

## The equilibrium geometries and molecular energies of all the studied species.

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[Ru(CL)6]4-  
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E(RI-PBE/def2-SVP)= -2853.74476436 a.u.  
E(RI-PBE/def2-SVP/COSMO(eps=80))= -2854.83387843 a.u.  
E(B3LYP/def2-TZVP)= -2855.60269579 a.u.

ru	-0.00001	-0.00001	0.00000
cl	-0.15712	-1.93405	-1.82564
cl	-0.74592	-1.72675	1.88663
cl	2.55637	-0.62273	0.43830
cl	-2.55652	0.62280	-0.43828
cl	0.74604	1.72681	-1.88653
cl	0.15718	1.93393	1.82552

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[Ru(CL)6]4- solvation geometry (eps=80)  
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ru	-0.00041	-0.00065	-0.00028
cl	2.02030	1.36620	0.33744
cl	-1.35483	1.72089	1.12399
cl	-0.38859	1.10862	-2.16456
cl	0.38903	-1.10457	2.16638
cl	1.35794	-1.72061	-1.12433
cl	-2.02267	-1.36868	-0.33813

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[Ru(CL)6]3-  
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E(RI-PBE/def2-SVP)= -2854.156632359 a.u.  
E(RI-PBE/def2-SVP/COSMO(eps=80))= -2854.781637493 a.u.  
E(B3LYP/def2-TZVP)= -2855.946910685 a.u.

ru	-0.00001	0.00004	0.00001
cl	1.46856	1.16564	1.59626
cl	-1.61840	-0.37613	1.80675
cl	-1.06759	2.17385	-0.54350
cl	1.06765	-2.17379	0.54309
cl	1.61842	0.37621	-1.80670
cl	-1.46861	-1.16588	-1.59592

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[Ru(CL)6]3- solvation geometry (eps=80)  
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ru	0.00006	0.00011	0.00034
cl	-0.92442	-1.41877	-1.71068
cl	0.93067	1.41136	-1.71402
cl	-2.02962	1.29402	-0.00746
cl	2.02991	-1.29359	0.00574
cl	-0.93107	-1.41262	1.71355
cl	0.92436	1.41930	1.71191

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[Ru(CN)6]4-  
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E(RI-PBE/def2-SVP)= -650.598700056 a.u.  
E(RI-PBE/def2-SVP/COSMO(eps=80))= -651.619044341 a.u.  
E(B3LYP/def2-TZVP)= -651.604918887 a.u.

ru	0.00003	0.00003	0.00000
c	1.61398	-0.88607	-0.95570
n	2.54481	-1.39697	-1.50708
c	-1.61392	0.88615	0.95569
n	-2.54467	1.39712	1.50714
c	0.46002	1.81083	-0.90216
n	0.72516	2.85507	-1.42254
c	-0.46004	-1.81082	0.90205
n	-0.72537	-2.85513	1.42216

c	1.21913	0.48977	1.60595
n	1.92187	0.77217	2.53220
c	-1.21914	-0.48983	-1.60585
n	-1.92203	-0.77248	-2.53189

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[Ru(CN)6]3-  
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E(RI-PBE/def2-SVP)= -650.902583407 a.u.  
E(RI-PBE/def2-SVP/COSMO(eps=80))= -651.470979003 a.u.  
E(B3LYP/def2-TZVP)= -651.882867220 a.u.

ru	-0.00001	0.00001	0.00001
c	1.25135	-1.14167	1.18834
n	1.96099	-1.80619	1.87090
c	-1.25137	1.14168	-1.18832
n	-1.96097	1.80614	-1.87098
c	1.62025	1.19260	-0.48040
n	2.54695	1.88565	-0.74822
c	-1.62024	-1.19264	0.48040
n	-2.54694	-1.88571	0.74815
c	-0.42878	1.16912	1.64906
n	-0.68197	1.85185	2.58747
c	0.42879	-1.16909	-1.64903
n	0.68202	-1.85179	-2.58746

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[Ru(H2O)6]2+  
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E(RI-PBE/def2-SVP)= -552.132240331 a.u.  
E(RI-PBE/def2-SVP/COSMO(eps=80))= -552.443253739 a.u.  
E(B3LYP/def2-TZVP)= -552.937946879 a.u.

ru	-0.00006	0.00007	0.00008
o	0.58313	1.79694	-0.98749
h	0.00752	2.55769	-0.74695
h	0.72285	1.85729	-1.95600
o	-1.84501	-0.39355	-0.99204
h	-1.96752	-0.30324	-1.96054
h	-2.21214	-1.27442	-0.75275
o	-1.26769	1.39942	0.98955
h	-2.21310	1.27805	0.74564
h	-1.25578	1.54783	1.95856
o	-0.58260	-1.79720	0.98735
h	-0.00735	-2.55818	0.74686
h	-0.72233	-1.85878	1.95574
o	1.84519	0.39304	0.99198
h	1.96726	0.30382	1.96064
h	2.21313	1.27342	0.75203
o	1.26735	-1.39907	-0.98975
h	2.21278	-1.27741	-0.74603
h	1.25553	-1.54699	-1.95886

