

Effect of Spin-Orbit Coupling on Reduction Potentials of Octahedral Ruthenium (II/III) and Osmium (II/III) Complexes.

(Supplementary Material)

*Martin Srnec,[§] Jakub Chalupský,[§] Miroslav Fojta,[‡] Lucie Zendlová,[§] Luděk Havran,[‡] Michal Hocek,[§]
Mojmír Kývala,^{§*} and Lubomír Rulíšek^{§*}*

Institute of Organic Chemistry and Biochemistry of the Academy of Sciences of the Czech Republic,
Centre for Complex Molecular Systems and Biomolecules, Gilead Sciences Research Center & IOCB,
Flemingovo náměstí 2, 166 10 Praha 6, Institute of Biophysics, Academy of Sciences of the Czech
Republic, Královopolská 135, 612 65 Brno, Czech Republic

E-mail: kyvala@uochb.cas.cz, lubos@uochb.cas.cz.

[§] Inst. Org. Chem. and Biochem. AS CR

[‡] Inst. of Biophysics, AS CR

* Corresponding authors. Tel.: +420-220-183-263, Fax: +420-220-183-578

Table S1 (Supporting Information): The calculated splittings of the $^2T_{2g}$ (or 2T_g) degenerate ground state into the $E_{(5/2)g}$ (or $E_{(1/2)g}$) and $G_{(3/2)g}$ states calculated using the CASSCF(5,3)/CASPT2/CASSI method and various contractions of the ANO-RCC basis set. All values are in cm^{-1} . All three complexes attain ideal octahedral (O_h) or T_h ($[\text{Ru}(\text{H}_2\text{O})_6]^{2+/3+}$ complexes) symmetry.

Complex	Basis set				
	MB	DZP	TZP/DZ	TZP/DZP	TZP
$[\text{Ru}(\text{H}_2\text{O})_6]^{2+/3+}$	1461	1585	1586	1573	1576
$[\text{RuCl}_6]^{4-/3-}$	1464	1554	1556	1547	1546
$[\text{Ru}(\text{CN})_6]^{4-/3-}$	1383	1350	1375	1354	1351
$[\text{Os}(\text{H}_2\text{O})_6]^{2+/3+}$	4799	5142	5111	5061	5070
$[\text{OsCl}_6]^{4-/3-}$	4725	4979	4988	4938	4926
$[\text{Os}(\text{CN})_6]^{4-/3-}$	4364	4135	4227	4155	4140
MB	Os[6s5p3d1f], Ru[5s4p2d], Cl[3s2p], O, N, C[2s1p], H[1s]				
DZP	Os[7s6p4d2f1g], Ru[6s5p3d1f], Cl[4s3p1d], O, N, C[3s2p1d], H[2s1p]				
TZP/DZ	Os[8s7p5d3f2g], Ru[7s6p4d2f1g], Cl[4s3p], O, N, C[3s2p], H[2s]				
TZP/DZP	Os[8s7p5d3f2g], Ru[7s6p4d2f1g], Cl[4s3p1d], O, N, C[3s2p1d], H[2s1p]				
TZP	Os[8s7p5d3f2g], Ru[7s6p4d2f1g], Cl[5s4p2d1f], O, N, C[4s3p2d1f], H[3s2p1d]				

Table S2 (Supporting Information): The calculated one-component relativistic (without SOC) and two-component relativistic (with SOC) energy splittings of the ideally degenerate $^2T_{2g}$ state into three Kramers' doublets (CASSCF(5,3)/CASPT2/CASSI). The reference energy (0 cm⁻¹) is the energy of the one-component relativistic ground state (1^2A) for the one-component relativistic calculations (columns 2, 3) and the energy of the relativistic ground state ($1E_{1/2}$) for the relativistic calculations (columns 4, 5). The energy difference between the two ground states (1^2A and $1E_{1/2}$) is then shown in the last column (in mV) and it corresponds to the shift in the reduction potential originating in SOC. An effect of basis set contraction is demonstrated.

Complex	Basis set	2^2A	3^2A	$2E_{1/2}$	$3E_{1/2}$	ΔE^0 (mV)
[Ru(H ₂ O) ₆] ^{2+/3+}	TZP/DZ	3946	5064	4024	5426	-18
	TZP/DZP	3996	5131	4068	5485	-18
[RuCl ₆] ^{4-/3-}	TZP/DZ	134	206	1514	1626	-116
	TZP/DZP	92	214	1500	1613	-116
[Ru(NH ₃) ₆] ^{2+/3+}	MB	415	429	1402	1627	-90
	DZP	470	501	1473	1733	-92
	TZP/DZ	364	394	1485	1689	-100
	TZP/DZP	407	487	1467	1712	-94
	TZP	445	513	1467	1727	-92
[Ru(en) ₃] ^{2+/3+}	TZP/DZ	1234	1247	1749	2148	-59
	TZP/DZP	1284	1326	1770	2186	-56
[Ru(bipy) ₃] ^{2+/3+}	TZP/DZ	1857	1866	2151	2586	-42
	TZP/DZP	1821	1829	2120	2547	-42
[Ru(CN) ₆] ^{4-/3-}	TZP/DZ	286	294	1356	1495	-94
	TZP/DZP	286	296	1336	1474	-92
[Os(H ₂ O) ₆] ^{2+/3+}	TZP/DZ	4845	6389	6230	8672	-152
	TZP/DZP	4756	6324	6139	8591	-151
[OsCl ₆] ^{4-/3-}	TZP/DZ	78	194	4922	5024	-400
	TZP/DZP	202	272	4863	4970	-387
[Os(NH ₃) ₆] ^{2+/3+}	MB	663	702	4701	4999	-344
	DZP	681	761	4833	5158	-353
	TZP/DZ	610	638	4862	5125	-362
[Os(en) ₃] ^{2+/3+}	TZP/DZ	1609	1709	5012	5368	-292
	TZP/DZP	1721	1858	4975	5391	-280
[Os(bipy) ₃] ^{2+/3+}	TZP/DZ	2265	2281	5138	5445	-250
[Os(CN) ₆] ^{4-/3-}	TZP/DZ	293	305	4286	4367	-333

Table S3 (Supporting Information): The calculated CASSCF(5,5)/MRCI/TZV-DKH and CASSCF(6,5)/MRCI//TZV-DKH stabilizations of the doublet and singlet ground states, using MRCI natural orbitals (30 iterations were used). Orbitals are state-averaged over lowest singlet, triplet and quintet in the case of M^{2+} and over 3 lowest doublets, lowest quartet and sextet in the case of M^{3+} . Threshold for configuration selection of 10^{-5} a.u. for both the reference CASCI space and the MRCI space was used. All orbitals were correlated during MRCI calculations (frozen and deleted orbitals were not used). Energy stabilization values are in cm^{-1} .

