Electronic Supplementary Information

DFT Characterization on the Mechanism of Water Splitting Catalyzed by Single-Ru-substituted Polyoxometalates

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The material enclosed in the electronic supplementary information is organized as following:

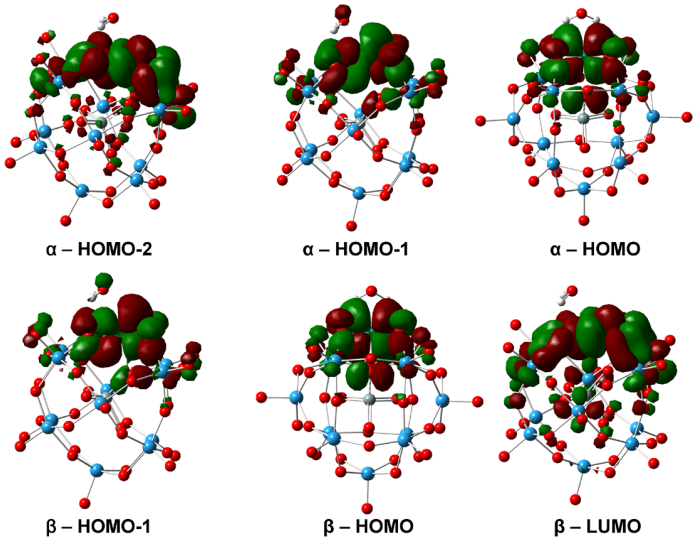

Fig. S1 Important HOMOs and LUMOs for $[Ru^{III}(H_2O)SiW_{11}O_{39}]^{5-}$ (**1**) complex computed at the B3LYP level in gas phase.

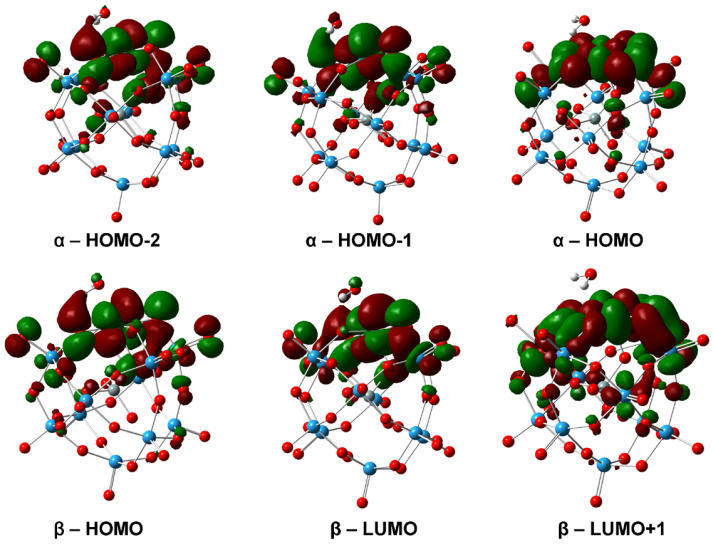

Fig. S2 Important HOMOs and LUMOs for $[Ru^{IV}(H_2O)SiW_{11}O_{39}]^{4-}$ (**2**) complex computed at the B3LYP level in gas phase.

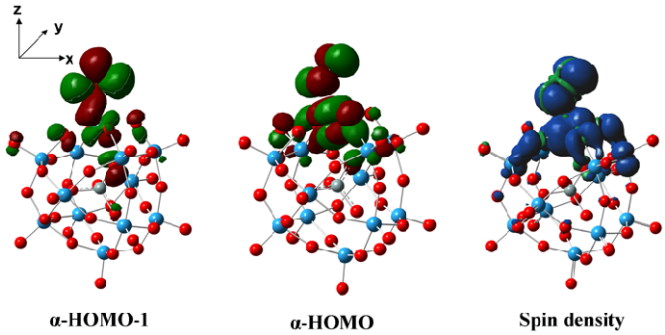

Fig. S3 The two highest singly occupied π* molecular orbitals and the spin density distribution of $[Ru^{IV}(OO)SiW_{11}O_{39}]^{6-}$ (**5**).

Table S1 Calculated Mulliken atomic charges (e) of the Ru, O_a, O_w atoms in pathways **a**, **b**, and **c**

charge	atom	**3**$_{a/b/c}$	**TS1**$_{a/b/c}$	**4H**$_{a/b/c}$
	Ru	1.26	1.00	0.88
pathway **a**	O_a	-0.48	-0.43	-0.38
	O_w	-0.68	-0.50	-0.40
	Ru	1.26	1.13	0.83
pathway **b**	O_a	-0.55	-0.49	-0.33
	O_w	-0.71	-0.63	-0.39
	Ru	1.28	0.95	0.88
pathway **c**	O_a	-0.48	-0.41	-0.40
	O_{w1}	-0.70	-0.46	-0.38

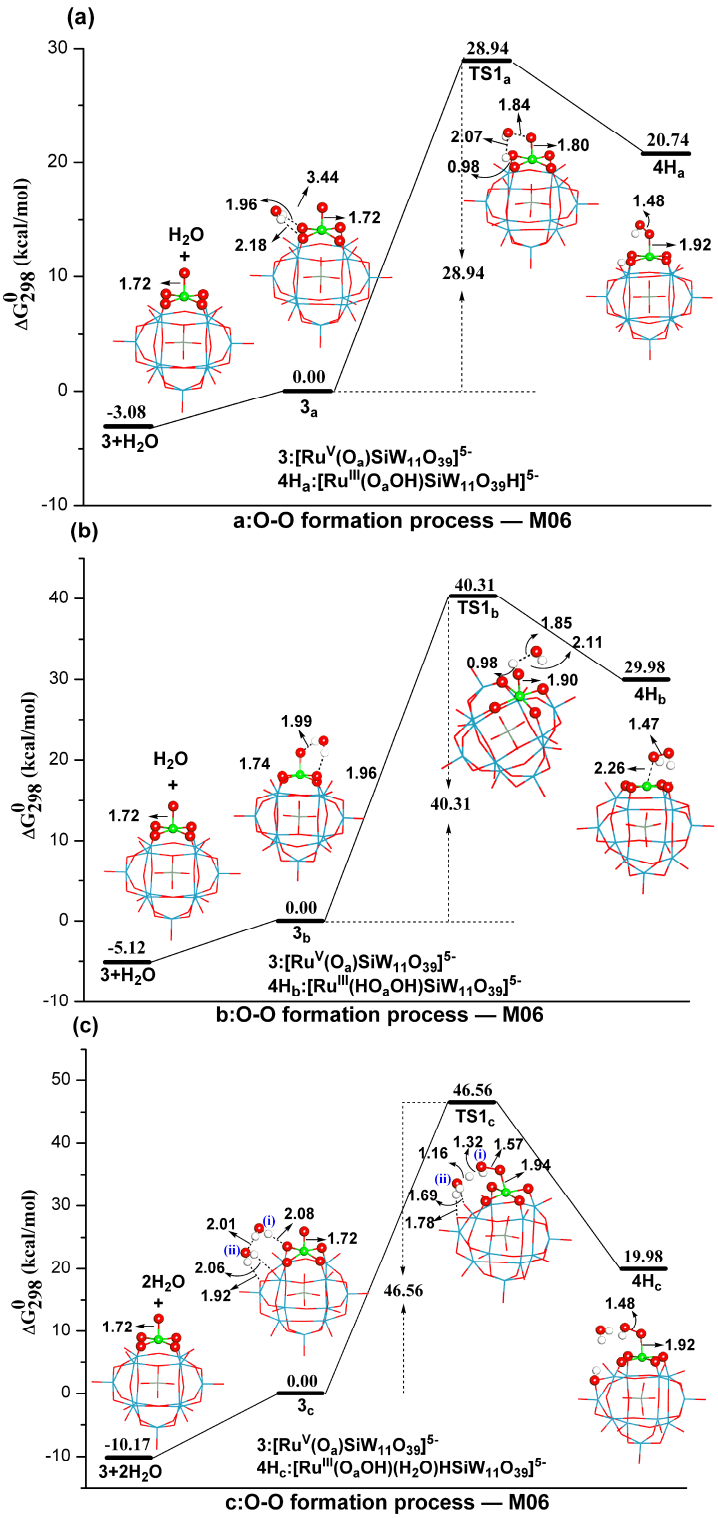

Fig. S4 Calculated energy profile for the O-O bond formation by pathways **a**, **b**, and **c**. The relative energies with solvation correction at UM06(SMD)/[6-311+g**/LANL2DZ(W, Ru)] level are given in kcal/mol.

Table S2 The Calculated relative energy of some important intermediates in different spin states at B3LYP(SMD)[6-311+g**/LANL2DZ(W, Ru)] level.

complex	Spin state	Relative energy (kcal/mol)
3	Doublet	0.00
	Quartet	5.86
4	Doublet	0.00
	Quartet	15.96
5	Triplet	0.00
	BS Singlet	9.53
	Singlet	9.43
	Quintet	21.49
	Singlet -η^2	9.85
6	Quartet	0.00
	Doublet	10.80
	Sextet	14.27
	Doublet -η^2	19.48

Optimized coordinates (xyz) optimized in gas phase

1($[Ru^{III}(H_2O)SiW_{11}O_{39}]^{5-}$) (Multiplicity = 2)

55

O	-0.942637	1.340786	-0.051960
Si	-0.000310	0.000027	-0.090963
O	1.058512	0.000297	1.162799
O	0.891903	-0.000788	-1.497081
Ru	-0.104476	-0.000843	-3.311269
O	1.328861	-1.408567	-3.650919
W	2.422000	-1.714387	-2.194344
O	1.072272	-2.940721	-1.464042
W	-0.113303	-3.545332	-0.104473
O	1.233749	-2.914030	1.134441
W	2.664293	-1.705380	1.553914
O	2.985699	-1.628601	-0.309766
O	-0.943142	-1.340305	-0.050810
O	3.556537	0.000249	1.777053
W	2.663329	1.707139	1.552967
O	1.786363	1.334250	3.254354
W	0.416774	0.000654	3.468897
O	1.786000	-1.332743	3.255261
O	2.986351	1.626739	-0.310747
W	2.423988	1.710306	-2.195330
O	1.329846	1.405381	-3.651511