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[Ru(H2O)6]3+  
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E(RI-PBE/def2-SVP)= -551.563961623 a.u.  
E(RI-PBE/def2-SVP/COSMO(eps=80))= -552.243323576 a.u.  
E(B3LYP/def2-TZVP)= -552.358928179 a.u.

ru	-0.00028	0.00003	0.00128
o	-0.18701	-0.18350	2.03606
h	0.53141	-0.05304	2.70174
h	-1.01179	-0.42951	2.52139
o	1.79569	-1.11389	0.03729
h	2.05134	-1.67077	0.81138
h	2.11649	-1.60310	-0.75816
o	1.24116	1.60830	0.25161
h	2.22686	1.53836	0.27988
h	0.98316	2.55368	0.37082
o	0.18700	0.18203	-2.03636
h	-0.52179	0.01385	-2.70366
h	0.99893	0.47212	-2.51854

o	-1.79523	1.11510	-0.03458
h	-2.07139	1.63115	-0.82969
h	-2.09511	1.64561	0.74235
o	-1.23995	-1.60813	-0.26142
h	-2.22672	-1.54446	-0.26623
h	-0.98006	-2.55541	-0.36209

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[Ru(NH3)6]2+  
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E(RI-PBE/def2-SVP)= -433.215085526 a.u.  
E(RI-PBE/def2-SVP/COSMO(eps=80))= -433.506305697 a.u.  
E(B3LYP/def2-TZVP)= -433.795042163 a.u.

ru	-0.00008	-0.00070	0.00005
n	-1.58271	1.45705	-0.19712
n	-1.46535	-1.56665	0.24885
n	-0.02491	-0.31390	-2.13602
n	0.02474	0.31829	2.13504
n	1.46743	1.56620	-0.24733
h	0.50475	-0.41807	2.68202
h	2.06507	-1.46117	1.11144
h	-1.93177	-1.87649	-0.62219
h	-0.44537	-1.20953	-2.44036
h	1.12110	2.52280	-0.05505
h	-1.30878	2.33832	-0.66663
h	0.49137	1.19040	2.43904
h	-0.90764	0.37375	2.58159
h	1.28671	-2.44185	0.07278
h	2.35519	-1.35179	-0.48256
h	-0.54892	0.39686	-2.67571
h	0.90575	-0.32321	-2.58932
h	-1.10053	-2.44631	0.65466
h	2.29766	1.48111	0.36446
h	1.87150	1.64313	-1.19684
h	-2.40188	1.13711	-0.74244
h	-1.99635	1.77931	0.69488
h	-2.25624	-1.32705	0.87134

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[Ru(NH3)6]3+  
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E(RI-PBE/def2-SVP)= -432.685665186 a.u.  
E(RI-PBE/def2-SVP/COSMO(eps=80))= -433.338159496 a.u.  
E(B3LYP/def2-TZVP)= -433.259939811 a.u.

ru	-0.00002	-0.00241	0.00034
n	-1.16132	1.35780	-1.22723
n	-1.09486	-1.68795	-0.79554
n	1.40878	-0.16699	-1.63193
n	-1.40856	0.16336	1.63259
n	1.06429	1.69851	0.82579
h	-1.33836	-0.58323	2.34957
h	0.95472	-1.38324	2.20449
h	-0.84212	-1.96426	-1.76316
h	1.39208	-1.07138	-2.14010
h	0.58083	2.60821	0.70208
h	-0.72706	2.29106	-1.35622
h	-1.35134	1.04763	2.17214
h	-2.40508	0.12180	1.34268
h	1.16246	-2.34647	0.89442
h	2.20647	-1.13154	1.19543
h	1.30036	0.54959	-2.37421
h	2.40362	-0.07425	-1.34802
h	-1.01295	-2.56571	-0.24843
h	1.24232	1.64741	1.84676
h	2.00377	1.86924	0.41837
h	-1.34327	1.02899	-2.19465
h	-2.10632	1.58318	-0.86079
h	-2.12057	-1.53413	-0.85122

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[Ru(en)3]2+  
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E(RI-PBE/def2-SVP)= -664.989851398 a.u.  
E(RI-PBE/def2-SVP/COSMO(eps=80))= -665.257909599 a.u.  
E(B3LYP/def2-TZVP)= -665.947605742 a.u.