Ground state	$\Delta E_{\text{stab}} (\text{cm}^{-1})$			
	$1^1\text{A}(=\text{S}_0)$	$1^2\text{A}(=\text{D}_1)$	$1^2\text{A}(=\text{D}_1)$	$1^2\text{A}(=\text{D}_1)$
interacting states	$\text{S}_{1-15}, \text{T}_{1-10}, \mathbf{5}_{1-5}$	$\text{D}_2\text{-D}_3$	$\text{D}_{2-15}, \text{Q}_{1-10}, \mathbf{6}_1$	$\text{D}_{4-15}, \text{Q}_{1-10}, \mathbf{6}_1$
$[\text{Ru}(\text{NH}_3)_6]^{2+/3+}$	-232	-791	-1126	-335
$[\text{Os}(\text{NH}_3)_6]^{2+/3+}$	-2129	-2508	-5319	-2811

Table S4 (Supporting Information): The calculated CASSCF(5,5)/RAS(9:2,2/5/2,2)/MRCI/TZV-DKH (and CASSCF(6,5)/RAS(10:2,2/5/2,2)/MRCI/TZV-DKH) stabilizations of the doublet and singlet ground states. CASSCF(5,5) is state-averaged (over the three lowest doublets) for M^{3+} complexes and CASSCF(6,5) is state-specific (for the lowest singlet) for M^{2+} complexes. Threshold for configuration selection of 10^{-5} a.u. for both the reference RAS space and the CISD space was used. An orbital window from -3 to 3 a.u. for the Ru complexes and from -1.9 to 2 a.u. for the Os complexes was used for the MRCI calculations. Energy stabilization values are in cm^{-1} .

Ground state	$\Delta E_{\text{stab}} (\text{cm}^{-1})$					
	$1^1\text{A}(=\text{S}_0)$	$1^1\text{A}(=\text{S}_0)$	$1^1\text{A}(=\text{S}_0)$	$1^2\text{A}(=\text{D}_1)$	$1^2\text{A}(=\text{D}_1)$	$1^2\text{A}(=\text{D}_1)$
interacting states	$\text{S}_{1-15}, \text{T}_{1-10}, \text{S}_{1-5}$	$\text{S}_{1-25}, \text{T}_{1-20}, \text{S}_{1-15}$	$\text{S}_{1-35}, \text{T}_{1-30}, \text{S}_{1-25}$	$\text{D}_{2-15}, \text{Q}_{1-10}, \text{D}_{1-5}$	$\text{D}_{2-25}, \text{Q}_{1-20}, \text{D}_{1-15}$	$\text{D}_{2-35}, \text{Q}_{1-30}, \text{D}_{1-25}$
$[\text{Ru}(\text{NH}_3)_6]^{2+/3+}$	-223	-224	-223	-679	-629	-653
$[\text{Ru}(\text{H}_2\text{O})_6]^{2+/3+}$	-372	-370	-372	-544	-544	-544
$[\text{Ru}(\text{CN})_6]^{4-/3-}$	-19	-29	-29	-925	-1034	-
$[\text{Os}(\text{NH}_3)_6]^{2+/3+}$	-1616	-1646	-1673	-5309	-5309	-5345
$[\text{Os}(\text{H}_2\text{O})_6]^{2+/3+}$	-2651	-2756	-2782	-4487	-4582	-4606
$[\text{Os}(\text{CN})_6]^{4-/3-}$	-86	-91	-99	-2527	-2549	-2580

Supporting Information: The equilibrium geometries and molecular energies of all the studied species.

[Ru(Cl)6]4-

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.
E(ZPE-RTlnq(trans)q(rot)q(vib)= -113.97 kJ.mol⁻¹

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

[Ru(Cl)6]3-

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.
E(ZPE-RTlnq(trans)q(rot)q(vib)= -93.27 kJ.mol⁻¹

E[CASSCF/ANO_RCC/TZP/DZ] = -7292.99768936 -7292.99701929 -7292.99675910
E[CASPT2/ANO_RCC/TZP/DZ] = -7294.17486625 -7294.17425433 -7294.17392900
E[QDPT-SOC/CASPT2/TZP/DZ] = -7294.17911911 -7294.17222160 -7294.17170887

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

[Ru(CN)6]4-

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.
E(ZPE-RTlnq(trans)q(rot)q(vib)= 14.86 kJ.mol⁻¹

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

[Ru(CN)6]3-

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.
E(ZPE-RTlnq(trans)q(rot)q(vib)= 9.76 kJ.mol⁻¹

E[CASSCF/ANO_RCC/TZP/DZ] = -5081.19764608 -5081.19612942 -5081.19608670
E[CASPT2/ANO_RCC/TZP/DZ] = -5082.82299703 -5082.82169534 -5082.82165663
E[QDPT-SOC/CASPT2/TZP/DZ] = -5082.82644694 -5082.82026732 -5082.81963474

ru	-0.00001	0.00001	0.00001
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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

[Ru(H2O)6]2+

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.
E(ZPE-RTlnq(trans)q(rot)q(vib))= 292.47 kJ.mol-1

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

[Ru(H2O)6]3+

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.
E(ZPE-RTlnq(trans)q(rot)q(vib))= 276.94 kJ.mol-1

E[CASSCF/ANO_RCC/TZP/DZ] = -4982.82471025 -4982.81115403 -4982.80683542
E[CASPT2/ANO_RCC/TZP/DZ] = -4984.23303239 -4984.21505457 -4984.20995737
E[QDPT-SOC/CASPT2/TZP/DZ] = -4984.23370000 -4984.21536670 -4984.20897714

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

[Ru(NH3)6]2+

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.
 E(ZPE-RTlnq(trans)q(rot)q(vib)= 481.64 kJ.mol⁻¹

ru	-0.000008	-0.000070	0.000005
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

[Ru(NH3)6]3+

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.
 E(ZPE-RTlnq(trans)q(rot)q(vib)= 489.39 kJ.mol⁻¹

E[CASSCF/ANO_RCC/TZP/DZ] = -4863.78632617 -4863.78472640 -4863.78467495
 E[CASPT2/ANO_RCC/TZP/DZ] = -4865.19293155 -4865.19127120 -4865.19113544
 E[QDPT-SOC/CASPT2/TZP/DZ] = -4865.19659954 -4865.18983485 -4865.18890379

ru	-0.000002	-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

[Ru(en)3]2+

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.

