-	-111.53	4.667	-	4.837
$[RuCp_2]^{0/+}$	-	-	-126.03	-	-	5.465
$[OsCp_2]^{0/+}$	-	-	-121.75	-	-	5.280
$[FeCp^*_2]^{0/+}$	-103.71	-103.50	-106.75	4.497	4.488	4.629
$[CoCp^*_2]^{0/+}$	-74.72	-	-77.73	3.240	-	3.371
$[NiCp^*_2]^{0/+}$	-	-	-91.42	-	-	3.964
$[RuCp^*_2]^{0/+}$	-	-	-111.38	-	-	4.830
$[OsCp^*_2]^{0/+}$	-	-	-114.15	-	-	4.950
$[Fe(bpy)_3]^{2+/3+}$	-122.88	-	-	5.328	-	-
$[Co(bpy)_3]^{2+/3+}$	-116.65	-	-	5.058	-	-
$[Os(bpy)_3]^{2+/3+}$	-119.44	-	-	5.180	-	-
$[Ir(bpy)_3]^{2+/3+}$	-79.82	-	-	3.461	-	-

Table 3: Single point calculations used to estimate the redox potential at a higher level of theory UB3LYP/LACVP/cc-pVTZ(-f) based on minimum energy structures obtained at the L1 [UB3LYP/LACVP/6-31G] level. The self-consistent field energies E_{SCF} are given for both levels of theory. The solvation free energies ΔG_{solv} in MeCN, DMSO, and DCM were obtained at the UB3LYP/LACVP/cc-pVTZ(-f) level.

	E_{SCF} (kcal/mol)	E_{SCF} (kcal/mol)	ΔG_{solv} (kcal/mol)		
Complex	LACVP / 6-31G	LACVP / cc-pVTZ(-f)	MeCN	DMSO	DCM
$[FeCp_2]^0$	-320289.90	-320433.87	-4.40	-4.33	-3.74
$[FeCp_2]^+$	-320124.32	-320268.04	-49.57	-49.77	-45.08
$[Ru(bpy)_3]^{2+}$	-991078.86	-991576.12	-125.54	-	-
$[Ru(bpy)_3]^{3+}$	-990803.72	-991294.77	-273.25	-	-
$[Ru(bpy)_3]^{2+} + 2BF_4^-$	-1523959.65	-1524774.16	-	-	-35.89
$[Ru(bpy)_3]^{3+} + 2BF_4^-$	-1523800.57	-1524608.24	-	-	-66.63
$[Ir(acac)_3]^0$	-715438.88	-715833.03	-14.40	-	-11.74
$[Ir(acac)_3]^+$	-715276.20	-715676.62	-42.40	-	-38.09
$[CoCp_2]^0$	-333861.82	-334001.96	-4.48	-	-3.76
$[CoCp_2]^+$	-333730.07	-333871.79	-49.59	-	-45.12
$[NiCp_2]^0$	-349068.97	-349207.10	-4.11	-	-3.50
$[NiCp_2]^+$	-348915.69	-349053.87	-49.01	-	-44.49
$[RuCp_2]^0$	-301758.89	-301906.08	-	-	-3.46
$[RuCp_2]^+$	-301591.86	-301738.12	-	-	-43.56
$[OsCp_2]^0$	-299968.65	-300121.18	-	-	-3.61
$[OsCp_2]^+$	-299804.73	-299956.42	-	-	-43.64
$[FeCp^*_2]^0$	-566953.46	-567232.11	-2.03	-2.05	-1.72
$[FeCp^*_2]^+$	-566812.76	-567089.59	-38.34	-38.58	-34.92
$[CoCp^*_2]^0$	-580523.92	-580799.46	-2.10	-	-1.76
$[CoCp^*_2]^+$	-580419.44	-580694.13	-38.39	-	-34.99
$[NiCp^*_2]^0$	-595727.68	-596001.73	-	-	-1.90
$[NiCp^*_2]^+$	-595605.15	-595875.84	-	-	-34.88
$[RuCp^*_2]^0$	-548421.96	-548703.28	-	-	-1.72
$[RuCp^*_2]^+$	-548277.05	-548555.23	-	-	-34.79
$[OsCp^*_2]^0$	-546634.65	-546921.35	-	-	-1.63
$[OsCp^*_2]^+$	-546488.90	-546771.46	-	-	-34.86
$[Fe(bpy)_3]^{2+}$	-1009616.90	-1010115.66	-126.98	-	-
$[Fe(bpy)_3]^{3+}$	-1009345.73	-1009837.90	-276.12	-	-

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Table 3 – Continued

Complex	E_{SCF} (kcal/mol) LACVP/6-31G	E_{SCF} (kcal/mol) LACVP/cc-pVTZ(-f)	ΔG_{solv} (kcal/mol) MeCN	DMSO	DCM
$[Co(bpy)_3]^{2+}$	-1023188.55	-1023690.74	-124.70	-	-
$[Co(bpy)_3]^{3+}$	-1022926.24	-1023418.49	-277.03	-	-
$[Os(bpy)_3]^{2+}$	-989302.92	-989799.40	-125.83	-	-
$[Os(bpy)_3]^{3+}$	-989036.04	-989527.38	-273.28	-	-
$[Ir(bpy)_3]^{2+}$	-997839.44	-998334.42	-126.77	-	-
$[Ir(bpy)_3]^{3+}$	-997615.73	-998108.82	-273.71	-	-

Table 4: Calculated changes in free energy ΔG and absolute redox potentials E^{abs} in MeCN, DMSO, and DCM at the L2 [UB3LYP/LACVP/6-31G/cc-pVTZ(-f)] level of theory.

Couple	ΔG (kcal/mol) MeCN	DMSO	DCM	E^{abs} (V) MeCN	DMSO	DCM
$[FeCp_2]^{0/+}$	-119.53	-119.26	-123.36	5.183	5.172	5.350
$[Ru(bpy)_3]^{2+/3+}$	-133.79	-	-	5.802	-	-
$[Ru(bpy)_3]^{2+/3+} + 2BF_4^-$	-	-	-136.30	-	-	5.910
$[Ir(acac)_3]^{0/+}$	-127.44	-	-129.09	5.526	-	5.598
$[CoCp_2]^{0/+}$	-88.39	-	-92.14	3.833	-	3.996
$[NiCp_2]^{0/+}$	-107.64	-	-111.55	4.668	-	4.837
$[RuCp_2]^{0/+}$	-	-	-126.87	-	-	5.502
$[OsCp_2]^{0/+}$	-	-	-122.47	-	-	5.311
$[FeCp^*_2]^{0/+}$	-104.92	-104.70	-108.03	4.550	4.540	4.685
$[CoCp^*_2]^{0/+}$	-74.90	-	-77.97	3.248	-	3.381
$[NiCp^*_2]^{0/+}$	-	-	-94.05	-	-	4.078
$[RuCp^*_2]^{0/+}$	-	-	-113.87	-	-	4.938
$[OsCp^*_2]^{0/+}$	-	-	-117.56	-	-	5.098
$[Fe(bpy)_3]^{2+/3+}$	-129.70	-	-	5.624	-	-
$[Co(bpy)_3]^{2+/3+}$	-126.99	-	-	5.507	-	-
$[Os(bpy)_3]^{2+/3+}$	-124.81	-	-	5.412	-	-
$[Ir(bpy)_3]^{2+/3+}$	-82.16	-	-	3.563	-	-

Table 5: Calculated free energies G_g and enthalpies H_g in the gas phase and solvation free energies ΔG_{solv} in MeCN, DMSO, and DCM at the L3 [UB3LYP/LACVP/6-311G*] level of theory.

Complex	G_g (kcal/mol)	H_g (kcal/mol)	ΔG_{solv} (kcal/mol) MeCN	DMSO	DCM
$[FeCp_2]^0$	-320319.41	-320293.29	-4.51	-4.48	-3.87
$[FeCp_2]^+$	-320155.49	-320128.47	-50.02	-50.23	-45.49
$[Ru(bpy)_3]^{2+}$	-991232.13	-991176.29	-125.96	-	-
$[Ru(bpy)_3]^{3+}$	-990950.62	-990894.45	-273.79	-	-
$[Ru(bpy)_3]^{2+} + 2BF_4^-$	-1524368.06	-1524294.42	-	-	-35.01
$[Ru(bpy)_3]^{3+} + 2BF_4^-$	-1524201.83	-1524131.36	-	-	-65.20
$[Ir(acac)_3]^0$	-715593.74	-715540.40	-14.03	-	-11.40
$[Ir(acac)_3]^+$	-715424.90	-715373.22	-53.53	-	-49.15
$[CoCp_2]^0$	-333890.51	-333862.62	-4.66	-	-3.96
$[CoCp_2]^+$	-333756.76	-333730.65	-49.88	-	-45.35
$[NiCp_2]^0$	-349097.93	-349066.83	-4.60	-	-3.83
$[NiCp_2]^+$	-348943.57	-348913.16	-49.46	-	-44.90
$[RuCp_2]^0$	-301790.42	-301763.68	-	-	-3.81
$[RuCp_2]^+$	-301624.61	-301596.89	-	-	-44.13
$[OsCp_2]^0$	-300004.30	-299977.36	-	-	-4.03
$[OsCp_2]^+$	-299838.67	-299812.57	-	-	-44.23
$[FeCp^*_2]^0$	-566927.18	-566879.26	-2.32	-2.33	-1.97
$[FeCp^*_2]^+$	-566785.24	-566734.32	-38.88	-39.06	-35.36
$[CoCp^*_2]^0$	-580498.03	-580446.15	-2.31	-	-1.97
$[CoCp^*_2]^+$	-580388.01	-580339.96	-38.78	-	-35.29
$[NiCp^*_2]^0$	-595703.47	-595648.56	-	-	-2.10
$[NiCp^*_2]^+$	-595575.78	-595523.32	-	-	-35.10
$[RuCp^*_2]^0$	-548397.39	-548348.77	-	-	-1.84
$[RuCp^*_2]^+$	-548248.82	-548199.83	-	-	-35.04
$[OsCp^*_2]^0$	-546613.27	-546564.73	-	-	-1.89
$[OsCp^*_2]^+$	-546463.49	-546416.15	-	-	-35.01
$[Fe(bpy)_3]^{2+}$	-1009771.57	-1009716.38	-127.16	-	-
$[Fe(bpy)_3]^{3+}$	-1009489.58	-1009435.29	-276.83	-	-
$[Co(bpy)_3]^{2+}$	-1023342.35	-1023284.84	-126.57	-	-
$[Co(bpy)_3]^{3+}$	-1023071.99	-1023017.98	-277.50	-	-
$[Os(bpy)_3]^{2+}$	-989454.29	-989398.52	-126.28	-	-

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Table 5 – Continued

Complex	G_g (kcal/mol)	H_g (kcal/mol)	ΔG_{solv} (kcal/mol) MeCN	DMSO	DCM
$[Os(bpy)_3]^{3+}$	-989181.96	-989125.84	-273.96	-	-
$[Ir(bpy)_3]^{2+}$	-997992.41	-997936.22	-127.02	-	-
$[Ir(bpy)_3]^{3+}$	-997761.49	-997706.34	-274.37	-	-

Table 6: Calculated changes in free energy ΔG and absolute redox potentials E^{abs} in MeCN, DMSO, and DCM at the L3 [UB3LYP/LACVP/6-311G*] level of theory.

Couple	ΔG (kcal/mol) MeCN	DMSO	DCM	E^{abs} (V) MeCN	DMSO	DCM
$[FeCp_2]^{0/+}$	-118.41	-118.17	-122.30	5.135	5.124	5.303
$[Ru(bpy)_3]^{2+/3+}$	-133.68	-	-	5.797	-	-
$[Ru(bpy)_3]^{2+/3+} + 2BF_4^-$	-	-	-136.04	-	-	5.899
$[Ir(acac)_3]^{0/+}$	-129.33	-	-131.09	5.608	-	5.685
$[CoCp_2]^{0/+}$	-88.54	-	-92.36	3.839	-	4.005
$[NiCp_2]^{0/+}$	-109.51	-	-113.29	4.749	-	4.913
$[RuCp_2]^{0/+}$	-	-	-125.49	-	-	5.442
$[OsCp_2]^{0/+}$	-	-	-125.42	-	-	5.439
$[FeCp^*_2]^{0/+}$	-105.38	-105.21	-108.55	4.570	4.562	4.707
$[CoCp^*_2]^{0/+}$	-73.55	-	-76.71	3.189	-	3.326
$[NiCp^*_2]^{0/+}$	-	-	-94.70	-	-	4.107
$[RuCp^*_2]^{0/+}$	-	-	-115.37	-	-	5.003
$[OsCp^*_2]^{0/+}$	-	-	-116.65	-	-	5.058
$[Fe(bpy)_3]^{2+/3+}$	-132.33	-	-	5.738	-	-
$[Co(bpy)_3]^{2+/3+}$	-119.44	-	-	5.179	-	-
$[Os(bpy)_3]^{2+/3+}$	-124.66	-	-	5.406	-	-
$[Ir(bpy)_3]^{2+/3+}$	-83.57	-	-	3.624	-	-

Table 7: Single point calculations used to estimate the redox potential at a higher level of theory UB3LYP/LACVP/cc-pVTZ(-f) based on minimum energy structures obtained at the L3 [UB3LYP/LACVP/6-311G*] level. The self-consistent field energies E_{SCF} are given for both levels of theory. The solvation free energies ΔG_{solv} in MeCN, DMSO, and DCM were obtained at the UB3LYP/LACVP/cc-pVTZ(-f) level.