c	-0.77681	-1.36943	2.55521
c	0.72409	-1.57441	2.45199
n	1.11791	-1.53791	1.00725
ru	0.00031	-0.00006	-0.00005
n	-1.11774	-1.52687	-1.02342
c	-0.72561	-1.54644	-2.46896
c	0.77535	-1.34134	-2.57107
n	1.14450	-0.09692	-1.82356
n	-1.14383	-0.11575	1.82223
n	1.13607	1.63856	0.82022
c	0.34984	2.90757	0.69030
c	-0.35089	2.91567	-0.65672
n	-1.13534	1.64728	-0.80307
h	-0.96325	0.68353	2.45371
h	-2.17009	-0.10171	1.70269
h	0.94677	-2.47927	0.60982
h	2.14459	-1.44126	0.95239
h	0.96556	0.70999	-2.44573
h	2.17073	-0.08621	-1.70356
h	-0.94552	-2.47273	-0.63728
h	-1.09761	-1.33744	3.61753
h	-1.31760	-2.21589	2.08214
h	1.02717	-2.52425	2.94076
h	1.26404	-0.75952	2.97832
h	1.09529	-1.29705	-3.63320
h	1.31571	-2.19398	-2.10869
h	-1.02960	-2.49036	-2.96849
h	-1.26559	-0.72497	-2.98488
h	1.43291	1.54229	1.80552
h	2.02835	1.76060	0.31340
h	-1.43001	1.56244	-1.79007
h	-2.02881	1.76232	-0.29672
h	-0.39587	2.94109	1.51308
h	0.99069	3.80670	0.80576
h	-0.99313	3.81524	-0.76062
h	0.39478	2.96093	-1.47896
h	-2.14443	-1.43152	-0.96619

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[Ru(en)3]3+  
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E(RI-PBE/def2-SVP)= -664.490424726 a.u.  
E(RI-PBE/def2-SVP/COSMO(eps=80))= -665.084386759 a.u.  
E(B3LYP/def2-TZVP)= -665.445735025 a.u.

c	-0.78029	-1.30902	2.62046
c	0.71787	-1.51876	2.52803
n	1.11050	-1.50992	1.07102
ru	-0.00014	-0.00068	0.00035
n	-1.10884	-1.55971	-0.99817
c	-0.71652	-1.63675	-2.45313
c	0.78127	-1.42947	-2.55547
n	1.13412	-0.15461	-1.82956
n	-1.13513	-0.07079	1.83475
n	1.09813	1.67573	0.81330
c	0.32663	2.95648	0.61140
c	-0.32584	2.92184	-0.75545
n	-1.10062	1.63456	-0.88996
h	-0.96743	0.75895	2.43149
h	-2.16222	-0.05803	1.69288
h	0.96266	-2.45987	0.68567
h	2.13844	-1.38866	1.01034
h	0.96383	0.64552	-2.46458
h	2.16128	-0.13332	-1.68927
h	-0.96100	-2.49061	-0.56841
h	-1.11094	-1.21279	3.67592
h	-1.33834	-2.16601	2.18886
h	1.02411	-2.47003	3.01186
h	1.27385	-0.70882	3.04447
h	1.11198	-1.38305	-3.61424
h	1.34058	-2.26405	-2.08349
h	-1.02136	-2.61027	-2.89133

h	-1.27394	-0.85306	-3.00731
h	1.36303	1.60314	1.81148
h	2.01114	1.77111	0.33153
h	-1.37019	1.51313	-1.88214
h	-2.01101	1.75570	-0.40877
h	-0.43194	3.03522	1.41877
h	0.99170	3.83934	0.71639
h	-0.98842	3.79986	-0.90616
h	0.43302	2.95643	-1.56588
h	-2.13684	-1.43624	-0.94318

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[Ru(bipy)3]2+  
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E(RI-PBE/def2-SVP)= -1577.93863300 a.u.  
E(RI-PBE/def2-SVP/COSMO(eps=80))= -1578.13363616 a.u.  
E(B3LYP/def2-TZVP)= -1580.36813925 a.u.