E(ZPE-RTlnq(trans)q(rot)q(vib)= 783.65 kJ.mol⁻¹

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

[Ru(en)3]3+

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.
E(ZPE-RTlnq(trans)q(rot)q(vib)= 784.38 kJ.mol⁻¹

E[CASSCF/ANO_RCC/TZP/DZ] = -5094.42624778 -5094.41987920 -5094.41980429
E[CASPT2/ANO_RCC/TZP/DZ] = -5096.37836324 -5096.37274235 -5096.37268178
E[QDPT-SOC/CASPT2/TZP/DZ] = -5096.38051367 -5096.37254573 -5096.37072796

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

[Ru(bipy)3]2+

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.
E(ZPE-RTlnq(trans)q(rot)q(vib)= 1083.28 kJ.mol-1

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

[Ru(bipy)3]3+

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.
 E(ZPE-RTlnq(trans)q(rot)q(vib)= 1082.77 kJ.mol⁻¹

E[CASSCF/ANO_RCC/TZP/DZ] = -6003.15155892 -6003.14188553 -6003.14186099
 E[CASPT2/ANO_RCC/TZP/DZ] = -6006.76938100 -6006.76092178 -6006.76087859
 E[QDPT-SOC/CASPT2/TZP/DZ] = -6006.77092189 -6006.76112097 -6006.75913851

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

[Os(CL)6]4-

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.
E(ZPE-RTlnq(trans)q(rot)q(vib))= -118.30 kJ.mol⁻¹

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]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.
E(ZPE-RTlnq(trans)q(rot)q(vib))= -95.90 kJ.mol⁻¹

E[CASSCF/ANO_RCC/TZP/DZ] = -20003.27580839 -20003.27527120 -20003.27496369
E[CASPT2/ANO_RCC/TZP/DZ] = -20004.42321211 -20004.42285612 -20004.42232608
E[QDPT-SOC/CASPT2/TZP/DZ] = -20004.43790304 -20004.41547833 -20004.41501295

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(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.
E(ZPE-RTlnq(trans)q(rot)q(vib))= 14.62 kJ.mol⁻¹

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.
E(ZPE-RTlnq(trans)q(rot)q(vib))= 9.73 kJ.mol⁻¹

E[CASSCF/ANO_RCC/TZP/DZ] = -17791.52088309 -17791.51939015 -17791.51934765
E[CASPT2/ANO_RCC/TZP/DZ] = -17793.11264801 -17793.11131449 -17793.11125685

E[QDPT-SOC/CASPT2/TZP/DZ] = -17793.12488249 -17793.10535309 -17793.10498377

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.
E(ZPE-RTlnq(trans)q(rot)q(vib))= 295.27 kJ.mol-1

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.
E(ZPE-RTlnq(trans)q(rot)q(vib))= 276.50 kJ.mol-1

E[CASSCF/ANO_RCC/TZP/DZ] = -17693.08964211 -17693.07230071 -17693.06623354
E[CASPT2/ANO_RCC/TZP/DZ] = -17695.60532808 -17695.58325129 -17695.57621667
E[QDPT-SOC/CASPT2/TZP/DZ] = -17695.61089869 -17695.58251326 -17695.57138410

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.
E(ZPE-RTlnq(trans)q(rot)q(vib)= 490.56 kJ.mol-1

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.
E(ZPE-RTlnq(trans)q(rot)q(vib)= 491.17 kJ.mol-1

E[CASSCF/ANO_RCC/TZP/DZ] = -17574.07057646 -17574.06802908 -17574.06792255
E[CASPT2/ANO_RCC/TZP/DZ] = -17575.02083548 -17575.01805696 -17575.01792923
E[QDPT-SOC/CASPT2/TZP/DZ] = -17575.03410839 -17575.01195702 -17575.01075626

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.
 E(ZPE-RTlnq(trans)q(rot)q(vib)= 782.73 kJ.mol⁻¹

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.
 E(ZPE-RTlnq(trans)q(rot)q(vib)= 784.44 kJ.mol⁻¹

E[CASSCF/ANO_RCC/TZP/DZ] = -17804.71331454 -17804.70543031 -17804.70518089
 E[CASPT2/ANO_RCC/TZP/DZ] = -17806.18908052 -17806.18174795 -17806.18129173
 E[QDPT-SOC/CASPT2/TZP/DZ] = -17806.19980481 -17806.17696887 -17806.17534651

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.
 E(ZPE-RTlnq(trans)q(rot)q(vib)= 1081.09 kJ.mol-1

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.
E(ZPE-RTlnq(trans)q(rot)q(vib))= 1082.02 kJ.mol⁻¹

E[CASSCF/ANO_RCC/TZP/DZ] = -18713.44266979 -18713.43143117 -18713.43136505
E[CASPT2/ANO_RCC/TZP/DZ] = -18717.03707963 -18717.02675917 -18717.02668755
E[QDPT-SOC/CASPT2/TZP/DZ] = -18717.04624920 -18717.02283811 -18717.02143904

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

Three systems with 12, 14, and 27 water molecules in the second solvation sphere. The water molecules were added using the LeaP program from Amber suite, TIP3P water model (taken as a snapshot from the molecular dynamics) with a solvation shell 3.81 Å and closeness parameter 0.8. This yielded 12 water molecules for [Ru(H₂O)₆]^{2+/3+}, 14 water molecules for [Ru(NH₃)₆]^{2+/3+} and 27 water molecules for [Ru(bipy)₃]^{2+/3+}.

