Supplementary material for "A comparison between artificial and natural water oxidation."

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Coordinates for the ruthenium blue dimer

BD_0^{4+}, 1 additional H_2O, ^3A

Ru1	-0.04306682	0.26929534	0.09915598
Ru2	0.20616382	-0.14256944	3.88823935
O3	1.83585513	1.40568121	0.63735396
O4	1.52526521	1.56853187	3.44656832
O5	-0.14467509	-0.17654273	1.99749894
N6	1.17908896	-1.38844233	-0.43722436
C7	1.52609696	-2.39338333	0.39264879
C8	2.25535289	-3.49632187	-0.03647775
C9	2.64363688	-3.56601934	-1.37520231
C10	2.28174474	-2.53297019	-2.23596201
C11	1.54126114	-1.45010011	-1.75104437
C12	1.07787080	-0.33361401	-2.60163644
C13	1.37101776	-0.23285456	-3.96431220
C14	0.87965626	0.84139884	-4.70413511
C15	0.10328673	1.80259744	-4.05833215
C16	-0.15315904	1.65008717	-2.69998436
N17	0.31673162	0.61214277	-1.97869042
N18	-1.83079948	-0.64774441	-0.38933687
C19	-1.97348125	-1.96048275	-0.65950210
C20	-3.19071522	-2.51354801	-1.04342269
C21	-4.30309996	-1.68029353	-1.15185074
C22	-4.15946844	-0.32475040	-0.86214464

C23	-2.91359547	0.17886602	-0.48081050
C24	-2.66691571	1.59933363	-0.15762224
C25	-3.64821799	2.59485076	-0.23233665
C26	-3.31544908	3.91429311	0.07181339
C27	-2.00531004	4.21472998	0.45098653
C28	-1.07484092	3.18254409	0.51113446
N29	-1.39061818	1.90447751	0.21834281
H30	1.18532123	-2.28697719	1.41452370
H31	2.50677491	-4.28664472	0.66271496
H32	3.21078570	-4.41362319	-1.74866918
H33	2.56632378	-2.58273929	-3.28012939
H34	1.97495949	-0.98584474	-4.45620039
H35	1.09824765	0.92204667	-5.76488144
H36	-0.30551334	2.65393641	-4.59328298
H37	-0.75597036	2.37374340	-2.16618431
H38	-1.08417595	-2.56954312	-0.56627000
H39	-3.25629733	-3.57517443	-1.25827999
H40	-5.26754847	-2.07493540	-1.45759753
H41	-5.01800652	0.33115884	-0.94128262
H42	-4.65804131	2.35335062	-0.54258326
H43	-4.06573842	4.69682656	0.00347650
H44	-1.70417730	5.23064983	0.68576965
H45	-0.04008975	3.37636432	0.76952038
N46	-1.44618589	1.10340747	4.38481859
C47	-2.42521100	1.45371299	3.52767494
C48	-3.52117468	2.21301673	3.91871852

C49	-3.61015873	2.62940905	5.24769570
C50	-2.60478103	2.26122436	6.13684509
C51	-1.52833362	1.48835376	5.68963557
C52	-0.44143433	1.01762683	6.57189301
C53	-0.35651875	1.34196401	7.92814849
C54	0.69827482	0.84607067	8.69399091
C55	1.65336006	0.03707366	8.08127828
C56	1.51634160	-0.24907113	6.72726348
N57	0.49693235	0.22111162	5.98177673
H58	-2.30286736	1.09240740	2.51551567
H59	-4.29121109	2.46646287	3.19818959
H60	-4.45204371	3.22246772	5.59231866
H61	-2.67069599	2.56593936	7.17399472
H62	-1.10143547	1.97469974	8.39423826
H63	0.77063135	1.08990677	9.74971185
H64	2.49276168	-0.36939417	8.63609804
H65	2.24136561	-0.87060963	6.21832439
N66	1.82578042	-1.49545617	3.82326053
C67	3.11449823	-1.16764883	3.59934975
C68	4.14501791	-2.09608800	3.70178457
C69	3.82865912	-3.40964579	4.05560791
C70	2.49723865	-3.74795567	4.29432012
C71	1.50177153	-2.77232007	4.17537549
C72	0.06684748	-3.01727239	4.43404431
C73	-0.45646066	-4.26780340	4.76990517
C74	-1.82296338	-4.40789567	5.00844693

C75	-2.64579582	-3.28796081	4.89752289
C76	-2.07314449	-2.06656307	4.55783615
N77	-0.75194026	-1.92804003	4.33331786
H78	3.30324139	-0.12574829	3.36590490
H79	5.17127872	-1.79090731	3.52434423
H80	4.60797773	-4.15927236	4.15864211
H81	2.24669660	-4.76042391	4.58796089
H82	0.19267380	-5.13175828	4.85256877
H83	-3.71419754	-3.35121754	5.07633877
H84	-2.23434664	-5.37611314	5.27806683
H85	-2.67261220	-1.17046882	4.46378810
H86	2.60684741	0.82568273	0.50390036
H87	2.04566162	2.25872331	0.13348043
H88	1.59063676	1.68147164	2.46906865
H89	1.32036659	2.43192228	3.84459872
O90	2.33852754	3.74482164	-0.45477695
H91	2.41205660	3.93421749	-1.40551659
H92	3.01366478	4.30589646	-0.03412477

BD_1^{5+}, 1 additional H_2O, ^2A

Ru1	0.02027903	0.18806953	0.07830038
Ru2	0.06028104	-0.04690503	3.91053354
O3	2.10440126	0.74586520	0.31531494
O4	0.58962407	2.10557285	3.73349318
O5	-0.12300254	-0.09282532	1.92216870

N6	0.75666034	-1.75310404	-0.45120067
C7	0.92012207	-2.77255251	0.42004954
C8	1.36298869	-4.02629485	0.01613071
C9	1.64944816	-4.23915348	-1.33467777
C10	1.47984859	-3.18918376	-2.23538926
C11	1.02738913	-1.94776192	-1.77608488
C12	0.80560391	-0.78586886	-2.65750449
C13	1.03628977	-0.81006409	-4.03493578
C14	0.79866154	0.33415133	-4.79901887
C15	0.33897498	1.48770644	-4.16193978
C16	0.12662443	1.45431947	-2.78842100
N17	0.34797180	0.34799838	-2.04436557
N18	-1.96150651	-0.21229436	-0.38338005
C19	-2.45360860	-1.44389504	-0.64168322
C20	-3.76076397	-1.63899446	-1.07340734
C21	-4.58304620	-0.52490616	-1.25320478
C22	-4.07610992	0.74632536	-0.97567289
C23	-2.75867858	0.89034908	-0.53700966
C24	-2.12984412	2.18799065	-0.22088974
C25	-2.79288652	3.41630966	-0.29580253
C26	-2.10242212	4.59132043	0.00925046
C27	-0.75994548	4.51502633	0.38973153
C28	-0.14877613	3.26573400	0.45048086
N29	-0.81597992	2.13048397	0.15353156
H30	0.67650179	-2.55201461	1.45228450
H31	1.47630280	-4.82354214	0.74327791

H32	1.99519000	-5.20794227	-1.68482773
H33	1.69481026	-3.34508332	-3.28584933
H34	1.39603667	-1.70900379	-4.52115132
H35	0.97059022	0.32192563	-5.87199246
H36	0.14199397	2.40023448	-4.71649215
H37	-0.22917675	2.33121251	-2.26357736
H38	-1.77530516	-2.27546326	-0.50018462
H39	-4.11831308	-2.64406976	-1.27517039
H40	-5.60401067	-0.63999643	-1.60750883
H41	-4.70797908	1.61615034	-1.11638395
H42	-3.83219015	3.46864044	-0.59947154
H43	-2.60508372	5.55264041	-0.05818132
H44	-0.18937330	5.40902094	0.62253212
H45	0.89616343	3.15899187	0.71500372
N46	-1.90745197	0.64512149	4.38398110
C47	-2.92439491	0.79229815	3.50871554
C48	-4.19106123	1.20733299	3.90565620
C49	-4.41812287	1.48328901	5.25605121
C50	-3.37012199	1.33150869	6.16361747
C51	-2.11758100	0.90611244	5.70898253
C52	-0.95497823	0.69944147	6.59527201
C53	-0.98224658	0.92800391	7.97157902
C54	0.16131288	0.70619859	8.74228646
C55	1.32353307	0.25647226	8.11309532
C56	1.29761545	0.03781816	6.74159571
N57	0.19154787	0.25115526	5.98965684

H58	-2.69376731	0.55517461	2.47634928
H59	-4.98701996	1.30495471	3.17473827
H60	-5.39635745	1.80606679	5.60204686
H61	-3.53986271	1.53768982	7.21358980
H62	-1.88722824	1.27791361	8.45458880
H63	0.14136341	0.88312861	9.81447179
H64	2.23659830	0.07465978	8.67180956
H65	2.17915621	-0.31191084	6.22118961
N66	2.02379566	-0.82977118	3.78592157
C67	3.13636652	-0.13147435	3.48412082
C68	4.40912619	-0.68748838	3.58383744
C69	4.53241698	-2.01553402	4.00149452
C70	3.38007415	-2.74737486	4.29296796
C71	2.12835246	-2.13315412	4.18030550
C72	0.84650776	-2.80276590	4.46835637
C73	0.72758095	-4.12971553	4.88401750
C74	-0.53550435	-4.67522425	5.12350211
C75	-1.66875727	-3.88122776	4.92946560
C76	-1.50153474	-2.56281003	4.52463450
N77	-0.27667560	-2.03187615	4.30121033
H78	2.98593508	0.89123975	3.15615436
H79	5.28427508	-0.08813687	3.35203883
H80	5.51172085	-2.47569086	4.10283505
H81	3.46744079	-3.77790600	4.61734307
H82	1.61135264	-4.74013294	5.03349851
H83	-2.66762637	-4.27026318	5.10176537

H84	-0.63079534	-5.70447327	5.45948404
H85	-2.34749583	-1.90376963	4.37854717
H86	2.69789781	0.00823937	0.08892816
H87	2.48949433	1.56877340	-0.14365235
H88	-0.17867777	2.69455614	3.85456954
H89	1.26517224	2.43043150	4.35889928
O90	3.11843074	2.92666669	-0.70662873
H91	3.28065705	3.09139790	-1.65216856
H92	3.87948752	3.33066374	-0.25212059

BD_1^{4+}, 1 additional H_2O, ^2A

Ru1	-0.16079426	0.11920865	0.06535631
Ru2	0.16491134	-0.04653581	3.82141915
O3	1.70755029	1.01042270	0.65030363
O4	1.17518897	1.52634871	3.17519024
O5	-0.35237279	-0.35827340	1.84046999
N6	0.94844087	-1.59405600	-0.51430150
C7	1.16822726	-2.65308430	0.28849589
C8	1.87480296	-3.77031095	-0.14158778
C9	2.37611450	-3.78860433	-1.44387590
C10	2.15128818	-2.69098162	-2.27178286
C11	1.42774670	-1.59580972	-1.78874835
C12	1.11649044	-0.40066689	-2.60015860
C13	1.52672127	-0.24255439	-3.92568372
C14	1.18168840	0.91578187	-4.62248471

C15	0.43828730	1.90132657	-3.97426931
C16	0.06030094	1.68960349	-2.65373508
N17	0.37909274	0.56603286	-1.97995202
N18	-2.00011908	-0.59773689	-0.61079865
C19	-2.24797925	-1.87368738	-0.96769518
C20	-3.48295191	-2.27587881	-1.46552039
C21	-4.49187311	-1.32344548	-1.60519466
C22	-4.23682505	-0.00403007	-1.22978901
C23	-2.98202405	0.34511254	-0.72874676
C24	-2.62516737	1.70934106	-0.28356213
C25	-3.49307307	2.80400483	-0.34864653
C26	-3.06284993	4.05049870	0.10780018
C27	-1.77603531	4.17907403	0.63513815
C28	-0.95564373	3.05651622	0.67307369
N29	-1.36465464	1.85630874	0.21780507
H30	0.75198525	-2.58023180	1.28580821
H31	2.02232072	-4.60995956	0.52927223
H32	2.92948491	-4.64635854	-1.81479479
H33	2.53120608	-2.69902947	-3.28570504
H34	2.10638863	-1.01084178	-4.42211171
H35	1.49135189	1.04367625	-5.65561971
H36	0.15301465	2.81908342	-4.47807557
H37	-0.51248055	2.43226326	-2.11335456
H38	-1.43236516	-2.57501132	-0.84671823
H39	-3.64192646	-3.31344697	-1.74079409
H40	-5.46558194	-1.59976970	-1.99915942