n	-1.77359	-1.04969	0.16847
c	-2.81917	-0.58365	-0.59254
c	-4.08285	-1.20106	-0.54485
c	-4.28905	-2.30571	0.28849
c	-3.21570	-2.77262	1.06307
c	-1.98270	-2.12016	0.97558
c	-2.49898	0.58038	-1.43505
n	-1.21291	1.04854	-1.30672
c	-0.83312	2.11910	-2.04858
c	-1.69567	2.76958	-2.93530
c	-3.01134	2.30048	-3.07206
c	-3.41073	1.19575	-2.31257
ru	-0.00022	0.00036	-0.00001
n	1.73652	1.05035	-0.39566
c	2.49114	0.58403	-1.44582
c	3.70681	1.20058	-1.79564
c	4.16457	2.30441	-1.06821
c	3.38793	2.77151	0.00355
c	2.18881	2.12005	0.30597
c	1.92243	-0.57918	-2.14628
n	0.74102	-1.04685	-1.62191
c	0.14736	-2.11673	-2.20822
c	0.68857	-2.76711	-3.32065
c	1.89577	-2.29876	-3.86207
c	2.51343	-1.19456	-3.26528
n	1.03611	-1.04706	1.45113
c	1.84469	-2.11348	1.22791
c	2.54231	-2.76159	2.25103
c	2.40824	-2.29451	3.56776
c	1.57789	-1.19427	3.80669
c	0.89946	-0.58109	2.73710
c	0.00439	0.57865	2.88198
n	-0.52879	1.04630	1.70447
c	-1.36584	2.11329	1.74768
c	-1.70641	2.76017	2.93898
c	-1.16580	2.29138	4.14641
c	-0.30320	1.19062	4.11123
h	1.92356	-2.45301	0.18577
h	-1.41316	2.77550	5.10241
h	0.13041	0.80346	5.04300
h	-1.76796	2.45426	0.78340
h	-2.38915	3.62137	2.91202
h	1.45858	-0.80853	4.82799
h	2.94371	-2.77941	4.39703
h	3.18249	-3.62212	2.00977
h	-3.71657	2.78751	-3.76127
h	-1.33207	3.63374	-3.50943
h	0.20290	2.46047	-1.91412
h	-4.43434	0.80828	-2.40384
h	-4.90769	-0.81544	-1.15886
h	-5.27334	-2.79429	0.33314
h	-3.32542	-3.63655	1.73401
h	-1.11952	-2.45965	1.56508
h	5.11394	2.79209	-1.33352
h	3.70298	3.63462	0.60715
h	1.55403	2.45983	1.13637
h	4.29751	0.81487	-2.63734
h	3.45736	-0.80762	-3.67232
h	2.34981	-2.78577	-4.73739

h	0.16293	-3.63072	-3.75244
h	-0.79503	-2.45758	-1.75660

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[Ru(bipy)3]3+  
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E(RI-PBE/def2-SVP)= -1577.49164400 a.u.  
E(RI-PBE/def2-SVP/COSMO(eps=80))= -1577.91882538 a.u.  
E(B3LYP/def2-TZVP)= -1579.92914565 a.u.

n	1.81288	-1.02436	-0.06044
c	2.78125	-0.56751	0.80377
c	4.05154	-1.17100	0.84000
c	4.33676	-2.24588	-0.01136
c	3.33997	-2.69868	-0.89124
c	2.09632	-2.05959	-0.89061
c	2.38084	0.57139	1.64521
n	1.09847	1.02621	1.44050
c	0.63241	2.06088	2.18408
c	1.41631	2.70123	3.14841
c	2.72865	2.25052	3.36553
c	3.21031	1.17627	2.60703
ru	0.00047	-0.00034	-0.00033
n	-1.79704	1.02487	0.23200
c	-2.61476	0.56891	1.24017
c	-3.86059	1.17591	1.48163
c	-4.27558	2.25338	0.68932
c	-3.43275	2.70456	-0.33945
c	-2.20755	2.06187	-0.54053
c	-2.08616	-0.57195	2.00466
n	-0.85305	-1.02656	1.59747
c	-0.27496	-2.06288	2.25600
c	-0.89642	-2.70625	3.33071
c	-2.15810	-2.25681	3.75373
c	-2.75318	-1.18005	3.08406
n	-0.95551	-1.02733	-1.53853
c	-1.81235	-2.06543	-1.36712
c	-2.43173	-2.70941	-2.44244
c	-2.16902	-2.25881	-3.74646
c	-1.29389	-1.18038	-3.92706
c	-0.69313	-0.57178	-2.80995
c	0.23071	0.57122	-2.88526
n	0.69577	1.02631	-1.67286
c	1.56900	2.06426	-1.64218
c	2.00517	2.70909	-2.80361
c	1.53407	2.25947	-4.04797
c	0.64167	1.18071	-4.08478
h	-1.99287	-2.39213	-0.33293
h	1.85986	2.74303	-4.98165
h	0.26671	0.81357	-5.04988
h	1.91561	2.38989	-0.65094
h	2.70589	3.55348	-2.72640
h	-1.08101	-0.81277	-4.94030
h	-2.64267	-2.74116	-4.61522
h	-3.11083	-3.55365	-2.25289
h	3.37074	2.72968	4.12047
h	0.99660	3.54263	3.71919
h	-0.39830	2.38743	1.98546
h	4.23290	0.80844	2.76746
h	4.82127	-0.80145	1.53100
h	5.32810	-2.72385	0.01027
h	3.51844	-3.54070	-1.57609
h	1.29179	-2.38696	-1.56408
h	-5.24846	2.73490	0.87201
h	-3.71670	3.54850	-0.98529
h	-1.52187	2.38827	-1.33548
h	-4.51012	0.80799	2.28781
h	-3.73768	-0.81325	3.40512
h	-2.67346	-2.73874	4.59857
h	-0.39183	-3.54906	3.82557
h	0.71165	-2.38793	1.89643

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[Os(CL)6]4-  
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E(RI-PBE/def2-SVP)= -2849.51796748 a.u.  
E(RI-PBE/def2-SVP/COSMO(eps=80))= -2850.60606882 a.u.  
E(B3LYP/def2-TZVP)= -2851.35374396 a.u.