[Ru(H₂O)₆]²⁺{12H₂O}

E(RI-PBE/def2-SVP)= -1467.89392878 a.u.
E(RI-PBE/def2-SVP/COSMO(eps=80))= -1468.13947142 a.u.
E(B3LYP/def2-TZVP)= -1470.37297331 a.u.
E(ZPE-RTlnq(trans)q(rot)q(vib))= 983.82 kJ.mol⁻¹

ru	0.30730	0.06258	-0.27287
o	-0.94265	0.80362	-1.85069
h	-0.85317	1.79214	-1.88901
h	-1.91141	0.62090	-1.67778
o	-1.13995	0.10314	1.28556
h	-1.84998	-0.58311	1.51677
h	-1.65629	0.94311	1.23786
o	0.61158	2.03771	0.46354
h	0.54657	2.71084	-0.25984
h	1.50314	2.09690	0.91031
o	1.64457	-0.78353	1.15231
h	1.15688	-1.44349	1.70258
h	2.03953	-0.07815	1.72825
o	1.89352	0.25230	-1.69580
h	2.79989	0.25435	-1.28154
h	1.87704	-0.46406	-2.37753
o	-0.05457	-1.95435	-0.93408
h	0.36576	-2.09980	-1.82130
h	-1.09457	-2.12573	-1.06867
o	-3.46861	0.18771	-1.10279
h	-3.54835	0.79155	-0.30965
h	-4.27224	0.32938	-1.63871
o	4.32489	0.72235	-0.46535
h	5.02793	-0.00186	-0.36811
h	4.76809	1.43314	-0.96854
o	-2.51678	-2.40774	-1.11003
h	-2.67705	-2.99722	-0.32771
h	-3.01347	-1.56398	-0.95128
o	-0.45643	3.50599	-1.54356
h	-1.19671	4.00706	-1.11173
h	-0.12221	4.07388	-2.26376
o	-2.37750	-3.78341	1.26780
h	-1.38711	-3.71508	1.43604
h	-2.65675	-4.68820	1.50254
o	-3.15346	-1.37566	2.07533
h	-3.01678	-2.34932	1.89218
h	-3.20191	-1.32176	3.04819
o	1.17120	-1.79986	-3.39770
h	0.53621	-1.42247	-4.03954
h	1.64947	-2.49431	-3.89217
o	0.24089	-3.18209	1.39536
h	0.27510	-2.87211	0.43507
h	0.90551	-3.89428	1.46733
o	-2.59777	4.56081	-0.07863
h	-2.31702	5.19266	0.61487
h	-3.31268	5.03120	-0.55494
o	-3.20767	1.99116	0.89437
h	-3.80340	2.02851	1.66722
h	-3.07322	2.93125	0.60538
o	6.13806	-1.18151	-0.24211
h	6.72272	-1.41991	-0.98530
h	6.70488	-1.26319	0.54838
o	2.92171	1.50133	1.68264
h	3.59246	1.27048	0.97000
h	3.40565	1.93217	2.41141

[Ru(H₂O)₆]³⁺{12H₂O}

E(RI-PBE/def2-SVP)= -1467.51460567 a.u.
E(RI-PBE/def2-SVP/COSMO(eps=80))= -1467.99588610 a.u.
E(B3LYP/def2-TZVP)= -1469.96141999 a.u.
E(ZPE-RTlnq(trans)q(rot)q(vib))= 985.94 kJ.mol⁻¹

ru	0.31968	0.00356	-0.05619
o	-0.85566	0.91762	-1.44934
h	-0.78395	1.92174	-1.40692
h	-1.85728	0.65147	-1.45215
o	-1.15074	0.07876	1.30640
h	-2.06456	-0.47471	1.60581
h	-1.03563	0.88935	1.84743
o	0.73597	1.85449	0.85628
h	0.54035	2.65530	0.28927
h	1.64967	1.87303	1.28387
o	1.54423	-0.94362	1.26184
h	1.23766	-1.83413	1.62618
h	2.14772	-0.37369	1.82762
o	1.87826	0.08692	-1.39671
h	2.82298	0.32185	-1.08577
h	1.89748	-0.62072	-2.10404
o	-0.16826	-1.89742	-0.82410
h	0.23670	-2.03741	-1.72455
h	-1.27839	-2.09405	-0.90033
o	-3.33443	0.23932	-1.24587
h	-3.67718	0.91341	-0.55076
h	-3.92315	0.31683	-2.02436
o	4.24226	0.79941	-0.44608
h	5.03804	0.14096	-0.53775
h	4.57183	1.63064	-0.84642
o	-2.56386	-2.35735	-0.88498
h	-2.76231	-2.90889	-0.08367
h	-3.08580	-1.50999	-0.84743
o	-0.42824	3.50484	-0.91248
h	-1.25116	4.00189	-0.62033
h	0.01206	4.08457	-1.56728
o	-2.39280	-3.60017	1.59034
h	-1.40607	-3.66597	1.71978
h	-2.78789	-4.43368	1.91797
o	-3.16528	-1.14894	1.95254
h	-2.95768	-2.13863	2.01990
h	-3.60918	-0.88112	2.78103
o	1.34496	-1.90312	-3.13747
h	0.96345	-1.62431	-3.99683
h	1.90536	-2.67650	-3.35906
o	0.37256	-3.29736	1.41700
h	0.28127	-3.06919	0.44626
h	0.91585	-4.11088	1.46875
o	-2.83392	4.58221	-0.15552
h	-2.83010	5.20315	0.60456
h	-3.31006	5.07688	-0.85693
o	-3.91600	2.03407	0.53689
h	-4.82320	2.09502	0.89620
h	-3.67172	2.96306	0.29321
o	6.19524	-0.85921	-0.69974
h	6.74312	-0.87432	-1.50945
h	6.82943	-1.01973	0.02699
o	3.02159	1.11410	1.90609
h	3.67778	1.04845	1.14252
h	3.50423	1.44361	2.69108