O	3.599082	2.793496	-2.861870
O	1.074170	2.939124	-1.466497
W	-0.112390	3.545661	-0.109868
O	-1.639827	3.471537	-1.276738
W	-2.711008	1.862357	-1.595417
O	-3.200988	-0.000252	-1.413944
W	-2.710721	-1.864459	-1.594511
O	-1.640878	-3.472037	-1.273703
O	3.301777	-0.002236	-2.442777
O	3.906444	2.780300	2.099179
O	1.234581	2.914902	1.131929
O	0.186222	5.249809	-0.120045
O	-1.375882	3.455144	1.377109
W	-2.367727	1.873850	1.824349
O	-3.387410	2.131092	0.233730
O	-3.461351	2.497919	3.010543
O	-0.886877	1.301723	2.924868
O	-2.823551	0.001651	1.788106
W	-2.369881	-1.869927	1.825420
O	-3.388659	-2.129343	0.234932
O	-4.048050	2.533943	-2.473315
O	-1.572251	1.374827	-2.975146
O	0.238077	0.001411	5.190030
O	-0.887758	-1.299163	2.925863
O	3.906668	-2.778935	2.101006
O	3.596370	-2.798829	-2.860134
O	-1.572841	-1.376079	-2.974398
O	-3.463828	-2.492566	3.012073
O	-1.378034	-3.452840	1.380125
O	0.184371	-5.249650	-0.113519
O	-4.048045	-2.535970	-2.472023
O	-1.442163	-0.000770	-5.216433
H	-1.857106	-0.761610	-4.748427
H	-1.855402	0.761518	-4.749173

2([$Ru^{IV}(H_2O)SiW_{11}O_{39}$]$^{4-}$) (Multiplicity = 3)

55

O	1.203460	-1.126622	-0.065511
Si	0.029366	0.004321	-0.072467
O	-1.011160	-0.195760	1.166803
O	-0.860793	-0.155166	-1.485438
Ru	0.030990	-0.052673	-3.290934
O	-1.637537	1.046250	-3.652771
W	-2.750168	1.197863	-2.173792

O	-1.668017	2.658781	-1.495242
W	-0.597612	3.509677	-0.155521
O	-1.762212	2.628461	1.102644
W	-2.917948	1.166003	1.567495
O	-3.247487	0.990737	-0.293230
O	0.674231	1.504582	-0.066128
O	-3.443403	-0.683689	1.827088
W	-2.237835	-2.176413	1.652089
O	-1.422801	-1.611671	3.302604
W	-0.341280	-0.018374	3.469035
O	-1.950610	1.000625	3.250907
O	-2.619944	-2.204405	-0.248037
W	-2.082295	-2.189640	-2.077957
O	-1.021071	-1.639529	-3.594610
O	-2.989538	-3.483140	-2.758270
O	-0.476089	-3.074601	-1.423340
W	0.819885	-3.454462	-0.065799
O	2.283330	-3.111207	-1.269647
W	3.000448	-1.342653	-1.636164
O	3.071269	0.592735	-1.507076
W	2.248752	2.323576	-1.634964
O	0.879675	3.683261	-1.382150
O	-3.232667	-0.688079	-2.392355
O	-3.228673	-3.464295	2.219950
O	-0.621416	-3.076677	1.169543
O	0.841659	-5.175794	-0.057474
O	2.055654	-3.082238	1.385424
W	2.732715	-1.326268	1.782157
O	3.753134	-1.410407	0.171852
O	3.940637	-1.695461	2.951170
O	1.180919	-1.027756	2.897386
O	2.806085	0.603984	1.706493
W	1.977558	2.334539	1.755868
O	2.913840	2.773772	0.100104
O	4.416579	-1.724990	-2.545249
O	1.748909	-1.118578	-3.006064
O	-0.134918	0.043117	5.176473
O	0.670994	1.519223	2.888168
O	-4.334122	1.974990	2.118763
O	-4.121267	1.997910	-2.841761
O	1.087717	1.528076	-2.958219
O	2.958088	3.185429	2.885879
O	0.706263	3.694032	1.277358
O	-1.223486	5.112730	-0.183196

O	3.349979	3.174695	-2.655799
O	1.191836	0.049860	-5.232617
H	1.521877	0.938312	-5.000133
H	1.822837	-0.551300	-4.760739

3($[Ru^{V}(O_a)SiW_{11}O_{39}]^{5-}$) (Multiplicity = 2)

53

O	-0.836447	-0.607876	-1.402387
O	-0.760914	-0.428056	1.294097
O	1.520171	-0.638061	-0.119546
O	0.075064	1.628045	-0.204247
W	-3.107346	-0.048728	-1.927131
W	-1.294385	-2.918698	-1.705102
W	0.012713	0.191413	3.477818
W	-2.982890	0.217704	1.827913
W	-1.156493	-2.650077	2.022890
W	1.168132	3.038949	1.381277
W	1.082060	2.744760	-2.003392
W	-1.822453	3.060293	-0.258592
W	3.196441	-0.099931	1.509741
W	3.068125	-0.379180	-1.918676
W	2.005339	-2.944249	0.077426
O	-2.974410	-1.988147	-1.909798
O	-0.688148	-2.250938	-3.345270
O	-2.233003	0.056115	-3.546223
O	-2.796145	-1.663450	2.277548
O	-1.870233	0.569382	3.397075
O	-0.449425	-1.680438	3.545860
O	3.121335	-2.234743	-1.321231
O	3.149650	-2.022160	1.343052
O	4.014761	0.005290	-0.173462
O	-0.629513	3.631563	-1.647429
O	-0.550116	3.824807	1.000089
O	1.718641	3.604557	-0.388935
O	-4.748502	0.160826	-2.434371
O	-1.752525	-4.516973	-2.184927
O	0.333030	0.485355	5.152208
O	-4.548460	0.526289	2.498220
O	-1.575707	-4.146367	2.784436
O	4.555361	0.091224	2.563503
O	4.475832	-0.323291	-2.927937
O	2.654634	-4.543860	0.189564
O	1.878793	4.293514	2.336771
O	1.703231	3.824067	-3.206882

O	-2.995827	4.330257	-0.309170
O	2.514318	1.476335	-1.830959
O	0.150458	1.482802	-3.057201
O	1.744097	-0.715468	-3.127430
O	2.559201	1.719174	1.349626
O	0.344425	1.937340	2.708398
O	1.729543	-0.262103	2.795800
O	-2.482801	1.960575	1.175278
O	-2.596309	1.757764	-1.427405
O	-3.366024	-0.219043	0.043969
O	0.644088	-2.978663	1.451107
O	0.555281	-3.185383	-1.137616
O	-1.645770	-2.968856	0.207514
Si	-0.000297	-0.013662	-0.103127
Ru	-0.215598	-0.337676	-3.572196
O	-0.023389	-0.327094	-5.284458

4 (Multiplicity = 2**)**

55

O	1.336253	-0.012641	1.056991
O	0.415242	-0.644254	-1.400822
O	-1.199742	-0.863348	0.749851
O	-0.476581	1.565929	-0.148330
W	3.438803	1.076966	0.593303
W	2.496268	-2.018923	1.723349
W	-1.111455	-0.859552	-3.235969
W	2.114601	0.207517	-2.830976
W	1.185080	-2.871568	-1.701545
W	-2.352170	2.220111	-1.514600
W	-1.176088	2.979693	1.637646
W	0.869278	3.259458	-1.100394
W	-3.374708	-1.169502	-0.263930
W	-2.178663	-0.342528	2.887658
W	-1.065017	-3.156459	1.255133
O	3.832641	-0.761389	1.046657
O	2.307123	-1.059433	3.264227
O	3.119450	1.524430	2.348548
O	2.338304	-1.716346	-2.757115
O	0.544874	-0.136820	-3.932682
O	-0.173775	-2.545375	-3.056750
O	-1.886175	-2.294985	2.750246
O	-2.737274	-2.907791	0.292768
O	-3.669640	-0.719994	1.516174
O	0.010366	4.007341	0.435390

O	-0.859469	3.348789	-1.994700
O	-2.503031	3.148003	0.107516
O	5.036007	1.729583	0.385656
O	3.507457	-3.328383	2.257350
O	-1.971356	-1.146597	-4.720525
O	3.264785	0.596899	-4.076746
O	1.756556	-4.427302	-2.230498
O	-4.979829	-1.579227	-0.792929
O	-3.225247	-0.282752	4.280747
O	-1.252860	-4.817743	1.730407
O	-3.617117	2.961249	-2.449244
O	-1.806696	4.278211	2.611563
O	1.608994	4.690094	-1.753601
O	-2.247239	1.462542	2.191267
O	0.228241	2.386997	2.603908
O	-0.554930	-0.071921	3.591954
O	-3.254328	0.693737	-0.759166
O	-1.654299	0.913256	-2.787767
O	-2.352034	-1.441521	-1.919294
O	1.371566	1.933389	-2.415722
O	2.290113	2.531073	-0.044465
O	3.125126	0.398784	-1.257607
O	-0.214460	-3.348946	-0.479707
O	0.697209	-2.769809	1.893793
O	2.241954	-2.533612	-0.181876
Si	0.013757	0.007300	0.057739
Ru	1.316059	0.730628	3.094187
O	1.628133	1.305755	4.915718
O	2.978513	1.907349	5.082290
H	3.279338	1.898540	4.143735

3_a(Multiplicity = 2**)**

56

O	0.498373	1.092213	-1.220768
O	-0.605739	0.808651	1.230175
O	-1.162302	-0.964310	-0.699598
O	1.295997	-0.902252	0.385650
W	2.111527	2.785560	-0.802425
W	-0.945888	2.672035	-2.298884
W	-1.496437	-0.276067	3.174791
W	0.614039	2.324357	2.588820
W	-2.458171	2.285056	1.126158
W	1.173989	-2.649806	2.028776
W	2.571842	-2.275208	-1.093661

W	3.246568	-0.031770	1.399518
W	-2.235883	-2.737806	0.491947
W	-0.823527	-2.335548	-2.575160
W	-3.246117	-0.187332	-1.535700
O	0.609523	3.648732	-1.623732
O	0.059502	1.964280	-3.674158
O	2.586231	1.963489	-2.444391
O	-1.104440	3.145941	2.195112
O	-0.334808	1.150474	3.787687
O	-2.741259	1.088204	2.646708
O	-2.527037	-1.433667	-2.823728
O	-3.612019	-1.727040	-0.417881
O	-1.717556	-3.423391	-1.237226
O	3.806649	-1.299005	0.084944
O	2.669014	-1.537643	2.492299
O	2.145594	-3.325608	0.570737
O	3.261041	4.076145	-0.790145
O	-1.782877	3.936290	-3.130709
O	-2.175967	-0.772883	4.685198
O	1.244760	3.474734	3.715698
O	-3.776281	3.380171	1.363216
O	-3.169649	-4.067214	1.083295
O	-0.871855	-3.409320	-3.931430
O	-4.816424	0.079716	-2.208264
O	1.354306	-3.926464	3.181031
O	3.657463	-3.427737	-1.794424
O	4.759255	0.320997	2.156185
O	0.858020	-2.834513	-1.738396
O	2.628344	-0.908639	-2.322073
O	0.069717	-0.842871	-3.280670
O	-0.492773	-3.138171	1.158037
O	0.026298	-1.406447	3.005130
O	-2.351492	-1.489974	1.946999
O	2.026731	1.057282	2.463504
O	3.096082	1.361736	0.115818
O	1.258943	3.006220	0.913738
O	-3.278582	0.916396	0.024093
O	-2.226666	1.225362	-2.347578
O	-1.673089	2.911231	-0.461969
Si	0.006536	0.008316	-0.069104
Ru	1.435222	0.526082	-3.199665
O	2.141934	0.426292	-4.769917
O	5.098883	0.685276	-3.032125
H	4.412045	1.349750	-2.834652