H41	-5.01693231	0.74141451	-1.33127095
H42	-4.49005969	2.69655477	-0.75949809
H43	-3.72518145	4.90961461	0.05016608
H44	-1.40940243	5.13195980	1.00319158
H45	0.04993128	3.09462974	1.07329477
N46	-1.57808730	1.02363993	4.31503491
C47	-2.64687973	1.17492729	3.50724217
C48	-3.80131840	1.82698042	3.92142234
C49	-3.85111992	2.34914644	5.21579991
C50	-2.74994675	2.19002862	6.05273365
C51	-1.61813401	1.51353772	5.58777088
C52	-0.42124502	1.25228784	6.40724078
C53	-0.26221406	1.70330992	7.71997554
C54	0.90574286	1.39709257	8.41775159
C55	1.89663741	0.64634413	7.78479576
C56	1.68629134	0.22470516	6.47646850
N57	0.55588209	0.51464780	5.80056813
H58	-2.54940179	0.74118206	2.51968850
H59	-4.64696732	1.91722105	3.24812556
H60	-4.73730869	2.86440296	5.57448525
H61	-2.78358559	2.57939870	7.06306948
H62	-1.03624603	2.29007793	8.20003918
H63	1.03928054	1.74237350	9.43874171
H64	2.82162657	0.38933685	8.29085357
H65	2.43193498	-0.35336747	5.94630754
N66	1.88334132	-1.29608341	3.63559302

C67	3.08028650	-0.87818181	3.18094588
C68	4.19966181	-1.70501115	3.17787612
C69	4.07325210	-3.00718673	3.66205806
C70	2.83254277	-3.43970994	4.12970839
C71	1.74194509	-2.56493731	4.11245016
C72	0.39707527	-2.91805991	4.61876544
C73	0.06999951	-4.17435531	5.13513772
C74	-1.21791741	-4.41393190	5.61247828
C75	-2.16096611	-3.38759845	5.56145126
C76	-1.77820891	-2.15649768	5.04076311
N77	-0.53441195	-1.92291637	4.57578683
H78	3.12048395	0.14682807	2.83632925
H79	5.15037484	-1.32583691	2.81751088
H80	4.92868407	-3.67607600	3.68810726
H81	2.72744884	-4.44463526	4.52174116
H82	0.81069189	-4.96428276	5.17682817
H83	-3.17341182	-3.53081782	5.92462655
H84	-1.47646759	-5.38607297	6.02204174
H85	-2.47612492	-1.33001776	4.98798036
H86	2.13679226	1.70224442	0.06538890
H87	1.60943320	1.36826446	1.57886155
H88	1.14698613	2.30722438	3.75436626
O89	2.90004748	2.78628220	-0.93964079
H90	3.75385180	2.50056511	-1.30673763
H91	3.03139079	3.72301643	-0.71518432

BD_2^{5+}, 1 additional H_2O, ^1A

Ru1	-0.22834522	0.17673423	0.07968550
Ru2	0.21050283	-0.08395807	3.73852288
O3	1.61381826	1.15653733	0.59658509
O4	1.31538347	1.47393756	3.21415059
O5	-0.34019429	-0.26493872	1.89801931
N6	0.93617238	-1.51993978	-0.45883423
C7	1.13221165	-2.58566859	0.34608550
C8	1.87724319	-3.68584259	-0.06077587
C9	2.44497496	-3.68306172	-1.33724280
C10	2.23687110	-2.58266332	-2.16607501
C11	1.46794257	-1.50667446	-1.71201410
C12	1.14102919	-0.32792636	-2.53023559
C13	1.58942498	-0.14539842	-3.83861979
C14	1.21422452	0.99628096	-4.55047084
C15	0.39847606	1.94288703	-3.92862774
C16	-0.01644573	1.71714105	-2.62275547
N17	0.33110029	0.60426525	-1.93372025
N18	-2.01226673	-0.64949592	-0.59407281
C19	-2.18824710	-1.94941051	-0.92308220
C20	-3.38814575	-2.42248029	-1.44217025
C21	-4.43802492	-1.52371227	-1.63855726
C22	-4.25734174	-0.18074948	-1.29412005
C23	-3.03747833	0.24468974	-0.77040145
C24	-2.74799385	1.63727195	-0.37848702

C25	-3.65767030	2.69210702	-0.49379836
C26	-3.27386890	3.97900638	-0.10809289
C27	-1.98753321	4.18974517	0.40108386
C28	-1.12107839	3.10709448	0.49428566
N29	-1.49005473	1.86323204	0.11251341
H30	0.66545075	-2.53670247	1.32195490
H31	2.00323887	-4.53228207	0.60648277
H32	3.03152155	-4.52761402	-1.68865300
H33	2.66058374	-2.57568566	-3.16358858
H34	2.22389692	-0.88444932	-4.31299761
H35	1.55529784	1.14101597	-5.57222086
H36	0.08327113	2.84489497	-4.44423710
H37	-0.64301960	2.43445262	-2.11239039
H38	-1.34604530	-2.60953556	-0.76450396
H39	-3.48871821	-3.47378536	-1.69444258
H40	-5.38453910	-1.85754770	-2.05586322
H41	-5.06904706	0.52213464	-1.44508777
H42	-4.65180026	2.52570604	-0.89310873
H43	-3.96979843	4.80791061	-0.21055234
H44	-1.65814982	5.17764561	0.70901069
H45	-0.10893617	3.21152844	0.86667125
N46	-1.46224565	1.07957408	4.35491946
C47	-2.54730001	1.30201678	3.57911024
C48	-3.65991628	1.98551042	4.05060582
C49	-3.65707325	2.45751992	5.36642753
C50	-2.54269920	2.21898441	6.16642836

C51	-1.45014100	1.51680415	5.64698767
C52	-0.24987660	1.17253755	6.42282427
C53	-0.02596219	1.59675608	7.73310768
C54	1.14973313	1.23555865	8.39273639
C55	2.08641000	0.45455672	7.71567723
C56	1.81606443	0.05720554	6.41107494
N57	0.67234997	0.39564673	5.77336252
H58	-2.49929517	0.90714367	2.57232950
H59	-4.51711101	2.13892944	3.40321996
H60	-4.51298364	2.99275447	5.76863901
H61	-2.53711651	2.56476451	7.19335979
H62	-0.75674135	2.21311700	8.24405515
H63	1.33022298	1.56442722	9.41267548
H64	3.01900978	0.15464654	8.18412237
H65	2.53039164	-0.53708471	5.86091882
N66	1.87250915	-1.35618589	3.68992994
C67	3.10807994	-0.95447220	3.30985545
C68	4.20146588	-1.80864353	3.38206185
C69	4.01209742	-3.10712511	3.86835160
C70	2.73427992	-3.51676755	4.26056527
C71	1.66440585	-2.62258617	4.17305631
C72	0.28529100	-2.92967107	4.60156547
C73	-0.10832815	-4.15694374	5.13652562
C74	-1.43319378	-4.34545510	5.53889090
C75	-2.34321247	-3.29791199	5.39087854
C76	-1.89639278	-2.09374409	4.85597703

N77	-0.61724234	-1.91074620	4.46568241
H78	3.18960169	0.07185881	2.97247552
H79	5.18319933	-1.45627053	3.08048275
H80	4.85217671	-3.79156861	3.95594454
H81	2.58775988	-4.51719621	4.65192920
H82	0.60433237	-4.96476944	5.25681285
H83	-3.38085205	-3.40423275	5.69183706
H84	-1.74359898	-5.29517973	5.96641596
H85	-2.56826318	-1.25386346	4.73047609
H86	2.05204651	1.86111592	0.01297973
H87	1.60889160	1.45117234	1.54851024
H88	1.11450169	2.29287243	3.70255679
O89	2.80965524	2.92471152	-0.94058406
H90	3.70119952	2.68611248	-1.25077317
H91	2.86310374	3.87915435	-0.75702127

BD_2^{4+}, 1 additional H_2O, ^5A

Ru1	0.08710668	0.03433595	-0.00428850
Ru2	-0.12297215	-0.08363857	3.78357741
O3	1.73615259	0.10367626	0.69132174
O4	1.74838133	0.78388942	3.27432116
O5	-0.61915407	-0.10525778	2.00453271
N6	0.01197247	-2.05234943	-0.28608060
C7	-0.50564123	-2.93394768	0.59099060
C8	-0.55853203	-4.29514949	0.31989402

C9	-0.05366301	-4.75714320	-0.89748273
C10	0.47370309	-3.84215223	-1.80580832
C11	0.49262688	-2.48224882	-1.48600428
C12	0.98364942	-1.42970321	-2.39523648
C13	1.56110173	-1.69099281	-3.63826939
C14	1.99423165	-0.63092126	-4.43543218
C15	1.84092679	0.67393985	-3.97009801
C16	1.26065372	0.87735642	-2.72249420
N17	0.83737013	-0.14498058	-1.95515122
H18	-0.88520768	-2.50795393	1.51142621
H19	-0.99371760	-4.97764629	1.04200655
H20	-0.07918537	-5.81444123	-1.14416093
H21	0.85327254	-4.18997665	-2.75896823
H22	1.68253771	-2.70933246	-3.98716969
H23	2.44791380	-0.82521484	-5.40274330
H24	2.16895825	1.52627152	-4.55595204
H25	1.13592471	1.87256865	-2.31760398
N26	-0.08680872	2.16907532	-0.11197568
C27	0.89689217	3.01102345	0.26697625
C28	0.81362034	4.38410780	0.06842842
C29	-0.32626667	4.90503277	-0.54545028
C30	-1.34587054	4.03623434	-0.93071340
C31	-1.21033258	2.66093915	-0.70887333
C32	-2.23587968	1.66955637	-1.10929449
C33	-3.43640477	2.02270714	-1.73213619
C34	-4.34821022	1.02718615	-2.08281702

C35	-4.04470196	-0.30282289	-1.79471977
C36	-2.83247199	-0.58911352	-1.17476007
N37	-1.94464721	0.36654745	-0.84097826
H38	1.76691053	2.55474491	0.72280414
H39	1.63404698	5.02328859	0.37731902
H40	-0.41963509	5.97116134	-0.73074318
H41	-2.22997124	4.43133988	-1.41591080
H42	-3.66569049	3.05749444	-1.95502784
H43	-5.27972801	1.28978231	-2.57548225
H44	-4.72712808	-1.10658412	-2.05050965
H45	-2.55325617	-1.60965923	-0.93909720
N46	-1.05682875	1.78747616	4.16618571
C47	-1.80282246	2.45127590	3.26018766
C48	-2.46066307	3.63500917	3.57129673
C49	-2.34245408	4.14953319	4.86335438
C50	-1.56985513	3.46306922	5.79751785
C51	-0.93001573	2.27415661	5.43245482
C52	-0.09899386	1.47314610	6.35669514
C53	0.16933862	1.84998731	7.67383004
C54	0.97930569	1.04409914	8.47401334
C55	1.51542061	-0.12424317	7.93443215
C56	1.21150787	-0.45034681	6.61695582
N57	0.41837854	0.31929366	5.84526670
H58	-1.86313551	1.99437927	2.27969325
H59	-3.06012596	4.13680691	2.81910052
H60	-2.84837714	5.06852395	5.14471951

H61	-1.47881707	3.85032978	6.80529629
H62	-0.24364392	2.76412109	8.08304081
H63	1.18977047	1.32985035	9.50048414
H64	2.15768395	-0.77496874	8.51880392
H65	1.61210035	-1.34539951	6.15891079
N66	-1.70364697	-1.25520776	4.49122417
C67	-2.94558936	-0.80690065	4.76222774
C68	-3.93085631	-1.63504999	5.28818917
C69	-3.61741065	-2.96944201	5.54802715
C70	-2.33405491	-3.43646100	5.26113764
C71	-1.38320545	-2.56364618	4.72765878
C72	-0.00392452	-2.96685131	4.37947690
C73	0.51124590	-4.24835640	4.58655945
C74	1.82937449	-4.52938609	4.22339246
C75	2.61015728	-3.52293622	3.65347759
C76	2.05000254	-2.26161310	3.47535433
N77	0.77782140	-1.99180195	3.83023847
H78	-3.13933051	0.23631762	4.54690380
H79	-4.91914548	-1.23596749	5.49224858
H80	-4.36080669	-3.64089698	5.96804530
H81	-2.08404586	-4.47238950	5.45705219
H82	-0.09767971	-5.02291696	5.03840083
H83	2.24008509	-5.52083300	4.39204680
H84	3.64022247	-3.70152147	3.36246161
H85	2.61837540	-1.43875869	3.06131521
H86	1.89787953	0.61842969	2.30399288

H87	2.00202470	1.73712221	3.45816712
O88	2.75166533	3.21441603	3.43331773
H89	3.72187611	3.16111948	3.48476920
H90	2.51742133	4.00166368	3.95157956