[Ru(NH3)6]2+{14H2O}

E(RI-PBE/def2-SVP)= -1501.48804213 a.u.
E(RI-PBE/def2-SVP/COSMO(eps=80))= -1501.71862571 a.u.
E(B3LYP/def2-TZVP)= -1504.05334892 a.u.
E(ZPE-RTlnq(trans)q(rot)q(vib)= 1259.17 kJ.mol⁻¹

n	1.74838	-1.75466	-0.27133
ru	0.25717	-0.19822	-0.47281
n	-1.15165	1.40064	-0.65438
n	-1.26242	-1.70606	-0.44461
n	0.37901	-0.32086	-2.61859
n	0.08420	-0.03961	1.65515
n	1.79696	1.32434	-0.49365
h	0.82015	-0.52622	2.19576
h	1.87252	-2.06467	0.71161
h	-1.42593	-2.12814	-1.38151
h	-0.14193	-1.13600	-3.00105
h	1.80935	1.96307	0.32416
h	-1.05187	1.90752	-1.55471

h	0.08960	0.97400	1.91026
h	-0.81254	-0.36883	2.05790
h	1.57140	-2.61461	-0.82193
h	2.69069	-1.43228	-0.56021
h	-0.00993	0.52597	-3.08284
h	1.33583	-0.41782	-2.99507
h	-1.00056	-2.50429	0.15799
h	2.75316	0.92541	-0.54416
h	1.74236	1.96402	-1.30671
h	-2.16526	1.18846	-0.59380
h	-0.97466	2.08538	0.11033
h	-2.19249	-1.41700	-0.08095
o	1.82571	3.58371	-3.06489
h	2.46317	3.56550	-3.80504
h	1.80068	4.52473	-2.80287
o	-2.72713	2.55320	3.31208
h	-2.96274	3.00044	4.14662
h	-3.40583	2.89676	2.61013
o	3.71025	4.05564	3.89880
h	4.61005	4.41743	3.79385
h	3.36936	4.50350	4.69592
o	2.08378	-2.15160	2.75216
h	2.93115	-1.98593	3.20776
h	1.67252	-2.85446	3.29068
o	-4.32998	3.32331	1.45218
h	-4.35859	2.61545	0.73983
h	-5.26275	3.50830	1.66485
o	-3.90146	-0.97242	0.95104
h	-4.61441	-1.60701	1.14959
h	-3.53089	-0.67559	1.84745
o	1.10917	-4.38959	-2.25389
h	1.81558	-4.60231	-2.89502
h	0.91957	-5.24816	-1.82705
o	-2.70537	-0.09785	3.12064
h	-2.73910	0.90686	3.25662
h	-2.87018	-0.48178	4.00133
o	-4.22375	1.31620	-0.30840
h	-4.77957	1.24439	-1.10591
h	-4.25769	0.41479	0.14268
o	-0.58422	2.33369	-3.45036
h	0.23215	2.89693	-3.44063
h	-1.14726	2.69515	-4.15855
o	2.06691	3.76727	1.76180
h	2.67806	3.84770	2.54945
h	2.08476	4.65906	1.36780
o	-1.01949	-2.87067	-3.13892
h	-1.57185	-3.25495	-3.84362
h	-0.31273	-3.54002	-2.94927
o	4.39921	-0.30337	-0.82293
h	4.93431	-0.29169	-1.63957
h	5.06909	-0.34098	-0.11396
o	-0.42576	2.75997	1.81499
h	0.39311	3.28384	2.01286
h	-1.11838	2.91599	2.50251

[Ru(NH3)6]3+{14H2O}

E(RI-PBE/def2-SVP)= -1501.14224933 a.u.
E(RI-PBE/def2-SVP/COSMO(eps=80))= -1501.60633611 a.u.
E(B3LYP/def2-TZVP)= -1503.67635666 a.u.
E(ZPE-RTlnq(trans)q(rot)q(vib)= 1292.69 kJ.mol⁻¹

n	1.72936	-1.70020	-0.25946
ru	0.23242	-0.15025	-0.43033
n	-1.17692	1.41263	-0.60036
n	-1.29227	-1.64016	-0.39613
n	0.35529	-0.26004	-2.56100
n	0.06608	-0.06972	1.66930
n	1.79565	1.33807	-0.49078
h	0.81253	-0.56789	2.19178
h	1.83202	-2.03060	0.72426
h	-1.41587	-2.07731	-1.34003
h	-0.16647	-1.08928	-2.93471
h	1.81920	2.02133	0.30294
h	-1.03577	1.95063	-1.48257
h	0.06857	0.96322	1.92169
h	-0.84465	-0.38033	2.07327

h	1.54970	-2.54691	-0.83537
h	2.67735	-1.36309	-0.52878
h	-0.06010	0.60078	-2.99952
h	1.31348	-0.33414	-2.93554
h	-1.04187	-2.42133	0.23022
h	2.74218	0.90500	-0.51417
h	1.75973	1.94367	-1.33335
h	-2.19875	1.19388	-0.57843
h	-1.00883	2.06346	0.20886
h	-2.24038	-1.34425	-0.06163
o	1.85538	3.46279	-3.05408
h	2.47141	3.39509	-3.81202
h	1.86500	4.41815	-2.84109
o	-2.68305	2.42637	3.32643
h	-2.91485	2.83751	4.18198
h	-3.34608	2.81350	2.62899
o	3.65452	3.88546	3.58884
h	4.57244	4.19951	3.47576
h	3.34431	4.34932	4.39051
o	2.01391	-2.12074	2.67145
h	2.87951	-1.96966	3.10083
h	1.63395	-2.85764	3.19070
o	-4.13627	3.29992	1.41980
h	-4.27142	2.60436	0.71770
h	-4.99532	3.74643	1.53773
o	-3.85181	-1.01361	0.87455
h	-4.55786	-1.67331	1.01830
h	-3.51568	-0.73972	1.79201
o	1.12270	-4.22897	-2.18363
h	1.81000	-4.44718	-2.84664
h	0.92705	-5.09641	-1.77291
o	-2.60481	-0.19861	3.03733
h	-2.69156	0.80021	3.22881
h	-2.76276	-0.63849	3.89543
o	-4.10979	1.27915	-0.39891
h	-4.73497	1.28819	-1.14911
h	-4.23489	0.39403	0.06214
o	-0.57412	2.30841	-3.30826
h	0.25077	2.86404	-3.38174
h	-1.18069	2.61920	-4.00742
o	1.99184	3.61289	1.54421
h	2.64045	3.69785	2.31772
h	2.01190	4.49973	1.13559
o	-0.99937	-2.72874	-3.02986
h	-1.59849	-3.05492	-3.72870
h	-0.30851	-3.43252	-2.89170
o	4.30635	-0.29083	-0.76018
h	4.83877	-0.29919	-1.58079
h	4.98199	-0.33203	-0.05413
o	-0.43855	2.60383	1.86283
h	0.35897	3.19340	1.96529
h	-1.14436	2.78853	2.54303