H	4.608258	-0.112138	-2.770503

$TS1_a$ (Multiplicity = 2**)**

56

O	0.719312	1.114821	1.086244
O	0.878744	-0.102235	-1.321553
O	-0.036393	-1.434070	0.831850
O	-1.530098	0.504116	-0.288029
W	1.111138	3.428188	0.527881
W	2.945602	0.939313	1.976241
W	0.393501	-1.593163	-3.140872
W	1.239837	1.696415	-2.815612
W	3.184252	-0.714713	-1.400819
W	-2.973618	-0.707023	-1.833414
W	-3.347266	0.709894	1.233895
W	-2.045433	2.553350	-1.335033
W	-1.004875	-3.395075	-0.147616
W	-1.114349	-1.841821	2.918453
W	1.879252	-2.629917	1.497066
O	2.769765	2.720014	1.167486
O	1.940710	1.431448	3.409862
O	0.360717	3.494885	2.207575
O	2.957336	0.784254	-2.568948
O	0.735403	0.150694	-3.886670
O	2.238810	-1.773796	-2.790871
O	0.585222	-2.729362	2.957903
O	0.721375	-3.880688	0.561304
O	-1.685246	-3.254420	1.594789
O	-3.278920	2.325668	0.130152
O	-3.076923	1.146821	-2.256588
O	-4.055458	-0.231284	-0.217193
O	1.509068	5.092673	0.280128
O	4.544255	1.027269	2.631275
O	0.235014	-2.541568	-4.578481
O	1.680027	2.796838	-4.075990
O	4.809470	-1.173627	-1.776639
O	-1.591563	-4.951555	-0.620661
O	-1.895884	-2.527135	4.303615
O	3.064629	-3.726768	2.113953
O	-4.246644	-1.354620	-2.807645
O	-4.788214	1.021915	2.135950
O	-2.741512	3.941951	-2.095259
O	-2.593548	-0.767833	2.069978
O	-2.071537	1.810645	2.428464

O	-0.487378	-0.272318	3.553927
O	-2.395354	-2.232057	-0.818750
O	-1.471004	-0.961203	-2.912908
O	-0.065632	-2.824744	-1.774153
O	-0.613453	2.102376	-2.560086
O	-0.718801	3.322393	-0.248156
O	1.571237	2.693678	-1.253124
O	2.640909	-2.125487	-0.172698
O	2.511606	-0.947350	2.161534
O	3.389612	0.360446	0.098080
Si	0.006319	0.022583	0.069362
Ru	-0.088502	1.661399	3.060045
O	-0.533972	2.421886	4.625231
O	-1.585022	3.888817	4.244983
H	-0.913854	4.174457	3.593219
H	-2.320919	2.712859	2.702177

$4H_a$ (Multiplicity = 2**)**

56

O	-1.371590	-0.398130	0.930593
O	-0.358312	-0.043486	-1.543863
O	0.455142	1.508215	0.506325
O	1.202273	-1.071980	0.382666
W	-2.589022	-2.458298	0.748994
W	-3.453375	0.849721	0.854421
W	1.193672	0.477073	-3.302156
W	-1.098015	-1.982315	-2.690668
W	-2.033286	1.286887	-2.596882
W	3.360860	-1.031442	-0.695067
W	2.252679	-1.391907	2.496107
W	1.000665	-3.402178	0.013956
W	2.407668	2.565880	-0.404595
W	1.015104	2.186211	2.739452
W	-0.830546	3.449985	0.165458
O	-3.867695	-1.049670	0.555744
O	-3.165803	0.558661	2.627471
O	-2.449251	-2.244826	2.573816
O	-2.211478	-0.506904	-3.283753
O	0.321632	-1.177799	-3.759157
O	-0.403289	1.398765	-3.717334
O	-0.058350	3.573569	1.941225
O	0.954556	3.823884	-0.512716
O	2.483068	2.767106	1.448147
O	1.768500	-3.153145	1.777580

O	2.745976	-2.844233	-0.681889
O	3.658551	-1.292831	1.277876
O	-3.589290	-3.867043	0.668943
O	-5.037693	1.541154	0.869461
O	2.119198	0.776378	-4.732186
O	-1.629805	-3.212117	-3.785133
O	-3.130023	2.130549	-3.635341
O	3.717036	3.570145	-0.922149
O	1.653032	2.996642	4.132523
O	-1.523633	5.029922	0.060266
O	4.996991	-1.237887	-1.215418
O	3.088415	-1.874903	3.931222
O	1.165257	-5.117685	-0.134237
O	2.010479	0.427771	2.747709
O	0.283231	-1.615025	3.155288
O	-0.367466	1.268546	3.409327
O	3.277969	0.835427	-0.287884
O	2.473687	-0.656487	-2.290290
O	1.770454	1.841061	-2.125035
O	0.265350	-2.919813	-1.685096
O	-0.754279	-3.228339	0.722549
O	-2.199069	-2.241070	-1.195719
O	-1.271815	2.720984	-1.554444
O	-2.296249	2.416119	0.826743
O	-3.086985	0.886702	-1.115743
Si	-0.015586	-0.004239	0.066611
Ru	-1.459548	-0.451956	3.100545
O	-1.805403	-0.624876	4.985087
O	-2.763036	-1.709998	5.280443
H	-2.856616	-2.109943	4.385879
H	-0.021200	-2.483139	2.841176

3_b (Multiplicity = 2**)**

56

O	1.387727	-0.620416	0.746935
O	-0.212862	-0.662430	-1.430810
O	-1.269118	-0.348583	1.024004
O	0.169676	1.628373	-0.095311
W	3.577710	-0.459834	-0.203012
W	1.693103	-2.951491	1.157206
W	-2.042538	-0.111857	-2.878957
W	1.338273	-0.468672	-3.219987
W	-0.517317	-2.976964	-1.858617
W	-1.482791	3.070434	-1.032711

W	0.489913	3.064936	1.736925
W	1.890807	2.692175	-1.345630
W	-3.515280	0.350859	0.536889
W	-1.465846	0.332610	3.297397
W	-2.012601	-2.534435	1.524718
O	3.276714	-2.318630	0.227129
O	2.224521	-2.042170	2.705095
O	3.825421	-0.033684	1.598073
O	0.758974	-2.321284	-3.147656
O	-0.426769	-0.068737	-3.932891
O	-1.877198	-2.033412	-2.868741
O	-2.034060	-1.525124	3.165273
O	-3.572904	-1.532921	0.979089
O	-3.197256	0.736478	2.346107
O	1.767495	3.589081	0.339982
O	0.204189	3.557902	-1.810377
O	-0.869046	3.876011	0.615597
O	5.221586	-0.501375	-0.732620
O	2.183354	-4.559245	1.560805
O	-3.236007	0.085129	-4.114416
O	2.256012	-0.502274	-4.685601
O	-0.758736	-4.583631	-2.451506
O	-5.205621	0.691186	0.407984
O	-2.006746	0.718782	4.896536
O	-2.759463	-3.996087	2.067833
O	-2.488889	4.340215	-1.636121
O	0.768960	4.350396	2.860818
O	2.995285	3.729076	-2.177703
O	-0.882476	2.054109	2.609481
O	1.737904	1.765334	2.308446
O	0.279295	-0.127016	3.576051
O	-2.728522	2.023140	-0.004203
O	-1.695211	1.721618	-2.376278
O	-3.089262	-0.192210	-1.295252
O	1.489694	1.371975	-2.695674
O	3.057597	1.373165	-0.609952
O	2.644504	-0.826287	-1.900565
O	-1.687497	-2.931406	-0.335878
O	-0.151023	-2.925511	1.759279
O	0.890573	-3.214629	-0.596990
Si	0.014047	-0.002437	0.056649
Ru	2.155808	-0.059412	2.784125
O	2.987302	0.130327	4.301317
O	5.777071	0.320570	3.669938

H	5.419064	0.244440	2.763911
H	4.933045	0.263104	4.151362

$TS1_b$ (Multiplicity = 2**)**

56

O	1.033456	-0.761383	1.097251
O	-0.384406	-1.030659	-1.163659
O	-1.347799	0.458608	0.856851
O	0.759444	1.333910	-0.559627
W	3.153912	-1.692870	0.397539
W	0.529977	-2.727541	2.360536
W	-1.910140	-0.473137	-2.920760
W	1.133576	-1.978992	-2.726708
W	-1.437261	-3.125678	-0.813879
W	-0.279858	2.807793	-2.148064
W	1.553175	3.182602	0.752953
W	2.739115	1.284214	-1.841497
W	-3.191477	1.612107	-0.115846
W	-1.315512	1.926610	2.724278
W	-2.800828	-1.051096	1.965741
O	2.272859	-2.998380	1.474514
O	1.366435	-1.600710	3.567679
O	3.469168	-0.646865	2.014430
O	-0.006382	-3.410564	-2.078554
O	-0.346632	-1.344365	-3.739198
O	-2.383011	-2.218048	-2.262275
O	-2.479015	0.422778	3.160025
O	-3.907967	0.141022	0.928901
O	-2.780213	2.499551	1.502759
O	2.913171	2.717619	-0.602585
O	1.468729	2.367270	-2.829567
O	0.523717	3.879954	-0.833493
O	4.718708	-2.399521	0.211978
O	0.404626	-4.180573	3.289552
O	-2.928926	-0.363829	-4.313756
O	2.022662	-2.821852	-3.946863
O	-2.212553	-4.670241	-0.878250
O	-4.656665	2.409328	-0.570952
O	-1.663415	2.967391	4.064421
O	-4.019989	-1.902563	2.846334
O	-0.776952	3.996713	-3.300395
O	2.162702	4.707931	1.299885
O	4.154718	1.530963	-2.801826
O	-0.135602	3.032241	1.645942