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os      0.00000  0.00000  0.00000
cl     -1.06507 -1.59141 -1.87865
cl     -2.03968 -0.58465  1.64130
cl      1.38407 -2.08614  0.97311
cl     -1.38409  2.08619 -0.97311
cl      2.03970  0.58465 -1.64129
cl      1.06506  1.59137  1.87863
```

-----  
[Os(CL)6]4- solvation geometry (eps=80)  
-----

```
os     -0.00016 -0.00052  0.00049
cl     -0.30256  2.26696 -0.97650
cl      1.60665 -0.56577 -1.81542
cl      1.88052  0.85151  1.39317
cl     -1.87801 -0.84937 -1.39786
cl     -1.60798  0.56933  1.81563
cl      0.30225 -2.26990  0.97834
```

-----  
[Os(CL)6]3-  
-----

E(RI-PBE/def2-SVP)= -2849.94639486 a.u.  
E(RI-PBE/def2-SVP/COSMO(eps=80))= -2850.57145190 a.u.  
E(B3LYP/def2-TZVP)= -2851.72278720 a.u.

```
os      0.00000  0.00000  0.00000
cl      1.30018 -1.88513 -0.98746
cl     -1.60660 -0.16002 -1.87441
cl     -1.32420 -1.65679  1.30459
cl      1.32420  1.65679 -1.30459
cl      1.60660  0.16002  1.87441
cl     -1.30018  1.88513  0.98746
```

-----  
[Os(CL)6]3- solvation geometry (eps=80)  
-----

```
os     -0.00005 -0.00028 -0.00009
cl      1.04053  1.74002  1.33896
cl     -1.06013  1.72342 -1.34508
cl      1.93308  0.00924 -1.45927
cl     -1.93328 -0.00736  1.45899
cl      1.06092 -1.72279  1.34623
cl     -1.04087 -1.74102 -1.33933
```

-----  
[Os(CN)6]4-  
-----

E(RI-PBE/def2-SVP)= -646.424680365 a.u.  
E(RI-PBE/def2-SVP/COSMO(eps=80))= -647.442980616 a.u.  
E(B3LYP/def2-TZVP)= -647.411090986 a.u.