[Ru(bipy)3]2+{27H2O}

E(RI-PBE/def2-SVP)= -3638.00429979 a.u.
E(RI-PBE/def2-SVP/COSMO(eps=80))= -3638.23088204 a.u.
E(B3LYP/def2-TZVP)= -3644.25107783 a.u.
E(ZPE-RTlnq(trans)q(rot)q(vib)= 2541.47 kJ.mol⁻¹

n	-1.29586	-1.38491	-1.78158
c	-1.55030	-0.87835	-3.03260
c	-2.34687	-1.58014	-3.95208
c	-2.90393	-2.81129	-3.59082
c	-2.65990	-3.31378	-2.30499
c	-1.85039	-2.57206	-1.43891
c	-0.89363	0.40582	-3.32522
n	-0.19329	0.94951	-2.27400
c	0.51911	2.08587	-2.48046
c	0.52792	2.75445	-3.70808
c	-0.21668	2.23391	-4.77842
c	-0.92115	1.03891	-4.58252
ru	-0.11119	-0.21630	-0.57028
n	1.16397	1.01803	0.47568
c	2.49700	0.83576	0.21403
c	3.47801	1.57682	0.88917
c	3.10183	2.49954	1.86731

c	1.73699	2.69439	2.12054
c	0.80170	1.94253	1.40019
c	2.79759	-0.15577	-0.82900
n	1.70906	-0.84193	-1.31338
c	1.89728	-1.76759	-2.28755
c	3.16566	-2.05248	-2.80943
c	4.28034	-1.34287	-2.33749
c	4.08999	-0.38131	-1.33690
n	-0.12613	-1.43917	1.08463
c	0.80349	-2.38615	1.36479
c	0.84305	-3.06959	2.58238
c	-0.12272	-2.77081	3.55806
c	-1.10680	-1.82198	3.26169
c	-1.09276	-1.16609	2.01801
c	-2.05896	-0.13491	1.61637
n	-1.80952	0.44301	0.39532
c	-2.64975	1.40785	-0.05106
c	-3.74966	1.84882	0.68833
c	-4.01285	1.26525	1.93823
c	-3.15595	0.26111	2.40146
h	1.53998	-2.58085	0.57256
h	-4.86714	1.58870	2.55996
h	-3.32382	-0.20243	3.38588
h	-2.40176	1.84328	-1.03019
h	-4.36703	2.67794	0.31699
h	-1.87055	-1.55749	4.00636
h	-0.09093	-3.23208	4.55725
h	1.66065	-3.77673	2.78605
h	-0.24058	2.71871	-5.76921
h	1.15367	3.65226	-3.80787
h	1.14743	2.44589	-1.65333
h	-1.42578	0.55360	-5.43141
h	-2.48174	-1.18167	-4.96609
h	-3.49124	-3.37946	-4.32585
h	-3.05100	-4.27358	-1.91933
h	-1.62944	-2.95448	-0.43193
h	3.88641	3.05417	2.40166
h	1.36560	3.38857	2.89061
h	-0.27464	2.09857	1.56165
h	4.53547	1.44742	0.63563
h	4.92528	0.25308	-1.00320
h	5.29058	-1.50137	-2.74410
h	3.23571	-2.81606	-3.59732
h	1.01775	-2.29601	-2.69874
o	0.26436	-2.65745	6.72431
h	-0.19133	-1.76672	6.79078
h	0.21163	-3.04280	7.61817
o	-0.97609	-0.24889	6.65122
h	-0.89913	0.31149	7.44594
h	-0.50981	0.29681	5.86611
o	0.07005	0.96896	4.71904
h	-0.07385	1.96170	4.65970
h	1.04657	0.81023	4.61170
o	2.82135	-2.19517	5.91681
h	2.77207	-1.26966	5.56610
h	1.89644	-2.39280	6.24424
o	2.70607	0.20392	4.45842
h	2.90657	-0.33795	3.64590
h	3.54563	0.72037	4.52530
o	3.71210	-3.48764	3.88724
h	4.46276	-4.03075	4.19065
h	3.32166	-3.05767	4.74862
o	-3.38210	-0.83844	5.67127
h	-3.51420	-1.76637	5.94185
h	-2.50983	-0.57353	6.10717
o	-0.28426	3.59788	4.40784
h	-0.91068	3.83498	3.64719
h	-0.42995	4.26893	5.09715
o	7.45328	0.28430	-2.34767
h	8.33836	-0.01810	-2.06747
h	7.60517	0.62637	-3.24956
o	3.57027	3.20286	-1.70368
h	4.47695	2.84638	-1.50934
h	3.59144	4.05548	-1.23235
o	4.07624	-1.28970	2.64326
h	4.02589	-2.23227	3.08030
h	3.99969	-1.41692	1.67991
o	6.52273	2.37359	1.84026
h	6.80151	3.18854	2.29352