O	2.308254	2.014158	1.944478
O	0.166468	1.000808	3.284036
O	-1.868669	2.628348	-1.051495
O	-0.941304	1.167652	-2.977220
O	-2.977294	0.333131	-1.574989
O	1.944036	-0.263699	-2.737839
O	3.339756	-0.006950	-0.566284
O	2.246130	-2.298113	-1.150896
O	-2.574882	-2.160106	0.418972
O	-1.189395	-1.911321	2.613097
O	-0.247638	-3.317042	0.633888
Si	0.007219	0.008628	0.045799
Ru	1.937218	0.185387	2.787389
O	2.820925	0.811137	4.352472
O	4.933497	0.794217	4.258059
H	4.831536	0.282698	3.434608
H	3.297592	1.639029	4.135083

4H$_b$(Multiplicity = 2**)**

56

O	1.075973	0.424741	1.241279
O	0.843264	-0.720969	-1.154251
O	-1.107529	-1.033631	0.683790
O	-0.761979	1.347491	-0.501367
W	2.941054	1.944988	0.924363
W	2.442569	-1.056797	2.518588
W	-0.157379	-1.624213	-3.124904
W	2.542729	0.336262	-2.437918
W	2.174180	-2.664548	-0.859394
W	-2.362049	1.278142	-2.311392
W	-2.211043	2.774080	0.783466
W	0.334075	3.189279	-1.485478
W	-2.883069	-2.015428	-0.598222
W	-2.610858	-0.504926	2.482467
W	-0.563174	-3.122689	1.633759
O	3.583981	0.425822	1.881377
O	1.686967	0.087325	3.750180
O	2.034808	2.578348	2.477549
O	3.207494	-1.413742	-1.901217
O	1.401001	-0.577163	-3.675468
O	1.084627	-2.927992	-2.464273
O	-1.844024	-2.274872	2.793658
O	-2.010464	-3.435398	0.393394
O	-3.641160	-1.402200	1.007462

O	-0.998637	3.887995	-0.316077
O	-1.124153	2.685111	-2.692941
O	-3.098239	2.363016	-0.925798
O	4.322703	2.983796	0.936830
O	3.567127	-1.933782	3.500134
O	-0.590056	-2.328551	-4.644919
O	3.815531	0.835080	-3.498237
O	3.177567	-4.070239	-0.966820
O	-4.210527	-2.885284	-1.286454
O	-3.867666	-0.493920	3.677905
O	-0.472105	-4.681499	2.377018
O	-3.529096	1.519641	-3.564500
O	-3.305220	3.986894	1.360506
O	0.855081	4.644606	-2.262170
O	-2.929774	1.154021	1.494510
O	-0.918893	2.778676	2.126279
O	-1.236862	0.322844	3.333660
O	-3.062147	-0.287813	-1.404804
O	-1.153950	0.022248	-3.134807
O	-1.504312	-2.282496	-1.969343
O	1.388675	1.845293	-2.438201
O	1.625788	2.992399	-0.113576
O	3.167536	1.006976	-0.735641
O	0.674795	-3.306947	0.170158
O	0.886813	-2.198991	2.515412
O	2.766839	-1.862530	0.741946
Si	-0.005892	0.001264	0.049922
Ru	0.419951	1.453532	2.914908
O	-0.030524	2.980423	4.520629
O	1.075640	3.943823	4.495033
H	1.608190	3.569139	3.724105
H	-0.643267	3.342380	3.823443

3_c (Multiplicity = 2**)**

59

O	-0.595420	0.967135	1.253221
O	0.850163	0.925459	-1.029056
O	1.065236	-1.080913	0.753847
O	-1.178873	-0.795386	-0.698197
W	-2.157450	2.739842	0.883178
W	0.733710	2.362642	2.638548
W	1.959530	0.055807	-2.967423
W	-0.149181	2.661696	-2.299052
W	2.731379	2.294021	-0.525894

W	-0.875275	-2.312411	-2.523020
W	-2.602526	-2.261547	0.394843
W	-2.970879	0.297215	-1.848896
W	2.235932	-2.759453	-0.501676
W	0.458955	-2.661547	2.441315
W	3.041116	-0.498784	1.910231
O	-0.702431	3.458069	1.937410
O	-0.464110	1.465688	3.754767
O	-2.863736	1.822761	2.333588
O	1.547215	3.338076	-1.624906
O	0.929273	1.574968	-3.522119
O	3.178121	1.284996	-2.121080
O	2.149977	-1.878544	2.942803
O	3.520087	-1.892817	0.651929
O	1.495237	-3.608158	1.005324
O	-3.736952	-1.072410	-0.748101
O	-2.313086	-1.128303	-3.000325
O	-2.101325	-3.130363	-1.251055
O	-3.214140	4.102882	0.817435
O	1.445747	3.454619	3.773865
O	2.835264	-0.293380	-4.416189
O	-0.579410	3.958892	-3.358356
O	4.094840	3.353719	-0.442244
O	3.211887	-4.026173	-1.158244
O	0.363701	-3.987849	3.549409
O	4.510591	-0.377389	2.812439
O	-0.964701	-3.460347	-3.811436
O	-3.896875	-3.287138	0.945696
O	-4.360109	0.794772	-2.745598
O	-1.086711	-2.985610	1.252766
O	-2.681760	-0.891558	1.693804
O	-0.522770	-1.380165	3.284679
O	0.581705	-2.989537	-1.476004
O	0.377781	-1.041449	-3.198185
O	2.541570	-1.325415	-1.786545
O	-1.589833	1.421301	-2.581837
O	-2.989338	1.516383	-0.379003
O	-0.999089	3.125249	-0.693029
O	3.333768	0.789161	0.515896
O	1.954713	0.843941	2.719575
O	1.735721	2.786344	1.019426
Si	0.041494	0.005953	0.067187
Ru	-1.800492	0.194090	3.016262
O	-2.700462	-0.069374	4.457226

O	-5.782534	0.974891	2.579868
H	-4.849536	1.247215	2.512627
H	-5.833470	0.196352	1.993252
O	-6.103572	-1.363244	0.747722
H	-5.559705	-2.084251	1.111487
H	-5.472604	-1.026518	0.077638

$TS1_c$ (Multiplicity = 2**)**

59

O	0.48662400	-0.93376300	1.32011100
O	-0.90475600	-0.93209500	-0.97534300
O	-0.94696600	1.23179900	0.66030600
O	1.25676400	0.66662100	-0.75694200
W	1.91445400	-2.91459600	1.03107100
W	-0.85597100	-2.09334200	2.89389700
W	-2.02191000	-0.13546700	-2.93098700
W	-0.04335500	-2.80447300	-2.16458300
W	-2.83811100	-2.16127700	-0.31126200
W	1.02452500	2.01134700	-2.73250400
W	2.73531600	2.17169100	0.19741700
W	2.97903200	-0.64856000	-1.80187400
W	-1.99341600	2.88953400	-0.69925200
W	-0.22151800	2.88795300	2.25766500
W	-2.94800800	0.85630200	1.86419000
O	0.47066100	-3.38054300	2.18422100
O	0.42944000	-1.31415200	3.92743400
O	2.77485600	-1.92593300	2.37192400
O	-1.77235200	-3.32651100	-1.39146600
O	-1.07581800	-1.75197000	-3.42151200
O	-3.27227800	-1.21002700	-1.99831700
O	-1.95094800	2.24320400	2.80119900
O	-3.33256000	2.19382400	0.51859400
O	-1.20099400	3.79453900	0.73770900
O	3.87453900	0.70019200	-0.81184500
O	2.39519400	0.70215100	-3.07911400
O	2.32887900	2.86516100	-1.54924900
O	2.87746700	-4.35249300	1.04456300
O	-1.68524900	-3.07828900	4.05343000
O	-2.88297600	0.18393200	-4.39931200
O	0.28110700	-4.20199500	-3.13522600
O	-4.28484800	-3.09988000	-0.14763800
O	-2.88807800	4.16787400	-1.45037600
O	-0.03135200	4.26986100	3.29020100
O	-4.41858600	0.91213900	2.77515400

O	1.18186600	3.02973500	-4.12361900
O	4.22037300	3.03266800	0.65537700
O	4.30863400	-1.34942600	-2.66337500
O	1.34267400	3.11502300	0.99935100
O	2.76501900	0.92712800	1.51537300
O	0.69579600	1.60060900	3.11777500
O	-0.34842800	2.90305500	-1.70943700
O	-0.32272200	0.80367300	-3.26445400
O	-2.43583000	1.37868900	-1.86948300
O	1.47240500	-1.71670600	-2.47925400
O	2.85826500	-1.78102400	-0.28331900
O	0.76124200	-3.26601500	-0.50025800
O	-3.32586200	-0.50273400	0.58287600
O	-1.95303900	-0.50009600	2.80733900
O	-1.89077900	-2.57871000	1.23713200
Si	-0.02989300	0.00768200	0.05308300
Ru	1.77488500	-0.15827300	2.83637200
O	3.18851600	0.20403000	4.10786800
O	4.48401700	-0.36569000	3.42556700
H	4.03332100	-1.17698700	3.00422100
H	4.86904600	0.31984600	2.36507000
O	5.38608800	0.78596200	1.43269400
H	5.08087900	1.75015900	1.34703200
H	4.91533300	0.43853900	0.60727200

4H$_e$(Multiplicity = 2**)**

59

O	0.352953	-0.813641	1.421733
O	-1.509260	-0.445980	-0.479834
O	0.041680	1.617066	0.337623
O	1.112948	-0.380502	-1.127275
W	0.479496	-3.202961	1.604343
W	-0.888496	-0.682002	3.459730
W	-2.539757	0.405460	-2.435852
W	-2.241371	-2.667842	-0.996284
W	-3.501079	-0.085393	0.803832
W	1.072299	0.535666	-3.329917
W	3.456877	0.200250	-0.887020
W	1.304260	-2.613306	-2.016193
W	-0.413722	3.298512	-1.302553
W	1.958657	2.859182	1.160129
W	-1.370195	2.715591	1.907327
O	-0.665771	-2.569318	3.019641
O	0.838043	-0.509805	3.983558