```
os      0.00000  0.00000  0.00000
c       1.47733 -1.44562  0.33295
n       2.32233 -2.27268  0.52305
c      -1.47734  1.44562 -0.33295
n      -2.32233  2.27269 -0.52305
c       0.73436  0.30516 -1.93659
n       1.15427  0.47963 -3.04447
c      -0.73436 -0.30517  1.93659
n      -1.15422 -0.47969  3.04449
c       1.28820  1.48408  0.72229
n       2.02478  2.33312  1.13554
c      -1.28821 -1.48407 -0.72229
n      -2.02479 -2.33311 -1.13555
```

-----  
[Os(CN)6]3-  
-----

-----

E(RI-PBE/def2-SVP)= -646.732445535 a.u.  
E(RI-PBE/def2-SVP/COSMO(eps=80))= -647.300052754 a.u.  
E(B3LYP/def2-TZVP)= -647.693453793 a.u.

os	0.00001	0.00000	0.00000
c	0.58188	-1.19474	1.60738
n	0.91042	-1.88629	2.51701
c	-0.58186	1.19473	-1.60741
n	-0.91062	1.88625	-2.51697
c	1.71029	1.15696	0.29306
n	2.67851	1.82674	0.45888
c	-1.71029	-1.15693	-0.29307
n	-2.67856	-1.82661	-0.45895
c	-1.08004	1.18901	1.32978
n	-1.69095	1.87740	2.08245
c	1.08006	-1.18903	-1.32978
n	1.69099	-1.87753	-2.08232

-----  
[Os(H2O)6]2+  
-----

E(RI-PBE/def2-SVP)= -547.919335057 a.u.  
E(RI-PBE/def2-SVP/COSMO(eps=80))= -548.229109072 a.u.  
E(B3LYP/def2-TZVP)= -548.685697770 a.u.

os	0.00002	0.00000	0.00000
o	-0.20804	1.92864	-0.92525
h	-1.05207	2.36773	-0.66789
h	-0.12672	2.03958	-1.89634
o	-1.56730	-1.14263	-0.92639
h	-1.69812	-1.12534	-1.89827
h	-1.52316	-2.09398	-0.67262
o	-1.77378	0.78354	0.92682
h	-2.57526	0.27040	0.67063
h	-1.82871	0.90962	1.89790
o	0.20775	-1.92872	0.92528
h	1.05186	-2.36827	0.66910
h	0.12442	-2.04019	1.89615
o	1.56762	1.14249	0.92635
h	1.69934	1.12325	1.89809
h	1.52291	2.09432	0.67450
o	1.77363	-0.78332	-0.92704
h	2.57504	-0.27101	-0.66891
h	1.82932	-0.90669	-1.89842

-----  
[Os(H2O)6]3+  
-----

E(RI-PBE/def2-SVP)= -547.371089520 a.u.  
E(RI-PBE/def2-SVP/COSMO(eps=80))= -548.046736938 a.u.  
E(B3LYP/def2-TZVP)= -548.136285249 a.u.

os	-0.00012	0.00002	0.00044
o	-0.17368	-0.09753	2.06476
h	0.56006	0.00758	2.71769
h	-1.00747	-0.25583	2.57049
o	1.80449	-1.14739	0.07216
h	2.05996	-1.67320	0.86757
h	2.11579	-1.67657	-0.70095
o	1.30977	1.59382	0.17325
h	2.29319	1.49500	0.20068
h	1.08224	2.55084	0.25315
o	0.17383	0.09682	-2.06549
h	-0.55578	-0.03121	-2.71892
h	1.00205	0.28453	-2.57015
o	-1.80426	1.14804	-0.06988
h	-2.07957	1.64072	-0.87972
h	-2.09651	1.70882	0.68819
o	-1.30878	-1.59403	-0.17946
h	-2.29288	-1.49868	-0.18840
h	-1.07992	-2.55161	-0.24838



-----  
 [Os(NH3)6]2+  
 -----

E(RI-PBE/def2-SVP) = -429.016031958 a.u.  
 E(RI-PBE/def2-SVP/COSMO(eps=80)) = -429.305760845 a.u.  
 E(B3LYP/def2-TZVP) = -429.559855857 a.u.

os	0.00002	-0.00019	0.00009
n	-1.40600	1.46094	-0.79168
n	-1.41234	-1.60714	-0.39396
n	0.83787	-0.26711	-1.99016
n	-0.83872	0.27088	1.98922
n	1.41945	1.60669	0.38657
h	-0.60299	-0.47312	2.67071
h	1.47436	-1.48232	1.83230
h	-1.48309	-1.90071	-1.38540
h	0.58912	-1.15874	-2.45562
h	1.01312	2.56001	0.40021
h	-0.98978	2.36991	-1.06548
h	-0.55146	1.14046	2.47256
h	-1.87335	0.30444	2.02981
h	1.19549	-2.44728	0.55328
h	2.38144	-1.34053	0.49372
h	0.56239	0.45157	-2.68307
h	1.87272	-0.25971	-2.03712
h	-1.22014	-2.49427	0.10591
h	1.91218	1.54253	1.29506
h	2.19155	1.68752	-0.29877
h	-1.90952	1.16194	-1.64574
h	-2.16890	1.73400	-0.14712
h	-2.39407	-1.39984	-0.13846

-----  
 [Os(NH3)6]3+  
 -----

E(RI-PBE/def2-SVP) = -428.500720328 a.u.  
 E(RI-PBE/def2-SVP/COSMO(eps=80)) = -429.150705492 a.u.  
 E(B3LYP/def2-TZVP) = -429.045196883 a.u.