h	6.19382	1.77464	2.56465
o	5.43450	0.71396	3.76609
h	5.10007	-0.10150	3.27845
h	6.08058	0.36811	4.41140
o	6.06221	2.21408	-0.87518
h	6.37165	2.28676	0.06411
h	6.69037	1.61019	-1.34025
o	-5.92966	4.68058	3.72360
h	-6.14659	3.71656	3.91792
h	-5.71127	5.06854	4.58942
o	-6.34512	2.08636	4.05801
h	-7.23335	1.75573	3.83039
h	-6.07432	1.54347	4.87091
o	-4.15512	4.77890	1.82118
h	-4.82005	4.74584	2.59574
h	-4.34708	5.62766	1.38320
o	-3.10420	-5.67585	-0.37609
h	-2.94026	-6.53642	-0.84118
h	-4.03594	-5.75392	-0.10131
o	-1.65746	4.11099	2.23382
h	-2.63443	4.38101	2.11652
h	-1.16337	4.78274	1.72941
o	-5.67614	0.55396	6.07891
h	-4.81269	0.06248	5.96928
h	-5.65502	0.91438	6.98295
o	-2.72143	-8.05910	-1.75266
h	-2.41298	-8.82648	-1.23525
h	-3.48497	-8.40890	-2.24860
o	-0.73100	3.00452	-8.01499
h	-1.11253	3.86012	-8.36728
h	0.15852	2.98344	-8.41649
o	0.30302	-3.66498	-4.10674
h	-0.26837	-3.63371	-4.92536
h	-0.07274	-4.42522	-3.62677
o	-1.28092	-1.08914	-7.04262
h	-0.31448	-0.96098	-7.06044
h	-1.61879	-0.44853	-7.75604
o	-2.02866	0.74711	-8.75574
h	-2.98278	0.94379	-8.75531
h	-1.58630	1.61279	-8.50969
o	-1.41088	-3.66327	-6.25221
h	-1.16501	-4.25552	-6.98609
h	-1.45940	-2.75662	-6.66905
o	-1.57899	5.30512	-9.12761
h	-2.03942	5.31357	-9.98699
h	-1.93882	6.07457	-8.65001

[Ru(bipy)3]3+{27H2O}

E(RI-PBE/def2-SVP)= -3637.64731414 a.u.
E(RI-PBE/def2-SVP/COSMO(eps=80))= -3638.03221992 a.u.
E(B3LYP/def2-TZVP)= -3643.89477506 a.u.
E(ZPE-RTlnq(trans)q(rot)q(vib)= 2558.05 kJ.mol-1

n	-1.35865	-1.35250	-1.75902
c	-1.58007	-0.86253	-3.02462
c	-2.37599	-1.56901	-3.93779
c	-2.94907	-2.78802	-3.55727
c	-2.73141	-3.27334	-2.25955
c	-1.93512	-2.52189	-1.39103
c	-0.90110	0.40436	-3.33160
n	-0.18731	0.94913	-2.29101
c	0.55690	2.06283	-2.50387
c	0.57236	2.71791	-3.73931
c	-0.18168	2.19815	-4.80392
c	-0.91042	1.01882	-4.59788
ru	-0.13620	-0.20389	-0.55882
n	1.14329	1.03233	0.50079
c	2.47449	0.83823	0.23402
c	3.45539	1.56482	0.92138
c	3.07783	2.48693	1.90048
c	1.71474	2.69698	2.14588
c	0.77420	1.95115	1.42609
c	2.77485	-0.14162	-0.81826
n	1.69186	-0.81605	-1.32685
c	1.86775	-1.72072	-2.32125
c	3.13819	-1.99646	-2.84363

c	4.25143	-1.29695	-2.35267
c	4.06714	-0.35995	-1.32758
n	-0.12264	-1.40460	1.12392
c	0.85271	-2.29654	1.42828
c	0.89422	-2.97116	2.65015
c	-0.11207	-2.71408	3.59749
c	-1.13103	-1.80946	3.27974
c	-1.11697	-1.15594	2.03547
c	-2.09588	-0.14304	1.62457
n	-1.85911	0.43490	0.39996
c	-2.71085	1.38121	-0.06277
c	-3.81755	1.80972	0.67401
c	-4.07182	1.22877	1.92804
c	-3.20124	0.24058	2.40333
h	1.62143	-2.45624	0.65964
h	-4.93475	1.54478	2.54794
h	-3.36407	-0.21660	3.39248
h	-2.47042	1.81182	-1.04599
h	-4.44613	2.62910	0.30038
h	-1.91686	-1.57298	4.01285
h	-0.07990	-3.16575	4.60307
h	1.74479	-3.63343	2.87997
h	-0.19475	2.67228	-5.80291
h	1.21002	3.60592	-3.85127
h	1.19724	2.41930	-1.68331
h	-1.41122	0.52697	-5.44695
h	-2.49311	-1.19015	-4.96159
h	-3.53423	-3.36096	-4.29015
h	-3.13161	-4.23100	-1.86780
h	-1.73493	-2.88515	-0.37252
h	3.86981	3.03376	2.43306
h	1.34131	3.39353	2.91359
h	-0.30116	2.12461	1.58105
h	4.51333	1.42732	0.67353
h	4.90584	0.26726	-0.97701
h	5.26098	-1.44660	-2.76529
h	3.21242	-2.74465	-3.64580
h	0.98879	-2.25163	-2.73770
o	0.26972	-2.67474	6.70942
h	-0.18765	-1.79146	6.82178
h	0.21371	-3.11710	7.57706
o	-0.96596	-0.25871	6.64585
h	-0.89273	0.32427	7.42540
h	-0.49412	0.24803	5.85960
o	0.09856	0.89172	4.63596
h	-0.05976	1.88372	4.59472
h	1.07891	0.75707	4.54245
o	2.79705	-2.20179	5.83820
h	2.75552	-1.27659	5.49044
h	1.88965	-2.39226	6.21372
o	2.77621	0.18592	4.33765
h	3.02437	-0.36817	3.55125
h	3.62457	0.67930	4.46812
o	3.74771	-3.53362	3.87819
h	4.41621	-4.16791	4.19842
h	3.34504	-3.09212	4.72883
o	-3.36580	-0.85866	5.62810
h	-3.55483	-1.75505	5.96588
h	-2.51090	-0.59185	6.09339
o	-0.31852	3.52012	4.36696
h	-0.93767	3.78220	3.61002
h	-0.43981	4.18486	5.06784
o	7.52553	0.36466	-2.40177
h	8.38991	0.00642	-2.12056
h	7.71967	0.75834	-3.27466
o	3.58915	3.09075	-1.68188
h	4.50104	2.75207	-1.47207
h	3.66796	4.03644	-1.45793
o	4.30518	-1.36355	2.65740
h	4.20373	-2.29101	3.11848
h	4.47099	-1.55186	1.71584
o	6.35392	2.50014	1.87984
h	6.88918	3.20451	2.28707
h	6.17788	1.84879	2.61226
o	5.51391	0.71821	3.83353
h	5.27120	-0.14489	3.37876
h	6.15098	0.46827	4.53085
o	6.02259	2.03582	-0.80149
h	6.36635	2.22529	0.11121