	E_{SCF} (kcal/mol)	E_{SCF} (kcal/mol)	ΔG_{solv} (kcal/mol)		
Complex	LACVP / 6-311G*	LACVP / cc-pVTZ(-f)	MeCN	DMSO	DCM
$[FeCp_2]^0$	-320404.17	-320437.14	-4.28	-4.25	-3.63
$[FeCp_2]^+$	-320238.26	-320272.22	-49.92	-50.10	-45.39
$[Ru(bpy)_3]^{2+}$	-991498.61	-991578.97	-125.46	-	-
$[Ru(bpy)_3]^{3+}$	-991217.14	-991297.64	-273.37	-	-
$[Ru(bpy)_3]^{2+} + 2BF_4^-$	-1524643.25	-1524775.68	-	-	-34.79
$[Ru(bpy)_3]^{3+} + 2BF_4^-$	-1524479.40	-1524611.25	-	-	-64.85
$[Ir(acac)_3]^0$	-715771.31	-715837.45	-13.08	-	-10.58
$[Ir(acac)_3]^+$	-715602.22	-715675.94	-46.84	-	-42.57
$[CoCp_2]^0$	-333972.70	-334003.49	-4.38	-	-3.69
$[CoCp_2]^+$	-333842.59	-333873.92	-49.78	-	-45.25
$[NiCp_2]^0$	-349177.44	-349208.20	-4.06	-	-3.38
$[NiCp_2]^+$	-349024.36	-349053.98	-49.29	-	-44.76
$[RuCp_2]^0$	-301874.42	-301907.79	-	-	-3.39
$[RuCp_2]^+$	-301706.51	-301740.31	-	-	-43.91
$[OsCp_2]^0$	-300088.18	-300123.18	-	-	-3.59
$[OsCp_2]^+$	-299923.09	-299958.92	-	-	-43.94
$[FeCp^*_2]^0$	-567175.13	-567234.59	-1.95	-1.96	-1.62
$[FeCp^*_2]^+$	-567031.56	-567091.63	-38.49	-38.68	-35.02
$[CoCp^*_2]^0$	-580742.41	-580800.97	-2.03	-	-1.69
$[CoCp^*_2]^+$	-580636.82	-580695.89	-38.55	-	-35.10
$[NiCp^*_2]^0$	-595943.86	-596002.47	-	-	-1.73
$[NiCp^*_2]^+$	-595818.57	-595877.35	-	-	-34.93
$[RuCp^*_2]^0$	-548644.21	-548704.75	-	-	-1.55
$[RuCp^*_2]^+$	-548495.57	-548557.48	-	-	-34.81
$[OsCp^*_2]^0$	-546860.24	-546922.65	-	-	-1.54
$[OsCp^*_2]^+$	-546711.44	-546775.04	-	-	-34.82
$[Fe(bpy)_3]^{2+}$	-1010039.18	-1010118.79	-126.57	-	-
$[Fe(bpy)_3]^{3+}$	-1009760.67	-1009840.93	-276.34	-	-

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Table 7 – Continued

Complex	E_{SCF} (kcal/mol) LACVP/6-311G*	E_{SCF} (kcal/mol) LACVP/cc-pVTZ(-f)	ΔG_{solv} (kcal/mol) MeCN	DMSO	DCM
$[Co(bpy)_3]^{2+}$	-1023607.06	-1023687.44	-125.99	-	-
$[Co(bpy)_3]^{3+}$	-1023341.45	-1023421.39	-277.01	-	-
$[Os(bpy)_3]^{2+}$	-989720.79	-989802.06	-125.77	-	-
$[Os(bpy)_3]^{3+}$	-989448.67	-989529.54	-273.59	-	-
$[Ir(bpy)_3]^{2+}$	-998256.82	-998299.59	-163.73	-	-
$[Ir(bpy)_3]^{3+}$	-998029.67	-998111.37	-273.95	-	-

Table 8: Calculated changes in free energy ΔG and absolute redox potentials E^{abs} in MeCN, DMSO, and DCM at the L4 [UB3LYP/LACVP/6-311G*/cc-pVTZ(-f)] level of theory.

Couple	ΔG (kcal/mol) MeCN	DMSO	DCM	E^{abs} (V) MeCN	DMSO	DCM
$[FeCp_2]^{0/+}$	-117.29	-117.08	-121.18	5.086	5.077	5.255
$[Ru(bpy)_3]^{2+/3+}$	-133.46	-	-	5.787	-	-
$[Ru(bpy)_3]^{2+/3+} + 2BF_4^-$	-	-	-136.75	-	-	5.930
$[Ir(acac)_3]^{0/+}$	-127.51	-	-129.29	5.530	-	5.606
$[CoCp_2]^{0/+}$	-87.81	-	-91.66	3.808	-	3.975
$[NiCp_2]^{0/+}$	-110.27	-	-114.12	4.782	-	4.949
$[RuCp_2]^{0/+}$	-	-	-124.86	-	-	5.414
$[OsCp_2]^{0/+}$	-	-	-124.46	-	-	5.397
$[FeCp^*_2]^{0/+}$	-104.78	-104.60	-107.93	4.544	4.536	4.680
$[CoCp^*_2]^{0/+}$	-72.99	-	-76.10	3.165	-	3.300
$[NiCp^*_2]^{0/+}$	-	-	-94.32	-	-	4.090
$[RuCp^*_2]^{0/+}$	-	-	-113.94	-	-	4.941
$[OsCp^*_2]^{0/+}$	-	-	-115.31	-	-	5.000
$[Fe(bpy)_3]^{2+/3+}$	-131.56	-	-	5.705	-	-
$[Co(bpy)_3]^{2+/3+}$	-119.78	-	-	5.194	-	-
$[Os(bpy)_3]^{2+/3+}$	-124.92	-	-	5.417	-	-
$[Ir(bpy)_3]^{2+/3+}$	-81.77	-	-	3.546	-	-

Table 9: Calculated free energies G_g and enthalpies H_g in the gas phase and solvation free energies ΔG_{solv} in MeCN, DMSO, and DCM at the L5 [UB3LYP/LACVP/cc-pVTZ(-f)] level of theory.

Complex	G_g (kcal/mol)	H_g (kcal/mol)	ΔG_{solv} (kcal/mol) MeCN	DMSO	DCM
$[FeCp_2]^0$	-320351.70	-320325.74	-4.18	-4.16	-3.54
$[FeCp_2]^+$	-320188.67	-320161.91	-49.92	-50.08	-45.36
$[Ru(bpy)_3]^{2+}$	-991312.92	-991256.05	-125.87	-	-
$[Ru(bpy)_3]^{3+}$	-991031.25	-990974.41	-273.80	-	-
$[Ru(bpy)_3]^{2+} + 2BF_4^-$	-1524501.90	-1524428.61	-	-	-36.69
$[Ru(bpy)_3]^{3+} + 2BF_4^-$	-1524338.31	-1524263.23	-	-	-68.14
$[Ir(acac)_3]^0$	-715660.85	-715606.71	-12.85	-	-10.07
$[Ir(acac)_3]^+$	-715492.22	-715440.64	-55.12	-	-50.88
$[CoCp_2]^0$	-333921.35	-333893.24	-4.29	-	-3.59
$[CoCp_2]^+$	-333787.44	-333761.53	-49.89	-	-45.37
$[NiCp_2]^0$	-349127.99	-349097.17	-3.98	-	-3.61
$[NiCp_2]^+$	-348972.67	-348943.26	-49.34	-	-44.77
$[RuCp_2]^0$	-301823.21	-301796.63	-	-	-3.22
$[RuCp_2]^+$	-301656.25	-301628.75	-	-	-43.91
$[OsCp_2]^0$	-300039.11	-300012.30	-	-	-3.48
$[OsCp_2]^+$	-299878.72	-299847.58	-	-	-43.95
$[FeCp^*_2]^0$	-566987.71	-566939.30	-1.89	-1.87	-1.59
$[FeCp^*_2]^+$	-566847.22	-566796.32	-38.57	-38.84	-35.09
$[CoCp^*_2]^0$	-580558.43	-580506.43	-1.99	-	-1.67
$[CoCp^*_2]^+$	-580447.97	-580399.54	-38.58	-	-35.11
$[NiCp^*_2]^0$	-595761.33	-595708.02	-	-	-1.70
$[NiCp^*_2]^+$	-595634.36	-595582.72	-	-	-35.00
$[RuCp^*_2]^0$	-548458.70	-548409.75	-	-	-1.53
$[RuCp^*_2]^+$	-548311.65	-548263.89	-	-	-34.83
$[OsCp^*_2]^0$	-546676.18	-546627.56	-	-	-1.50
$[OsCp^*_2]^+$	-546530.38	-546479.89	-	-	-34.84
$[Fe(bpy)_3]^{2+}$	-1009849.75	-1009794.10	-127.51	-	-
$[Fe(bpy)_3]^{3+}$	-1009569.72	-1009514.83	-277.86	-	-
$[Co(bpy)_3]^{2+}$	-1023421.96	-1023363.98	-126.33	-	-
$[Co(bpy)_3]^{3+}$	-1023152.17	-1023097.44	-277.73	-	-
$[Os(bpy)_3]^{2+}$	-989535.44	-989478.59	-126.14	-	-

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Table 9 – Continued

Complex	G_g (kcal/mol)	H_g (kcal/mol)	ΔG_{solv} (kcal/mol) MeCN	DMSO	DCM
$[Os(bpy)_3]^{3+}$	-989263.08	-989206.18	-274.40	-	-
$[Ir(bpy)_3]^{2+}$	-998073.40	-998017.53	-127.06	-	-
$[Ir(bpy)_3]^{3+}$	-997842.95	-997787.09	-274.90	-	-

Table 10: Calculated changes in free energy ΔG and absolute redox potentials E^{abs} in MeCN, DMSO, and DCM at the L5 [UB3LYP/LACVP/cc-pVTZ(-f)] level of theory.

Couple	ΔG (kcal/mol) MeCN	DMSO	DCM	E^{abs} (V) MeCN	DMSO	DCM
$[FeCp_2]^{0/+}$	-117.29	-117.11	-121.21	5.086	5.078	5.256
$[Ru(bpy)_3]^{2+/3+}$	-133.75	-	-	5.800	-	-
$[Ru(bpy)_3]^{2+/3+} + 2BF_4^-$	-	-	-132.15	-	-	5.730
$[Ir(acac)_3]^{0/+}$	-126.37	-	-127.83	5.480	-	5.543
$[CoCp_2]^{0/+}$	-88.30	-	-92.13	3.829	-	3.995
$[NiCp_2]^{0/+}$	-109.95	-	-114.15	4.768	-	4.950
$[RuCp_2]^{0/+}$	-	-	-126.27	-	-	5.476
$[OsCp_2]^{0/+}$	-	-	-119.92	-	-	5.200
$[FeCp^*_2]^{0/+}$	-103.80	-103.52	-106.99	4.501	4.489	4.640
$[CoCp^*_2]^{0/+}$	-73.87	-	-77.02	3.203	-	3.340
$[NiCp^*_2]^{0/+}$	-	-	-93.67	-	-	4.062
$[RuCp^*_2]^{0/+}$	-	-	-113.75	-	-	4.933
$[OsCp^*_2]^{0/+}$	-	-	-112.46	-	-	4.877
$[Fe(bpy)_3]^{2+/3+}$	-129.69	-	-	5.624	-	-
$[Co(bpy)_3]^{2+/3+}$	-118.40	-	-	5.134	-	-
$[Os(bpy)_3]^{2+/3+}$	-124.09	-	-	5.381	-	-
$[Ir(bpy)_3]^{2+/3+}$	-82.61	-	-	3.582	-	-

Table 11: Minimum energy geometries of all the benchmark transition-metal complexes obtained at the L3 (UB3LYP/LACVP/6-311G*) level of theory.

$[FeCp_2]^0$

Atom	x (Å)	y (Å)	z (Å)
Fe	0.0000175681	-0.0005004744	-0.0000067873
C	-1.6911504037	-1.0618451643	0.5860808515
C	-1.6905961831	0.2286447753	1.1914271502
H	-1.6618979423	0.4322603565	2.2522184118
C	-1.6906129551	1.2031568044	0.1511268583
H	-1.6619560711	2.2749653696	0.2851417943
C	-1.6915598384	-0.8849082506	-0.8282776111
H	-1.6639028641	-1.6732601930	-1.5667304381
C	-1.6913006427	0.5148914078	-1.0971260318
H	-1.6631165966	0.9734643513	-2.0751208637
C	1.6919141375	-1.2028515770	-0.1510996560
C	1.6918515553	-0.5145621443	1.0971373898
H	1.6636553636	-0.9731638928	2.0751194383
C	1.6907172718	0.8852349551	0.8282618002
H	1.6613720139	1.6735382180	1.5666957677
C	1.6909088373	-0.2283676377	-1.1914201806
H	1.6618442911	-0.4320564424	-2.2521848414
C	1.6901464514	1.0621367436	-0.5861005576
H	1.6603870118	2.0080543347	-1.1075599874
H	-1.6631331495	-2.0078344451	1.1075131713
H	1.6639013963	-2.2746844736	-0.2850759877

$[FeCp_2]^+$

Atom	x (Å)	y (Å)	z (Å)
Fe	0.0000034693	-0.0000688001	-0.0007172715
C	1.7149542459	0.4889062372	-1.1110286813
C	1.7142467408	1.2083043493	0.1216409494
H	1.6888072273	2.2829528848	0.2296184111
C	1.7132905927	0.2580533874	1.1864608320

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Table 11 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	1.6861846792	0.4871987981	2.2419329898
C	1.7148754349	-0.9058468749	-0.8081455329
H	1.6899898961	-1.7117419922	-1.5272468333
C	1.7137714983	-1.0484797716	0.6118460946
H	1.6871852484	-1.9813068259	1.1562611755
C	-1.7148293492	-0.2579468504	-1.1859693066
C	-1.7144204644	1.0485481810	-0.6113018560
H	-1.6878513102	1.9813696214	-1.1557280118
C	-1.7138052135	0.9058615773	0.8086883091
H	-1.6874444625	1.7117141455	1.5277765827
C	-1.7146018073	-1.2082402965	-0.1212141128
H	-1.6889572163	-2.2828742147	-0.2292936831
C	-1.7136618993	-0.4889196314	1.1115114715
H	-1.6857589634	-0.9237840464	2.1001514900
H	1.6887981515	0.9237103352	-2.0997481296
H	-1.6884679108	-0.4870397470	-2.2414794573

[Ru(bpy)$_3$]$^{2+}$

Atom	x (Å)	y (Å)	z (Å)
Ru	-0.4345490479	-0.0870275959	-0.0236999257
C	1.0657223930	-0.2924155616	2.5359991852
C	-1.1852250484	0.1126831786	2.9778203338
C	1.3456695076	-0.2959508783	3.9035427990
C	-0.9693328267	0.1182433765	4.3480707770
H	-2.1744112483	0.2684534141	2.5682434046
C	0.3227048862	-0.0893644857	4.8198904811
H	2.3549395655	-0.4563927211	4.2578583544
H	-1.7996230252	0.2836081707	5.0234538428
H	0.5326984769	-0.0902343042	5.8829753536
C	0.7735745791	2.7663849227	0.0759224654
C	-1.5531411096	2.6682858172	0.0176537780
C	0.7661762643	4.1524810976	0.1292727565
H	1.7032050360	2.2129064795	0.0733446677

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Table 11 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	-1.6249306791	4.0613016391	0.0718603727
C	-0.4582730971	4.8126927318	0.1285074089
H	1.7025481800	4.6949219417	0.1718154823
H	-2.5831200932	4.5630883715	0.0725811070
H	-0.5063812386	5.8943898459	0.1717834748
C	-3.5176379095	-0.4023618673	-0.1190219962
C	-2.7396271963	1.7921176166	-0.0480491990
C	-4.8406167464	0.0125797316	-0.1612185891
H	-3.2621617583	-1.4536484455	-0.1262248348
C	-4.0502587493	2.2706367318	-0.0906655108
C	-5.1118138098	1.3769090378	-0.1477749109
H	-5.6345998827	-0.7226379881	-0.2049452041
H	-4.2479513550	3.3339993429	-0.0819593576
H	-6.1318361785	1.7411452243	-0.1817818660
C	-0.7901784508	-3.0703457923	0.7427045651
C	-0.7859769653	-2.6196507702	-1.5426645091
C	-0.9499037260	-4.4313478086	0.5273101519
H	-0.7270698881	-2.6677409092	1.7449156174
C	-0.9446833967	-3.9779417697	-1.8227760766
C	-1.0275431760	-4.8940863438	-0.7822446110
H	-1.0099967351	-5.1069229993	1.3716387965
H	-1.0018618236	-4.3255748988	-2.8454199108
H	-1.1501270183	-5.9500963850	-0.9921738983
C	2.5203742716	-0.6247992929	-0.7926866697
C	2.0886991720	-0.5074478415	1.4934087430
C	3.8672827197	-0.8782003458	-0.5786456634
H	2.1169453905	-0.5601925930	-1.7945058994
C	3.4327406674	-0.7613453191	1.7721702320
C	4.3320441364	-0.9490978791	0.7305923440
H	4.5301726491	-1.0173220456	-1.4236894769
H	3.7816213056	-0.8159737521	2.7945262876
H	5.3766476821	-1.1476711424	0.9394561220
C	-0.4127381827	0.6927790956	-3.0244118659