os	0.00000	-0.00156	0.00024
n	-1.17599	1.37270	-1.23138
n	-1.16150	-1.69949	-0.71643
n	1.34496	-0.25193	-1.69701
n	-1.34513	0.25010	1.69730
n	1.14150	1.71116	0.74173
h	-1.27201	-0.47721	2.43437
h	0.99506	-1.36461	2.22215
h	-0.95124	-2.00837	-1.68484
h	1.28988	-1.16908	-2.18037
h	0.67968	2.63101	0.60750
h	-0.72678	2.29318	-1.39911
h	-1.24914	1.14690	2.21147
h	-2.35405	0.22821	1.44855
h	1.13147	-2.36938	0.93566
h	2.21753	-1.17996	1.16813
h	1.23118	0.44567	-2.45708
h	2.35351	-0.17898	-1.45646
h	-1.08274	-2.56637	-0.15086
h	1.35863	1.68997	1.75660
h	2.07013	1.84744	0.29741
h	-1.40386	1.03057	-2.18466
h	-2.10188	1.63315	-0.83948
h	-2.18611	-1.52839	-0.74455

-----  
 [Os(en)3]2+  
 -----

E(RI-PBE/def2-SVP) = -660.790344207 a.u.  
 E(RI-PBE/def2-SVP/COSMO(eps=80)) = -661.057174103 a.u.  
 E(B3LYP/def2-TZVP) = -661.713942830 a.u.

c	-0.76644	-1.40959	2.56738
c	0.72815	-1.64288	2.43751
n	1.10081	-1.58565	0.98474

os	-0.00019	0.00034	-0.00010
n	-1.10099	-1.54504	-1.04797
c	-0.72699	-1.54496	-2.50161
c	0.76754	-1.30577	-2.62115
n	1.11975	-0.06070	-1.86116
n	-1.12034	-0.13593	1.85703
n	1.12512	1.65297	0.85781
c	0.34304	2.92929	0.73700
c	-0.34265	2.95724	-0.61709
n	-1.12446	1.68670	-0.79106
h	-0.92619	0.64790	2.50528
h	-2.14767	-0.10732	1.74888
h	0.91498	-2.52234	0.57816
h	2.12798	-1.50235	0.91909
h	0.92444	0.74791	-2.47803
h	2.14707	-0.03459	-1.75219
h	-0.91485	-2.49675	-0.67852
h	-1.06975	-1.38412	3.63454
h	-1.33222	-2.23563	2.08809
h	1.01823	-2.60943	2.89965
h	1.29445	-0.84900	2.96785
h	1.07166	-1.23834	-3.68626
h	1.33365	-2.14947	-2.17405
h	-1.01600	-2.49286	-3.00159
h	-1.29330	-0.73120	-3.00084
h	1.40560	1.54337	1.84705
h	2.02755	1.78344	0.37111
h	-1.40389	1.61780	-1.78428
h	-2.02724	1.79706	-0.30028
h	-0.41029	2.95268	1.55284
h	0.98851	3.82209	0.86976
h	-0.98838	3.85463	-0.71279
h	0.41062	3.01466	-1.43115
h	-2.12831	-1.46481	-0.98031

-----  
[Os(en)3]3+  
-----

E(RI-PBE/def2-SVP)= -660.302961281 a.u.  
E(RI-PBE/def2-SVP/COSMO(eps=80))= -660.894773071 a.u.  
E(B3LYP/def2-TZVP)= -661.230224638 a.u.

c	-0.77604	-1.33560	2.63120
c	0.71808	-1.56743	2.52205
n	1.10113	-1.54820	1.05940
os	0.00038	-0.00031	0.00013
n	-1.10034	-1.57672	-1.01635
c	-0.72023	-1.63258	-2.47867
c	0.77385	-1.40464	-2.59612
n	1.12239	-0.13225	-1.85746
n	-1.12198	-0.08183	1.86049
n	1.09954	1.68823	0.83477
c	0.32530	2.97228	0.64367
c	-0.32710	2.95376	-0.72392
n	-1.09980	1.66422	-0.88070
h	-0.95162	0.73771	2.47145
h	-2.15033	-0.06161	1.72547
h	0.94732	-2.49687	0.67122
h	2.13057	-1.43803	0.99981
h	0.95374	0.67185	-2.48897
h	2.15078	-0.11122	-1.72290
h	-0.94472	-2.51517	-0.60451
h	-1.09360	-1.24473	3.69057
h	-1.35188	-2.17734	2.19359
h	1.01193	-2.52915	2.99153
h	1.29180	-0.77125	3.04032
h	1.08969	-1.34032	-3.65792
h	1.34962	-2.23592	-2.13881
h	-1.01557	-2.60541	-2.92366
h	-1.29457	-0.84915	-3.01534
h	1.35951	1.61014	1.83413
h	2.01722	1.79581	0.36383
h	-1.35892	1.55909	-1.87782
h	-2.01811	1.78329	-0.41367
h	-0.43344	3.03935	1.45164
h	0.98962	3.85401	0.75686
h	-0.99243	3.83135	-0.86056

h	0.43157	3.00033	-1.53354
h	-2.12975	-1.46626	-0.95715

-----  
[Os(bipy)3]2+  
-----

E(RI-PBE/def2-SVP)= -1573.74981835 a.u.  
E(RI-PBE/def2-SVP/COSMO(eps=80))= -1573.94603038 a.u.  
E(B3LYP/def2-TZVP)= -1576.14953027 a.u.

n	1.79075	-1.04019	0.23904
c	2.64029	-0.57850	1.22009
c	3.88365	-1.19497	1.45197
c	4.27581	-2.29243	0.67898
c	3.40450	-2.75458	-0.32067
c	2.18210	-2.10672	-0.50880