BD_3^{5+}, 1 additional H_2O, ^2A

Ru1	0.03851965	0.10914064	0.03869057
Ru2	-0.09344386	-0.12917958	3.74727088
O3	1.74082151	0.28587393	0.59003610
O4	1.82302832	0.72784086	3.30016134
O5	-0.53644764	-0.10534356	1.93508783
N6	0.08374447	-1.99403562	-0.29304559
C7	-0.41078856	-2.90304500	0.57721481
C8	-0.42510376	-4.26038706	0.28750442
C9	0.08902487	-4.69709114	-0.93713363
C10	0.58600114	-3.75602949	-1.83560703
C11	0.56625212	-2.39809453	-1.50296139
C12	1.00462878	-1.32537192	-2.40448381
C13	1.61769218	-1.55066937	-3.63714040
C14	2.01578164	-0.47026489	-4.42591008
C15	1.78813123	0.82300236	-3.95716839
C16	1.17614896	0.99470210	-2.71955229
N17	0.78086070	-0.05132180	-1.96203401
H18	-0.80308966	-2.50707430	1.50480564
H19	-0.83823515	-4.96317649	1.00359143

H20	0.09147611	-5.75255552	-1.19588965
H21	0.96773917	-4.08038745	-2.79681209
H22	1.79935551	-2.56165466	-3.98351241
H23	2.49954927	-0.63952294	-5.38411506
H24	2.08114364	1.69506404	-4.53408948
H25	1.00202401	1.98549653	-2.32673471
N26	-0.20736734	2.18568074	-0.21074768
C27	0.76881932	3.08075060	0.08461286
C28	0.64414506	4.42781704	-0.21783980
C29	-0.52344502	4.86930577	-0.85374254
C30	-1.52733413	3.94821774	-1.15694405
C31	-1.35782389	2.59674967	-0.83821823
C32	-2.34475797	1.54745353	-1.16108014
C33	-3.54939295	1.80623903	-1.81970469
C34	-4.42062241	0.74992071	-2.10099242
C35	-4.06941223	-0.54086771	-1.70651493
C36	-2.85351254	-0.73490166	-1.05383429
N37	-2.00571729	0.27866117	-0.78667917
H38	1.66247737	2.67845416	0.54798283
H39	1.45155916	5.11303028	0.02214727
H40	-0.64472874	5.91566058	-1.12280573
H41	-2.42622089	4.28552643	-1.65961788
H42	-3.81531199	2.81110842	-2.12630879
H43	-5.35514272	0.93735833	-2.62307743
H44	-4.71824054	-1.38800843	-1.90661127
H45	-2.54299263	-1.72443619	-0.73982506

N46	-0.99709364	1.76571609	4.14021912
C47	-1.75141153	2.43724399	3.24229274
C48	-2.37291910	3.63894592	3.55795198
C49	-2.21207534	4.16659419	4.84159368
C50	-1.43674336	3.46962341	5.76585577
C51	-0.83590396	2.26103889	5.39936981
C52	-0.01830744	1.44054024	6.30839385
C53	0.27635722	1.80253817	7.62284058
C54	1.07638535	0.97447493	8.41266727
C55	1.57740220	-0.20484787	7.85965754
C56	1.25170488	-0.52188598	6.54660340
N57	0.46139373	0.26975715	5.78353469
H58	-1.85118259	1.97648818	2.26733183
H59	-2.97900267	4.14743822	2.81507328
H60	-2.68846207	5.10167151	5.12339674
H61	-1.31421735	3.86419587	6.76789224
H62	-0.11021968	2.72525485	8.04013903
H63	1.30615727	1.25085285	9.43839999
H64	2.20996631	-0.87539239	8.43346576
H65	1.62889017	-1.42560123	6.09032415
N66	-1.71259663	-1.23073714	4.43960946
C67	-2.94745419	-0.73448276	4.67778536
C68	-3.96170989	-1.51744041	5.21744205
C69	-3.69029016	-2.85105823	5.53145254
C70	-2.41447643	-3.36569187	5.28137533
C71	-1.43101695	-2.54235518	4.73237867

C72	-0.05540886	-2.98435139	4.43509610
C73	0.43448752	-4.26671222	4.68681931
C74	1.76459314	-4.57244179	4.38242043
C75	2.58531250	-3.58825173	3.82219127
C76	2.05465247	-2.32314278	3.59621224
N77	0.76648263	-2.03214399	3.89152518
H78	-3.11103444	0.30521971	4.42539609
H79	-4.94135079	-1.08315568	5.39321218
H80	-4.45839908	-3.48450405	5.96760437
H81	-2.19744983	-4.39986072	5.52398140
H82	-0.20108567	-5.02451524	5.13168821
H83	2.15517202	-5.56515238	4.59195700
H84	3.62454433	-3.78936140	3.57991626
H85	2.65107763	-1.51065087	3.19983059
H86	2.03008257	0.69338913	2.33982134
H87	2.24642094	1.56916869	3.68444445
O88	3.22826978	2.76996585	4.03546043
H89	4.17524432	2.58990050	4.16909570
H90	3.08274345	3.66766359	4.37666838

BD_3^{4+}, 1 additional H_2O, ^6A

Ru1	0.08731096	-0.15464660	0.07632951
Ru2	-0.05313216	0.00879440	3.77992344
O3	1.85552595	-0.38209709	0.71102193
O4	1.46025882	0.83019566	3.29115202

O5	-0.57489849	-0.21923630	1.85577199
N6	-0.23423472	-2.20093777	-0.31765752
C7	-0.77964673	-3.05885551	0.56890929
C8	-0.98696321	-4.39656802	0.25828117
C9	-0.61314557	-4.85709597	-1.00620387
C10	-0.04864280	-3.96609143	-1.91812064
C11	0.13479901	-2.62825416	-1.55975150
C12	0.71080297	-1.60450901	-2.45796651
C13	1.13531264	-1.86991756	-3.76047409
C14	1.66497991	-0.83915020	-4.53885139
C15	1.76622203	0.43989060	-3.99426963
C16	1.32838407	0.64525351	-2.69007508
N17	0.80660104	-0.34516346	-1.94204856
H18	-1.04887890	-2.63380386	1.52867581
H19	-1.43555771	-5.06127045	0.98888123
H20	-0.76218312	-5.89658042	-1.28405613
H21	0.23977170	-4.31762196	-2.90164853
H22	1.05627653	-2.86733109	-4.17678014
H23	1.99423472	-1.03784004	-5.55467825
H24	2.17792791	1.26687553	-4.56358757
H25	1.39585984	1.62043718	-2.22377322
N26	0.19484833	1.96407310	0.07500713
C27	1.21914523	2.65304741	0.61856251
C28	1.30705311	4.03701304	0.50199231
C29	0.30898753	4.71923956	-0.19553218
C30	-0.76018801	4.00270908	-0.73593956

C31	-0.80647876	2.61416628	-0.58525530
C32	-1.90869749	1.76370071	-1.08234735
C33	-3.02215378	2.25838411	-1.76437264
C34	-4.03124445	1.38435556	-2.16888192
C35	-3.91245052	0.02641980	-1.87273399
C36	-2.77815564	-0.41187324	-1.19795201
N37	-1.79808345	0.43060070	-0.81476771
H38	1.95349932	2.06648025	1.15784645
H39	2.14667664	4.56182528	0.94633182
H40	0.35706255	5.79772669	-0.31621845
H41	-1.54423979	4.52664558	-1.26988272
H42	-3.10893026	3.31573223	-1.98580667
H43	-4.89714140	1.76168113	-2.70521733
H44	-4.67948471	-0.68515853	-2.16083512
H45	-2.64221460	-1.45751947	-0.95058164
N46	-1.16964015	1.78654856	4.07061967
C47	-1.97453342	2.34579206	3.14563641
C48	-2.71394271	3.49165600	3.40901979
C49	-2.61302201	4.07948751	4.67163824
C50	-1.78538308	3.49631301	5.62790321
C51	-1.06877464	2.33860919	5.31233050
C52	-0.19383670	1.62933947	6.26572588
C53	0.06680358	2.07984245	7.56068973
C54	0.91291934	1.34707579	8.39283426
C55	1.48816960	0.17435479	7.90758325
C56	1.19536053	-0.22668908	6.60812572

N57	0.36901101	0.47484800	5.80950811
H58	-2.01306738	1.83749095	2.18972675
H59	-3.36041650	3.91026200	2.64505960
H60	-3.17681709	4.97556083	4.91407132
H61	-1.70999195	3.93856893	6.61407971
H62	-0.37733217	2.99866581	7.92465654
H63	1.12158624	1.69294683	9.40089628
H64	2.15859932	-0.42281104	8.51700994
H65	1.63354420	-1.12256954	6.18942833
N66	-1.69307955	-1.31154122	4.50200658
C67	-2.96364444	-0.94746079	4.75315019
C68	-3.89120299	-1.81235979	5.32675334
C69	-3.48063491	-3.10333675	5.65664664
C70	-2.16608540	-3.48724684	5.39055595
C71	-1.28378686	-2.57281304	4.80869100
C72	0.12816679	-2.89471297	4.48628361
C73	0.71473443	-4.13898069	4.73699577
C74	2.05361824	-4.35497885	4.41201683
C75	2.78887985	-3.32282099	3.82726766
C76	2.16148833	-2.10340383	3.59658743
N77	0.86820807	-1.89769533	3.92163474
H78	-3.23517198	0.06818669	4.48764287
H79	-4.90542170	-1.47572104	5.51536507
H80	-4.17059454	-3.80471520	6.11675691
H81	-1.84145137	-4.48892777	5.64661264
H82	0.14089478	-4.93511866	5.19638176

H83	2.51528099	-5.31590739	4.62035323
H84	3.83461382	-3.45076966	3.56751817
H85	2.67475328	-1.25691720	3.15614521
H86	2.62404535	-0.38971375	0.05122338
O87	3.96249809	-0.35733175	-0.93076051
H88	4.64570727	0.31181363	-0.75236321
H89	4.45862483	-1.17967464	-1.08301712

BD_4^{5+}, 1 additional H_2O, ^5A

Ru1	0.13474869	-0.15482419	0.09920464
Ru2	-0.14185285	-0.00255009	3.78862662
O3	1.81237840	0.26034086	0.83841677
O4	1.30688532	0.90256544	3.57662971
O5	-0.58243612	-0.38649292	1.89519173
N6	0.55317462	-2.19167365	-0.27641905
C7	0.25338514	-3.20283254	0.56977385
C8	0.50146285	-4.52862680	0.23954635
C9	1.07953052	-4.81956347	-1.00038754
C10	1.38787029	-3.77407383	-1.87137449
C11	1.11290997	-2.45606630	-1.49635735
C12	1.38073225	-1.28558995	-2.35003146
C13	1.97324511	-1.36196177	-3.61040196
C14	2.19789290	-0.19597469	-4.34696161
C15	1.83066252	1.03296719	-3.79786826
C16	1.24318032	1.05551108	-2.53819025

N17	1.00988089	-0.07353464	-1.83337589
H18	-0.19990761	-2.91543752	1.51090156
H19	0.24018048	-5.31990652	0.93486479
H20	1.28174492	-5.84737332	-1.29042338
H21	1.82919115	-3.99313914	-2.83677576
H22	2.26330627	-2.31983147	-4.02708569
H23	2.65698618	-0.25124258	-5.33062277
H24	1.99610385	1.96393060	-4.33161040
H25	0.95397317	1.98997399	-2.07725718
N26	-0.48721359	1.87615549	-0.04563629
C27	0.22784902	2.91306157	0.44373644
C28	-0.13124086	4.23238343	0.19089156
C29	-1.26063846	4.48363999	-0.59405024
C30	-2.00628387	3.40875896	-1.08292297
C31	-1.60547026	2.09915305	-0.79816379
C32	-2.32197699	0.89379929	-1.25850168
C33	-3.50395925	0.93004654	-1.99784411
C34	-4.12949619	-0.26313654	-2.36875266
C35	-3.56139337	-1.47673939	-1.97725252
C36	-2.37743398	-1.45733855	-1.24863253
N37	-1.76526467	-0.30430124	-0.89704508
H38	1.09949649	2.65686560	1.03561979
H39	0.47133622	5.04209747	0.59173686
H40	-1.55690985	5.50326802	-0.82677432
H41	-2.88277178	3.59689641	-1.69250170
H42	-3.94461137	1.87618826	-2.29112098