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Table 11 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	-0.6937578545	-1.5773789492	-2.5842505735
C	-0.4937624030	0.4908469400	-4.3944097667
H	-0.2632471944	1.6826442929	-2.6140587749
C	-0.7848047387	-1.8432572858	-3.9516030275
C	-0.6848718188	-0.8035043642	-4.8669327453
H	-0.4095563414	1.3338255367	-5.0690720471
H	-0.9355102195	-2.8538076357	-4.3065683653
H	-0.7557564726	-1.0022806710	-5.9298171690
N	-0.3506443072	2.0311095173	0.0201941034
N	-2.4840019430	0.4555152103	-0.0623146189
N	-0.5078385534	-0.3076813468	-2.1312885408
N	-0.7097922238	-2.1763518063	-0.2582386964
N	1.6430352779	-0.4409947770	0.2093271486
N	-0.2014297022	-0.0879600481	2.0837006102

[Ru(bpy)$_3$]$^{3+}$

Atom	x (Å)	y (Å)	z (Å)
Ru	-0.4359577294	-0.0882030161	-0.0221442875
C	1.0737122059	-0.2695936525	2.5372222797
C	-1.1754016730	0.2214757460	2.9676350043
C	1.3503007262	-0.2465160599	3.9034554756
C	-0.9570239649	0.2497731689	4.3366254894
H	-2.1595578338	0.4003841462	2.5556445460
C	0.3294753252	0.0126077897	4.8121068183
H	2.3534149919	-0.4272031505	4.2657406113
H	-1.7807076392	0.4551578201	5.0090152389
H	0.5386967895	0.0306680827	5.8754035433
C	0.7772792217	2.7516752274	0.1844480794
C	-1.5586602631	2.6675815837	0.0382560245
C	0.7710828163	4.1366391950	0.2520139518
H	1.7048871658	2.1955995209	0.2100670885
C	-1.6229674299	4.0583995037	0.1092595914
C	-0.4514766027	4.8009575052	0.2149132330

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Table 11 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	1.7066802141	4.6758686960	0.3332500806
H	-2.5768007594	4.5680630061	0.0844390942
H	-0.4956351643	5.8825123533	0.2694842970
C	-3.5075140110	-0.4140482188	-0.2205670343
C	-2.7411568785	1.7938624839	-0.0692916304
C	-4.8299299221	-0.0015217496	-0.2817778853
H	-3.2483594353	-1.4639389753	-0.2508811802
C	-4.0521306104	2.2636338374	-0.1341310842
C	-5.1061838905	1.3620030955	-0.2390153176
H	-5.6202483800	-0.7374640814	-0.3625140932
H	-4.2592842486	3.3249445694	-0.1049162075
H	-6.1273889052	1.7217076734	-0.2885570753
C	-0.6833835404	-3.0770920705	0.7465003108
C	-0.7639672091	-2.6224727679	-1.5493375757
C	-0.8261043826	-4.4393959446	0.5304839017
H	-0.5942652863	-2.6771120796	1.7477043264
C	-0.9029696645	-3.9822611350	-1.8237657783
C	-0.9367965472	-4.8993950566	-0.7784861587
H	-0.8480671909	-5.1187498769	1.3735275861
H	-0.9841829569	-4.3331488860	-2.8437915574
H	-1.0461345306	-5.9575380008	-0.9860066587
C	2.4902939600	-0.7334379577	-0.8001722929
C	2.0859795087	-0.5288177802	1.4973538589
C	3.8337396926	-1.0038498998	-0.5884034543
H	2.0795596495	-0.6958922694	-1.8002811947
C	3.4260868230	-0.8022224078	1.7675439263
C	4.3090122582	-1.0399680865	0.7193027114
H	4.4866496949	-1.1825232564	-1.4336912771
H	3.7876386572	-0.8331466591	2.7865968382
H	5.3520549627	-1.2522060272	0.9235250793
C	-0.5167257282	0.7197455402	-3.0088688678
C	-0.7129464430	-1.5754329038	-2.5858243737
C	-0.6091836110	0.5239553668	-4.3784599610

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Table 11 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	-0.3961274993	1.7113733330	-2.5936603567
C	-0.8174764747	-1.8283435483	-3.9528227222
C	-0.7635175345	-0.7735526925	-4.8580540694
H	-0.5618601369	1.3736524975	-5.0481587763
H	-0.9416497709	-2.8388318221	-4.3184173925
H	-0.8431704530	-0.9646137737	-5.9219391571
N	-0.3535633295	2.0296690135	0.0728664285
N	-2.4849615326	0.4547561946	-0.1095892503
N	-0.5591386531	-0.2992077946	-2.1297809552
N	-0.6597123898	-2.1851724200	-0.2616763740
N	1.6343327300	-0.4937475138	0.2109400172
N	-0.1921708277	-0.0382851062	2.0852734966

$[Ru(bpy)_3]^{2+}$ + 2BF_4^-

Atom	x (Å)	y (Å)	z (Å)
Ru	-0.6749235476	-0.6425000169	-0.3904868694
C	1.1451530317	-0.5929840757	1.9425656843
C	-1.0539722528	-0.4942573415	2.6818524063
C	1.6084853146	-0.4673154516	3.2498151206
C	-0.6554312411	-0.3934142015	4.0060093921
H	-2.1017737976	-0.5130749000	2.4121376073
C	0.7018524533	-0.3748606598	4.2936315389
H	2.6664060916	-0.4946610907	3.4596042941
H	-1.4022067940	-0.3486895736	4.7890878568
H	1.0569691444	-0.3228011747	5.3158280527
C	0.1970327746	2.3329028243	-0.2648169885
C	-2.0856502295	1.9459230960	-0.1001708153
C	0.0243364510	3.7014568042	-0.1243967131
H	1.1802617873	1.9059578322	-0.4107226610
C	-2.3227754192	3.3081029820	0.0637240654
C	-1.2604680423	4.1977340414	0.0408604849
H	0.8836919430	4.3581602766	-0.1769606377
H	-3.3315739508	3.6835249061	0.1454218439

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Table 11 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	-1.4466736845	5.2625713872	0.1093244504
C	-3.6808793228	-1.3303375524	-0.1311332093
C	-3.1593498159	0.9389798290	-0.1241049165
C	-5.0392246521	-1.0705695824	-0.0700318191
H	-3.3005625057	-2.3429143337	-0.1515490946
C	-4.5168190467	1.2645979569	-0.1142258638
C	-5.4640950030	0.2560613653	-0.0794712231
H	-5.7427551802	-1.8937424293	-0.0355600854
H	-4.8233232158	2.2988992430	-0.1766972110
H	-6.5207902039	0.4981398279	-0.0720474951
C	-0.6751764672	-3.6470674859	0.3497287637
C	-0.9383196391	-3.1981419106	-1.9199006343
C	-0.6397690411	-5.0187689274	0.1240365656
H	-0.5802640176	-3.2608573380	1.3514142965
C	-0.9270450764	-4.5615327122	-2.2072011311
C	-0.7605680442	-5.4822889916	-1.1772960592
H	-0.4703736405	-5.6778159972	0.9665086715
H	-1.0245406704	-4.9043476708	-3.2290267662
H	-0.7179974272	-6.5433645911	-1.3967830056
C	2.1899795256	-0.7859062625	-1.5410590611
C	2.0384797996	-0.7425170266	0.7814262694
C	3.5690241993	-0.9009833361	-1.4987643225
H	1.6553480386	-0.7439197424	-2.4804955517
C	3.4195437437	-0.9160286901	0.8908112975
C	4.1925426742	-0.9873736232	-0.2562039294
H	4.1324002704	-0.9445260922	-2.4230971110
H	3.8690490419	-1.0564680633	1.8635572912
H	5.2653638923	-1.1245569243	-0.1839210318
C	-1.0196689841	0.1402696366	-3.3651114435
C	-1.0978668243	-2.1474932322	-2.9392773005
C	-1.3303349447	-0.0480317291	-4.7076995925
H	-0.8551751211	1.1326345958	-2.9789532102
C	-1.3950140557	-2.4017538862	-4.2767962422

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Table 11 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	-1.5298447284	-1.3410405916	-5.1677024262
H	-1.4517936887	0.8253636626	-5.3363733764
H	-1.5420858773	-3.4177422186	-4.6193329222
H	-1.7929546557	-1.5291729581	-6.2027821372
N	-0.8247415855	1.4660318894	-0.2542443138
N	-2.7548926580	-0.3553090855	-0.1657067556
N	-0.9375610890	-0.8724423952	-2.4907757685
N	-0.7899276199	-2.7523855419	-0.6422298603
N	1.4335489168	-0.7141455867	-0.4320085568
N	-0.1844440447	-0.5865676959	1.6664003600
B	1.6017962766	-3.7753064538	2.7785932207
F	2.5626031182	-3.1201842431	3.5703911251
F	0.2881352886	-3.2796757474	3.1185706094
F	1.8602493505	-3.4545848071	1.4106683529
F	1.6117130149	-5.1544163024	2.9376143046
B	-2.5957922626	3.0535188870	-3.2173769029
F	-1.1986884256	3.0431433278	-2.8495147773
F	-3.2432411862	4.0976196600	-2.5427080941
F	-2.6826568513	3.1517123304	-4.6035098446
F	-3.1782714678	1.8176793061	-2.7987073732

$[Ru(bpy)_3]^{3+}$ + 2BF_4^-

Atom	x (Å)	y (Å)	z (Å)
Ru	-0.6201252103	-0.4876627839	-0.2647834941
C	1.1100951485	-0.5026718559	2.1500192133
C	-1.1144819987	-0.2260293285	2.7956344942
C	1.5160714184	-0.4841814905	3.4835930792
C	-0.7694792148	-0.1973435969	4.1369584894
H	-2.1453327724	-0.1362800645	2.4790261715
C	0.5713232751	-0.3309120535	4.4846369298
H	2.5530537811	-0.6461301613	3.7389313418
H	-1.5416229427	-0.0841792850	4.8875433848
H	0.8754835935	-0.3361008353	5.5245226292

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Table 11 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	0.4274895182	2.4397537608	-0.1838053582
C	-1.8895954571	2.1908610353	-0.0687132165
C	0.3271406790	3.8208728170	-0.1442993047
H	1.3889707166	1.9481760005	-0.2539814410
C	-2.0524304990	3.5749967885	-0.0337198968
C	-0.9377736978	4.3965217863	-0.0715249672
H	1.2243390459	4.4257896888	-0.1835841996
H	-3.0426246319	4.0066307955	-0.0352601987
H	-1.0559552831	5.4735372795	-0.0642741000
C	-3.6594030571	-0.9906602742	-0.2641830210
C	-3.0142836902	1.2443314096	-0.0630471486
C	-5.0020808585	-0.6520907524	-0.2381968888
H	-3.3447677893	-2.0196372043	-0.3607947542
C	-4.3468535713	1.6393087216	-0.0150123120
C	-5.3501963099	0.6867201822	-0.1154624271
H	-5.7506043359	-1.4289073961	-0.3291747493
H	-4.6070639355	2.6845359502	0.0352215383
H	-6.3878859491	0.9968707671	-0.1238996137
C	-0.9119942242	-3.4348162750	0.5587840163
C	-0.9891197682	-3.0257601078	-1.7423847667
C	-1.0362296899	-4.8045732505	0.3664759493
H	-0.7741687249	-3.0383315492	1.5510885313
C	-1.1037185224	-4.3885994257	-1.9925495120
C	-1.1214950553	-5.2872628688	-0.9294037244
H	-0.9876386288	-5.4599952630	1.2259069533
H	-1.1658292730	-4.7536740856	-3.0087176778
H	-1.1852501490	-6.3521172579	-1.1198207326
C	2.2370011801	-1.0363862849	-1.2756432956
C	2.0368373695	-0.7001045623	1.0262956707
C	3.6006450468	-1.2544077716	-1.1704337702
H	1.7359324446	-1.0843401977	-2.2315333856
C	3.4050131622	-0.8901508901	1.1872577098
C	4.1928623571	-1.1829435732	0.0836304223

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Table 11 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	4.1737346516	-1.4906689878	-2.0579593289
H	3.8480963078	-0.8787227513	2.1702873331
H	5.2499993341	-1.3790428466	0.2140995987
C	-0.7015266974	0.2853636790	-3.2373169799
C	-0.9693903384	-1.9936789385	-2.7885106944
C	-0.8569068033	0.0826140103	-4.6021795115
H	-0.5871613524	1.2839493325	-2.8498620427
C	-1.1464521327	-2.2512414021	-4.1432285635
C	-1.0962667480	-1.2033806964	-5.0583752045
H	-0.8646550024	0.9408526837	-5.2608288499
H	-1.3352900798	-3.2591692442	-4.4870368446
H	-1.2591455429	-1.3949963109	-6.1123867860
N	-0.6517051441	1.6409019801	-0.1507753138
N	-2.6850464990	-0.0719805049	-0.1677369736
N	-0.7601659866	-0.7197064056	-2.3529274183
N	-0.8841047365	-2.5681611336	-0.4630730870
N	1.4703127025	-0.7547733036	-0.2100568425
N	-0.2008759774	-0.3781042260	1.8229556809
B	1.9225790118	-3.8759837299	1.9171205786
F	0.8856013953	-3.2221028065	2.6922142049
F	1.7835872293	-5.2396774299	2.0535601368
F	1.7354038201	-3.5139610981	0.5332186090
F	3.1632607359	-3.3780760759	2.3420059804
B	-3.3143950291	2.0931462468	-3.2476755157
F	-2.0609912097	2.6839288466	-2.8223669342
F	-3.2958689828	0.6998038153	-2.8756314203
F	-4.3533601646	2.7256795876	-2.5478420495
F	-3.4115418497	2.1977441217	-4.6177862778

[Ir(acac)$_3$]^0

Atom	x (Å)	y (Å)	z (Å)
Ir	-1.6418909081	-2.6272029149	-0.2791770567
O	-0.5642379483	-4.0477614487	-1.2914444910

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Table 11 – Continued

Atom	x (Å)	y (Å)	z (Å)
O	-2.5055066126	-1.8959502221	-1.9887792009
O	-2.7443886990	-1.2774723862	0.8011900305
O	-0.0813825640	-1.3224538754	-0.5370767537
O	-0.7621169826	-3.2643570298	1.4595787220
O	-3.1939897276	-3.9574792099	-0.1184565739
C	-0.0834610331	-0.1393977696	-0.0625935397
C	-1.1080661404	0.4675635282	0.6792066448
C	-2.3341883235	-0.0988286703	1.0593793897
H	-0.9318503519	1.4872721680	0.9958704979
C	-3.3028464645	-4.7789390138	0.8497022132
C	-1.2468726054	-4.1993757185	2.1775581466
C	-2.4219276781	-4.9256540484	1.9318926415
H	-2.6781407030	-5.6843355265	2.6598119160
C	-0.6205040382	-4.1860783956	-2.5573312143
C	-2.2640586645	-2.3750285884	-3.1446700974
C	-1.3974053491	-3.4348535808	-3.4519904622
H	-1.3173778779	-3.7014753137	-4.4977366112
C	-3.0156107306	-1.6855526070	-4.2588993859
H	-2.7275023046	-0.6312554159	-4.2947347029
H	-2.8287804389	-2.1373105724	-5.2329389912
H	-4.0873447345	-1.7174617913	-4.0475987512
C	0.2634998688	-5.2893626634	-3.0889456973
H	-0.0133060340	-6.2369427570	-2.6192038983
H	0.1968900498	-5.3953769945	-4.1716064028
H	1.3015799637	-5.0863905097	-2.8126667797
C	1.1754930360	0.6392682738	-0.3627361890
H	1.3249741936	0.6887877466	-1.4445320560
H	1.1488643736	1.6515141213	0.0404170343
H	2.0362842629	0.1106389536	0.0554419813
C	-3.3126267973	0.7240408702	1.8638917751
H	-3.4998977213	0.2327966194	2.8227067234
H	-2.9565948741	1.7375687509	2.0479193220
H	-4.2683486021	0.7697587325	1.3356583904