O	2.021903	-2.654707	2.428809
O	-3.611125	-1.911278	0.064078
O	-2.798238	-1.503507	-2.453857
O	-3.843921	0.500067	-1.037213
O	0.396152	3.445758	2.139580
O	-1.447577	3.742949	0.236343
O	1.152748	3.824698	-0.416598
O	3.267424	-1.882551	-1.559880
O	1.378520	-1.430577	-3.473722
O	2.887232	0.586498	-2.714482
O	0.521898	-4.899999	1.929315
O	-1.708205	-0.782288	4.979109
O	-3.501277	0.855322	-3.800714
O	-2.983425	-4.156209	-1.469984
O	-5.095410	0.026640	1.464170
O	-0.715362	4.673589	-2.305617
O	3.107424	4.065795	1.628994
O	-2.249497	3.778008	2.947481
O	1.284644	0.970222	-4.990016
O	5.180990	0.304505	-1.101298
O	1.846984	-4.079437	-2.756821
O	2.962877	1.881428	-0.289893
O	3.362041	-0.597997	0.737319
O	2.318583	1.490914	2.262826
O	0.682402	2.182630	-2.514055
O	-0.794440	0.135924	-3.251775
O	-1.820908	2.087615	-1.877715
O	-0.527768	-2.795176	-2.037577
O	1.328294	-3.091781	-0.161992
O	-1.186603	-3.149908	0.456113
O	-2.802449	1.648703	1.167112
O	-1.018102	1.241484	3.035216
O	-2.482193	-0.730385	2.221998
Si	-0.005501	0.000320	0.027414
Ru	2.240208	-0.564272	2.453457
O	3.767097	-0.661765	3.615862
O	4.556936	-1.885465	3.326290
H	3.841796	-2.462814	2.974539
H	5.778577	-1.360394	1.763223
O	6.500468	-1.227088	1.121087
H	6.077112	-0.688642	0.429600
H	3.485032	-2.341972	-0.732760

4_{ox}(Multiplicity = 3)

55

O	1.193448	-0.131328	1.184319
O	0.544842	-0.613352	-1.370334
O	-1.323813	-0.821112	0.564123
O	-0.380639	1.592368	-0.141995
W	3.382175	0.855521	1.014833
W	2.150713	-2.225012	1.885475
W	-0.756189	-0.671467	-3.367221
W	2.438494	0.197514	-2.550419
W	1.231653	-2.865058	-1.681194
W	-2.019942	2.399973	-1.678376
W	-1.222522	2.974818	1.600753
W	1.163408	3.253342	-0.828892
W	-3.360942	-0.957692	-0.694605
W	-2.520893	-0.345616	2.595906
W	-1.371111	-3.142173	0.982023
O	3.614545	-0.993736	1.522698
O	1.777948	-1.252465	3.455703
O	2.804186	1.246990	2.780923
O	2.570229	-1.731770	-2.506411
O	1.015291	-0.018851	-3.834446
O	0.074803	-2.415154	-3.157655
O	-2.301045	-2.289234	2.419875
O	-2.889454	-2.754564	-0.147232
O	-3.837927	-0.565701	1.070588
O	0.175472	3.970869	0.640915
O	-0.434437	3.477331	-1.906546
O	-2.318184	3.278824	-0.019265
O	5.007026	1.438938	1.099432
O	3.011275	-3.575870	2.536345
O	-1.440895	-0.852838	-4.945258
O	3.752930	0.572474	-3.610412
O	1.789049	-4.420768	-2.191975
O	-4.906912	-1.248862	-1.413009
O	-3.690041	-0.276193	3.872672
O	-1.688415	-4.800074	1.355809
O	-3.125721	3.248866	-2.701608
O	-1.860170	4.246390	2.587440
O	2.052463	4.651697	-1.322237
O	-2.379468	1.495311	2.020643
O	0.070550	2.218050	2.685005
O	-0.944916	-0.182757	3.486230
O	-3.084416	0.911484	-1.082811
O	-1.248623	1.119509	-2.914415

O	-2.168859	-1.223934	-2.231253
O	1.755529	1.935059	-2.116327
O	2.405911	2.401267	0.363078
O	3.278094	0.266224	-0.829686
O	-0.303934	-3.308202	-0.630031
O	0.324146	-2.863680	1.851203
O	2.133541	-2.643168	-0.006373
Si	-0.005115	0.005841	0.047384
Ru	0.970435	0.527174	3.206692
O	1.105349	1.018959	5.078485
O	2.378970	1.641600	5.396714
H	2.812264	1.646733	4.505909

TS2 (Multiplicity = 3)

55

O	0.933068	-0.009849	1.441954
O	0.952373	-0.472985	-1.200702
O	-1.276839	-0.994729	0.234271
O	-0.530391	1.539226	-0.199453
W	2.951298	1.186752	1.672683
W	1.888130	-1.988086	2.417746
W	0.139361	-0.691101	-3.447641
W	2.921488	0.615280	-2.002542
W	1.998618	-2.587425	-1.288424
W	-1.847756	2.167169	-2.102578
W	-1.973728	2.737063	1.304634
W	0.866951	3.395074	-0.490814
W	-2.956829	-1.360913	-1.482205
W	-3.000694	-0.751426	1.918316
W	-1.122217	-3.311815	0.608538
O	3.249748	-0.563621	2.370866
O	1.062869	-1.168305	3.837904
O	1.829777	1.502943	3.413360
O	3.326551	-1.250953	-1.817444
O	1.906550	0.261569	-3.530398
O	1.179650	-2.249435	-3.039741
O	-2.472759	-2.639663	1.784910
O	-2.372515	-3.089928	-0.848140
O	-3.876509	-1.094667	0.109382
O	-0.514318	3.937986	0.681684
O	-0.383715	3.438502	-1.950867
O	-2.643931	2.943077	-0.596304
O	4.347516	2.013193	2.272911
O	2.769081	-3.249788	3.208973

O	-0.110356	-0.895195	-5.147348
O	4.387257	1.208006	-2.703420
O	2.874963	-4.030937	-1.665620
O	-4.233879	-1.823719	-2.551946
O	-4.445501	-0.897105	2.864111
O	-1.295092	-5.010162	0.881287
O	-2.754256	2.896979	-3.381621
O	-3.029094	3.906670	2.027167
O	1.678280	4.903164	-0.731190
O	-2.992401	1.108094	1.378737
O	-0.958436	2.185584	2.700140
O	-1.738995	-0.404127	3.165645
O	-2.818327	0.525442	-1.807162
O	-0.628276	1.019240	-3.104575
O	-1.402161	-1.452386	-2.712504
O	1.975280	2.207221	-1.597399
O	1.895467	2.625681	0.961021
O	3.435925	0.737348	-0.039973
O	0.311503	-3.271466	-0.698313
O	0.262733	-2.867758	1.872769
O	2.414781	-2.312005	0.520891
Si	0.011527	0.010707	0.063180
Ru	0.064277	0.549076	3.381319
O	-0.301682	1.072864	5.303441
O	0.629330	1.882147	5.805574
H	1.882222	1.979127	4.263513

4_{ox}-H_2O(Multiplicity = 3)

58

O	0.769628	-0.884278	1.192752
O	-0.927800	-1.008634	-0.880804
O	-0.977500	1.112775	0.777349
O	1.093870	0.771368	-0.898165
W	2.259076	-2.712526	0.707166
W	-0.309397	-2.172537	2.907523
W	-2.332903	-0.270538	-2.668944
W	-0.064744	-2.770967	-2.223465
W	-2.639002	-2.405212	-0.024438
W	0.513770	2.147516	-2.770913
W	2.644263	2.408911	-0.093496
W	2.761577	-0.333709	-2.161909
W	-2.336911	2.695261	-0.403336
W	-0.183830	2.807499	2.266073
W	-2.768105	0.570901	2.219412

O	1.068186	-3.310084	2.064289
O	1.040129	-1.242747	3.768788
O	3.168541	-1.597869	1.973086
O	-1.594872	-3.473277	-1.228176
O	-1.318796	-1.823166	-3.307693
O	-3.350305	-1.502316	-1.612689
O	-1.768759	2.006375	3.045832
O	-3.442439	1.866597	0.970260
O	-1.446352	3.645809	0.952491
O	3.607367	1.132805	-1.289451
O	1.893974	0.951574	-3.351324
O	1.820242	3.086641	-1.752086
O	3.378009	-4.026611	0.614907
O	-0.858913	-3.221877	4.167538
O	-3.391312	-0.044746	-4.017624
O	0.274173	-4.127770	-3.240395
O	-3.950323	-3.485021	0.300702
O	-3.431875	3.896213	-0.992971
O	0.018104	4.175970	3.307017
O	-4.105977	0.473240	3.309426
O	0.375805	3.178760	-4.151496
O	3.873436	3.616201	0.082645
O	4.040294	-0.862367	-3.197254
O	1.181369	3.111274	0.896482
O	3.026287	1.253132	1.302693
O	0.925668	1.558220	3.005959
O	-0.857611	2.870614	-1.595141
O	-0.807934	0.800087	-3.156242
O	-2.813688	1.161351	-1.530139
O	1.322901	-1.562864	-2.676084
O	2.967383	-1.474579	-0.661444
O	0.998724	-3.171702	-0.655321
O	-3.161285	-0.827317	0.977400
O	-1.537421	-0.705850	3.011236
O	-1.457327	-2.751658	1.401306
Si	-0.017260	0.005956	0.036020
Ru	2.137459	-0.010491	2.588106
O	3.350411	0.455068	4.020158
O	4.731613	0.682401	3.722260
H	4.857753	0.447323	2.764040
O	5.446186	-0.296335	1.216326
H	4.750515	-0.969349	1.401403
H	4.969952	0.276680	0.590503

TS2' (Multiplicity = 3)

58

O	0.972285	-0.762359	1.137318
O	-0.957892	-1.123051	-0.694149
O	-0.933057	1.113681	0.810387
O	0.929710	0.751799	-1.087203
W	2.479471	-2.540195	0.567656
W	0.197241	-1.955653	3.061420
W	-2.627689	-0.589381	-2.326535
W	-0.177182	-2.930969	-2.031016
W	-2.450301	-2.538908	0.472024
W	0.030940	1.956512	-2.964718
W	2.459937	2.527027	-0.597902
W	2.488436	-0.341724	-2.474369
W	-2.531796	2.530924	-0.289618
W	-0.070615	2.967844	2.073648
W	-2.494774	0.591546	2.504647
O	1.554650	-3.074782	2.123271
O	1.577996	-0.901430	3.690395
O	3.528767	-1.264454	1.648191
O	-1.492764	-3.641818	-0.783513
O	-1.603641	-2.141682	-2.996520
O	-3.409768	-1.811179	-1.070475
O	-1.500416	2.133946	3.095279
O	-3.404078	1.737135	1.266574
O	-1.549518	3.625021	0.867704
O	3.329155	1.237710	-1.849345
O	1.386592	0.786390	-3.635764
O	1.377572	3.035719	-2.184183
O	3.676718	-3.777051	0.420978
O	-0.124674	-2.950265	4.439571
O	-3.864016	-0.531713	-3.534411
O	0.124020	-4.338909	-2.988600
O	-3.633481	-3.667199	1.036614
O	-3.773184	3.614451	-0.813567
O	0.143167	4.432894	2.972628
O	-3.678609	0.499892	3.760590
O	-0.341340	2.869954	-4.384350
O	3.618237	3.813257	-0.676532
O	3.658879	-0.883222	-3.625774
O	1.089311	3.228501	0.518635
O	3.100422	1.504858	0.798148
O	1.196034	1.871640	2.773902
O	-1.240990	2.687751	-1.678521