H43	-5.04652940	-0.24070981	-2.95170977
H44	-4.02167585	-2.42572106	-2.23494071
H45	-1.90328499	-2.37736842	-0.93227546
N46	-1.55584148	1.54170903	3.95778470
C47	-2.41495087	1.90108455	2.97599911
C48	-3.34986864	2.90928568	3.15525589
C49	-3.39789420	3.57603260	4.38466239
C50	-2.51910222	3.19831052	5.39811063
C51	-1.60367437	2.16621910	5.17910318
C52	-0.67514506	1.66539968	6.20327872
C53	-0.53651806	2.22138254	7.47729734
C54	0.37967213	1.67383923	8.37787869
C55	1.14630071	0.57783309	7.98208547
C56	0.97045975	0.06338874	6.69913503
N57	0.07539949	0.58586033	5.84215492
H58	-2.33481760	1.34164001	2.05227208
H59	-4.03512226	3.16434991	2.35371040
H60	-4.11828964	4.37113925	4.55827988
H61	-2.56122062	3.69879260	6.35882839
H62	-1.12713554	3.08112340	7.77275815
H63	0.49610167	2.10408294	9.36905757
H64	1.87864311	0.12796281	8.64584524
H65	1.56145498	-0.77267794	6.34796121
N66	-1.44768573	-1.47992052	4.70200170
C67	-2.73639845	-1.23672837	5.03846047
C68	-3.52446255	-2.18922492	5.67228053

C69	-2.95995881	-3.42750165	5.98939076
C70	-1.62876704	-3.67463651	5.64853267
C71	-0.88098658	-2.68293411	5.01150305
C72	0.53863318	-2.82748406	4.64325834
C73	1.31593221	-3.95010912	4.94345264
C74	2.66588438	-3.97410910	4.58842139
C75	3.21342825	-2.87282218	3.92758058
C76	2.39531328	-1.78182067	3.64734960
N77	1.09277348	-1.76216455	3.99859223
H78	-3.13867669	-0.26709713	4.77610969
H79	-4.55851527	-1.96024223	5.91215870
H80	-3.54372205	-4.18904339	6.50011644
H81	-1.18292434	-4.63230959	5.89242947
H82	0.88406262	-4.79416763	5.46948416
H83	3.28030609	-4.83522957	4.83815974
H84	4.26306680	-2.84434321	3.65140759
H85	2.77168814	-0.89405863	3.15304467
H86	2.66964970	0.47473827	0.29355835
O87	3.95661381	0.81850390	-0.50092606
H88	4.68455561	0.17315637	-0.55120547
H89	4.39329720	1.67590003	-0.34568299

BD_4^{4+}, ^1A

Ru1	-0.56209509	-1.85974874	0.14287514
Ru2	0.41145909	1.82958898	-0.02579966

O3	-0.59114610	-2.24315041	-1.56190061
O4	2.13988152	1.65238641	0.17716660
O5	-0.17047633	0.01035056	0.11997491
N6	1.47503327	-2.40648801	0.34091918
C7	2.51184579	-1.55065752	0.24127543
C8	3.83215649	-1.97959347	0.30178321
C9	4.08818547	-3.34104190	0.46654978
C10	3.01504096	-4.22552855	0.56473120
C11	1.70602542	-3.74400632	0.49503355
N12	-0.69203444	-3.97686124	0.46359837
C13	-1.83292558	-4.69222157	0.47223395
C14	-1.83257332	-6.07612431	0.60678221
C15	-0.61077962	-6.73773380	0.73333038
C16	0.57023636	-5.99595124	0.71034237
C17	0.51286059	-4.60764266	0.56587182
N18	-1.05858695	-1.87294957	2.28439768
C19	-0.17263652	-2.08175318	3.27583398
C20	-0.55720690	-2.15700226	4.61009816
C21	-1.91041404	-2.01484746	4.92092063
C22	-2.82630356	-1.79431876	3.89221514
C23	-2.38076158	-1.73062317	2.56930433
N24	-2.67994936	-1.54452582	0.18191919
C25	-3.42310157	-1.44331751	-0.93793479
C26	-4.80893469	-1.32593077	-0.89141491
C27	-5.43926930	-1.31308143	0.35360988
C28	-4.66647597	-1.42225467	1.51084983

C29	-3.27777879	-1.54529930	1.40663791
N30	0.14234518	2.23302754	2.05528433
C31	1.11211686	2.02301913	2.96590136
C32	0.96561607	2.39634567	4.29808557
C33	-0.22496868	3.00619148	4.69409442
C34	-1.22621102	3.22285016	3.74669413
C35	-1.02431862	2.83417254	2.41960032
N36	-1.61477836	2.68108136	0.08913237
C37	-2.41853530	2.90061990	-0.96932034
C38	-3.65191427	3.53055781	-0.84119437
C39	-4.05881822	3.94970029	0.42697766
C40	-3.22748370	3.71805911	1.52351210
C41	-1.99716797	3.08262489	1.33211244
N42	0.85832779	3.86343760	-0.53079715
C43	1.03708493	4.86302414	0.35357590
C44	1.43142650	6.13608161	-0.04260997
C45	1.65188013	6.37687754	-1.39865660
C46	1.47700621	5.33609700	-2.31004985
C47	1.08402210	4.07448042	-1.85872168
N48	0.54233797	1.73897718	-2.13594158
C49	0.37868126	0.61867786	-2.86780885
C50	0.56178222	0.60404935	-4.24519392
C51	0.93055835	1.78782572	-4.88487937
C52	1.10145120	2.94503553	-4.12591898
C53	0.90733577	2.90681943	-2.74347177
H54	2.26453969	-0.50465978	0.10991473

H55	4.63782899	-1.25816296	0.21445713
H56	5.10730476	-3.71372921	0.51396403
H57	3.20471938	-5.28524036	0.68639255
H58	-2.75682395	-4.14015797	0.35781741
H59	-2.77276281	-6.61807280	0.60491442
H60	-0.57412196	-7.81800107	0.84035290
H61	1.52362295	-6.50323409	0.79518847
H62	0.86463776	-2.19532889	2.98091822
H63	0.18616750	-2.33559243	5.38047058
H64	-2.25316434	-2.08314211	5.94949749
H65	-3.87859505	-1.69082803	4.12820836
H66	-2.88323393	-1.48654405	-1.87747101
H67	-5.37623707	-1.26516484	-1.81478117
H68	-6.52040303	-1.23513776	0.42619958
H69	-5.15031918	-1.43163194	2.48037301
H70	2.02707573	1.57418019	2.59539744
H71	1.77800926	2.22885959	4.99803723
H72	-0.37011617	3.32512365	5.72233175
H73	-2.14652708	3.71229007	4.04315316
H74	-2.05239921	2.56479280	-1.93317564
H75	-4.26948301	3.69777440	-1.71796648
H76	-5.00863832	4.45940474	0.56198206
H77	-3.53528212	4.04762255	2.50869999
H78	0.87117851	4.62782865	1.39676312
H79	1.56871556	6.91421989	0.70115268
H80	1.96361096	7.35796123	-1.74517894

H81	1.65806463	5.51289541	-3.36328237
H82	0.09825038	-0.27624811	-2.32566886
H83	0.42373730	-0.31941072	-4.79799800
H84	1.08753858	1.81312854	-5.95937902
H85	1.39182333	3.86712995	-4.61511212

$BD_{TS4\text{-}5}^{4+}$, ^{3}A

Ru1	-0.48429200	-1.57242900	0.42700600
Ru2	-0.01107400	1.73633400	-0.65112600
O3	0.54248700	-1.42667000	-1.00899300
O4	0.44323100	0.44570100	-1.81292400
O5	-0.64889100	0.35925900	0.59570800
N6	1.04701400	-1.69394900	1.87869100
C7	1.45884700	-0.65225600	2.63092400
C8	2.42012600	-0.79560600	3.62313900
C9	2.97867800	-2.05817200	3.83803700
C10	2.54770700	-3.13398400	3.06313700
C11	1.56809800	-2.93988000	2.08467700
N12	-0.02299100	-3.67736900	0.43577800
C13	-0.58749600	-4.60542000	-0.35831700
C14	-0.16173600	-5.93080800	-0.37122100
C15	0.89291500	-6.30315800	0.46129000
C16	1.48393400	-5.33836600	1.27935900
C17	1.01216400	-4.02469000	1.25383700
N18	-2.06397600	-2.09685400	1.85132200

C19	-1.91172300	-2.19490700	3.18751600
C20	-2.95800000	-2.54302100	4.03539000
C21	-4.20918400	-2.80710100	3.47751000
C22	-4.37082900	-2.70563200	2.09454600
C23	-3.28312700	-2.35042000	1.29389500
N24	-2.21881100	-1.81291900	-0.80369100
C25	-2.18458800	-1.69820700	-2.14814700
C26	-3.29058100	-1.99538300	-2.93897800
C27	-4.46522800	-2.42216400	-2.31760100
C28	-4.49677300	-2.53438500	-0.92700700
C29	-3.35709300	-2.22780800	-0.17700300
N30	1.98843600	1.84018700	0.08386700
C31	2.97688400	1.04740900	-0.38551700
C32	4.30098200	1.21595900	0.00403200
C33	4.60948100	2.23814600	0.90411700
C34	3.58484400	3.05219900	1.38754400
C35	2.26761100	2.84469600	0.96531400
N36	-0.07888000	3.37840100	0.83536200
C37	-1.16627100	4.09122800	1.18472500
C38	-1.11650400	5.13462800	2.10510800
C39	0.11062800	5.45293400	2.68546000
C40	1.24004800	4.71246500	2.33155100
C41	1.12485400	3.67639700	1.40156600
N42	0.37805300	3.19013800	-2.17919800
C43	1.59965200	3.61215600	-2.55585900
C44	1.78843300	4.48619200	-3.62277400

C45	0.67332100	4.93001400	-4.33133000
C46	-0.59290400	4.48568000	-3.94656400
C47	-0.72294800	3.61166100	-2.86631000
N48	-1.95445400	2.17267700	-1.37836000
C49	-3.09104900	1.67660000	-0.84515400
C50	-4.34643100	2.05997800	-1.29933900
C51	-4.42890400	2.98489900	-2.34326100
C52	-3.25426600	3.50036200	-2.88849800
C53	-2.01515100	3.08877500	-2.38875000
H54	0.98084100	0.29709500	2.42045400
H55	2.71648700	0.06049100	4.21956600
H56	3.73116600	-2.20903200	4.60643800
H57	2.96389100	-4.11907000	3.23636000
H58	-1.39156400	-4.27277200	-1.00200200
H59	-0.64610800	-6.64599500	-1.02772900
H60	1.25714500	-7.32605000	0.47336500
H61	2.31091100	-5.61701500	1.92142400
H62	-0.92511300	-1.98231800	3.58036800
H63	-2.78957400	-2.60589600	5.10532500
H64	-5.04910100	-3.08892300	4.10555200
H65	-5.34084500	-2.90572800	1.65546100
H66	-1.24378300	-1.37526100	-2.57890400
H67	-3.21860800	-1.90730000	-4.01808900
H68	-5.34328800	-2.67635100	-2.90404900
H69	-5.40029000	-2.87896900	-0.43836400
H70	2.67992500	0.28622700	-1.09810600

H71	5.06914600	0.56805500	-0.40529600
H72	5.63469100	2.40974300	1.21892300
H73	3.82062900	3.85567500	2.07485300
H74	-2.10039000	3.81332200	0.71138800
H75	-2.01985900	5.68161900	2.35363700
H76	0.19284100	6.26390700	3.40288100
H77	2.19575600	4.95284200	2.78159100
H78	2.44239000	3.23400500	-1.99320500
H79	2.79219700	4.80012300	-3.88918700
H80	0.78214800	5.60617000	-5.17396200
H81	-1.46522900	4.81691600	-4.49715100
H82	-2.96207600	0.97448200	-0.03054200
H83	-5.23832700	1.65059100	-0.83732800
H84	-5.39308600	3.31132600	-2.72164900
H85	-3.30958000	4.23090500	-3.68648900

BD_5^{4+}, ^3A

Ru1	-0.51410925	-1.58298803	0.36426306
Ru2	0.13874593	1.57830075	-0.90240414
O3	0.56021679	-1.31606257	-1.38529003
O4	0.54608631	-0.13515165	-1.98524418
O5	-0.59297907	0.27157654	0.35916551
N6	1.22943721	-1.68165227	1.57670445
C7	1.67830928	-0.66250346	2.33862952
C8	2.76911128	-0.80260707	3.18766124

C9	3.41999825	-2.03683769	3.24670539
C10	2.95124239	-3.08883850	2.46321357
C11	1.84154631	-2.89679123	1.63449109
N12	0.06937346	-3.63940999	0.18214712
C13	-0.55508748	-4.56707713	-0.57211936
C14	-0.06668400	-5.85968755	-0.72303765
C15	1.11890980	-6.20602313	-0.07689030
C16	1.77088922	-5.24747883	0.70047276
C17	1.23222198	-3.96666738	0.82046742
N18	-1.82691214	-2.01400075	1.95809416
C19	-1.49816425	-2.03129077	3.26624133
C20	-2.42350095	-2.32954496	4.26011332
C21	-3.73498058	-2.62253187	3.88730671
C22	-4.07657621	-2.60351699	2.53411612
C23	-3.10882077	-2.29829031	1.57643359
N24	-2.32385710	-1.91419352	-0.67236693
C25	-2.46260457	-1.89372220	-2.01556816
C26	-3.66234711	-2.22650891	-2.63436015
C27	-4.75001464	-2.59068958	-1.83747039
C28	-4.60417631	-2.60902515	-0.45014605
C29	-3.37539675	-2.27000287	0.12252360
N30	2.14821287	1.68164760	-0.21848681
C31	3.12717669	0.80821807	-0.53974466
C32	4.44823706	1.00687610	-0.15373843
C33	4.76703427	2.14518747	0.58955939
C34	3.75541116	3.04627770	0.92349543