c	2.13511	0.57723	1.97571
n	0.90362	1.03877	1.56559
c	0.36176	2.10455	2.21377
c	1.00258	2.75168	3.27211
c	2.25953	2.28980	3.69495
c	2.82450	1.19315	3.03637
os	-0.00007	-0.00042	0.00009
n	-1.80663	1.04022	-0.00036
c	-2.77834	0.57888	0.86014
c	-4.04111	1.19585	0.92623
c	-4.32734	2.29325	0.10819
c	-3.33180	2.75482	-0.76804
c	-2.09551	2.10659	-0.79345
c	-2.37789	-0.57712	1.67566
n	-1.10373	-1.04007	1.43123
c	-0.65275	-2.10648	2.14486
c	-1.42781	-2.75307	3.10960
c	-2.72907	-2.28989	3.36327
c	-3.20144	-1.19258	2.63628
n	-0.68941	-1.03871	-1.67114
c	-1.53429	-2.10410	-1.63750
c	-1.98315	-2.75012	-2.79112
c	-1.55187	-2.28742	-4.04496
c	-0.68457	-1.19126	-4.09043
c	-0.26344	-0.57650	-2.89689
c	0.64496	0.57805	-2.83600
n	0.90470	1.03902	-1.56415
c	1.73746	2.10415	-1.41760
c	2.33511	2.75125	-2.50077
c	2.07407	2.28978	-3.80107
c	1.22076	1.19377	-3.96245
h	-1.84828	-2.44067	-0.63967
h	2.52914	2.77625	-4.67603
h	1.00212	0.81162	-4.96862
h	1.91639	2.44004	-0.38660
h	2.99886	3.60861	-2.31916
h	-0.33449	-0.80803	-5.05822
h	-1.88671	-2.77289	-4.97306
h	-2.66508	-3.60757	-2.70006
h	2.79110	2.77637	4.52558
h	0.51452	3.60955	3.75633
h	-0.62086	2.44088	1.85439
h	3.80550	0.81077	3.34868
h	4.54777	-0.81221	2.23853
h	5.24629	-2.77932	0.85318
h	3.66497	-3.61290	-0.95627
h	1.47422	-2.44280	-1.27930
h	-5.31200	2.78080	0.15282
h	-3.50592	3.61323	-1.43245
h	-1.29196	2.44238	-1.46373
h	-4.80308	0.81364	1.61860
h	-4.21457	-0.80925	2.81712
h	-3.36573	-2.77596	4.11669
h	-1.00852	-3.61136	3.65373
h	0.36804	-2.44339	1.91710

-----  
[Os(bipy)3]3+  
-----

E(RI-PBE/def2-SVP) = -1573.30912334 a.u.  
 E(RI-PBE/def2-SVP/COSMO(eps=80)) = -1573.73994464 a.u.  
 E(B3LYP/def2-TZVP) = -1575.71882795 a.u.

n	1.48906	-1.01454	1.06747
c	1.73498	-0.56520	2.34709
c	2.71234	-1.18288	3.14792
c	3.44564	-2.26486	2.64639
c	3.19015	-2.71061	1.33904
c	2.21391	-2.05928	0.58128
c	0.91336	0.57826	2.77181
n	0.00698	1.02431	1.83340
c	-0.81714	2.05907	2.14873
c	-0.76658	2.70652	3.38590
c	0.15996	2.26763	4.34714
c	1.00258	1.19374	4.03385
os	-0.00034	0.00331	-0.00029
n	-1.59249	1.01272	-0.91870
c	-2.85798	0.56729	-0.59983
c	-3.99461	1.17041	-1.16947
c	-3.84539	2.23084	-2.07296
c	-2.55034	2.67162	-2.39410
c	-1.45460	2.03777	-1.80346
c	-2.89986	-0.56286	0.33988
n	-1.66860	-1.01385	0.76345
c	-1.60724	-2.04611	1.64504
c	-2.75179	-2.68377	2.12941
c	-4.01265	-2.23424	1.70302
c	-4.08327	-1.16473	0.80285
n	0.17900	-1.02378	-1.81833
c	-0.60521	-2.06590	-2.20353
c	-0.44375	-2.71074	-3.43303
c	0.55310	-2.25769	-4.31371
c	1.35654	-1.17727	-3.92788
c	1.15896	-0.56995	-2.67516
c	1.94761	0.56515	-2.17459
n	1.58509	1.02003	-0.92594
c	2.27386	2.05561	-0.37376
c	3.32735	2.69280	-1.03365
c	3.70131	2.24121	-2.31079
c	3.00468	1.16789	-2.88007
h	-1.37549	-2.39329	-1.49060
h	4.52952	2.71822	-2.85688
h	3.28813	0.79844	-3.87524
h	1.95359	2.38399	0.62512
h	3.84518	3.53278	-0.54762
h	2.13866	-0.80683	-4.60453
h	0.70153	-2.73939	-5.29227
h	-1.09651	-3.55738	-3.69274
h	0.22455	2.75497	5.33190
h	-1.44915	3.54484	3.58920
h	-1.52758	2.37873	1.37317
h	1.72901	0.83381	4.77488
h	2.90178	-0.81986	4.16763
h	4.21013	-2.75497	3.26956
h	3.74100	-3.55785	0.90430
h	1.98482	-2.38248	-0.44554
h	-4.73053	2.70555	-2.52342
h	-2.38551	3.50147	-3.09706
h	-0.42728	2.35831	-2.02704
h	-4.99949	0.81040	-0.91118
h	-5.06110	-0.79837	0.46223
h	-4.93387	-2.71134	2.07110
h	-2.65060	-3.52280	2.83402
h	-0.60394	-2.37054	1.95685