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Table 11 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	-0.4264226438	-4.5110017800	3.4068125954
H	-0.3418342241	-3.6137816545	4.0260519306
H	-0.8543434691	-5.3164172328	4.0036576647
H	0.5871042526	-4.7883676428	3.1050782947
C	-4.5283809875	-5.6580681834	0.7675444335
H	-4.5118031555	-6.2205469801	-0.1697037555
H	-4.6002906026	-6.3565096787	1.6011171229
H	-5.4235041097	-5.0308288840	0.7484877286

[Ir(acac)$_3$]$^+$

Atom	x (Å)	y (Å)	z (Å)
Ir	-1.6512683105	-2.6036923167	-0.1819741503
O	-0.6516180558	-4.0509889301	-1.1689091642
O	-2.4383857882	-1.8294566264	-1.8690216730
O	-2.6355671692	-1.1609413267	0.8719578946
O	-0.0623799811	-1.3994653274	-0.3827739122
O	-0.8904764745	-3.3438050993	1.5595733755
O	-3.2350894985	-3.8217489816	-0.0277755408
C	-0.1027042025	-0.1106380513	-0.2729770396
C	-1.1769106295	0.6163860506	0.2351714441
C	-2.3428916861	0.0783191287	0.8259383353
H	-1.0588768207	1.6901899966	0.2912084555
C	-3.2563126920	-4.9073220063	0.6757982600
C	-1.2159187477	-4.4711555751	2.0559141436
C	-2.2972551688	-5.2687951488	1.6188080967
H	-2.4606637259	-6.1947479313	2.1531391377
C	-0.6681005226	-4.1900105035	-2.4458501656
C	-2.2362392575	-2.3136074896	-3.0419315795
C	-1.4082024735	-3.4057570477	-3.3437845723
H	-1.3293639561	-3.6714660406	-4.3889403468
C	-2.9758568167	-1.5953831033	-4.1343719424
H	-2.6843178380	-0.5414392413	-4.1429576744
H	-2.7874095888	-2.0263075748	-5.1164774358

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Table 11 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	-4.0487679311	-1.6281371183	-3.9269955484
C	0.2033917863	-5.3043501107	-2.9501078332
H	-0.0390758455	-6.2302399658	-2.4236735805
H	0.0989317329	-5.4603300763	-4.0224345803
H	1.2485960130	-5.0734002387	-2.7252067651
C	1.1635283842	0.5730291161	-0.6990723834
H	1.4131488912	0.2821659047	-1.7225625018
H	1.0868181233	1.6576066551	-0.6407159060
H	1.9878413092	0.2394124288	-0.0625346976
C	-3.3050515118	0.9853254000	1.5372513097
H	-3.0415134894	1.0275351073	2.5994294913
H	-3.2696692542	2.0006323338	1.1424718480
H	-4.3182127312	0.5914195331	1.4623164889
C	-0.4051018410	-4.9001978816	3.2445762975
H	-0.8311744648	-4.4561600166	4.1504759229
H	-0.4113648665	-5.9830537178	3.3677448137
H	0.6195565837	-4.5420503432	3.1500091804
C	-4.4664898199	-5.7614115716	0.4343123791
H	-4.5389110623	-6.0058416260	-0.6288031199
H	-4.4448766873	-6.6821310562	1.0152981470
H	-5.3666444763	-5.1968503357	0.6936217844

[CoCp$_2$]^0

Atom	x (Å)	y (Å)	z (Å)
Co	-0.0000018437	-0.0003144572	0.0000183167
C	-1.8195443386	-1.0617489906	0.5967546669
C	-1.7763505597	0.2165244825	1.1888933980
H	-1.7626184590	0.4298018481	2.2484742456
C	-1.7893852730	1.2050572783	0.1355188394
H	-1.7770037757	2.2761342386	0.2796485552
C	-1.7495017894	-0.8742239452	-0.8179035309
H	-1.7355409812	-1.6621874986	-1.5580973690
C	-1.8196369919	0.5304491250	-1.0973633293

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Table 11 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	-1.8029148401	0.9838826838	-2.0777584246
C	1.7900074610	-1.2049186606	-0.1354798915
C	1.8200574137	-0.5303007720	1.0973657245
H	1.8034741933	-0.9836756187	2.0777999115
C	1.7487711401	0.8743540793	0.8178364027
H	1.7344873758	1.6623548469	1.5580278171
C	1.7764519031	-0.2164119374	-1.1888852726
H	1.7630767802	-0.4297681552	-2.2484402745
C	1.8192731718	1.0618864182	-0.5968433424
H	1.7978727611	2.0095461633	-1.1148949002
H	-1.7989456176	-2.0094204366	1.1147962429
H	1.7784978470	-2.2759887358	-0.2796219756

[CoCp$_2$]$^+$

Atom	x (Å)	y (Å)	z (Å)
Co	-0.0000325329	-0.0000527241	-0.0005452439
C	1.6871128465	0.4884444975	-1.1101651624
C	1.6862100116	1.2069302354	0.1214292064
H	1.6615372169	2.2815364780	0.2295072086
C	1.6857404409	0.2576697351	1.1853702363
H	1.6604701459	0.4869960262	2.2407558460
C	1.6867609819	-0.9048740915	-0.8073523444
H	1.6627402404	-1.7108032124	-1.5263510612
C	1.6860832606	-1.0475044293	0.6113529026
H	1.6611622103	-1.9803663120	1.1556028648
C	-1.6869125363	-0.2575776660	-1.1850512380
C	-1.6865359952	1.0475749879	-0.6109621178
H	-1.6626598097	1.9804738292	-1.1551948381
C	-1.6857647769	0.9048716916	0.8077455699
H	-1.6613193380	1.7107701783	1.5267565080
C	-1.6863569880	-1.2068993455	-0.1211502631
H	-1.6623885779	-2.2815095156	-0.2293262529
C	-1.6859515836	-0.4884697253	1.1104862129

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Table 11 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	-1.6614074030	-0.9233343943	2.0990803822
H	1.6630960969	0.9232464717	-2.0988091272
H	-1.6633780577	-0.4868645699	-2.2404875939

[NiCp$_2$]^0

Atom	x (Å)	y (Å)	z (Å)
Ni	-0.0000082011	-0.0004134488	-0.0000007809
C	-1.8907574579	-1.0598806600	0.5850212214
C	-1.8906412890	0.2280770916	1.1891382529
H	-1.8865878317	0.4319518833	2.2507030060
C	-1.8909649562	1.2006150834	0.1508914807
H	-1.8871522226	2.2732281531	0.2850350414
C	-1.8912207910	-0.8833335236	-0.8265772415
H	-1.8876806764	-1.6722633824	-1.5655653457
C	-1.8913431444	0.5137458504	-1.0949053331
H	-1.8878613696	0.9728185975	-2.0735808341
C	1.8916214481	-1.2005755752	-0.1508927913
C	1.8916850116	-0.5137065882	1.0948899217
H	1.8873190605	-0.9727508752	2.0735660212
C	1.8908927287	0.8833624459	0.8265776043
H	1.8857207091	1.6722874961	1.5655882920
C	1.8908384055	-0.2280454404	-1.1891369386
H	1.8857554747	-0.4319101147	-2.2507149270
C	1.8903507878	1.0599145771	-0.5850223123
H	1.8847347941	2.0065550687	-1.1069642443
H	-1.8868269841	-2.0064987576	1.1069570043
H	1.8872522601	-2.2731862320	-0.2850259655

[NiCp$_2$]$^+$

Atom	x (Å)	y (Å)	z (Å)
Ni	-0.0001396838	-0.0001272800	-0.0006823542
C	1.7772364796	0.4730066207	-1.1157568315

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Table 11 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	1.7835466788	1.2074017243	0.1415724416
H	1.7860097461	2.2837274408	0.2369438923
C	1.8100587101	0.2765455698	1.1912102252
H	1.8101680568	0.4976598072	2.2483085573
C	1.8106462612	-0.9016515477	-0.8226147516
H	1.8096098286	-1.7119420071	-1.5365000792
C	1.7490296413	-1.0352623172	0.6040343458
H	1.7400385170	-1.9684293190	1.1496507017
C	-1.8112425899	-0.2763674019	-1.1904660156
C	-1.7495172491	1.0354385178	-0.6032800564
H	-1.7405506987	1.9686658062	-1.1488867081
C	-1.8096586699	0.9018090504	0.8234882973
H	-1.8064350614	1.7121020841	1.5374051303
C	-1.7837199032	-1.2073134958	-0.1408351735
H	-1.7858790892	-2.2837182029	-0.2361795610
C	-1.7760452120	-0.4729083748	1.1165636758
H	-1.7754584076	-0.9191850453	2.1008238260
H	1.7783958413	0.9192102056	-2.0999585264
H	-1.8115958945	-0.4974111501	-2.2476012578

[RuCp$_2$]^0

Atom	x (Å)	y (Å)	z (Å)
Ru	0.0000703629	-0.0003233228	-0.0000071416
C	-1.8735924340	-1.0649513677	0.5877477407
C	-1.8734474410	0.2290982822	1.1947202916
H	-1.8806301370	0.4328098683	2.2554968153
C	-1.8737707225	1.2062488985	0.1515886736
H	-1.8811601421	2.2780558038	0.2856453062
C	-1.8740983812	-0.8875497495	-0.8305382976
H	-1.8820756190	-1.6758517650	-1.5689998386
C	-1.8741734538	0.5161250204	-1.1000793925
H	-1.8820430728	0.9747960037	-2.0780201571
C	1.8740542302	-1.2062435837	-0.1515692628

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Table 11 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	1.8741299925	-0.5160801616	1.1000988654
H	1.8845861273	-0.9747309059	2.0780323441
C	1.8733757224	0.8876130074	0.8305374980
H	1.8832665786	1.6759262957	1.5689736433
C	1.8733563018	-0.2291025427	-1.1947235936
H	1.8830699426	-0.4328226865	-2.2554851674
C	1.8729050988	1.0649646611	-0.5877683908
H	1.8821870514	2.0108628353	-1.1093053185
H	-1.8808415651	-2.0108733572	1.1092752189
H	1.8842606995	-2.2780430200	-0.2856096037

[RuCp$_2$]$^+$

Atom	x (Å)	y (Å)	z (Å)
Ru	0.0000151268	-0.0001121699	-0.0010900824
C	1.9082284678	0.4896016477	-1.1121260625
C	1.9074436210	1.2097585135	0.1222021628
H	1.9018569150	2.2847633148	0.2302636128
C	1.9066687338	0.2583254047	1.1884931478
H	1.9004358108	0.4877149511	2.2442849986
C	1.9080615103	-0.9068878597	-0.8087159038
H	1.9032877385	-1.7130857973	-1.5280283608
C	1.9070963606	-1.0498336747	0.6131676069
H	1.9013984246	-1.9830885784	1.1575680861
C	-1.9082747166	-0.2581740554	-1.1874205191
C	-1.9076633880	1.0499644367	-0.6120569473
H	-1.9048465206	1.9832563388	-1.1564472548
C	-1.9065060692	0.9069935820	0.8098356161
H	-1.9029087538	1.7131800963	1.5291816717
C	-1.9076801341	-1.2096378633	-0.1211737702
H	-1.9046742562	-2.2846630526	-0.2292815643
C	-1.9065472094	-0.4895298478	1.1131883327
H	-1.9026343303	-0.9245078896	2.1022179881
H	1.9029648258	0.9245396359	-2.1011620521

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Table 11 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	-1.9055681444	-0.4875728385	-2.2432517617

[OsCp$_2$]^0

Atom	x (Å)	y (Å)	z (Å)
Os	0.0000490037	-0.0004350797	0.0000066619
C	-1.8608317422	-1.0682315321	0.5894778726
C	-1.8603304147	0.2297367184	1.1982950266
H	-1.8721031529	0.4333001867	2.2586201575
C	-1.8605554879	1.2098769279	0.1519613140
H	-1.8725345829	2.2812180989	0.2858935566
C	-1.8612108199	-0.8903317842	-0.8331081118
H	-1.8739633894	-1.6783344404	-1.5712039701
C	-1.8610094759	0.5176195566	-1.1035315038
H	-1.8736051440	0.9760620851	-2.0810500743
C	1.8613256035	-1.2098811934	-0.1520041685
C	1.8613697789	-0.5176441353	1.1035077413
H	1.8749484368	-0.9760779907	2.0810200170
C	1.8606577383	0.8903183190	0.8331094673
H	1.8735362973	1.6783255480	1.5712054153
C	1.8603421008	-0.2297388009	-1.1983428113
H	1.8727989135	-0.4332729361	-2.2586697473
C	1.8598874088	1.0682485849	-0.5894984693
H	1.8719198385	2.0137835661	-1.1107621750
H	-1.8734541930	-2.0137394942	1.1107599668
H	1.8747930483	-2.2812027058	-0.2859540310

[OsCp$_2$]$^+$

Atom	x (Å)	y (Å)	z (Å)
Os	-0.0000123003	-0.0001599533	-0.0013118993
C	1.8861083284	0.4912280644	-1.1157895205
C	1.8847888762	1.2137295671	0.1226309195
H	1.8869872745	2.2884106459	0.2304323620

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Table 11 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	1.8836470024	0.2592247518	1.1925706727
H	1.8849289514	0.4884725472	2.2480295991
C	1.8858572463	-0.9098351981	-0.8113536593
H	1.8891978414	-1.7157194130	-1.5304597091
C	1.8843383408	-1.0532480063	0.6152906306
H	1.8863728412	-1.9861627435	1.1595662333
C	-1.8861766070	-0.2589450522	-1.1913149736
C	-1.8853751252	1.0534463764	-0.6139979532
H	-1.8885253108	1.9863838430	-1.1582238049
C	-1.8838564072	0.9099801855	0.8126451955
H	-1.8857673627	1.7158454888	1.5317604007
C	-1.8852485692	-1.2135369902	-0.1214843514
H	-1.8882194077	-2.2881974431	-0.2294054842
C	-1.8837204555	-0.4911481667	1.1170430248
H	-1.8855673631	-0.9260215492	2.1056803164
H	1.8895312165	0.9260532415	-2.1044588750
H	-1.8899231069	-0.4881026971	-2.2467866754

[FeCp*$_2$]^0

Atom	x (Å)	y (Å)	z (Å)
Fe	-0.0003450413	-0.0000604799	0.0005600756
C	1.6970922795	1.0385146547	-0.6230913479
C	1.7018968992	0.8981098834	0.8030880535
C	1.6923190170	-0.5016727329	1.1102858922
C	1.6816343204	-1.2263489889	-0.1260623695
C	1.6844215082	-0.2744260700	-1.1973452356
C	-1.6920833784	0.5588278970	-1.0832178804
C	-1.6820172270	1.2186328871	0.1889178968
C	-1.6861077223	0.2126364367	1.2095848352
C	-1.6985856183	-1.0688808400	0.5682344036
C	-1.7022419665	-0.8549033728	-0.8488052317
C	-1.7629477128	0.4577819496	2.6876948729
C	-1.7543933159	2.7003849030	0.4126759215