C35	2.44477273	2.80029761	0.50395491
N36	0.12222245	3.39377837	0.18572511
C37	-0.94387304	4.20429611	0.35631587
C38	-0.87987473	5.36894935	1.11310217
C39	0.33143903	5.71334389	1.71164455
C40	1.43782474	4.88018699	1.53396105
C41	1.31792591	3.72301306	0.76359602
N42	0.54816719	2.53045756	-2.72640796
C43	1.78719575	2.73894624	-3.22198478
C44	1.99927537	3.32428140	-4.46411984
C45	0.89407479	3.69721191	-5.22946649
C46	-0.38630066	3.46616943	-4.72730109
C47	-0.54413040	2.87667686	-3.47286797
N48	-1.80549618	1.90596685	-1.68044625
C49	-2.95169282	1.61242987	-1.03422825
C50	-4.19788357	1.96193606	-1.54179374
C51	-4.26174250	2.63775505	-2.76240887
C52	-3.07753205	2.94199553	-3.42949518
C53	-1.85126606	2.57137404	-2.86825909
H54	1.13042904	0.26881884	2.25491063
H55	3.09146973	0.03440777	3.79822642
H56	4.27212475	-2.18532436	3.90368722
H57	3.43632134	-4.05618678	2.51727956
H58	-1.46798515	-4.25937088	-1.06455175
H59	-0.60764841	-6.57257784	-1.33687735
H60	1.53418045	-7.20485151	-0.17478121

H61	2.69524605	-5.50680182	1.20277009
H62	-0.46967503	-1.79970625	3.51020658
H63	-2.11599809	-2.33363148	5.30079486
H64	-4.48444615	-2.86470759	4.63526979
H65	-5.09401738	-2.83017069	2.23892098
H66	-1.58277359	-1.62026369	-2.58606362
H67	-3.73378831	-2.21326753	-3.71722270
H68	-5.69876012	-2.86883139	-2.28782590
H69	-5.44059599	-2.90433185	0.17244256
H70	2.83063378	-0.05007748	-1.13072223
H71	5.20962338	0.29107440	-0.44665089
H72	5.79130357	2.33945370	0.89485468
H73	3.99822276	3.94081093	1.48430452
H74	-1.86449898	3.90057424	-0.12379790
H75	-1.76336090	5.98937131	1.22391155
H76	0.41945163	6.61794314	2.30642506
H77	2.38248981	5.14239034	1.99480606
H78	2.61712141	2.43061267	-2.60125634
H79	3.01268313	3.48040288	-4.81925224
H80	1.02338574	4.15407310	-6.20632848
H81	-1.25182942	3.73776625	-5.32012789
H82	-2.84058693	1.09579533	-0.08782938
H83	-5.09723546	1.71940392	-0.98492488
H84	-5.21754029	2.93370312	-3.18517984
H85	-3.11298365	3.47867902	-4.37026381

$BD_{TS5\text{-}6}{}^{4+}$, 1 additional H_2O, ^5A

Ru1	-0.06568000	0.07542500	0.15153100
Ru2	-0.13858700	0.01251000	3.81144800
O3	2.76662000	-0.09714300	-0.30891800
O4	1.34805100	1.05431900	2.83483100
O5	1.44605100	1.03303800	1.53965300
O6	-0.69089000	-0.34652300	2.06668500
N7	0.45093000	-1.95167100	-0.19119100
C8	0.39889300	-2.93894000	0.72149200
C9	0.75597500	-4.24936200	0.42264300
C10	1.18287200	-4.54797000	-0.87122300
C11	1.22587500	-3.52756400	-1.81956100
C12	0.85133100	-2.22897000	-1.46288100
C13	0.83872400	-1.09668900	-2.41050000
C14	1.19529800	-1.21955500	-3.75407300
C15	1.17401000	-0.10174600	-4.58796200
C16	0.79827300	1.12852700	-4.05342700
C17	0.44527300	1.19205300	-2.70956800
N18	0.45333500	0.11196300	-1.90480200
H19	0.04485600	-2.64999600	1.70261900
H20	0.69189000	-5.01718900	1.18587600
H21	1.46876100	-5.55899500	-1.14491900
H22	1.54433100	-3.75298800	-2.82982400
H23	1.49212800	-2.17917100	-4.15875500
H24	1.44889300	-0.19475600	-5.63414200

H25	0.77370400	2.02826800	-4.65908000
H26	0.15593700	2.13127600	-2.25983800
N27	-2.02840800	-0.15992400	-0.44271900
C28	-2.63191200	-1.35952900	-0.57848600
C29	-3.93580300	-1.48136400	-1.04448200
C30	-4.64148400	-0.32436300	-1.37708400
C31	-4.02449300	0.91570000	-1.21314400
C32	-2.71252900	0.98662100	-0.73887900
C33	-1.98531700	2.24689200	-0.50661700
C34	-2.49722100	3.51023400	-0.81720800
C35	-1.72232000	4.64574500	-0.57743700
C36	-0.45023600	4.49141000	-0.02553400
C37	0.00620500	3.20671500	0.26297000
H38	-2.04542900	-2.22840900	-0.31355600
H39	-4.37905000	-2.46615100	-1.14786500
H40	-5.65816700	-0.38269500	-1.75405300
H41	-4.56811100	1.82085600	-1.45659400
H42	-3.48099800	3.61534000	-1.25955600
H43	-2.10467000	5.63079900	-0.82786700
H44	0.18935100	5.34557800	0.17114700
H45	0.99132400	3.03570100	0.67897400
N46	-1.32114500	1.76813600	4.05817100
C47	-2.34270400	2.11035400	3.24921600
C48	-3.13768200	3.22519900	3.48918900
C49	-2.86093800	4.01830900	4.60432700
C50	-1.80248300	3.66589200	5.43866000

C51	-1.03960400	2.52862700	5.15287500
C52	0.07388700	2.05774500	6.00017500
C53	0.54333100	2.75730000	7.11284000
C54	1.59734400	2.23753200	7.86600200
C55	2.16417700	1.02169800	7.48575600
C56	1.65751900	0.37175000	6.36541300
N57	0.63612900	0.86722500	5.63750900
H58	2.07764300	-0.56898100	6.03464200
H59	2.98578700	0.58084000	8.04022700
H60	1.96767600	2.77743600	8.73222100
H61	0.10155200	3.70453800	7.39701600
H62	-1.58832800	4.26809200	6.31327000
H63	-3.46357800	4.89313200	4.82895400
H64	-3.96090800	3.45864500	2.82274900
H65	-2.51073700	1.45361100	2.40437300
N66	-1.45689000	-1.26053000	4.86361400
C67	-2.71862600	-0.95332000	5.22358400
C68	-3.51926600	-1.82737600	5.95169600
C69	-2.99279000	-3.06454600	6.32228300
C70	-1.68735200	-3.38666500	5.94684300
C71	-0.92869700	-2.47141400	5.21513600
C72	0.46021500	-2.72377100	4.77769300
C73	1.18323900	-3.87627600	5.10007700
C74	2.49941000	-4.01466400	4.65699600
C75	3.07037800	-2.99907800	3.88735800
C76	2.30612200	-1.87367600	3.59515300

N77	1.03727700	-1.73724300	4.03147700
H78	-3.08407500	0.01887000	4.91846300
H79	-4.52866800	-1.53656900	6.22266300
H80	-3.58508100	-3.77125200	6.89574500
H81	-1.27269500	-4.34687600	6.22936400
H82	0.73717800	-4.65724400	5.70427900
H83	3.07021300	-4.90121900	4.91707600
H84	4.09145400	-3.06671000	3.52710500
H85	2.70380500	-1.05313300	3.00995100
H86	3.21535800	0.46865100	0.33749300
H87	3.27760800	0.02414600	-1.15091700
N88	-0.73871100	2.10901700	0.02954100
O89	4.21852200	0.18316400	-2.62802900
H90	4.92433000	-0.47367300	-2.75007100
H91	4.63715400	1.02941300	-2.85747500

BD_6^{4+}, 1 additional H_2O, ^3A

Ru1	0.60045631	1.89350704	-0.97780810
Ru2	0.07595079	-1.87195749	-0.43840349
O3	0.45581136	1.36220737	-2.87614930
O4	1.29188719	-2.00643828	-2.17888709
O5	0.29694761	-0.02627048	-0.38657368
N6	1.72168967	-2.38399782	0.81507401
C7	2.51212433	-1.48418723	1.43350173
C8	3.54249480	-1.86789507	2.28344844

C9	3.76328648	-3.22903448	2.50155172
C10	2.94955701	-4.15862319	1.85842612
C11	1.92751531	-3.71656753	1.01195071
N12	0.06961585	-4.02749309	-0.48922104
C13	-0.77538077	-4.79192930	-1.21173430
C14	-0.73712536	-6.18120264	-1.18046543
C15	0.21170157	-6.80593650	-0.37166865
C16	1.09808801	-6.01856638	0.36255348
C17	1.01708335	-4.62679773	0.28766950
N18	-1.36993194	-1.99777823	1.05813168
C19	-1.11497861	-2.05856082	2.38054248
C20	-2.12375233	-2.24623616	3.31872616
C21	-3.43759836	-2.38420945	2.87009366
C22	-3.70116057	-2.31198829	1.50195049
C23	-2.65289370	-2.11309781	0.60121553
N24	-1.68811889	-1.78622365	-1.58161417
C25	-1.73900068	-1.64500903	-2.92050264
C26	-2.94165581	-1.72199594	-3.61811020
C27	-4.11707905	-1.96177018	-2.90512141
C28	-4.06028347	-2.09909919	-1.51628475
C29	-2.82961838	-2.00116700	-0.86402216
N30	2.72157741	1.71837434	-0.67672517
C31	3.59288931	1.22616284	-1.57780788
C32	4.96947727	1.24449267	-1.36997233
C33	5.46131126	1.78847246	-0.18328490
C34	4.56116385	2.29726906	0.75306647

C35	3.18856959	2.26208776	0.48526029
N36	0.87897002	2.75353929	0.96641212
C37	-0.10978670	3.27484350	1.72042749
C38	0.13228039	3.88872738	2.94410712
C39	1.44885306	3.97448518	3.39770122
C40	2.47295757	3.43811615	2.61729825
C41	2.16880597	2.82921411	1.39709789
N42	0.71442075	3.84415154	-1.76314082
C43	1.85994713	4.49725166	-2.04657314
C44	1.87115216	5.73597055	-2.67698617
C45	0.65558677	6.31896669	-3.03419371
C46	-0.53079769	5.64607822	-2.74275564
C47	-0.48310420	4.40575791	-2.10405533
N48	-1.44515421	2.41815474	-1.15921758
C49	-2.48234103	1.66760307	-0.74611859
C50	-3.80224636	2.07647275	-0.89232188
C51	-4.06016247	3.30622256	-1.49990130
C52	-2.98813084	4.08604492	-1.92444695
C53	-1.68017771	3.62830574	-1.73867628
H54	2.28655398	-0.44420886	1.23146453
H55	4.15444974	-1.11526563	2.76911245
H56	4.55520166	-3.56446679	3.16486198
H57	3.11231745	-5.21656436	2.02234223
H58	-1.49325083	-4.27055048	-1.83096002
H59	-1.43882274	-6.75464311	-1.77755936
H60	0.26715626	-7.88920125	-0.31500027

H61	1.84536026	-6.49587180	0.98496506
H62	-0.07832980	-1.95608414	2.67616405
H63	-1.87843645	-2.29130349	4.37490276
H64	-4.24933874	-2.54607701	3.57347000
H65	-4.72000168	-2.41646525	1.14803664
H66	-0.79342510	-1.48340313	-3.42374164
H67	-2.94692073	-1.60786236	-4.69731539
H68	-5.06945151	-2.04608830	-3.42086710
H69	-4.96940409	-2.28965390	-0.95717660
H70	3.15884959	0.83276976	-2.49030251
H71	5.63628107	0.85720714	-2.13361537
H72	6.52979180	1.83112662	0.00765704
H73	4.93370173	2.73811932	1.67006541
H74	-1.11321594	3.19370560	1.32050826
H75	-0.69204998	4.29871337	3.51859292
H76	1.67985690	4.45856038	4.34221616
H77	3.49805831	3.51072570	2.96071424
H78	2.78160479	4.00484434	-1.76658247
H79	2.81690758	6.22466330	-2.88713415
H80	0.62834237	7.28230278	-3.53487531
H81	-1.48006257	6.08851907	-3.01944873
H82	-2.22104782	0.72471746	-0.28209799
H83	-4.61009745	1.44773853	-0.53358377
H84	-5.07828599	3.65955834	-1.63388522
H85	-3.17435822	5.04882318	-2.38492491
O86	1.17022147	0.40768563	-3.37851155