O	-1.253439	0.513009	-3.086304
O	-3.053905	0.878700	-1.230231
O	1.080292	-1.693677	-2.711889
O	2.951061	-1.343417	-0.930603
O	1.125662	-3.171769	-0.579883
O	-2.943510	-0.928322	1.425022
O	-1.097711	-0.562424	3.222872
O	-1.072024	-2.716340	1.746678
Si	-0.004525	0.001291	0.035718
Ru	2.419524	0.314937	2.312588
O	3.749981	1.046766	3.592408
O	5.085730	1.042196	3.322388
H	5.291226	0.568825	2.178780
O	5.457636	0.051505	1.131600
H	4.586663	-0.730179	1.308806
H	4.968136	0.652647	0.536352

5([Ru^{IV}(η^2-OO)$SiW_{11}O_{39}$]$^{6-}$) (Multiplicity = 1**)**

54

O	-1.159817	-0.002885	1.307967
O	-0.723988	-0.001129	-1.390810
O	0.918156	1.349620	0.248632
O	0.923820	-1.345958	0.247913
W	-2.863140	-1.730521	1.476736
W	-2.869786	1.717505	1.479728
W	0.534949	0.003370	-3.480702
W	-2.152840	-1.707466	-2.224783
W	-2.161770	1.698962	-2.223013
W	2.807394	-1.871961	-1.172876
W	2.150917	-1.844281	2.214686
W	0.114624	-3.564676	0.063891
W	2.799760	1.884762	-1.170957
W	2.142135	1.852699	2.215682
W	0.098670	3.564733	0.065681
O	-3.767091	-0.008404	1.444076
O	-2.261989	1.455537	3.173356
O	-2.255483	-1.468823	3.170578
O	-2.966370	-0.004886	-2.682705
O	-0.861559	-1.325630	-3.632016
O	-0.866938	1.326549	-3.629988
O	1.264071	3.505082	1.580035
O	1.697562	3.464347	-1.046031
O	3.351870	2.147152	0.594517
O	1.279150	-3.501445	1.576836

O	1.711296	-3.456026	-1.049974
O	3.360841	-2.134324	0.591675
O	-4.191315	-2.817713	1.755444
O	-4.202521	2.798845	1.759492
O	1.142157	0.005512	-5.110047
O	-3.220163	-2.781723	-3.081563
O	-3.233103	2.770373	-3.078341
O	4.156762	2.517120	-2.055356
O	3.229044	2.533722	3.395362
O	-0.202320	5.274666	-0.013344
O	4.166508	-2.497776	-2.058695
O	3.241680	-2.522662	3.392394
O	-0.179627	-5.275668	-0.017411
O	2.712255	0.004526	2.105189
O	0.708233	-1.398974	3.189884
O	0.701382	1.397093	3.189213
O	3.232893	0.007272	-1.061621
O	1.634201	-1.296302	-2.631722
O	1.629440	1.306656	-2.630637
O	-0.877666	-2.931640	-1.473925
O	-1.379657	-2.956074	1.082614
O	-2.921377	-1.623150	-0.514101
O	-0.890003	2.929159	-1.470700
O	-1.391858	2.949275	1.086453
O	-2.927917	1.611965	-0.511789
Si	-0.011114	-0.000084	0.094251
Ru	-0.806338	-0.003982	3.439090
O	-0.152703	-0.001090	5.351895
O	-1.531975	-0.009062	5.309660

5([$Ru^{IV}(\eta^1$-OO)$SiW_{11}O_{39}]^{6-}$) (Multiplicity = 1)

54

O	1.181464	-0.403379	1.180093
O	0.643775	-0.089556	-1.455550
O	-1.242800	-1.066080	0.206335
O	-0.516177	1.518459	0.357319
W	3.263217	0.772668	1.476238
W	2.336880	-2.504307	1.212026
W	-0.594990	0.408189	-3.452616
W	2.491866	1.209680	-2.203372
W	1.542133	-2.054967	-2.439124
W	-2.212729	2.639349	-0.931511
W	-1.510734	2.183008	2.401012
W	0.873130	3.437492	0.290550

W	-3.234699	-0.964214	-1.167777
W	-2.544867	-1.359640	2.205994
W	-1.069879	-3.385401	-0.143253
O	3.688030	-1.114195	1.250006
O	1.869626	-2.185102	2.958471
O	2.666495	0.531384	3.167104
O	2.780388	-0.605748	-2.817530
O	1.098425	1.311475	-3.582373
O	0.373234	-1.243094	-3.761402
O	-2.144738	-3.127356	1.416184
O	-2.601262	-2.785742	-1.191134
O	-3.803173	-1.192694	0.591386
O	-0.224699	3.569449	1.860298
O	-0.731652	3.861084	-0.734563
O	-2.625954	2.906298	0.889486
O	4.843394	1.444748	1.754831
O	3.315249	-3.930013	1.386148
O	-1.227608	0.690322	-5.047953
O	3.782008	2.019555	-3.043880
O	2.256044	-3.311986	-3.406725
O	-4.728352	-1.136182	-2.041228
O	-3.784623	-1.799976	3.349292
O	-1.242717	-5.104272	-0.335052
O	-3.376632	3.681031	-1.694675
O	-2.313594	3.017712	3.700747
O	1.618506	5.007093	0.314694
O	-2.577993	0.572539	2.220777
O	-0.209554	1.244762	3.260391
O	-1.053807	-1.394685	3.203104
O	-3.135883	0.952971	-0.915501
O	-1.287321	1.899295	-2.475940
O	-1.981043	-0.606312	-2.629043
O	1.602304	2.681504	-1.323629
O	2.163302	2.375838	1.213447
O	3.247612	0.814779	-0.547979
O	0.016381	-2.941708	-1.692763
O	0.558212	-3.258774	0.839067
O	2.364196	-2.305842	-0.758319
Si	0.015868	-0.014213	0.066793
Ru	0.824059	-0.486304	3.352492
O	0.664659	-0.766794	5.179957
O	1.627406	-0.563450	6.054968

$[Ru^{IV}(\eta^1\text{-OO})SiW_{11}O_{39}]^{6-}$ (Multiplicity = 3**)**

54

O	1.075193	0.306364	1.292342
O	0.868603	-0.465674	-1.272952
O	-1.042550	-1.167933	0.495632
O	-0.820562	1.389383	-0.285407
W	2.811537	1.930070	1.286102
W	2.519299	-1.318289	2.271708
W	-0.113146	-1.019417	-3.374539
W	2.540253	0.856564	-2.316974
W	2.255232	-2.390709	-1.330587
W	-2.471856	1.562428	-2.037452
W	-2.250690	2.517066	1.277753
W	0.186990	3.408161	-0.974038
W	-2.786444	-2.012637	-0.949071
W	-2.563170	-1.004465	2.352307
W	-0.410109	-3.359508	1.083861
O	3.588506	0.256184	1.895993
O	1.723107	-0.506468	3.718590
O	1.975670	2.196436	2.891278
O	3.251273	-0.945837	-2.149475
O	1.395264	0.134523	-3.725171
O	1.170910	-2.405201	-2.948800
O	-1.729774	-2.787871	2.353036
O	-1.853779	-3.534331	-0.208543
O	-3.563525	-1.706567	0.726226
O	-1.140578	3.847017	0.333679
O	-1.270412	3.062473	-2.218165
O	-3.204971	2.363446	-0.512512
O	4.179716	2.994539	1.426708
O	3.699120	-2.326381	3.056097
O	-0.532040	-1.481192	-4.998344
O	3.783916	1.575069	-3.297960
O	3.317207	-3.723184	-1.679236
O	-4.080613	-2.817287	-1.785271
O	-3.848695	-1.267505	3.497920
O	-0.249708	-5.024226	1.555945
O	-3.659904	1.965739	-3.240439
O	-3.412588	3.579070	2.023040
O	0.631197	5.003640	-1.499371
O	-2.947968	0.755779	1.644877
O	-1.007102	2.301177	2.574865
O	-1.241870	-0.312390	3.371644
O	-3.072924	-0.171828	-1.446574
O	-1.196525	0.525395	-3.096933

O	-1.412690	-1.954727	-2.335191
O	1.293480	2.302638	-2.120520
O	1.498986	3.060172	0.365145
O	3.105482	1.246099	-0.570323
O	0.803816	-3.264939	-0.416788
O	0.998266	-2.536110	2.078472
O	2.829899	-1.834827	0.374255
Si	0.018235	0.013885	0.056126
Ru	0.379171	0.963133	3.281753
O	-0.053122	1.399994	5.215021
O	0.644401	2.332135	5.845456

$[Ru^{IV}(\eta^1\text{-}OO)SiW_{11}O_{39}]^{6-}$ (Multiplicity = 5**)**

54

O	1.160942	0.692917	1.090524
O	0.577436	-1.349013	-0.606154
O	-1.375431	-0.242051	0.894559
O	-0.289051	1.142502	-1.129712
W	3.471640	1.278394	0.398442
W	2.005554	-0.456461	2.988915
W	-0.666830	-2.694256	-2.190176
W	2.543208	-1.534263	-1.949670
W	1.167487	-3.273688	0.633285
W	-1.872881	0.769349	-2.920637
W	-1.128802	3.352032	-0.742760
W	1.339812	1.904987	-2.660413
W	-3.390776	-1.193755	-0.104682
W	-2.675831	1.438362	2.034706
W	-1.532758	-1.730140	2.696221
O	3.550603	0.149938	1.970254
O	1.697610	1.261805	3.613415
O	2.998145	2.730386	1.343002
O	2.559013	-3.015817	-0.683923
O	1.121979	-2.525477	-2.867023
O	0.051262	-3.882406	-0.841862
O	-2.540059	-0.188856	3.174885
O	-3.002022	-2.192687	1.493563
O	-3.934932	0.251921	0.937647
O	0.339795	3.432897	-2.038364
O	-0.225720	1.417012	-3.703833
O	-2.174211	2.498710	-2.248697
O	5.154819	1.588232	0.083101
O	2.791488	-1.155728	4.372878
O	-1.317266	-3.847840	-3.316909

O	3.889638	-1.978731	-2.957802
O	1.659818	-4.809781	1.284381
O	-4.919366	-1.884084	-0.561823
O	-3.929669	2.316293	2.866503
O	-1.923189	-2.758067	4.042099
O	-2.900259	0.766695	-4.322565
O	-1.805682	4.944297	-0.935013
O	2.276690	2.658814	-3.913901
O	-2.394310	2.475829	0.441006
O	0.009916	3.581081	0.659601
O	-1.175034	2.056150	2.794109
O	-3.022433	0.007126	-1.584779
O	-1.104528	-1.021269	-3.005674
O	-2.152943	-2.370671	-1.042110
O	1.895024	0.057157	-2.811143
O	2.545641	1.985969	-1.190155
O	3.316760	-0.433034	-0.669467
O	-0.436638	-2.917193	1.632512
O	0.137104	-0.955323	3.262983
O	2.001211	-2.038499	1.792220
Si	0.017568	0.051271	0.062536
Ru	0.914726	2.560856	2.226381
O	0.821597	4.175836	3.494490
O	1.851175	4.990340	3.637758