h	6.72488	1.55441	-1.30808
o	-5.86843	4.65376	3.66383
h	-6.11317	3.70595	3.89234
h	-5.78284	5.12512	4.51086
o	-6.35229	2.06849	3.99449
h	-7.27210	1.80535	3.80291
h	-6.10215	1.53371	4.81979
o	-4.12336	4.69124	1.76888
h	-4.77395	4.70002	2.56320
h	-4.32952	5.51412	1.28842
o	-3.23086	-5.63142	-0.43719
h	-3.02608	-6.50970	-0.86248
h	-4.14217	-5.75574	-0.11225
o	-1.62540	4.08322	2.15189
h	-2.61423	4.33797	2.04788
h	-1.15312	4.85248	1.78170
o	-5.69942	0.53943	6.01309
h	-4.82132	0.07574	5.94876
h	-5.79574	0.80894	6.94358
o	-2.74112	-8.01550	-1.69899
h	-2.40558	-8.76929	-1.17772
h	-3.47140	-8.40241	-2.21779
o	-0.67341	3.01518	-7.99263
h	-1.08633	3.86299	-8.34072
h	0.16107	2.95534	-8.49608
o	0.20301	-3.58254	-4.03888
h	-0.34775	-3.58809	-4.87596
h	0.12397	-4.50271	-3.72739
o	-1.29128	-1.07510	-7.00277
h	-0.33139	-1.03898	-7.17473
h	-1.66919	-0.43504	-7.70380
o	-2.00267	0.75736	-8.68230
h	-2.91523	0.94645	-8.96362
h	-1.58794	1.64052	-8.45354
o	-1.49917	-3.61411	-6.16003
h	-1.40371	-4.27286	-6.87221
h	-1.52271	-2.72874	-6.62586
o	-1.77418	5.21088	-9.06096
h	-1.90178	5.26500	-10.02641
h	-1.57832	6.12705	-8.79181

48486.8

24	4	-1	9	1	222.836	6.064	48906.8
25	4	-1	8	1	228.012	6.205	50042.8

Os/with_DKH2/Os2/Os2_h2o6/from_cas/ST5_5-15/Os2_h2o6.log
TRANSITION ENERGIES

The lowest energy is -17689.022616410 Eh

State	Mult	Irrep	Root	Block	mEh	eV	1/cm
0	1	-1	0	2	0.000	0.000	0.0
1	3	-1	1	1	87.553	2.382	19215.7
2	3	-1	0	1	92.632	2.521	20330.4
3	3	-1	2	1	93.722	2.550	20569.6
4	3	-1	4	1	108.290	2.947	23766.9
5	3	-1	3	1	108.470	2.952	23806.4
6	3	-1	5	1	110.660	3.011	24287.1
7	1	-1	2	2	116.379	3.167	25542.2
8	1	-1	1	2	119.483	3.251	26223.6
9	1	-1	3	2	119.920	3.263	26319.3
10	5	-1	2	0	133.101	3.622	29212.3
11	5	-1	1	0	139.442	3.794	30604.0
12	5	-1	0	0	147.496	4.014	32371.6
13	1	-1	5	2	150.028	4.082	32927.4
14	1	-1	4	2	150.752	4.102	33086.3
15	1	-1	6	2	158.244	4.306	34730.5
16	3	-1	8	1	204.266	5.558	44831.1
17	3	-1	6	1	205.459	5.591	45093.0
18	3	-1	9	1	216.387	5.888	47491.5
19	3	-1	7	1	220.410	5.998	48374.5
20	1	-1	7	2	226.887	6.174	49795.9
21	1	-1	10	2	238.488	6.490	52342.1
22	1	-1	8	2	238.747	6.497	52398.9
23	1	-1	12	2	239.273	6.511	52514.3
24	1	-1	11	2	242.536	6.600	53230.6
25	1	-1	9	2	244.306	6.648	53618.9

26	1	-1	14	2	256.936	6.992	56390.9
27	1	-1	13	2	257.032	6.994	56412.0
28	5	-1	3	0	266.073	7.240	58396.3
29	5	-1	4	0	266.145	7.242	58412.0

Os/with_DKH2/0s3/0s3_cn6/from_cas/DQ6_1-15/0s3_cn6.log
TRANSITION ENERGIES

The lowest energy is -17787.511222083 Eh

State	Mult	Irrep	Root	Block	mEh	eV	1/cm
0	2	-1	0	2	0.000	0.000	0.0
1	2	-1	2	2	1.313	0.036	288.2
2	2	-1	1	2	7.398	0.201	1623.6
3	4	-1	0	1	283.531	7.715	62227.9
4	4	-1	1	1	297.756	8.102	65349.9
5	2	-1	5	2	311.232	8.469	68307.5
6	2	-1	11	2	312.974	8.516	68689.8
7	2	-1	12	2	324.157	8.821	71144.2
8	2	-1	9	2	328.423	8.937	72080.5
9	2	-1	4	2	329.361	8.962	72286.4
10	2	-1	10	2	333.509	9.075	73196.8
11	2	-1	13	2	340.114	9.255	74646.3
12	2	-1	8	2	341.585	9.295	74969.3
13	4	-1	5	1	345.934	9.413	75923.7
14	2	-1	7	2	355.979	9.687	78128.4
15	2	-1	3	2	358.554	9.757	78693.5
16	2	-1	6	2	385.920	10.501	84699.6
17	4	-1	2	1	403.102	10.969	88470.6
18	4	-1	3	1	439.259	11.953	96406.3
19	4	-1	4	1	441.829	12.023	96970.2
20	2	-1	14	2	488.762	13.300	107270.8
21	4	-1	8	1	507.299	13.804	111339.2
22	4	-1	9	1	508.405	13.834	111582.0
23	4	-1	6	1	563.440	15.332	123660.7
24	4	-1	7	1	630.344	17.153	138344.6
25	6	-1	0	0	945.852	25.738	207590.6

Os/with_DKH2/0s2/0s2_cn6/from_cas/ST5_5-15/0s2_cn6.log
TRANSITION ENERGIES

The lowest energy is -17787.161819890 Eh

State	Mult	Irrep	Root	Block	mEh	eV	1/cm
0	1	-1	0	2	0.000	0.000	0.0
1	3	-1	0	1	258.444		