H87	1.49238362	-1.10954044	-2.54253262
H88	2.10201570	-2.60312140	-2.21602723
O89	3.22568599	-3.79478487	-2.34044565
H90	4.18319708	-3.62724528	-2.34065699
H91	3.08116260	-4.39287940	-3.09440117

$BD^*_{TS4\text{-}5}{}^{4+}$, 1 additional H_2O, ^5A

Ru1	2.17228100	-0.45718200	-0.54309800
Ru2	-0.82260600	1.79605600	-0.12251900
O3	0.98562400	-1.26671900	-1.64122000
O4	-1.32948100	0.56255100	-1.31946200
O5	1.02444300	0.97437000	0.06285500
N6	-1.64561800	0.83289800	1.57532800
C7	-0.94566600	0.05931600	2.42698200
C8	-1.52360900	-0.51201800	3.55402100
C9	-2.87699800	-0.27817500	3.80498800
C10	-3.59703100	0.53276900	2.93056000
C11	-2.96213500	1.09230600	1.81754400
N12	-2.82311500	2.56044700	-0.08162900
C13	-3.35302700	3.41447700	-0.97598700
C14	-4.69825300	3.77216600	-0.96245800
C15	-5.52960900	3.21642900	0.00770900
C16	-4.98372300	2.32600900	0.93251100
C17	-3.62516200	2.00952900	0.87362600
N18	-0.16452600	3.56966700	1.05413700

C19	-0.11634500	3.65696400	2.39497200
C20	0.24464000	4.82532900	3.06134900
C21	0.57112100	5.94919700	2.30406100
C22	0.53162800	5.86146900	0.91205500
C23	0.15835800	4.65869900	0.30549500
N24	-0.24873000	3.23453500	-1.61131700
C25	-0.36027100	3.00603800	-2.93666600
C26	-0.15502900	4.00227300	-3.88445700
C27	0.17623100	5.28500300	-3.44369300
C28	0.29889900	5.51976300	-2.07479400
C29	0.07936400	4.48114700	-1.16195000
N30	1.56293000	-1.85938300	0.97003600
C31	0.54422800	-2.72649300	0.80387200
C32	0.26904500	-3.72998800	1.72765700
C33	1.07744900	-3.83561600	2.86100800
C34	2.12552200	-2.93098900	3.03527600
C35	2.35995700	-1.94297100	2.07304400
N36	3.58185000	-0.12057600	1.08930200
C37	4.55597200	0.80804800	1.08291200
C38	5.46395000	0.94456600	2.12896700
C39	5.35709500	0.08490200	3.22195700
C40	4.34235000	-0.87299100	3.23407000
C41	3.46114700	-0.96078300	2.15349100
N42	3.65548900	-1.83456100	-1.34065000
C43	3.78681800	-3.13030700	-1.00630100
C44	4.69449900	-3.97660800	-1.63760700

C45	5.48848200	-3.46121000	-2.66065100
C46	5.34578800	-2.11932000	-3.01653300
C47	4.42015800	-1.31933400	-2.34260000
N48	3.22585900	0.73780200	-1.93109100
C49	3.00536600	2.05587800	-2.10523700
C50	3.73731100	2.81466500	-3.00981700
C51	4.72928800	2.18584300	-3.76408300
C52	4.96367100	0.82526600	-3.57499800
C53	4.20586300	0.10924700	-2.64396100
H54	0.09821800	-0.07821800	2.17843400
H55	-0.92431400	-1.12123300	4.22151300
H56	-3.36470600	-0.70830700	4.67452700
H57	-4.64197300	0.73783200	3.12844300
H58	-2.68314700	3.81426400	-1.72473500
H59	-5.07749100	4.46671600	-1.70447900
H60	-6.58564900	3.46552500	0.04603000
H61	-5.62190300	1.88082000	1.68615700
H62	-0.38044000	2.76254000	2.94684400
H63	0.26119000	4.84869900	4.14581000
H64	0.85128400	6.88183700	2.78423200
H65	0.78771900	6.73009900	0.31768600
H66	-0.63148400	1.99845100	-3.22338100
H67	-0.26782700	3.77539000	-4.93937100
H68	0.32796800	6.09470700	-4.15138700
H69	0.54385200	6.51505400	-1.72457100
H70	-0.03901900	-2.60149500	-0.10158700

H71	-0.55219800	-4.41643100	1.55017500
H72	0.90371000	-4.61557200	3.59657300
H73	2.76412600	-3.01351100	3.90675700
H74	4.60418800	1.45308100	0.21413400
H75	6.23646900	1.70461800	2.07923100
H76	6.05106100	0.15500300	4.05413900
H77	4.24926100	-1.54184000	4.08120600
H78	3.14293900	-3.49764100	-0.21752400
H79	4.76744200	-5.01483800	-1.33155100
H80	6.20611500	-4.09017100	-3.17862600
H81	5.95229600	-1.71181500	-3.81621900
H82	2.22845800	2.48315800	-1.48524800
H83	3.53644300	3.87495900	-3.11529000
H84	5.32214300	2.74528300	-4.48144600
H85	5.74427600	0.33394900	-4.14284400
O86	0.33108700	-0.51071900	-3.15016800
H87	0.11347200	-1.36354900	-3.68886800
H88	-0.48267100	-0.23716800	-2.64891900
O89	-0.20955100	-2.65792800	-4.49320100
H90	0.05311400	-2.71424900	-5.42788600
H91	-1.07407700	-3.09874100	-4.43738000

$BD^{*}_{5}{}^{4+}$, 1 additional H_2O, ^{3}A

Ru1	0.63385425	1.84057298	-1.07964887
Ru2	0.03414879	-1.90041249	-0.48453187

O3	0.41575220	1.41549455	-3.02129505
O4	1.12045383	-2.06550231	-2.05249331
O5	0.22653536	0.05141220	-0.52973279
N6	1.59675085	-2.27567799	0.87578462
C7	2.26403504	-1.32410787	1.56041883
C8	3.26217532	-1.63855928	2.47222504
C9	3.58489474	-2.98245309	2.67804860
C10	2.89609228	-3.96432210	1.97002654
C11	1.89477985	-3.59355265	1.06713162
N12	0.11135680	-4.02104267	-0.48768577
C13	-0.64662916	-4.83096356	-1.24930108
C14	-0.47962206	-6.21276367	-1.26195494
C15	0.51392947	-6.77559491	-0.46401908
C16	1.31016469	-5.93597826	0.31494571
C17	1.09607086	-4.55745280	0.28760364
N18	-1.49776149	-2.02217131	1.05887798
C19	-1.27119789	-2.07742165	2.38443536
C20	-2.28335690	-2.31327753	3.30942421
C21	-3.58237103	-2.50597835	2.84208677
C22	-3.82254818	-2.44094494	1.47007824
C23	-2.76494546	-2.19702689	0.59011056
N24	-1.78627814	-1.87635904	-1.59157979
C25	-1.83618632	-1.78802229	-2.93688265
C26	-3.02634344	-1.93226925	-3.64107154
C27	-4.20065118	-2.18179707	-2.92937265
C28	-4.14697774	-2.26721897	-1.53864559

C29	-2.92448062	-2.11159598	-0.87841791
N30	2.74653021	1.59737986	-0.86053290
C31	3.58268111	1.09181680	-1.78906383
C32	4.96322849	1.06243907	-1.61319172
C33	5.50013597	1.58452084	-0.43726201
C34	4.63709849	2.10898636	0.52467775
C35	3.25826022	2.10662070	0.29867016
N36	0.96724955	2.57058514	0.88311672
C37	0.00493536	3.02741055	1.70869191
C38	0.29400625	3.58187112	2.95104897
C39	1.62787072	3.67477563	3.34925753
C40	2.62510008	3.19734515	2.49911635
C41	2.27461410	2.64366171	1.26395270
N42	0.83996946	3.87731622	-1.73087509
C43	2.00465186	4.49556015	-2.00907216
C44	2.06402712	5.81535127	-2.44398941
C45	0.87369080	6.52388737	-2.60111485
C46	-0.33450255	5.88530520	-2.32385547
C47	-0.33147050	4.55736103	-1.89066407
N48	-1.38360081	2.51198384	-1.18289815
C49	-2.45359137	1.75749286	-0.86999690
C50	-3.75215060	2.24814754	-0.93450621
C51	-3.95202302	3.56769583	-1.34283857
C52	-2.84611400	4.34916923	-1.66811421
C53	-1.56105030	3.80279007	-1.58084784
H54	1.96410556	-0.30402780	1.35595631

H55	3.77384583	-0.85024061	3.01378166
H56	4.35923408	-3.26486310	3.38552267
H57	3.13577530	-5.00812402	2.13029913
H58	-1.39754182	-4.35641713	-1.86653654
H59	-1.11608703	-6.82679488	-1.89064609
H60	0.67509595	-7.84944846	-0.44966684
H61	2.09415362	-6.36168516	0.92988173
H62	-0.24702711	-1.93111208	2.70588442
H63	-2.05056870	-2.35258869	4.36867596
H64	-4.39808048	-2.70570902	3.53081931
H65	-4.82910123	-2.59094468	1.09847299
H66	-0.89168787	-1.62145206	-3.43918978
H67	-3.02360891	-1.86489383	-4.72398998
H68	-5.14586161	-2.31631563	-3.44732148
H69	-5.05240545	-2.46894031	-0.97831052
H70	3.12082071	0.71810466	-2.69362454
H71	5.59706966	0.64825539	-2.39052766
H72	6.57338152	1.59177515	-0.27027454
H73	5.04466745	2.52631307	1.43799938
H74	-1.01432436	2.94257755	1.35304378
H75	-0.51127462	3.94031667	3.58411855
H76	1.89118713	4.11478840	4.30682091
H77	3.66360598	3.26891396	2.79953319
H78	2.90658327	3.91086985	-1.88214914
H79	3.02606659	6.27099179	-2.65454880
H80	0.88188321	7.55650353	-2.93722115

H81	-1.26574823	6.42424759	-2.44845637
H82	-2.23555874	0.74364858	-0.55808623
H83	-4.58790508	1.61011332	-0.66766002
H84	-4.95243827	3.98583282	-1.40444564
H85	-2.98912447	5.37578424	-1.98209922
O86	1.13650069	0.38156249	-3.53882807
H87	0.88329671	0.36767640	-4.55044522
H88	1.30916597	-1.18595690	-2.44388375
O89	0.42729163	0.13147915	-5.98135114
H90	1.01796833	-0.37153948	-6.56972921
H91	0.10386063	0.88028697	-6.51179775

$BD^*_{TS5\text{-}6}{}^{4+}$, 1 additional H_2O, ^1A

Ru1	-0.14000500	-1.88468900	-0.67744300
Ru2	1.21937700	1.49447800	-0.78272500
O3	0.82516000	-1.97035600	-2.36803000
O4	0.78838400	0.91088500	-2.60711100
O5	0.44680800	-0.16816800	-0.15048400
N6	1.36899700	-2.90963100	0.43144400
C7	2.32089200	-2.27390300	1.14431900
C8	3.24820600	-2.95864400	1.91960800
C9	3.19058900	-4.35291500	1.96222800
C10	2.20473400	-5.00841000	1.22949900
C11	1.29522300	-4.26939700	0.46560700
N12	-0.61015300	-3.99896000	-0.96713900

C13	-1.60585900	-4.47588500	-1.73903000
C14	-1.85112100	-5.83700400	-1.88939600
C15	-1.03056700	-6.74352900	-1.21888000
C16	0.01193300	-6.25359600	-0.43400400
C17	0.20992800	-4.87494900	-0.32402600
N18	-1.64992700	-1.94952500	0.88213700
C19	-1.43238200	-2.26425100	2.17102600
C20	-2.46385900	-2.34637700	3.10335000
C21	-3.76849800	-2.09773200	2.67792100
C22	-3.99546900	-1.76475700	1.34115600
C23	-2.91806300	-1.69430600	0.45402900
N24	-1.90108100	-1.32719100	-1.70781500
C25	-1.92988100	-1.05767300	-3.02750200
C26	-3.11938400	-0.79049900	-3.69769600
C27	-4.31317100	-0.81520100	-2.97429500
C28	-4.27972300	-1.10068700	-1.60715900
C29	-3.05773900	-1.35813200	-0.98074700
N30	3.25433300	0.91770100	-0.47758300
C31	4.03079800	0.26619000	-1.36972800
C32	5.38568600	0.03788300	-1.15111900
C33	5.96124600	0.49585200	0.03425300
C34	5.15670900	1.15117000	0.96722600
C35	3.80013700	1.35513100	0.70037600
N36	1.59082600	2.14386500	1.22203600
C37	0.68215900	2.72201500	2.02901500
C38	1.01145500	3.23304800	3.28120900