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Table 11 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	-1.7993090041	-1.9206097012	-1.9003305335
C	-1.7771202536	1.2299787668	-2.4223282400
C	1.7789216922	-1.1022820552	2.4823848858
C	1.7995223909	2.0172860453	1.7974419379
C	1.7607695061	-0.5957255798	-2.6608417747
C	1.7885279672	2.3297530577	-1.3814730306
C	-1.7907263968	-2.3979614658	1.2580931027
C	1.7541773349	-2.7176853759	-0.2728267614
H	1.2696629993	-3.0629317106	-1.1888301240
H	2.7955639816	-3.0604866788	-0.3113041919
H	1.2776431108	-3.2346858381	0.5628109080
H	1.2823749163	0.1713208203	-3.2739037383
H	2.8030437820	-0.6701098192	-2.9949258336
H	1.2803469027	-1.5477746978	-2.8962947668
H	1.3048936989	2.2654987707	-2.3585401727
H	1.3221628458	3.1561149755	-0.8405070907
H	2.8341555390	2.6107903046	-1.5580533652
H	1.3283999046	2.9320141959	1.4313919330
H	1.3241033151	1.7634078815	2.7474659803
H	2.8465489283	2.2603373545	2.0168669677
H	1.3113697120	-0.4667420372	3.2374723281
H	1.2936897991	-2.0795378609	2.5329117553
H	2.8234904603	-1.2461615972	2.7851742427
H	-1.2724147781	3.2599940123	-0.3920409318
H	-2.7957898252	3.0417434531	0.4623925524
H	-1.2753106805	2.9967390474	1.3482380198
H	-1.3063786901	0.6358578384	-3.2087422250
H	-2.8213501947	1.3867985378	-2.7197497332
H	-1.2942761834	2.2095387633	-2.4204506347
H	-1.2783901845	1.3941502859	2.9730384895
H	-2.8053212254	0.5198536663	3.0240184422
H	-1.2889257641	-0.3422743491	3.2603099871
H	-1.3237514380	-3.1946844637	0.6751417560

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Table 11 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	-1.3080139384	-2.3849556243	2.2378113554
H	-2.8364848864	-2.6877975355	1.4189689096
H	-1.3235132097	-1.6172810581	-2.8353609392
H	-1.3283288756	-2.8534313107	-1.5824764305
H	-2.8462167677	-2.1520554044	-2.1324982253

[FeCp*$_2$]$^+$

Atom	x (Å)	y (Å)	z (Å)
Fe	-0.0006363316	0.0002940940	-0.0006917407
C	1.7238500637	1.0474500599	-0.6145515666
C	1.7283082182	0.8916825665	0.8138662519
C	1.7183562969	-0.5147456350	1.1071732378
C	1.7077974842	-1.2283016179	-0.1398633616
C	1.7110604682	-0.2627299314	-1.2039772565
C	-1.7193268185	0.5492052917	-1.0925253297
C	-1.7090945616	1.2244574230	0.1756744438
C	-1.7129138118	0.2268910801	1.2097773875
C	-1.7258655589	-1.0646969882	0.5806764757
C	-1.7298758874	-0.8654815284	-0.8422823665
C	-1.7890416706	0.4875990697	2.6824602841
C	-1.7815472458	2.7056884906	0.3832388978
C	-1.8287773665	-1.9407473716	-1.8797418155
C	-1.8036401922	1.2052036959	-2.4361576979
C	1.8036605200	-1.1288173699	2.4704102240
C	1.8273099022	1.9982039340	1.8179904146
C	1.7871036484	-0.5692122106	-2.6678773635
C	1.8162741091	2.3445314166	-1.3572671218
C	-1.8185731632	-2.3836838676	1.2837151992
C	1.7809615697	-2.7151796575	-0.3021290439
H	1.3079768783	-3.0540831336	-1.2247564573
H	2.8274546429	-3.0363034003	-0.3413083033
H	1.3149501010	-3.2451059744	0.5295561287
H	1.3284457799	0.2101826820	-3.2777467722

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Table 11 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	2.8340731792	-0.6466108721	-2.9803916860
H	1.3082890666	-1.5170725499	-2.9168799699
H	1.3490592955	2.2914426878	-2.3414194157
H	1.3557466990	3.1679660748	-0.8098397735
H	2.8668250865	2.6117565898	-1.5146694479
H	1.3672917136	2.9211017102	1.4625656344
H	1.3637513401	1.7354812484	2.7697698053
H	2.8792686451	2.2227797822	2.0246149001
H	1.3454481467	-0.5012491152	3.2358094726
H	1.3302621917	-2.1106266381	2.5119454469
H	2.8527281570	-1.2663768573	2.7539546907
H	-1.3145637002	3.2607255577	-0.4313452691
H	-2.8279929533	3.0260249588	0.4307124527
H	-1.3100395954	3.0158203674	1.3165606879
H	-1.3489173034	0.5997269299	-3.2211777758
H	-2.8525417120	1.3552902972	-2.7141216649
H	-1.3269583331	2.1861372229	-2.4478375180
H	-1.3156392545	1.4300987877	2.9604026998
H	-2.8362211483	0.5495113556	2.9979731307
H	-1.3259754059	-0.3079192723	3.2675342938
H	-1.3619643607	-3.1909289705	0.7097540942
H	-1.3485840494	-2.3617213906	2.2677489672
H	-2.8692590008	-2.6533439703	1.4363489536
H	-1.3657502108	-1.6489285005	-2.8231426720
H	-1.3691075631	-2.8742817532	-1.5527499636
H	-2.8808653805	-2.1589428564	-2.0929014405

[CoCp*$_2$]^0

Atom	x (Å)	y (Å)	z (Å)
Co	-0.0002687538	0.0001492159	-0.0008814275
C	1.7523589993	1.0231558929	-0.6167767359
C	1.8193069953	0.8918628876	0.8093645220
C	1.7639407472	-0.4953390512	1.1043983274

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Table 11 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	1.7793725243	-1.2317310163	-0.1493096339
C	1.8031152982	-0.2966388916	-1.2051140195
C	-1.7609141729	0.5510840670	-1.0772206521
C	-1.7839715774	1.2247098076	0.2106621988
C	-1.8020087850	0.2376499672	1.2171201947
C	-1.7540406720	-1.0528755876	0.5634263778
C	-1.8197729246	-0.8508471436	-0.8524107731
C	-1.8792958141	0.4597302514	2.6988558499
C	-1.8534583852	2.7108333945	0.4050389227
C	-1.9195109534	-1.9231668124	-1.8971593059
C	-1.8363428786	1.2399398580	-2.4083909204
C	1.8408082129	-1.1179147475	2.4677988257
C	1.9183397927	2.0163618683	1.7977269124
C	1.8815569377	-0.5952554430	-2.6732833027
C	1.8325120168	2.3127984446	-1.3805501925
C	-1.8348466319	-2.3778120410	1.2641594459
C	1.8466204287	-2.7257378179	-0.2701518517
H	1.4634228885	-3.0751684046	-1.2313229067
H	2.8789641459	-3.0866707237	-0.1841609457
H	1.2696586457	-3.2257726227	0.5113354631
H	1.3214389067	0.1297859354	-3.2688974928
H	2.9175557298	-0.5701344510	-3.0334954091
H	1.4840774362	-1.5845905699	-2.9104315517
H	1.3282217334	2.2479827662	-2.3472684305
H	1.3822610442	3.1423717178	-0.8307928368
H	2.8752853335	2.5884374607	-1.5807868342
H	1.4049873097	2.9151825253	1.4477652340
H	1.4819486459	1.7511434574	2.7635836077
H	2.9625230050	2.2971802519	1.9842094904
H	1.4408416939	-0.4583800494	3.2409512108
H	1.2860415806	-2.0576504812	2.5208105173
H	2.8785338400	-1.3443840262	2.7422662622
H	-1.2680893459	3.2494159334	-0.3441594028

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Table 11 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	-2.8848030036	3.0761757084	0.3255116919
H	-1.4809306390	3.0119543402	1.3864639879
H	-1.4284099177	0.6222834296	-3.2115140666
H	-2.8746337660	1.4720628501	-2.6758527441
H	-1.2881061475	2.1847677280	-2.4120192882
H	-1.4985703432	1.4427594376	2.9846149952
H	-2.9132755969	0.3976767812	3.0603183991
H	-1.3039019060	-0.2844742164	3.2548911501
H	-1.3944225006	-3.1818172394	0.6704681536
H	-1.3214321628	-2.3630281736	2.2283703936
H	-2.8772840782	-2.6571767386	1.4610518894
H	-1.4756758718	-1.6121693139	-2.8457312572
H	-1.4136697334	-2.8418898730	-1.5902310489
H	-2.9641923726	-2.1877101979	-2.1036406366

$[CoCp^*_2]^+$

Atom	x (Å)	y (Å)	z (Å)
Co	-0.0055850997	0.0004381309	-0.0003677958
C	1.6911292256	1.0465947255	-0.6137203418
C	1.6957003297	0.8913065082	0.8130783282
C	1.6855696339	-0.5136596518	1.1063388103
C	1.6748116414	-1.2267045219	-0.1391965617
C	1.6781228507	-0.2623846235	-1.2022475618
C	-1.6964112740	0.5488291358	-1.0910609059
C	-1.6857324657	1.2230515623	0.1759170975
C	-1.6895908126	0.2264177741	1.2087164125
C	-1.7026073232	-1.0637592262	0.5799959871
C	-1.7069274334	-0.8644716578	-0.8413080252
C	-1.7699571861	0.4868814820	2.6807677723
C	-1.7611615926	2.7037420409	0.3838055767
C	-1.8085580501	-1.9388713468	-1.8789822941
C	-1.7851479384	1.2042738583	-2.4341876974
C	1.7748000584	-1.1269873238	2.4691353570

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Table 11 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	1.7973122867	1.9974626188	1.8168329209
C	1.7580204091	-0.5684611474	-2.6655402058
C	1.7871177257	2.3426301596	-1.3568441509
C	-1.7987437098	-2.3823568733	1.2824036226
C	1.7505302685	-2.7130929079	-0.3011457962
H	1.2801217984	-3.0529490464	-1.2245725836
H	2.7977884339	-3.0319146478	-0.3390298034
H	1.2854053666	-3.2438105310	0.5303557932
H	1.2972280020	0.2087233738	-3.2764081195
H	2.8061775750	-0.6400743074	-2.9755414849
H	1.2858094731	-1.5192088231	-2.9154160013
H	1.3183007573	2.2910961073	-2.3401551226
H	1.3325344089	3.1685029436	-0.8083988131
H	2.8386496807	2.6045958124	-1.5165811831
H	1.3402802050	2.9216475841	1.4613796833
H	1.3343780924	1.7357778693	2.7690472911
H	2.8500190522	2.2192481722	2.0228436681
H	1.3189574731	-0.4994018412	3.2357478962
H	1.3033288952	-2.1095179795	2.5122377163
H	2.8249451830	-1.2631612864	2.7493362183
H	-1.2953954941	3.2599441203	-0.4306145960
H	-2.8083315797	3.0215091480	0.4309706400
H	-1.2909320023	3.0145664046	1.3174282593
H	-1.3302679157	0.6001439030	-3.2201000957
H	-2.8351269577	1.3504870364	-2.7097706612
H	-1.3120962884	2.1868439966	-2.4468572850
H	-1.2971498594	1.4291180208	2.9603631921
H	-2.8181899271	0.5494995316	2.9923468361
H	-1.3096977603	-0.3091571869	3.2671659823
H	-1.3446379489	-3.1906798191	0.7081360733
H	-1.3291553431	-2.3618461517	2.2665776621
H	-2.8502486083	-2.6487507400	1.4346089016
H	-1.3442416976	-1.6481846266	-2.8220151202

Continued on Next Page...

Table 11 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	-1.3525527799	-2.8740987371	-1.5519698057
H	-2.8612456340	-2.1532404561	-2.0927010660

[NiCp*$_2$]^0

Atom	x (Å)	y (Å)	z (Å)
Ni	-0.0004134775	0.0001050893	-0.0000175834
C	1.8841291199	1.0756300096	-0.5463166235
C	1.8880178255	0.8331344403	0.8640556294
C	1.8760178242	-0.5831186635	1.0694827030
C	1.8646946026	-1.2160308051	-0.2140201923
C	1.8694166555	-0.1908712966	-1.2125202166
C	-1.8780626318	0.4818113973	-1.1171631543
C	-1.8657066875	1.2302778308	0.1025370731
C	-1.8697307409	0.3017070992	1.1914111902
C	-1.8841521707	-1.0208001010	0.6447460086
C	-1.8893070584	-0.9094205425	-0.7820310802
C	-1.9415326325	0.6537291309	2.6489878232
C	-1.9318539369	2.7254111633	0.2198153726
C	-1.9851546068	-2.0485758704	-1.7549934047
C	-1.9598375922	1.0548576857	-2.5023010728
C	1.9577544095	-1.2812599508	2.3959712977
C	1.9848418367	1.8782711164	1.9373310695
C	1.9430712829	-0.4069107644	-2.6962261463
C	1.9754274911	2.4191146584	-1.2098981262
C	-1.9731150807	-2.2976781500	1.4291435523
C	1.9327965796	-2.6938704551	-0.4687241531
H	1.4400450764	-2.9722432241	-1.4034619244
H	2.9712192504	-3.0409871797	-0.5400820893
H	1.4600486161	-3.2698421946	0.3305888171
H	1.4663391779	0.4034163919	-3.2530793805
H	2.9828122559	-0.4627396706	-3.0421906859
H	1.4574969512	-1.3376960871	-2.9995755957
H	1.4968303781	2.4244460485	-2.1922762015

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Table 11 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	1.5019276332	3.2037871916	-0.6148232140
H	3.0192477262	2.7208903901	-1.3625308051
H	1.5202429796	2.8201368626	1.6353316053
H	1.5007128957	1.5609257244	2.8641227347
H	3.0298807933	2.1035240746	2.1844394852
H	1.4900114626	-0.7001224094	3.1945375993
H	1.4678430305	-2.2577723479	2.3765785984
H	2.9993253388	-1.4529157907	2.6952746854
H	-1.4492013928	3.2248410515	-0.6237397437
H	-2.9697444350	3.0800655978	0.2488799661
H	-1.4475743171	3.0869507482	1.1302716995
H	-1.4806762679	0.4093158054	-3.2424042662
H	-3.0014610787	1.1866224229	-2.8210254485
H	-1.4812433145	2.0349484338	-2.5693096056
H	-1.4465117577	1.6032924219	2.8665554180
H	-2.9807372883	0.7511150300	2.9873414535
H	-1.4731695055	-0.1072365560	3.2780447607
H	-1.5095778356	-3.1353740637	0.9023068078
H	-1.4831236716	-2.2163050609	2.4024345151
H	-3.0162645345	-2.5794270597	1.6198622342
H	-1.5099803236	-1.8125811679	-2.7103613773
H	-1.5108357768	-2.9557160683	-1.3727758925
H	-3.0299981010	-2.3027318206	-1.9732277612

[NiCp*$_2$]$^+$

Atom	x (Å)	y (Å)	z (Å)
Ni	0.0011090767	0.0096170164	-0.0117155824
C	1.8004360296	1.0868515975	-0.5936405272
C	1.8142601872	0.9176271398	0.8045234675
C	1.7571234158	-0.5120267451	1.0759477658
C	1.7974757553	-1.2167341010	-0.1734795093
C	1.7614901629	-0.2420655702	-1.2083678680
C	-1.7576610253	0.5388706425	-1.0936714983

Continued on Next Page...