6([$Ru^{V}(\eta^{2}$-OO)$SiW_{11}O_{39}]^{5-}$) (Multiplicity = 2**)**

54

W	0.038340	3.562769	0.229996
W	0.108186	0.189866	-3.503271
W	0.192575	-3.554016	-0.098184
W	-2.682897	1.590293	1.912490
W	-2.357786	-1.670064	-2.061278
W	2.672340	-1.737443	-1.558551
W	2.365830	1.795645	1.977501
W	2.588918	2.005703	-1.412980
W	2.453306	-1.905002	1.882587
W	-2.660662	-1.844906	1.653407
W	-2.458760	1.727011	-1.835806
O	-0.989059	-0.070447	1.419015
O	0.927031	1.360013	0.164419
O	-0.891757	0.035013	-1.283183
O	0.974710	-1.329639	0.093245
O	2.941126	-0.039761	1.805171
O	-3.005731	1.559839	-0.037662

O	3.079660	0.150105	-1.414611
O	-2.964375	-1.677489	-0.241104
O	-1.123148	2.955094	-1.170514
O	-1.189675	-3.008260	1.100805
O	1.287700	1.492943	-2.743199
O	1.152536	-1.522860	3.095321
O	1.317953	-1.108587	-2.830503
O	0.941341	1.197420	2.990570
O	-1.008351	-2.879849	-1.480005
O	-1.297421	2.844455	1.431922
O	-3.555762	-0.159669	1.906895
O	3.354344	2.199382	0.328747
O	-3.267191	0.034211	-2.284425
O	3.436965	-2.073323	0.113685
O	-1.773364	-1.605935	3.289757
O	-1.323675	1.472303	-3.399625
O	1.515092	-3.524762	1.282536
O	1.503331	3.562287	-1.042529
O	1.363520	3.443104	1.605429
O	1.626025	-3.352371	-1.386122
O	-1.876926	1.175366	3.534457
O	-1.271295	-1.176639	-3.567674
O	0.323738	0.225515	5.262972
O	-0.317482	5.253885	0.282298
O	0.516925	0.277114	-5.180987
O	-0.082851	-5.256818	-0.216157
O	-3.969590	2.614807	2.446188
O	-3.495788	-2.724404	-2.826922
O	3.917360	-2.285550	-2.626580
O	3.485810	2.412596	3.145703
O	3.829783	2.713875	-2.387489
O	3.693652	-2.606775	2.868547
O	-3.887469	-2.972259	2.113603
O	-3.638224	2.808677	-2.493338
O	-0.551391	-0.801829	5.340488
Ru	-0.388520	-0.197539	3.432409
Si	0.016817	-0.001700	0.081678

6([$Ru^{V}(\eta^{1}$-OO)$SiW_{11}O_{39}]^{5-}$) (Multiplicity = 2**)**

54

O	1.001642	-0.214342	1.351971
O	0.771295	-0.501571	-1.305064
O	-1.377561	-0.866653	0.284427
O	-0.368428	1.596858	-0.074617

W	3.164527	0.792959	1.648276
W	1.865011	-2.350025	2.016377
W	-0.179753	-0.390628	-3.492340
W	2.827922	0.405809	-2.076091
W	1.526253	-2.717583	-1.691104
W	-1.750505	2.521779	-1.787123
W	-1.500067	2.836887	1.601175
W	1.252382	3.310395	-0.374043
W	-3.179250	-0.904177	-1.304543
W	-2.904743	-0.565030	2.114581
W	-1.454656	-3.209401	0.500455
O	3.346248	-1.114677	1.994105
O	1.208724	-1.503211	3.586339
O	2.311943	1.020152	3.267826
O	2.960188	-1.528102	-2.196898
O	1.615868	0.293972	-3.601483
O	0.608020	-2.154155	-3.289795
O	-2.633822	-2.482447	1.826468
O	-2.787111	-2.732081	-0.827120
O	-3.943217	-0.643812	0.390551
O	0.026823	3.891563	0.989471
O	-0.175711	3.625654	-1.654917
O	-2.325633	3.270772	-0.113924
O	4.757679	1.357695	2.015644
O	2.616269	-3.747789	2.700863
O	-0.606737	-0.443806	-5.167538
O	4.285429	0.858668	-2.890276
O	2.174291	-4.229810	-2.224502
O	-4.587045	-1.129843	-2.283193
O	-4.263085	-0.592570	3.189641
O	-1.802739	-4.893052	0.684291
O	-2.698485	3.456140	-2.890673
O	-2.288187	4.011093	2.597536
O	2.171905	4.755654	-0.605298
O	-2.675025	1.324775	1.736482
O	-0.368376	1.966020	2.833840
O	-1.490407	-0.478659	3.258351
O	-2.873198	0.999025	-1.477196
O	-0.783819	1.360718	-2.983892
O	-1.757680	-1.028380	-2.638217
O	2.051497	2.116239	-1.659630
O	2.306731	2.381821	0.921428
O	3.361947	0.337134	-0.271716
O	-0.152902	-3.241157	-0.931615

O	0.063592	-2.988783	1.650229
O	2.140765	-2.638356	0.126828
Si	-0.004171	0.000944	0.051819
Ru	0.414602	0.269913	3.369006
O	0.038281	0.500870	5.302412
O	0.946154	1.030648	6.069156

6 ($[Ru^{V}(\eta^{1}\text{-}OO)SiW_{11}O_{39}]^{5-}$) (Multiplicity = 4**)**

54

O	-1.078266	-0.538591	1.188452
O	-0.794371	0.226165	-1.362015
O	0.666444	1.399639	0.565670
O	1.180213	-1.142243	-0.137479
W	-2.361306	-2.559882	0.990843
W	-3.042061	0.670432	1.916291
W	0.267978	0.995106	-3.362926
W	-1.948490	-1.463351	-2.563784
W	-2.588274	1.754353	-1.650551
W	3.015581	-0.893234	-1.657694
W	2.639142	-1.900035	1.613310
W	0.795424	-3.348170	-0.878256
W	2.274937	2.646292	-0.688922
W	1.947766	1.625420	2.556549
W	-0.577616	3.364065	1.032728
O	-3.584544	-1.140793	1.497728
O	-2.223305	0.077537	3.473495
O	-1.645165	-2.533505	2.735314
O	-3.092444	0.087249	-2.517591
O	-0.854804	-0.502876	-3.843489
O	-1.358248	2.014646	-3.129463
O	0.675888	3.114547	2.463570
O	0.937101	3.886281	-0.074537
O	2.909854	2.538933	1.115875
O	2.019624	-3.450435	0.598476
O	2.256028	-2.652112	-1.938256
O	3.730811	-1.491857	-0.027913
O	-3.400310	-3.937436	1.077569
O	-4.509335	1.340858	2.538982
O	0.753197	1.534819	-4.932696
O	-2.844691	-2.481332	-3.636930
O	-3.894278	2.765738	-2.163910
O	3.430239	3.738437	-1.368462
O	2.908948	2.140230	3.900443
O	-1.196737	4.928604	1.429676

O	4.400191	-0.982344	-2.689974
O	3.905257	-2.617126	2.553760
O	0.807956	-4.998697	-1.392097
O	2.801166	-0.006374	2.025362
O	1.206815	-1.981103	2.734272
O	0.626580	0.584944	3.396392
O	3.080961	0.933868	-1.049311
O	1.659744	-0.211792	-2.892315
O	1.160618	2.249344	-2.209219
O	-0.424528	-2.556431	-2.146754
O	-0.708473	-3.320903	0.323756
O	-2.609473	-1.994752	-0.853871
O	-1.528113	2.962389	-0.603892
O	-1.848001	2.215213	1.870989
O	-3.220067	1.067060	-0.001967
Si	0.009102	-0.011002	0.047834
Ru	-0.522406	-0.982368	3.183395
O	-0.368766	-1.553028	5.114194
O	-0.989922	-2.532210	5.680598

6 ($[Ru^{V}(\eta^{1}\text{-}OO)SiW_{11}O_{39}]^{5-}$) (Multiplicity = 6**)**

54

O	1.522354	-0.138312	0.675757
O	-0.432625	-1.519159	-0.438552
O	-1.035691	0.608330	1.115000
O	0.074741	0.989836	-1.290885
W	3.538680	-0.744349	-0.348747
W	2.073514	-1.257780	2.660311
W	-2.451765	-2.070194	-1.492239
W	0.843115	-2.830445	-1.949256
W	-0.627782	-3.326355	1.085124
W	-1.813054	1.397075	-2.714316
W	0.602500	3.326656	-1.241653
W	1.474321	0.623679	-3.161244
W	-3.386743	0.875799	0.629583
W	-0.952710	2.816908	2.109602
W	-1.532418	-0.387041	3.183155
O	3.454724	-1.648194	1.377587
O	2.749410	0.485328	2.924892
O	3.978790	0.845759	0.457871
O	0.380162	-3.957533	-0.438582
O	-1.053314	-2.956924	-2.454930
O	-2.193158	-3.345406	-0.064586
O	-1.364399	1.514616	3.490987

O	-3.239283	0.000164	2.336848
O	-2.792382	2.478498	1.452296
O	1.592752	2.497429	-2.692638
O	-0.304288	1.012636	-3.845795
O	-0.986446	3.098048	-2.337058
O	5.080435	-1.294657	-0.913506
O	2.711633	-2.067953	4.049169
O	-3.847575	-2.749993	-2.256986
O	1.493520	-4.015493	-3.029012
O	-0.869777	-4.813720	1.934066
O	-5.092443	1.152356	0.562539
O	-1.273074	4.300330	2.943009
O	-2.086828	-0.884309	4.744503
O	-2.980224	1.874734	-3.897435
O	0.915390	4.997402	-1.560465
O	2.352049	0.626043	-4.651135
O	-0.533178	3.398502	0.311042
O	2.024336	2.913186	-0.051076
O	0.869149	2.619262	2.404090
O	-2.804413	1.555183	-1.081319
O	-2.150844	-0.486256	-2.559585
O	-3.234250	-0.854442	-0.224029
O	0.940518	-1.218009	-3.002026
O	2.842705	0.193229	-1.910722
O	2.368945	-2.209878	-1.052532
O	-1.523062	-2.061569	2.219827
O	0.346117	-0.629270	3.333361
O	0.983777	-2.674114	1.871761
Si	0.020809	-0.005344	0.016154
Ru	2.454763	1.817812	1.487204
O	4.498583	3.422921	2.497449
O	5.728721	3.531221	2.309956