C39	2.33468800	3.14344400	3.71202500
C40	3.27636600	2.53218400	2.88306200
C41	2.88287700	2.03337200	1.63851900
N42	1.86956900	3.40871400	-1.55881100
C43	3.14231400	3.74049800	-1.85275100
C44	3.48151300	4.93977800	-2.47210700
C45	2.46554800	5.83118900	-2.80956200
C46	1.14617800	5.49073300	-2.50993100
C47	0.86651500	4.27540600	-1.88322200
N48	-0.59630800	2.59949100	-0.97599700
C49	-1.79733300	2.13781700	-0.57512100
C50	-2.95916500	2.88869000	-0.70575400
C51	-2.87645100	4.16014500	-1.27670900
C52	-1.63376500	4.63675300	-1.68591900
C53	-0.49447400	3.84136200	-1.52345700
H54	2.30610000	-1.19362100	1.08532700
H55	3.99421000	-2.40869300	2.48289400
H56	3.89553100	-4.92210300	2.56056000
H57	2.14294100	-6.08923300	1.26211600
H58	-2.21768200	-3.74624700	-2.25200900
H59	-2.66780100	-6.17048300	-2.52097300
H60	-1.19234200	-7.81343600	-1.30861100
H61	0.66498900	-6.94795800	0.08042300
H62	-0.40338400	-2.45349700	2.45378200
H63	-2.24399000	-2.60665400	4.13337100
H64	-4.60093800	-2.16347500	3.37206900

H65	-5.00701800	-1.57210800	1.00364600
H66	-0.97137900	-1.09343400	-3.52787900
H67	-3.10612800	-0.58509900	-4.76292700
H68	-5.26299200	-0.62840300	-3.46685900
H69	-5.20583400	-1.13821200	-1.04587900
H70	3.53445900	-0.04716200	-2.27764800
H71	5.97311400	-0.47515600	-1.90527800
H72	7.01926000	0.35134100	0.23257800
H73	5.59464500	1.50914400	1.89114000
H74	-0.33118300	2.77898600	1.65213000
H75	0.24618200	3.69656700	3.89473100
H76	2.63376100	3.54149400	4.67696500
H77	4.30571700	2.45666900	3.21206800
H78	3.90739800	3.02338300	-1.59085900
H79	4.52246900	5.15809400	-2.68575300
H80	2.69002600	6.77394900	-3.29904200
H81	0.34625000	6.17236200	-2.77234200
H82	-1.79894100	1.14873300	-0.13456900
H83	-3.90559100	2.48743500	-0.36022200
H84	-3.76215000	4.77720900	-1.39354700
H85	-1.55537000	5.62789200	-2.11568200
O86	1.83098500	0.42895200	-3.38035600
H87	1.41176800	-0.35112100	-3.80821900
H88	1.46140700	-2.72994500	-2.42514400
O89	2.40142100	-4.21990500	-2.74339000
H90	3.36994400	-4.29161200	-2.75738000

H91	2.11515500	-4.69899900	-3.53928100

$BD^{H+}{}_{TS4\text{-}5}{}^{5+}$, 1 additional H_2O, ^5A

Ru1	0.00709900	0.06617100	-0.12290500
Ru2	0.10325700	-0.06165400	3.42398300
O3	1.68979000	-0.01462600	0.78619500
O4	1.71748000	0.15722500	2.64251900
O5	-0.77224500	-0.05932600	1.69656100
N6	-0.22965000	-1.97184600	-0.53212900
C7	-0.91058400	-2.83681800	0.25761900
C8	-1.10767000	-4.16119200	-0.10622700
C9	-0.58098700	-4.61192700	-1.32278800
C10	0.12042400	-3.71928300	-2.13554200
C11	0.28323800	-2.39126000	-1.73341800
C12	0.96724900	-1.36445900	-2.53742400
C13	1.56053700	-1.61439600	-3.77588900
C14	2.18688800	-0.57523700	-4.47082500
C15	2.21334300	0.69872200	-3.90241900
C16	1.60693700	0.89435000	-2.66415600
N17	0.98951100	-0.10530800	-1.99970600
N18	0.02416500	2.21242700	-0.21421600
C19	1.00255900	2.98412100	0.30973600
C20	1.07477500	4.35139000	0.06422400
C21	0.10437300	4.94231000	-0.74955000
C22	-0.91527700	4.14682500	-1.27434300

C23	-0.94233700	2.77629700	-0.99615500
C24	-1.96855300	1.85075100	-1.50211400
N25	-1.78495300	0.52996500	-1.18481500
C26	-2.70595900	-0.37989800	-1.58053400
C27	-3.83558000	-0.02746800	-2.31043100
C28	-4.02498600	1.31170800	-2.65547500
C29	-3.08235200	2.25509100	-2.23833600
H30	-1.30445200	-2.42554600	1.17919400
H31	-1.67083500	-4.82467400	0.54190000
H32	-0.72265700	-5.64121700	-1.64156300
H33	0.52158600	-4.06216300	-3.08219100
H34	1.54173000	-2.60794800	-4.20879500
H35	2.64716400	-0.76381500	-5.43695300
H36	2.69349500	1.53320700	-4.40404100
H37	1.61323500	1.86695900	-2.19044500
H38	-2.53212900	-1.40900600	-1.29936900
H39	-4.54714700	-0.79399800	-2.60127600
H40	-4.89094200	1.62147500	-3.23419300
H41	-3.22769800	3.29967800	-2.48819600
H42	-1.67181100	4.59554800	-1.90787900
H43	0.13997100	6.00435300	-0.97673300
H44	1.88278400	4.93490300	0.49431900
H45	1.73375300	2.47975500	0.92826100
N46	-0.40290400	1.94741500	3.83301900
C47	-1.24754800	2.68530100	3.07391600
C48	-1.64638200	3.96117900	3.44592200

C49	-1.15504600	4.49940300	4.64051700
C50	-0.29157100	3.73559400	5.42528100
C51	0.07184400	2.44883100	5.01657600
C52	0.92604200	1.54925300	5.80822800
C53	1.55371700	1.92189500	6.99817700
C54	2.34737800	0.99908500	7.68489200
C55	2.50128500	-0.28263700	7.15724600
C56	1.85509600	-0.60037500	5.96485800
N57	1.07771200	0.28569500	5.31117200
H58	1.96422900	-1.58045200	5.52025200
H59	3.11408100	-1.02973000	7.65182600
H60	2.83904000	1.28321000	8.61112300
H61	1.43754400	2.92367700	7.39503000
H62	0.07662300	4.13917000	6.36129600
H63	-1.45072400	5.49315500	4.96576800
H64	-2.33779100	4.51749400	2.82160100
H65	-1.60815500	2.21042600	2.16986300
N66	-1.60627200	-0.75320000	4.59375500
C67	-2.62164700	0.01964600	5.03691700
C68	-3.66727500	-0.48472000	5.80428200
C69	-3.66525200	-1.84036800	6.13356100
C70	-2.62094900	-2.64541100	5.67126400
C71	-1.59842500	-2.08497200	4.90382600
C72	-0.45866300	-2.85861700	4.37898000
C73	-0.23050400	-4.20757800	4.67265100
C74	0.89639900	-4.85266600	4.16200800

C75	1.78105000	-4.13595100	3.35083800
C76	1.51073800	-2.79878600	3.08534100
H77	2.17548500	-2.18986400	2.48535700
N78	0.41838000	-2.17576100	3.58441500
H79	2.67569100	-4.59730100	2.94470900
H80	1.08525400	-5.89467300	4.40560700
H81	-0.91234400	-4.75286600	5.31471200
H82	-2.61627900	-3.70124000	5.91530700
H83	-4.46001300	-2.26864900	6.73798100
H84	-4.46115900	0.17743100	6.13510200
H85	-2.59546600	1.06649800	4.76495800
H86	2.71261300	0.18583500	0.54151600
O87	4.04946200	0.51139000	0.11507400
H88	4.61676100	1.06890600	0.67946500
H89	4.63049200	-0.18974000	-0.23381400

$BD^{H+\ 5+}_{5}$, 1 additional H_2O, ^1A

Ru1	0.04814061	0.00956572	0.02894689
Ru2	-0.01767655	-0.02206770	3.50347152
O3	1.85442208	-0.02399828	1.36850675
O4	1.59164842	0.66738170	2.60383295
O5	-0.73519017	-0.16283026	1.70474831
H6	2.76915825	0.40472073	1.09258616
N7	0.14752458	-2.10886460	-0.21696844
C8	-0.55461903	-2.98610491	0.53355197

C9	-0.53169894	-4.35280249	0.27990771
C10	0.24494455	-4.83022922	-0.77908251
C11	0.96616036	-3.92165395	-1.55236185
C12	0.89797588	-2.55551921	-1.26239224
C13	1.57451903	-1.51195988	-2.05198784
C14	2.38573009	-1.78029430	-3.15526555
C15	2.97607410	-0.72636482	-3.85683030
C16	2.74821636	0.58441663	-3.43098782
C17	1.93533559	0.79948180	-2.32521559
N18	1.35004296	-0.21962807	-1.64978790
N19	-1.57897100	0.20646179	-1.21824481
C20	-2.33988938	-0.81986100	-1.66774725
C21	-3.42050106	-0.61493573	-2.51689615
C22	-3.72325064	0.68603823	-2.92479698
C23	-2.93803700	1.74570969	-2.46039362
C24	-1.86576305	1.49395412	-1.60533116
C25	-0.98339583	2.53984016	-1.06035141
C26	-1.08747224	3.89556845	-1.37716062
C27	-0.19028376	4.80801593	-0.81767435
C28	0.79346827	4.34683883	0.06235914
C29	0.85525891	2.98768619	0.34620858
N30	-0.00972624	2.10295799	-0.20250913
H31	-1.14875738	-2.56070076	1.33378574
H32	-1.12181072	-5.02734923	0.89250075
H33	0.28089998	-5.89175073	-1.00910008
H34	1.56085585	-4.28087663	-2.38426562

H35	2.55901829	-2.80033409	-3.47803076
H36	3.60308729	-0.92844396	-4.72147949
H37	3.18604234	1.43207218	-3.94966960
H38	1.73599116	1.80085274	-1.96874947
H39	-2.07310171	-1.81116299	-1.32930259
H40	-4.00850965	-1.46442303	-2.85130753
H41	-4.55754627	0.87723395	-3.59490653
H42	-3.16930717	2.75816889	-2.77108805
H43	-1.84966360	4.24676400	-2.06361219
H44	-0.25738943	5.86280570	-1.07171792
H45	1.50835401	5.02769112	0.51406822
H46	1.59852680	2.58163830	1.01998540
N47	-0.81356761	1.92217966	3.81377382
C48	-1.73638519	2.49041375	3.00269914
C49	-2.33434541	3.70436330	3.31088534
C50	-1.97040985	4.35633992	4.49380370
C51	-1.02471206	3.76598849	5.32879317
C52	-0.45838634	2.53519359	4.97952535
C53	0.49610409	1.80005214	5.82186923
C54	1.03197215	2.30848664	7.00592998
C55	1.93111616	1.54465340	7.75046081
C56	2.28042220	0.27769768	7.28456421
N57	0.83972693	0.55094110	5.38041837
C58	1.71857603	-0.18306582	6.09821849
H59	-1.99258843	1.93606246	2.10818581
H60	-3.08095914	4.12521303	2.64474017

H61	-2.42660202	5.30341674	4.76975431
H62	-0.75125985	4.25299923	6.25775530
H63	0.75848737	3.29801832	7.35295770
H64	2.35031673	1.93574512	8.67360712
H65	2.97741531	-0.35332769	7.82769525
H66	1.97781544	-1.15843445	5.71238851
C67	-2.78717920	-0.28999556	4.92342707
C68	-3.78360362	-0.92396641	5.66076989
C69	-3.57956736	-2.23863517	6.07716567
C70	-2.38786799	-2.87816389	5.72850730
C71	-1.42596738	-2.19644828	4.98149938
N72	-1.63461120	-0.90344164	4.58717756
C73	-0.13935441	-2.78315023	4.57409379
C74	0.29029043	-4.06172097	4.94000878
C75	1.54468027	-4.51875168	4.53617727
C76	2.35482316	-3.68834429	3.75307078
C77	1.88679585	-2.42810948	3.41169945
N78	0.66898210	-1.98294557	3.80759758
H79	-2.91529071	0.73016566	4.58753399
H80	-4.69644250	-0.38861593	5.90332436
H81	-4.33010526	-2.76120675	6.66418341
H82	-2.21998663	-3.90042300	6.04723527
H83	-0.33606526	-4.69631033	5.55613588
H84	1.88886723	-5.50438155	4.83906042
H85	3.34013110	-4.00618446	3.42624937
H86	2.47548049	-1.74413411	2.81535868