Table 11 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	-1.7957083046	1.2373959061	0.1589420584
C	-1.7591455852	0.2575465884	1.1889532684
C	-1.8014384631	-1.0682038440	0.5680455192
C	-1.8160739359	-0.8921839811	-0.8290357658
C	-1.8412819524	0.5131463418	2.6601742812
C	-1.8764654669	2.7225894101	0.3389027585
C	-1.9287202454	-1.9590766794	-1.8736040684
C	-1.8485596370	1.1656197811	-2.4482459150
C	1.8463506576	-1.1322642991	2.4335359813
C	1.9248808851	1.9902712347	1.8433315295
C	1.8448423468	-0.5051274181	-2.6782802136
C	1.9096631341	2.3753904823	-1.3468594138
C	-1.9100893539	-2.3598272343	1.3160087298
C	1.8789522152	-2.7027038539	-0.3463621641
H	1.4350063679	-3.0327545770	-1.2866703885
H	2.9234920075	-3.0320283766	-0.3525004052
H	1.3808603993	-3.2396475187	0.4625334643
H	1.3265212497	0.2547275401	-3.2653659217
H	2.8921649545	-0.4953125856	-3.0012574805
H	1.4370047936	-1.4801240476	-2.9475954707
H	1.3458186397	2.3581762880	-2.2811939341
H	1.5625278915	3.2265632722	-0.7600982598
H	2.9545480393	2.5722018929	-1.6113577334
H	1.5588720478	2.9520533844	1.4820215780
H	1.3739852204	1.7432689102	2.7525946842
H	2.9709948408	2.1334199612	2.1350789480
H	1.3632096254	-0.5247573322	3.2001796210
H	1.4088805448	-2.1309555411	2.4628871104
H	2.8976271493	-1.2354389022	2.7263211069
H	-1.3764749540	3.2631196748	-0.4664515492
H	-2.9208246168	3.0525191343	0.3444813792
H	-1.4342433455	3.0478040112	1.2816838399
H	-1.3669265710	0.5614066432	-3.2184743321

Continued on Next Page...

Table 11 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	-2.9002115111	1.2708747824	-2.7390284184
H	-1.4103777110	2.1641208807	-2.4734647549
H	-1.4350616654	1.4875542070	2.9339793507
H	-2.8883028599	0.4996664074	2.9840431829
H	-1.3210442171	-0.2487212035	3.2429195731
H	-1.5721101042	-3.2096772738	0.7221128912
H	-1.3378733746	-2.3497084884	2.2453919574
H	-2.9534297159	-2.5531892327	1.5890324910
H	-1.3740835250	-1.7099349094	-2.7800286727
H	-1.5680795061	-2.9242977123	-1.5161822674
H	-2.9746055097	-2.0960014680	-2.1690984347

[RuCp*$_2$]^0

Atom	x (Å)	y (Å)	z (Å)
Ru	-0.0003055712	0.0001090220	0.0002028145
C	1.8741086044	1.0401388242	-0.6271843298
C	1.8789565472	0.9010118576	0.8039387511
C	1.8694280817	-0.5029999454	1.1139471085
C	1.8587484688	-1.2316453473	-0.1255980736
C	1.8615678204	-0.2779359076	-1.2016755446
C	-1.8691950194	0.5631178069	-1.0853501939
C	-1.8587254254	1.2234967849	0.1918833428
C	-1.8623448660	0.2128343177	1.2146764951
C	-1.8750905110	-1.0721506801	0.5695591766
C	-1.8793129431	-0.8556304693	-0.8519211018
C	-1.9639113744	0.4559499119	2.6918212232
C	-1.9558599379	2.7036637760	0.4177289380
C	-2.0009062910	-1.9188955398	-1.9036916015
C	-1.9787586263	1.2356435658	-2.4222143862
C	1.9790700485	-1.1015027312	2.4855663537
C	2.0002052203	2.0202337737	1.7960081327
C	1.9622204682	-0.6014922271	-2.6633856791
C	1.9898519853	2.3291317559	-1.3865176659

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Table 11 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	-1.9915769256	-2.4007340524	1.2571908873
C	1.9555780542	-2.7219616360	-0.2702362241
H	1.4745809997	-3.0723691375	-1.1860189777
H	3.0018521140	-3.0509847493	-0.3063541784
H	1.4818916788	-3.2415465046	0.5654411600
H	1.4907965191	0.1655396859	-3.2816593507
H	3.0093455919	-0.6779154466	-2.9826963070
H	1.4812096192	-1.5525439287	-2.9017271688
H	1.5089376946	2.2673596328	-2.3650862270
H	1.5272823638	3.1593731592	-0.8484410785
H	3.0401810849	2.5974954503	-1.5569448138
H	1.5320190313	2.9371121593	1.4315501729
H	1.5280767327	1.7702785777	2.7485945884
H	3.0517586462	2.2535298919	2.0058999001
H	1.5149347904	-0.4662302873	3.2429973718
H	1.4959977491	-2.0794681064	2.5407813414
H	3.0280659747	-1.2403764406	2.7763724904
H	-1.4795300075	3.2684824788	-0.3865900361
H	-3.0022481364	3.0303692786	0.4686636533
H	-1.4777357713	3.0029237904	1.3528820486
H	-1.5143871958	0.6429638869	-3.2133558066
H	-3.0277958576	1.3898353484	-2.7050788085
H	-1.4960748515	2.2152887828	-2.4236218177
H	-1.4813799839	1.3915484309	2.9827125694
H	-3.0112373836	0.5166738072	3.0138074634
H	-1.4945861900	-0.3448408293	3.2673060602
H	-1.5286772042	-3.2002716894	0.6748180160
H	-1.5114089644	-2.3928425105	2.2381028320
H	-3.0420715696	-2.6778420853	1.4118634715
H	-1.5277975131	-1.6177443753	-2.8407993862
H	-1.5340580350	-2.8549506978	-1.5895883031
H	-3.0525580921	-2.1392048757	-2.1267366261

Continued on Next Page...

Table 11 – Continued

Atom	x (Å)	y (Å)	z (Å)

[RuCp*$_2$]$^+$

Atom	x (Å)	y (Å)	z (Å)
Ru	-0.0006382270	0.0002584016	-0.0007468636
C	1.9171731248	1.0468112843	-0.6167346439
C	1.9217463453	0.8917584217	0.8135854420
C	1.9116995589	-0.5164311837	1.1081544749
C	1.9008886862	-1.2317097918	-0.1400734975
C	1.9042391664	-0.2655634339	-1.2061226298
C	-1.9126294361	0.5523907792	-1.0927528303
C	-1.9018472074	1.2277297176	0.1775759380
C	-1.9055618641	0.2282009295	1.2123964281
C	-1.9187096089	-1.0648131364	0.5815864280
C	-1.9231187599	-0.8644205671	-0.8430636201
C	-1.9919545464	0.4880804897	2.6860538829
C	-1.9839201310	2.7097325378	0.3861792688
C	-2.0307705894	-1.9394447852	-1.8821192449
C	-2.0074748433	1.2092655298	-2.4367761861
C	2.0062887711	-1.1299182086	2.4725484630
C	2.0291018708	1.9995382202	1.8176419408
C	1.9902513995	-0.5728813377	-2.6706617982
C	2.0186039114	2.3439965545	-1.3609524428
C	-2.0206288006	-2.3850960858	1.2839343656
C	1.9828124188	-2.7196026340	-0.3012397182
H	1.5104872668	-3.0600153875	-1.2237143045
H	3.0306431238	-3.0367685133	-0.3387700589
H	1.5160568646	-3.2494793418	0.5301950337
H	1.5306019709	0.2049920766	-3.2818915673
H	3.0389225692	-0.6478629986	-2.9782599741
H	1.5132652370	-1.5215780424	-2.9204325486
H	1.5472292413	2.2924473584	-2.3433221291
H	1.5624174202	3.1694624351	-0.8127931320
H	3.0704611229	2.6047781378	-1.5207529221
H	1.5690499194	2.9226164420	1.4623887066

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Table 11 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	1.5652553458	1.7381714724	2.7697325283
H	3.0822393883	2.2213890540	2.0216917421
H	1.5495356855	-0.5017442873	3.2385034055
H	1.5314384517	-2.1110334909	2.5162033654
H	3.0567263086	-1.2668730456	2.7514467120
H	-1.5171120089	3.2661037718	-0.4277852171
H	-3.0318079102	3.0253540049	0.4337396283
H	-1.5117758250	3.0204594972	1.3191485648
H	-1.5532481698	0.6047807123	-3.2230335901
H	-3.0579533935	1.3575071703	-2.7096804922
H	-1.5303671938	2.1901603511	-2.4497537769
H	-1.5174183288	1.4294937811	2.9662305575
H	-3.0407410941	0.5502050501	2.9960980508
H	-1.5301118422	-0.3079071261	3.2717673173
H	-1.5654904205	-3.1928303073	0.7091742200
H	-1.5484726404	-2.3655353314	2.2671178432
H	-3.0725747143	-2.6500771511	1.4360350791
H	-1.5656323116	-1.6483495103	-2.8248963179
H	-1.5722198933	-2.8740283252	-1.5561863001
H	-3.0839678782	-2.1533273388	-2.0942138208

[OsCp*$_2$]^0

Atom	x (Å)	y (Å)	z (Å)
Os	-0.0000372947	0.0003102176	-0.0001432358
C	1.8699128086	1.0902672414	-0.5373563508
C	1.8732189409	0.8297938207	0.8807570425
C	1.8608822964	-0.5992861977	1.0713728504
C	1.8499165583	-1.2221046018	-0.2289691471
C	1.8556865660	-0.1778870198	-1.2231927398
C	-1.8631822360	0.4716906162	-1.1314273454
C	-1.8509892009	1.2397564531	0.0886998565
C	-1.8547406963	0.3168614708	1.1963297558
C	-1.8680769414	-1.0217958647	0.6608859959

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Table 11 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	-1.8736530178	-0.9260703257	-0.7778361819
C	-1.9725435385	0.6854767382	2.6457094592
C	-1.9657947445	2.7321792939	0.1878226977
C	-2.0164765825	-2.0736056415	-1.7335628232
C	-1.9929822121	1.0280375204	-2.5185594258
C	1.9886439740	-1.3123460559	2.3850775855
C	2.0159103210	1.8588301646	1.9630684640
C	1.9747826597	-0.3759614653	-2.7054623230
C	2.0079556010	2.4373037585	-1.1832092681
C	-2.0046477394	-2.2850285650	1.4585568797
C	1.9633499368	-2.6931962419	-0.4999982249
H	1.4882825755	-2.9674604307	-1.4440468474
H	3.0139094338	-3.0044380721	-0.5592948022
H	1.4915679345	-3.2863857095	0.2860412583
H	1.5112752092	0.4421164283	-3.2604949618
H	3.0264817806	-0.4269560631	-3.0143274412
H	1.4947875065	-1.3017570810	-3.0291902573
H	1.5337341152	2.4644880558	-2.1664233519
H	1.5501144860	3.2234021008	-0.5794024881
H	3.0635939531	2.7031610071	-1.3212860359
H	1.5555300797	2.8080618195	1.6814295653
H	1.5472939684	1.5334886333	2.8940262330
H	3.0725852262	2.0592807388	2.1807737607
H	1.5327452903	-0.7448609370	3.1989543904
H	1.5065447623	-2.2917212642	2.3613751383
H	3.0421673477	-1.4720046170	2.6472563883
H	-1.4957754078	3.2305444189	-0.6623740259
H	-3.0166774352	3.0470643692	0.2120648849
H	-1.4900747148	3.1147858360	1.0931221723
H	-1.5375399061	0.3702984557	-3.2616052800
H	-3.0469206407	1.1557623676	-2.7961306794
H	-1.5115440425	2.0039282444	-2.6091546132
H	-1.4909354652	1.6417719407	2.8594000926

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Table 11 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	-3.0239633621	0.7735545123	2.9471481148
H	-1.5099685327	-0.0633140722	3.2919223153
H	-1.5481404192	-3.1360646186	0.9490178388
H	-1.5283940332	-2.1980063168	2.4371983624
H	-3.0600006809	-2.5329006583	1.6286258470
H	-1.5503378510	-1.8574803354	-2.6970557818
H	-1.5535412266	-2.9828276257	-1.3447855227
H	-3.0731754373	-2.2997384215	-1.9243346861

[OsCp*$_2$]$^+$

Atom	x (Å)	y (Å)	z (Å)
Os	0.0001285141	0.0100951154	-0.0158184702
C	1.8988291107	1.0704495145	-0.6117733545
C	1.8974715547	0.8955314964	0.8211372433
C	1.8872990222	-0.5216190605	1.0973396274
C	1.8823550299	-1.2221810351	-0.1648607124
C	1.8895637724	-0.2381994143	-1.2206780307
C	-1.8954944361	0.5482222572	-1.1126921619
C	-1.8800554097	1.2429672977	0.1524464359
C	-1.8797229976	0.2539601488	1.2039870165
C	-1.8946043879	-1.0519290462	0.5884963048
C	-1.9045199782	-0.8697538678	-0.8433577876
C	-1.9826774085	0.5345271418	2.6736434644
C	-1.9833224666	2.7270389136	0.3416816044
C	-2.0360085661	-1.9581978612	-1.8668684451
C	-2.0139802006	1.1873716617	-2.4643348692
C	1.9997205990	-1.1540870845	2.4526134005
C	2.0235400269	1.9885208192	1.8403626708
C	2.0005985608	-0.5258400973	-2.6884718806
C	2.0234754931	2.3765929778	-1.3383773504
C	-2.0160840749	-2.3616919667	1.3090386126
C	1.9873496696	-2.7070535707	-0.3471109278
H	1.5211905577	-3.0398114235	-1.2752258038

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Table 11 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	3.0399980433	-3.0060969403	-0.3860294184
H	1.5248143540	-3.2545037727	0.4749252382
H	1.5484806323	0.2593575901	-3.2955137824
H	3.0545043243	-0.5946364307	-2.9775785736
H	1.5281211299	-1.4711772944	-2.9578154620
H	1.5565328686	2.3436411204	-2.3234584953
H	1.5736712454	3.1996753829	-0.7819562507
H	3.0800288567	2.6228204832	-1.4869732580
H	1.5711523065	2.9205843933	1.4997635106
H	1.5602007191	1.7186220400	2.7900506455
H	3.0804501458	2.1934024180	2.0402554709
H	1.5453032926	-0.5396828061	3.2307101750
H	1.5303029660	-2.1379592766	2.4857680607
H	3.0539402385	-1.2872470117	2.7170138275
H	-1.5234358856	3.2777008937	-0.4797135653
H	-3.0356143141	3.0266229511	0.3855871745
H	-1.5135895981	3.0553902036	1.2695253473
H	-1.5667590961	0.5749265632	-3.2481351738
H	-3.0693431170	1.3256211946	-2.7215282577
H	-1.5411069137	2.1696402420	-2.4961070537
H	-1.5082789134	1.4783659096	2.9448017514
H	-3.0349041791	0.6023686195	2.9689021467
H	-1.5276178890	-0.2539279373	3.2741924670
H	-1.5712598172	-3.1822747555	0.7449983722
H	-1.5424176174	-2.3346607464	2.2910613012
H	-3.0719130831	-2.6074009336	1.4634280582
H	-1.5820430872	-1.6821869185	-2.8193114173
H	-1.5775268719	-2.8904941089	-1.5350996475
H	-3.0939853184	-2.1656810067	-2.0583773133

[Fe(bpy)$_3$]$^{2+}$

Atom	x (Å)	y (Å)	z (Å)
Fe	-0.4346472826	-0.0893718802	-0.0209414836

Continued on Next Page...