TS3 (Multiplicity = 4**)**

57

O	1.591225	-0.410330	0.289549
O	-0.850493	-1.363261	-0.234141
O	-0.566389	0.825136	1.312290
O	-0.060311	0.970933	-1.322497
W	3.000343	-1.629134	-1.256570
W	2.343351	-1.820140	2.115399
W	-3.214078	-1.394007	-0.700593
W	-0.445222	-2.924923	-1.981929
W	-1.101681	-3.104807	1.361425

W	-2.118115	1.840956	-2.214525
W	0.997355	3.111942	-1.529944
W	0.655231	0.303995	-3.471671
W	-2.832608	1.632460	1.457479
W	0.283145	2.910111	2.121028
W	-0.693026	-0.079263	3.490884
O	3.152949	-2.480558	0.481562
O	3.454905	-0.338960	2.093123
O	3.992351	-0.185177	-0.656305
O	-0.719150	-3.930876	-0.350256
O	-2.360095	-2.580157	-1.953808
O	-2.869984	-2.723866	0.653701
O	-0.017526	1.714067	3.641486
O	-2.429641	0.717866	3.099055
O	-1.683067	3.040654	2.020553
O	1.306257	2.088563	-3.167306
O	-1.114571	1.091111	-3.675824
O	-0.869330	3.272097	-2.159006
O	4.171342	-2.503379	-2.181400
O	3.102378	-2.813472	3.310831
O	-4.879407	-1.711495	-1.041604
O	-0.395267	-4.212113	-3.136324
O	-1.457257	-4.507239	2.309644
O	-4.380728	2.304882	1.832625
O	0.601346	4.399768	2.946361
O	-0.922448	-0.458634	5.162083
O	-3.427114	2.581338	-3.067842
O	1.566085	4.674923	-2.014417
O	1.078468	0.109545	-5.136615
O	0.328191	3.425366	0.258284
O	2.520850	2.382590	-0.766276
O	1.996414	2.228295	1.910446
O	-2.583713	2.179506	-0.375720
O	-2.829259	0.071753	-1.868823
O	-3.322035	-0.071484	0.682329
O	-0.230406	-1.373038	-3.089740
O	2.160033	-0.473805	-2.593670
O	1.384601	-2.707635	-1.535396
O	-1.343734	-1.684030	2.625644
O	1.041986	-0.795061	3.164891
O	0.760544	-2.877960	1.653754
Si	-0.002201	0.017602	0.005911
Ru	3.016153	1.012177	0.649400
O	5.759976	1.282845	1.271122

O	6.635305	1.229835	0.409161
O	4.140688	3.782606	1.024685
H	3.418207	3.536853	1.634799
H	3.702847	3.619675	0.166384

3_a(Ge) (Multiplicity = 2)

56

O	0.526863	1.165239	-1.289538
O	-0.651298	0.847608	1.320815
O	-1.234957	-1.026935	-0.735214
O	1.382175	-0.958033	0.410043
W	2.098076	2.804285	-0.803168
W	-0.951027	2.677511	-2.298544
W	-1.502000	-0.285103	3.178708
W	0.598402	2.316396	2.607847
W	-2.467727	2.279755	1.147982
W	1.198828	-2.655727	2.024662
W	2.585014	-2.266816	-1.093108
W	3.257592	-0.032017	1.398822
W	-2.229367	-2.752804	0.476193
W	-0.828903	-2.333031	-2.586229
W	-3.253637	-0.203252	-1.533617
O	0.599034	3.679483	-1.625891
O	0.052997	1.990654	-3.689619
O	2.592685	2.001918	-2.454571
O	-1.126752	3.154829	2.223264
O	-0.347756	1.149540	3.819131
O	-2.765127	1.079780	2.670803
O	-2.537446	-1.444303	-2.846490
O	-3.629168	-1.757664	-0.432271
O	-1.715455	-3.447121	-1.261710
O	3.840489	-1.299310	0.089666
O	2.693031	-1.545467	2.504865
O	2.174472	-3.345588	0.576239
O	3.246478	4.095825	-0.763529
O	-1.811875	3.936826	-3.113982
O	-2.175232	-0.808172	4.683642
O	1.243807	3.469644	3.724118
O	-3.795692	3.367763	1.364682
O	-3.146994	-4.089485	1.077693
O	-0.847236	-3.396081	-3.951843
O	-4.822206	0.079068	-2.205212
O	1.355890	-3.930140	3.183326
O	3.664513	-3.416368	-1.809698

O	4.762459	0.345068	2.160291
O	0.861177	-2.807083	-1.727268
O	2.628525	-0.884181	-2.304168
O	0.069308	-0.817980	-3.259786
O	-0.474564	-3.121090	1.133074
O	0.032726	-1.397185	2.979836
O	-2.342517	-1.491854	1.926252
O	2.005498	1.043615	2.456098
O	3.073880	1.357589	0.112780
O	1.227101	2.983146	0.911624
O	-3.263679	0.890818	0.032627
O	-2.212245	1.209092	-2.333545
O	-1.667173	2.885399	-0.444660
Ru	1.441993	0.550238	-3.214592
O	2.157877	0.443976	-4.779492
O	5.112956	0.742801	-2.997837
H	4.406920	1.394709	-2.825345
H	4.643827	-0.059178	-2.713426
Ge	0.006889	0.010258	-0.066941

TS1$_a$(Ge) (Multiplicity = 2**)**

56

O	0.681163	1.226131	1.158489
O	0.939581	-0.039866	-1.415293
O	0.067257	-1.526714	0.870871
O	-1.662264	0.412670	-0.319957
W	0.868502	3.497674	0.557591
W	2.872712	1.142947	1.993109
W	0.517398	-1.542355	-3.158863
W	1.126345	1.793518	-2.818469
W	3.232821	-0.477609	-1.413544
W	-2.922721	-0.901200	-1.842451
W	-3.404946	0.466465	1.225955
W	-2.234550	2.409112	-1.330635
W	-0.756960	-3.468186	-0.161669
W	-0.980854	-1.944230	2.908477
W	2.061212	-2.510262	1.492429
O	2.580111	2.927249	1.200861
O	1.848130	1.563365	3.441997
O	0.110844	3.520749	2.241904
O	2.917197	1.014847	-2.577987
O	0.739185	0.227000	-3.914837
O	2.380772	-1.598930	-2.821175
O	0.778620	-2.716971	2.963725

O	1.003902	-3.847695	0.549849
O	-1.454446	-3.403855	1.582257
O	-3.468287	2.093405	0.128412
O	-3.172257	0.941450	-2.275284
O	-4.054653	-0.522875	-0.228386
O	1.131878	5.189182	0.294908
O	4.471445	1.327174	2.635270
O	0.411669	-2.503724	-4.596262
O	1.482540	2.947810	-4.060771
O	4.894513	-0.819413	-1.766055
O	-1.231482	-5.055493	-0.666783
O	-1.729434	-2.676794	4.291057
O	3.335566	-3.510756	2.103561
O	-4.132601	-1.652414	-2.827400
O	-4.856874	0.663043	2.148234
O	-3.008921	3.762478	-2.085088
O	-2.514228	-0.954113	2.034818
O	-2.187612	1.648919	2.414376
O	-0.463128	-0.328065	3.535928
O	-2.211230	-2.380514	-0.829352
O	-1.384673	-1.035455	-2.903486
O	0.152150	-2.790466	-1.774376
O	-0.756279	2.054185	-2.540996
O	-0.956418	3.228652	-0.218743
O	1.368024	2.780755	-1.225586
O	2.767650	-1.920909	-0.177933
O	2.552095	-0.772485	2.155880
O	3.324679	0.604485	0.098825
Ru	-0.205135	1.648198	3.093201
O	-0.742868	2.369313	4.653736
O	-1.886551	3.752409	4.228653
H	-1.216451	4.087980	3.595511
H	-2.503689	2.526705	2.706813
Ge	0.005782	0.025247	0.065348

$4H_a$(Ge) (Multiplicity = 2**)**

56

O	1.451894	-0.435480	-0.955917
O	0.351063	-0.044261	1.636795
O	-0.450563	1.586304	-0.544172
O	-1.280699	-1.110578	-0.400972
W	2.570412	-2.492560	-0.715569
W	3.476455	0.793073	-0.825663
W	-1.215868	0.506040	3.296887

W	1.037744	-1.983766	2.722016
W	2.020421	1.260676	2.627139
W	-3.382829	-0.990069	0.659403
W	-2.254655	-1.376210	-2.512195
W	-1.060791	-3.391137	-0.015155
W	-2.376439	2.609994	0.362113
W	-0.950807	2.200957	-2.752368
W	0.873865	3.445350	-0.167683
O	3.882009	-1.112554	-0.513280
O	3.229722	0.504814	-2.607596
O	2.466752	-2.298023	-2.546644
O	2.177455	-0.528447	3.336864
O	-0.380192	-1.163693	3.788861
O	0.384337	1.413290	3.743849
O	0.127935	3.591137	-1.961499
O	-0.912547	3.861434	0.489853
O	-2.444227	2.821243	-1.489151
O	-1.806210	-3.153633	-1.793879
O	-2.813504	-2.823269	0.663299
O	-3.683874	-1.258818	-1.322666
O	3.533129	-3.925238	-0.599146
O	5.064695	1.476327	-0.802540
O	-2.173182	0.829688	4.701288
O	1.542442	-3.231777	3.809460
O	3.125857	2.105785	3.655844
O	-3.682555	3.617356	0.883037
O	-1.567870	2.997904	-4.163206
O	1.605341	5.007648	-0.051871
O	-5.027572	-1.152066	1.170322
O	-3.063910	-1.838960	-3.969621
O	-1.227509	-5.105953	0.144184
O	-1.964862	0.442375	-2.741517
O	-0.262299	-1.617274	-3.122936
O	0.428323	1.254383	-3.390962
O	-3.244446	0.874551	0.236373
O	-2.488845	-0.621589	2.252794
O	-1.742900	1.860121	2.082548
O	-0.332608	-2.886983	1.686473
O	0.706078	-3.209506	-0.707051
O	2.140430	-2.238198	1.223730
O	1.274833	2.689975	1.551969
O	2.319831	2.365073	-0.815186
O	3.060913	0.831064	1.142360
Ru	1.508817	-0.488857	-3.101814

O	1.846605	-0.671365	-4.987846
O	2.775331	-1.783345	-5.277086
H	2.862270	-2.179464	-4.380378
H	0.025393	-2.488270	-2.800455
Ge	0.018501	-0.008499	-0.064412

The complete reference 37.

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