Table 11 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	0.9941471879	-0.2793075168	2.4635427884
C	-1.2561236670	0.1058565867	2.8814416280
C	1.2716911727	-0.2611849163	3.8309294240
C	-1.0505265349	0.1320061343	4.2542976208
H	-2.2458969129	0.2432661749	2.4679948693
C	0.2398063216	-0.0534815116	4.7379488890
H	2.2815445662	-0.4034699853	4.1914943289
H	-1.8871869967	0.2960433999	4.9218187017
H	0.4422628724	-0.0366647325	5.8023483174
C	0.8271562804	2.6556905947	0.0630055385
C	-1.4920379903	2.5821364050	0.0178432596
C	0.8342134050	4.0430084434	0.1245361591
H	1.7540236789	2.0984359431	0.0489911538
C	-1.5574643871	3.9742615463	0.0822083282
C	-0.3832168298	4.7149421814	0.1363884106
H	1.7758705191	4.5764894681	0.1634432656
H	-2.5120301183	4.4826556613	0.0938705592
H	-0.4203709554	5.7967780155	0.1872760030
C	-3.4315625034	-0.4882287264	-0.1002924571
C	-2.6781481043	1.7065544414	-0.0488382886
C	-4.7593075155	-0.0861350451	-0.1591305791
H	-3.1717128890	-1.5381645128	-0.0901702863
C	-3.9893808184	2.1789476689	-0.1102951304
C	-5.0429293664	1.2750596525	-0.1661545003
H	-5.5463497723	-0.8288060090	-0.1997526621
H	-4.1938849412	3.2409398149	-0.1186088605
H	-6.0658202265	1.6293005561	-0.2147842005
C	-0.7918978475	-2.9733736037	0.8107791064
C	-0.7746516875	-2.5461483644	-1.4707635765
C	-0.9399401342	-4.3387755423	0.6069325159
H	-0.7422989593	-2.5657718265	1.8113242394
C	-0.9184522201	-3.9063162954	-1.7465137871
C	-1.0021923720	-4.8141254200	-0.6981708553

Continued on Next Page...

Table 11 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	-1.0027261514	-5.0069835435	1.4566721145
H	-0.9620486436	-4.2611800950	-2.7672818858
H	-1.1137477797	-5.8729894341	-0.8991085577
C	2.4238313257	-0.5977098027	-0.8619530756
C	2.0159413252	-0.4968190428	1.4207423172
C	3.7717169097	-0.8647763552	-0.6622640671
H	2.0177424398	-0.5196408050	-1.8613263357
C	3.3577793254	-0.7657527805	1.6926372893
C	4.2470199511	-0.9523239835	0.6414787517
H	4.4262987190	-1.0012379437	-1.5140098478
H	3.7116072866	-0.8344561725	2.7124898089
H	5.2914187515	-1.1627485590	0.8392836964
C	-0.3882369204	0.7629448729	-2.9222227003
C	-0.6837003468	-1.5020320357	-2.5103358689
C	-0.4798589698	0.5785740606	-4.2952935448
H	-0.2254495273	1.7478834161	-2.5063755952
C	-0.7884149958	-1.7573162591	-3.8780322135
C	-0.6859844115	-0.7073394685	-4.7820806177
H	-0.3921011619	1.4284792573	-4.9604661858
H	-0.9524174886	-2.7628317114	-4.2411635155
H	-0.7665450716	-0.8922851235	-5.8466932120
N	-0.3015014917	1.9314318800	0.0097344932
N	-2.4065544424	0.3769592900	-0.0451108004
N	-0.4853247134	-0.2443817463	-2.0404200340
N	-0.7106943618	-2.0878214263	-0.1949795723
N	1.5568560757	-0.4152060778	0.1463771265
N	-0.2666516700	-0.0949142090	1.9970144154

[Fe(bpy)$_3$]$^{3+}$

Atom	x (Å)	y (Å)	z (Å)
Fe	-0.4362524564	-0.0884789202	-0.0215315556
C	0.9878239060	-0.2635813981	2.4497495338
C	-1.2708240996	0.1778641369	2.8479110326

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Table 11 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	1.2528379466	-0.2352652593	3.8173556744
C	-1.0687186266	0.2123736224	4.2205053509
H	-2.2554761407	0.3310675649	2.4298082365
C	0.2159092655	0.0048963991	4.7136450459
H	2.2566648180	-0.3961165477	4.1878867503
H	-1.9056898989	0.3996309471	4.8817641089
H	0.4108920432	0.0292952282	5.7796467961
C	0.8467784933	2.6190779211	0.1310004211
C	-1.4861320021	2.5684981668	0.0305202520
C	0.8590815534	4.0048665935	0.2015103090
H	1.7695471630	2.0569099891	0.1333713027
C	-1.5371549109	3.9592154453	0.1039808309
C	-0.3538739051	4.6867440816	0.1903758288
H	1.8035472559	4.5308588503	0.2645057557
H	-2.4871660400	4.4774558211	0.0965011478
H	-0.3819181985	5.7688384058	0.2482454912
C	-3.4016335292	-0.5186072042	-0.1681855645
C	-2.6673251237	1.6961188900	-0.0632207850
C	-4.7299237990	-0.1227241498	-0.2343789854
H	-3.1358183342	-1.5659137853	-0.1740699271
C	-3.9817442186	2.1538936932	-0.1322668407
C	-5.0251582139	1.2370652605	-0.2186147754
H	-5.5103964806	-0.8707632358	-0.2975501419
H	-4.1976831708	3.2142641455	-0.1213043277
H	-6.0513481070	1.5821263348	-0.2728529657
C	-0.7217578012	-2.9495712966	0.8360234075
C	-0.7581958091	-2.5353657822	-1.4622002104
C	-0.8598546320	-4.3160323378	0.6378291513
H	-0.6569233611	-2.5393223036	1.8335374606
C	-0.8923447968	-3.8975742439	-1.7236704465
C	-0.9440765827	-4.7988139165	-0.6645538541
H	-0.8989274892	-4.9810082270	1.4916005386
H	-0.9547589192	-4.2602388298	-2.7413418582

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Table 11 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	-1.0483408057	-5.8605687460	-0.8564320465
C	2.3784467936	-0.6603783098	-0.8886501612
C	2.0005527719	-0.5074782821	1.4110816023
C	3.7250015317	-0.9345370871	-0.6949295849
H	1.9645998372	-0.5981811056	-1.8849017100
C	3.3417952953	-0.7840828284	1.6679419669
C	4.2146596260	-1.0001757276	0.6060085990
H	4.3691042707	-1.0930887298	-1.5509831101
H	3.7096011867	-0.8348308578	2.6843157372
H	5.2599778971	-1.2166323607	0.7943465642
C	-0.4492447200	0.7979341366	-2.8874937787
C	-0.6933776497	-1.4918937735	-2.4974769431
C	-0.5445558273	0.6203146585	-4.2604546213
H	-0.3040955534	1.7822606530	-2.4659800609
C	-0.8005277808	-1.7316579352	-3.8660241235
C	-0.7257332571	-0.6664106258	-4.7583441598
H	-0.4778181064	1.4777883841	-4.9185041695
H	-0.9432969703	-2.7369345165	-4.2402853477
H	-0.8081855854	-0.8414487996	-5.8249194244
N	-0.2940071767	1.9120657446	0.0437864803
N	-2.3902043113	0.3637772771	-0.0808708923
N	-0.5176695775	-0.2289878678	-2.0215185499
N	-0.6747563575	-2.0744355026	-0.1843155016
N	1.5319950790	-0.4473356488	0.1348167508
N	-0.2720298897	-0.0574534925	1.9782255291

[Co(bpy)$_3$]$^{2+}$

Atom	x (Å)	y (Å)	z (Å)
Co	-0.4356057688	-0.0973419972	-0.0319921780
C	1.1258019729	-0.2923264269	2.4308670714
C	-1.1270872660	0.1092529978	2.8531340754
C	1.3992646242	-0.2441198522	3.7998953799
C	-0.9221153390	0.1574169800	4.2246184880

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Table 11 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	-2.1139720417	0.2418419651	2.4314579052
C	0.3704444585	-0.0191208764	4.7058452668
H	2.4104952001	-0.3701441672	4.1619920083
H	-1.7577467743	0.3336532883	4.8904619156
H	0.5778043255	0.0198696952	5.7690159622
C	0.6965329814	2.6512620603	0.0768522277
C	-1.6285578542	2.5716892079	0.0227841801
C	0.7059118241	4.0359108376	0.1668181914
H	1.6187766995	2.0870096564	0.0545753733
C	-1.6864823696	3.9638450615	0.1223219051
C	-0.5131735743	4.7041293129	0.1942603589
H	1.6475229824	4.5682846407	0.2183974161
H	-2.6403055836	4.4724782916	0.1548403475
H	-0.5531295440	5.7844111447	0.2731851582
C	-3.6745522538	-0.4376691929	-0.0572856000
C	-2.8438414715	1.7223067568	-0.0664380391
C	-4.9857205299	0.0027965707	-0.2017017249
H	-3.4493370307	-1.4965206251	0.0119385893
C	-4.1310313232	2.2431537123	-0.2219581018
C	-5.2132725735	1.3720048395	-0.2883275363
H	-5.8000148871	-0.7100066177	-0.2469033075
H	-4.3001237973	3.3087592603	-0.3011996774
H	-6.2182186956	1.7601891421	-0.4082563089
C	-0.7554862370	-2.9677182289	0.8181598161
C	-0.7697260095	-2.5434333724	-1.4656409773
C	-0.9292157216	-4.3311428333	0.6178118217
H	-0.6805425576	-2.5606788136	1.8169615707
C	-0.9422512714	-3.9004614885	-1.7372341726
C	-1.0219563074	-4.8058049522	-0.6855704179
H	-0.9887441086	-4.9976875685	1.4692427922
H	-1.0158714401	-4.2547605484	-2.7566853851
H	-1.1558654705	-5.8629499709	-0.8833706855
C	2.6777903406	-0.5895863436	-0.8476805937

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Table 11 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	2.1765329949	-0.5402807621	1.4109413549
C	3.9987963763	-0.9512863410	-0.6069060750
H	2.3165226063	-0.4503036741	-1.8609967470
C	3.4838388743	-0.9119267433	1.7347029640
C	4.4045804364	-1.1177212115	0.7127678995
H	4.6841843504	-1.0992497377	-1.4324768926
H	3.7894689379	-1.0527099287	2.7629271458
H	5.4228518649	-1.4061667617	0.9471419759
C	-0.4200426615	0.7715476873	-2.9113876289
C	-0.6812670279	-1.5007252613	-2.5052421783
C	-0.4824429031	0.5851659963	-4.2863298631
H	-0.2852395937	1.7591202611	-2.4927905136
C	-0.7535199396	-1.7576339323	-3.8741650748
C	-0.6546063096	-0.7045389161	-4.7759625187
H	-0.3977476897	1.4367825865	-4.9498952378
H	-0.8851514234	-2.7668559611	-4.2407229704
H	-0.7099620334	-0.8909227275	-5.8421782590
N	-0.4332634080	1.9292187560	0.0058438044
N	-2.6294412449	0.3932940033	0.0101903365
N	-0.5174946326	-0.2386585144	-2.0345578281
N	-0.6748133729	-2.0879347331	-0.1908784530
N	1.7876142761	-0.3872563414	0.1290383320
N	-0.1382642714	-0.1099897992	1.9716549697

[Co(bpy)$_3$]$^{3+}$

Atom	x (Å)	y (Å)	z (Å)
Co	-0.4368692158	-0.0902784456	-0.0228238802
C	0.9592605497	-0.2674679180	2.4259447355
C	-1.3069947668	0.1310518008	2.8216573083
C	1.2204870184	-0.2477983648	3.7946092728
C	-1.1079651671	0.1589865383	4.1957553419
H	-2.2937925668	0.2697357821	2.4048821123
C	0.1781484173	-0.0313487320	4.6908057540

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Table 11 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	2.2259380746	-0.3969373408	4.1657725608
H	-1.9501620329	0.3275901595	4.8556764020
H	0.3699526770	-0.0129087456	5.7576052462
C	0.8726789843	2.5871800661	0.0817081391
C	-1.4612329422	2.5405622042	0.0259603027
C	0.8878694473	3.9740390925	0.1501491099
H	1.7954673196	2.0259265196	0.0662479323
C	-1.5087977810	3.9314329859	0.0956457597
C	-0.3236141501	4.6579356279	0.1598037632
H	1.8349138699	4.4977700203	0.1948783649
H	-2.4581757954	4.4506069181	0.1028990651
H	-0.3487786772	5.7402700418	0.2155617647
C	-3.3811882227	-0.5445398783	-0.1259956246
C	-2.6442850094	1.6697653870	-0.0514305676
C	-4.7103842319	-0.1472977826	-0.1837507632
H	-3.1186857522	-1.5922239522	-0.1228337161
C	-3.9588735758	2.1282828405	-0.1091313186
C	-5.0044660930	1.2124544777	-0.1770445224
H	-5.4915475673	-0.8959833684	-0.2328067156
H	-4.1731768132	3.1889287390	-0.1044139231
H	-6.0310007899	1.5578800497	-0.2234699104
C	-0.7655125769	-2.9185929902	0.8625942639
C	-0.7617312903	-2.5127610745	-1.4366347003
C	-0.9071950447	-4.2860334800	0.6661237135
H	-0.7164760165	-2.5072853765	1.8601895921
C	-0.9011778668	-3.8745606457	-1.6959450465
C	-0.9737704147	-4.7727759274	-0.6355565056
H	-0.9630644743	-4.9472660331	1.5222719967
H	-0.9511430006	-4.2393986639	-2.7134234180
H	-1.0813461127	-5.8346566055	-0.8255243958
C	2.3605687580	-0.6098526159	-0.9125117928
C	1.9764936965	-0.4920863432	1.3874494215
C	3.7104853095	-0.8713232972	-0.7189695745

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Table 11 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	1.9503916136	-0.5385664070	-1.9091129677
C	3.3211301849	-0.7530238562	1.6438340163
C	4.1989830405	-0.9461080513	0.5814760368
H	4.3571756836	-1.0119189283	-1.5764054279
H	3.6874847741	-0.8091909840	2.6604833059
H	5.2468880669	-1.1508519176	0.7690699673
C	-0.4031879446	0.8124864630	-2.8639089808
C	-0.6814755822	-1.4724292831	-2.4728433229
C	-0.4950509185	0.6339537512	-4.2380479809
H	-0.2456184016	1.7956399245	-2.4451438252
C	-0.7826304547	-1.7131377740	-3.8414628771
C	-0.6901821767	-0.6506751611	-4.7354288279
H	-0.4143829028	1.4905446178	-4.8961419894
H	-0.9357522709	-2.7172634778	-4.2145112533
H	-0.7693477802	-0.8259781727	-5.8023303280
N	-0.2705727840	1.8831249740	0.0196611543
N	-2.3697306359	0.3378504421	-0.0596984735
N	-0.4922647670	-0.2120032903	-1.9987482918
N	-0.6952016035	-2.0492783604	-0.1598572409
N	1.5107924512	-0.4225817478	0.1115766530
N	-0.3021262780	-0.0778579031	1.9538825741

[Os(bpy)$_3$]$^{2+}$

Atom	x (Å)	y (Å)	z (Å)
Os	-0.4377591316	-0.0793860960	-0.0111792753
C	1.0705698179	-0.2816329817	2.5438811296
C	-1.1850007631	0.1321733401	2.9750819471
C	1.3433012902	-0.2797510746	3.9123688782
C	-0.9706702446	0.1436194305	4.3431424721
H	-2.1724633776	0.2873037151	2.5627607412
C	0.3191196444	-0.0656602106	4.8238301369
H	2.3517521996	-0.4420037801	4.2686463099
H	-1.8034924480	0.3152283174	5.0138714250

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Table 11 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	0.5239647486	-0.0616964898	5.8877268721
C	0.7728375998	2.7564668086	0.1022736304
C	-1.5580966753	2.6750895876	0.0329529967
C	0.7706205970	4.1400310012	0.1588257977
H	1.6990570500	2.1985690917	0.1014513071
C	-1.6188034060	4.0680522196	0.0889704075
C	-0.4489607579	4.8116292258	0.1532340762
H	1.7109117866	4.6751676194	0.2076848475
H	-2.5750980597	4.5737668509	0.0858425619
H	-0.4887348253	5.8933886856	0.1986806713
C	-3.5052054340	-0.3995672990	-0.1164019567
C	-2.7398068674	1.8032029421	-0.0393554388
C	-4.8268772094	0.0108666760	-0.1650692008
H	-3.2455217023	-1.4491834384	-0.1216872742
C	-4.0531702215	2.2722574249	-0.0877522974
C	-5.1090030975	1.3741671776	-0.1517326368
H	-5.6156899802	-0.7296273588	-0.2138707795
H	-4.2542855810	3.3351221659	-0.0787540535
H	-6.1311499959	1.7313145652	-0.1909566456
C	-0.7791211789	-3.0484915876	0.7580198299
C	-0.7797333525	-2.6111200134	-1.5338913289
C	-0.9317675526	-4.4085179403	0.5471731563
H	-0.7183342528	-2.6414370017	1.7578743207
C	-0.9322687483	-3.9716482054	-1.8040265402
C	-1.0090400583	-4.8821963603	-0.7597363575
H	-0.9872189983	-5.0787250232	1.3960873101
H	-0.9890142076	-4.3227442440	-2.8256631676
H	-1.1265591989	-5.9400471011	-0.9621972673
C	2.4977434282	-0.6256290579	-0.7896017317
C	2.0863270440	-0.5017064443	1.5037887945
C	3.8430369199	-0.8810361040	-0.5829794229
H	2.0880556842	-0.5614454788	-1.7881742944
C	3.4321793080	-0.7571197586	1.7696316827

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Table 11 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	4.3220236191	-0.9498456811	0.7224599457
H	4.4974470772	-1.0238530978	-1.4340405631
H	3.7871795590	-0.8091481081	2.7901629127
H	5.3680136887	-1.1501974768	0.9215326361
C	-0.4318105412	0.7071393888	-2.9954827797
C	-0.6948375828	-1.5719816105	-2.5707263161
C	-0.5107364339	0.5100364245	-4.3639129013
H	-0.2895934385	1.6954609716	-2.5806196230
C	-0.7813122775	-1.8277933378	-3.9397928287
C	-0.6896117306	-0.7829024077	-4.8482328387
H	-0.4336230240	1.3588590789	-5.0321086406
H	-0.9229160247	-2.8383534777	-4.2988806026
H	-0.7571824755	-0.9740972842	-5.9125330911
N	-0.3583998601	2.0226390143	0.0393591200
N	-2.4699992941	0.4645338593	-0.0533576342
N	-0.5183015236	-0.3013315267	-2.1023516996
N	-0.7038348405	-2.1533287555	-0.2495522329
N	1.6229261192	-0.4362084851	0.2208320700
N	-0.1970193698	-0.0760597771	2.0790966446

[Os(bpy)$_3$]$^{3+}$

Atom	x (Å)	y (Å)	z (Å)
Os	-0.4401569898	-0.0841758509	-0.0229313173
C	1.0716534953	-0.2700907815	2.5372400453
C	-1.1797310020	0.2241982722	2.9611884450
C	1.3415296545	-0.2546770051	3.9045133096
C	-0.9657900070	0.2431918010	4.3295903884
H	-2.1617628714	0.4077837299	2.5471607548
C	0.3181713893	0.0003785689	4.8105374804
H	2.3431074217	-0.4396017256	4.2690673873
H	-1.7921186751	0.4469463644	4.9994136250
H	0.5222492668	0.0112363747	5.8749869444
C	0.7761818774	2.7486369037	0.1813132786

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Table 11 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	-1.5618663687	2.6748958427	0.0392680599
C	0.7748272150	4.1324322689	0.2442092275
H	1.7015953546	2.1895502957	0.2071792331
C	-1.6187483386	4.0658366516	0.1071922621
C	-0.4445976000	4.8037153239	0.2077962923
H	1.7133836547	4.6672636767	0.3224187216
H	-2.5708233387	4.5789241293	0.0828819711
H	-0.4830022448	5.8857318263	0.2590766997
C	-3.5068097866	-0.4057391044	-0.2220005637
C	-2.7436277945	1.8043420910	-0.0640801700
C	-4.8284936901	0.0057429458	-0.2742550704
H	-3.2470805141	-1.4549213587	-0.2584730399
C	-4.0556672326	2.2709224669	-0.1204860383
C	-5.1085884308	1.3687675395	-0.2234724579
H	-5.6176437251	-0.7316385020	-0.3551305540
H	-4.2637061621	3.3319486766	-0.0854050449
H	-6.1309945487	1.7261948051	-0.2656843206
C	-0.6867882016	-3.0670887569	0.7485227586
C	-0.7621225098	-2.6221327258	-1.5507981208
C	-0.8294261105	-4.4286334988	0.5365006877
H	-0.6003949855	-2.6641080418	1.7484267314
C	-0.8992150458	-3.9829186612	-1.8188874717
C	-0.9362261087	-4.8957612511	-0.7708736691
H	-0.8535017944	-5.1041250355	1.3827887704
H	-0.9773039591	-4.3371781407	-2.8380253356
H	-1.0449100887	-5.9549677231	-0.9735682779
C	2.4811462683	-0.7277004642	-0.8012838567
C	2.0830315662	-0.5243070681	1.4989589194
C	3.8251060600	-0.9903074562	-0.5922232716
H	2.0682576825	-0.6924971276	-1.8001616172
C	3.4249806907	-0.7915012546	1.7640039711
C	4.3061128102	-1.0241327627	0.7139696588
H	4.4759528362	-1.1659971355	-1.4398691119

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Table 11 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	3.7888507378	-0.8202581154	2.7823483385
H	5.3511220308	-1.2304832419	0.9143734380
C	-0.5261376699	0.7200606753	-3.0050348407
C	-0.7099007506	-1.5783751557	-2.5864652733
C	-0.6100038480	0.5243468167	-4.3738389352
H	-0.4140918763	1.7119708783	-2.5889846809
C	-0.8058472535	-1.8288177637	-3.9540788734
C	-0.7532191294	-0.7734373376	-4.8576972200
H	-0.5653859136	1.3758240086	-5.0417467854
H	-0.9223123587	-2.8398010233	-4.3209426745
H	-0.8255492703	-0.9627782070	-5.9224785567
N	-0.3590960872	2.0262658755	0.0733309777
N	-2.4802199852	0.4637697102	-0.1112198948
N	-0.5656683311	-0.3006835883	-2.1225124583
N	-0.6602583685	-2.1742153814	-0.2635282570
N	1.6220646781	-0.4906981328	0.2125576649
N	-0.1933493202	-0.0336391532	2.0761816006

[Ir(bpy)$_3$]$^{2+}$

Atom	x (Å)	y (Å)	z (Å)
Ir	-0.4370461851	-0.0922999762	-0.0225712521
C	1.0467754686	-0.3081979942	2.5050710613
C	-1.2303720239	0.0937849113	2.9368950779
C	1.2977990435	-0.3558197699	3.8837740133
C	-1.0271544778	0.0663382188	4.3024014054
H	-2.2130537925	0.2619773386	2.5186261728
C	0.2664035187	-0.1689995856	4.7849164994
H	2.3005385090	-0.5395081557	4.2460629748
H	-1.8622542823	0.2248838957	4.9725880674
H	0.4597381186	-0.2045706897	5.8504062822
C	0.8118619336	2.7098574103	0.0597836968
C	-1.5382970910	2.6325257151	-0.0011734572
C	0.8154333314	4.0906303740	0.0745343207

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Table 11 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	1.7339364327	2.1455439968	0.0755819164
C	-1.5825772589	4.0339138875	0.0014081573
C	-0.4107318313	4.7662858258	0.0397587150
H	1.7563247751	4.6245385305	0.1117617613
H	-2.5350632431	4.5462457950	-0.0262558341
H	-0.4440799067	5.8492547943	0.0432483500
C	-3.4847247747	-0.4481684472	-0.1020027352
C	-2.7096275122	1.7714468279	-0.0290561993
C	-4.8036876919	-0.0394561857	-0.1106449784
H	-3.2212330152	-1.4965026858	-0.1251247600
C	-4.0339235537	2.2318618176	-0.0249311971
C	-5.0826730036	1.3322134257	-0.0659493821
H	-5.5941302738	-0.7778785037	-0.1506180685
H	-4.2385166694	3.2936590554	0.0099493524
H	-6.1063376436	1.6872130262	-0.0641799922
C	-0.8023536155	-3.0317396810	0.7821904174
C	-0.8009299576	-2.5902515397	-1.5280220080
C	-0.9947937606	-4.3831975381	0.5738560922
H	-0.7217856869	-2.6230107521	1.7798358681
C	-1.0073093840	-3.9525266768	-1.7868205096
C	-1.1043991940	-4.8516588364	-0.7411597792
H	-1.0579557345	-5.0532037058	1.4216555931
H	-1.0906389390	-4.3040958349	-2.8065692164
H	-1.2625694744	-5.9048612039	-0.9402103174
C	2.4781223843	-0.6068488969	-0.8343434179
C	2.0603853067	-0.4804106936	1.4771501539
C	3.8278758413	-0.8135216475	-0.6292450866
H	2.0611522380	-0.5664359399	-1.8310110039
C	3.4252082728	-0.6756177193	1.7325010375
C	4.3113613762	-0.8428035694	0.6848906441
H	4.4854189436	-0.9476053153	-1.4785515065
H	3.7884515858	-0.6958038490	2.7513919175
H	5.3659454194	-0.9948988784	0.8813787921

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Table 11 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	-0.3930490110	0.7289575180	-2.9794431932
C	-0.6736994715	-1.5671224483	-2.5538547235
C	-0.4358180170	0.5314292211	-4.3454999879
H	-0.2623137394	1.7161572255	-2.5584046134
C	-0.7118284854	-1.8163569213	-3.9329409492
C	-0.5940109181	-0.7722707826	-4.8314457981
H	-0.3465475874	1.3786518021	-5.0132895045
H	-0.8344622002	-2.8273551873	-4.2980118480
H	-0.6248871774	-0.9637548951	-5.8974134561
N	-0.3263824119	1.9873617480	0.0162312999
N	-2.4553996728	0.4223341183	-0.0553335027
N	-0.5006687677	-0.2844844237	-2.0959219670
N	-0.7131526373	-2.1466764722	-0.2317244135
N	1.6073114712	-0.4359172173	0.1816400854
N	-0.2311335255	-0.0940293034	2.0503917454

[Ir(bpy)$_3$]$^{3+}$

Atom	x (Å)	y (Å)	z (Å)
Ir	-0.4371007746	-0.0896089177	-0.0225239644
C	1.0475098208	-0.2799279623	2.5159300470
C	-1.2163584983	0.1398656476	2.9432042573
C	1.3169228177	-0.2738844238	3.8829954096
C	-1.0023519821	0.1550366609	4.3133103799
H	-2.2032808103	0.2938120644	2.5300121130
C	0.2869413923	-0.0544497296	4.7917337862
H	2.3227821131	-0.4381507538	4.2455961851
H	-1.8348237008	0.3278785708	4.9841532476
H	0.4910512355	-0.0483202181	5.8561829404
C	0.8030836404	2.7207348976	0.1029683954
C	-1.5363200856	2.6438979904	0.0262533435
C	0.8016576591	4.1064410771	0.1589820229
H	1.7285773617	2.1621480025	0.1039731343
C	-1.5936968815	4.0350127630	0.0814649692

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Table 11 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	-0.4180215052	4.7753684301	0.1492443477
H	1.7416511254	4.6420543510	0.2088419167
H	-2.5468717631	4.5465370212	0.0730014179
H	-0.4570298151	5.8576436654	0.1931420684
C	-3.4894317730	-0.4393456041	-0.1462320564
C	-2.7218177829	1.7710177385	-0.0515807435
C	-4.8125391278	-0.0264107278	-0.1927876254
H	-3.2306638770	-1.4888134007	-0.1588462758
C	-4.0335120554	2.2389797326	-0.0961280464
C	-5.0896408945	1.3365575583	-0.1677869009
H	-5.6030843864	-0.7646503580	-0.2470975497
H	-4.2390842861	3.3008805951	-0.0765813912
H	-6.1118361172	1.6952405075	-0.2033574645
C	-0.7614639652	-3.0417531761	0.7743715361
C	-0.7730782662	-2.6018134452	-1.5257105673
C	-0.9123837622	-4.4037513020	0.5612664893
H	-0.6985594919	-2.6360972944	1.7743392489
C	-0.9239986931	-3.9605699365	-1.7949627758
C	-0.9939425982	-4.8716493472	-0.7462159812
H	-0.9643748970	-5.0765033550	1.4083916025
H	-0.9868318518	-4.3149990730	-2.8151051381
H	-1.1108814714	-5.9297270677	-0.9500581980
C	2.4771622044	-0.6498683268	-0.8263292143
C	2.0663110975	-0.5071313638	1.4748529280
C	3.8243810136	-0.9035141800	-0.6166457947
H	2.0678273755	-0.5931707264	-1.8252157535
C	3.4107625188	-0.7586711380	1.7405304275
C	4.2994805706	-0.9596450279	0.6895683328
H	4.4803744209	-1.0523583455	-1.4654283082
H	3.7709994503	-0.8004785676	2.7596854459
H	5.3461327492	-1.1565603000	0.8906945930
C	-0.4377639234	0.7308785164	-2.9857391118
C	-0.6937690271	-1.5584524446	-2.5642136322

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Table 11 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	-0.5186070726	0.5344509995	-4.3562163545
H	-0.2970990538	1.7187448020	-2.5699827893
C	-0.7811968280	-1.8106130805	-3.9318142865
C	-0.6941060902	-0.7587468909	-4.8378122082
H	-0.4442019490	1.3831744102	-5.0248395096
H	-0.9180896470	-2.8196875857	-4.2968947329
H	-0.7624665969	-0.9492399357	-5.9026155627
N	-0.3330978050	2.0014212342	0.0369689949
N	-2.4652204607	0.4314918812	-0.0756125087
N	-0.5210643452	-0.2851760594	-2.1063512944
N	-0.6941017571	-2.1573447643	-0.2384807262
N	1.6146004555	-0.4540379563	0.1888188934
N	-0.2217303521	-0.0729731402	2.0611742328