O87	4.03441313	1.13590070	0.71646139
H88	4.47703871	1.68575419	1.38879946
H89	4.75611154	0.67411715	0.25183000

$BD^{H+}_{TS5\text{-}6}{}^{5+}$, 1 additional H_2O, ^1A

Ru1	0.20131300	-0.18961400	-0.12391800
Ru2	0.08073300	-0.15508600	3.71672200
O3	2.30913400	0.80917200	2.22567000
O4	2.01096100	-0.11686000	3.16502100
O5	-0.24726800	-0.22758100	1.68126000
H6	2.97339600	0.32051100	1.59823600
N7	0.29952800	-2.31535200	-0.33773600
C8	-0.11128200	-3.19175400	0.60456300
C9	-0.07785500	-4.56645900	0.40283500
C10	0.40119700	-5.05852200	-0.81357100
C11	0.82429800	-4.15387600	-1.78647400
C12	0.76034100	-2.77942000	-1.53560900
C13	1.14687600	-1.74951800	-2.51463200
C14	1.64859300	-2.04296300	-3.78323100
C15	1.98377100	-1.00719900	-4.65873300
C16	1.81713900	0.31173100	-4.23475400
C17	1.31423100	0.54679800	-2.95996400
N18	0.97611100	-0.45205000	-2.11172600
N19	-1.65894300	0.01018300	-0.91893800
C20	-2.50831300	-1.02509600	-1.10572400

C21	-3.74626300	-0.85025900	-1.71400300
C22	-4.11523200	0.42645600	-2.14340800
C23	-3.23681800	1.49293500	-1.93701900
C24	-2.00438000	1.27668900	-1.31928400
C25	-1.00675200	2.32689300	-1.05902800
C26	-1.14166200	3.66032600	-1.45238500
C27	-0.11205800	4.56637300	-1.18098700
C28	1.02882900	4.12198900	-0.50701000
C29	1.10783900	2.78276000	-0.13427700
N30	0.11933900	1.90550900	-0.40653300
H31	-0.47951600	-2.75630500	1.52457200
H32	-0.42799700	-5.23676700	1.18041000
H33	0.43794600	-6.12662000	-1.00854500
H34	1.18868600	-4.52521600	-2.73693600
H35	1.77911100	-3.07042900	-4.10171100
H36	2.36666800	-1.23101100	-5.65064700
H37	2.06629600	1.14983800	-4.87794700
H38	1.17974800	1.55832400	-2.60369200
H39	-2.17939300	-1.99564600	-0.76233000
H40	-4.39942500	-1.70648000	-1.85083800
H41	-5.07129700	0.59329600	-2.63222700
H42	-3.51621600	2.48847700	-2.26314300
H43	-2.02586800	3.99668700	-1.98216300
H44	-0.19974000	5.60150800	-1.50008500
H45	1.84999000	4.79487500	-0.28092600
H46	1.97184200	2.39112800	0.38772300

N47	-0.32941400	1.91971300	3.86358800
C48	-0.95866400	2.63952700	2.91050900
C49	-1.28205500	3.97861700	3.08841100
C50	-0.94404000	4.60249300	4.29363500
C51	-0.30380100	3.85786100	5.28106000
C52	-0.01194700	2.50877700	5.05227700
C53	0.60122100	1.62083100	6.04552600
C54	1.06044300	2.04688700	7.29237800
C55	1.64733700	1.13371800	8.16960700
C56	1.76764500	-0.19787700	7.76975500
N57	0.71467900	0.30810300	5.66920900
C58	1.29833700	-0.57091500	6.51510200
H59	-1.20149700	2.10470100	2.00122400
H60	-1.79579900	4.52188200	2.30254500
H61	-1.18610000	5.64698900	4.46809100
H62	-0.05353100	4.32350100	6.22696900
H63	0.97354400	3.08721700	7.58309000
H64	2.00747000	1.45945700	9.14140900
H65	2.21779200	-0.94532500	8.41544600
H66	1.38432600	-1.59390900	6.18064300
C67	-2.92232900	0.18019800	4.48761400
C68	-4.15672300	-0.21401800	4.99546100
C69	-4.32249200	-1.53663200	5.40478900
C70	-3.24636400	-2.42034900	5.28306100
C71	-2.03000200	-1.97061000	4.76773400
N72	-1.87842100	-0.66857500	4.37292500

C73	-0.83793800	-2.83208600	4.63075000
C74	-0.78701100	-4.16601800	5.04790100
C75	0.40206000	-4.88837500	4.92717500
C76	1.52687300	-4.26483600	4.37691800
C77	1.42299100	-2.93853200	3.97548300
N78	0.27071900	-2.23808800	4.09471500
H79	-2.75625100	1.20013000	4.16847700
H80	-4.96226200	0.50890200	5.07532800
H81	-5.26745000	-1.87930000	5.81692600
H82	-3.36611000	-3.44920400	5.60135500
H83	-1.65594800	-4.64102900	5.48794600
H84	0.45091000	-5.91782300	5.27179900
H85	2.47244700	-4.78871300	4.27807200
H86	2.27037100	-2.39815800	3.56932500
O87	3.32468200	-0.40410500	0.26668800
H88	4.03148900	0.13628000	-0.23278700
H89	3.73543000	-1.27551800	0.41095900
O90	5.12129700	1.08135700	-0.93577500
H91	5.79526900	1.52957400	-0.39457200
H92	5.60402700	0.78028600	-1.72542900

$BD^{H+\ 5+}_{6}$, 1 additional H_2O, ^1A

Ru1	-0.03289646	-0.00874112	0.03701358
Ru2	-0.01253519	-0.19936375	3.86009163
O3	1.69631906	1.28626903	0.35017375

O4	1.78408356	-1.03351186	3.75098857
O5	2.75993792	-0.26087003	3.13368216
O6	-0.15482180	-0.11114706	1.90269958
H7	2.32257506	0.86114714	0.96663313
H8	2.24707567	1.60964307	-0.45212441
H9	3.59236966	-0.69267576	3.43336084
N10	1.33190677	-1.62669951	-0.29644241
C11	1.77507816	-2.47050271	0.66078957
C12	2.64467975	-3.51819444	0.38059493
C13	3.07440820	-3.70400374	-0.93531562
C14	2.61956858	-2.83245124	-1.92372874
C15	1.74443407	-1.79449824	-1.58657659
C16	1.20848871	-0.83030405	-2.56373192
C17	0.97305274	0.09661735	-4.78291734
C18	1.51964181	-0.85915526	-3.92401423
C19	0.12556603	1.07271384	-4.25597548
C20	-0.15479633	1.05341146	-2.89579909
H21	-0.80784384	1.79536417	-2.45770389
N22	0.36341285	0.12263892	-2.05989631
H23	-0.31758088	1.83773604	-4.88635913
H24	1.20751097	0.07766884	-5.84399111
H25	2.18050131	-1.61880578	-4.32441330
H26	2.94689501	-2.96955893	-2.94713213
H27	3.75177201	-4.51439412	-1.19084167
H28	2.97851339	-4.17669082	1.17638195
H29	1.41425476	-2.27995332	1.66262141

N30	-1.73478555	-1.08255998	-0.44712883
C31	-1.76966471	-2.42143548	-0.63172979
C32	-2.91557794	-3.07296380	-1.07181103
C33	-4.06127221	-2.31789739	-1.33252067
C34	-4.02585313	-0.93637024	-1.13201461
C35	-2.85121689	-0.32676722	-0.69021518
C36	-2.70034095	1.12579154	-0.48250663
N37	-1.45391089	1.53806239	-0.10613001
C38	-1.19815885	2.85001265	0.07216438
C39	-2.17659477	3.82203684	-0.10993641
C40	-3.45949175	3.41877560	-0.49067730
C41	-3.72124602	2.05955207	-0.67549213
H42	-4.71195461	1.74174130	-0.98077122
H43	-4.24528269	4.15199884	-0.65296675
H44	-1.93400049	4.87092603	0.03114159
H45	-0.18106334	3.10484371	0.34794699
H46	-0.85464109	-2.96217088	-0.42794933
H47	-2.90191640	-4.14845569	-1.21982945
H48	-4.96940087	-2.79343921	-1.69384055
H49	-4.91016955	-0.34434148	-1.33798855
N50	0.88329709	1.68774515	4.31755464
C51	1.19275526	2.61698427	3.38600332
C52	1.77060449	3.83389014	3.72416422
C53	2.04228834	4.10446838	5.06763575
C54	1.72827699	3.14358074	6.02566178
C55	1.14782084	1.93342688	5.63158672

C56	0.78954215	0.85739831	6.56646011
C57	1.01745212	0.92770562	7.94221497
C58	0.67280589	-0.14781554	8.76147624
C59	0.10678481	-1.27919469	8.17643177
C60	-0.10246521	-1.29516440	6.80166123
N61	0.22195681	-0.25266314	6.00447048
H62	-0.53201558	-2.16544184	6.32874843
H63	-0.17103442	-2.14549250	8.76904836
H64	0.84887940	-0.10185728	9.83270517
H65	1.46710712	1.81032995	8.38114425
H66	1.93745045	3.34069399	7.06996362
H67	2.49357462	5.04661230	5.36650844
H68	2.00833486	4.55539843	2.94915340
H69	0.98150414	2.35387380	2.35815616
N70	-1.98540236	0.47421430	4.22724037
C71	-2.36115720	1.76061087	4.37453796
C72	-3.65309180	2.11659293	4.75134986
C73	-4.58820606	1.10692367	4.98150141
C74	-4.20303467	-0.22529965	4.81540976
C75	-2.89209605	-0.52510650	4.44069022
C76	-2.37841935	-1.90122878	4.28517380
C77	-3.15361723	-3.05110882	4.45328091
C78	-2.56168663	-4.31171291	4.35171711
H79	-0.69413562	-5.36904830	4.01723174
C80	-1.19240820	-4.40649600	4.08108252
C81	-0.46601306	-3.23449759	3.91530960

N82	-1.04479723	-2.01528875	4.00000001
H83	0.60437727	-3.24512416	3.74020323
H84	-3.15958361	-5.20727211	4.50026149
H85	-4.21059814	-2.97457940	4.68158173
H86	-4.92200208	-1.01557984	4.99937907
H87	-5.60084343	1.34753085	5.29400804
H88	-3.91075476	3.16367247	4.87724643
H89	-1.59890909	2.51003546	4.20018862
O90	3.09812705	2.11598652	-1.68691648
H91	3.08805116	3.06243956	-1.91675630
H92	4.02711786	1.84581167	-1.79916817

$BD^{H+}*_{TS4\text{-}6}{}^{5+}$, 1 additional H_2O, ^5A

Ru1	-0.02216200	0.01942300	-0.03058200
Ru2	0.09487300	0.06011000	3.92545400
O3	1.89361500	-0.07594300	0.30548300
O4	1.89758800	-0.15528300	3.56146000
O5	-0.33064200	0.09595800	1.85205900
C6	-0.72936600	-2.86014200	0.76759600
C7	-0.95126400	-4.21586000	0.57278400
C8	-0.75752400	-4.75584600	-0.70307900
C9	-0.35244600	-3.91620900	-1.74088900
C10	-0.14827400	-2.55514600	-1.49859700
N11	-0.33602800	-2.04780900	-0.23983400
C12	0.25758500	-1.58914100	-2.53143500

C13	0.49390000	-1.93239500	-3.86322100
C14	0.87884600	-0.94772700	-4.77742500
C15	1.02683100	0.36547300	-4.33084400
C16	0.77826300	0.65026400	-2.99129200
N17	0.39239400	-0.29583200	-2.10908100
N18	-2.05054600	0.45266900	-0.59751400
C19	-3.04197000	-0.46133700	-0.67249300
C20	-4.31630800	-0.14184100	-1.13023500
C21	-4.57930300	1.16964700	-1.52788400
C22	-3.55894300	2.11939800	-1.43863600
C23	-2.29796800	1.74496300	-0.97136500
C24	-1.16384200	2.67674000	-0.84275100
C25	-1.20356800	4.01944800	-1.23310800
C26	-0.06745900	4.81886000	-1.09533200
C27	1.09394400	4.26202900	-0.55182700
C28	1.08107500	2.92265800	-0.17763400
N29	-0.01752200	2.14758200	-0.32212900
H30	-0.86325700	-2.38359400	1.72961500
H31	-1.27150800	-4.83739300	1.40179000
H32	-0.92397000	-5.81293600	-0.89152300
H33	-0.20564600	-4.32675200	-2.73294500
H34	0.38116300	-2.95598900	-4.20104900
H35	1.06058500	-1.20735300	-5.81673600
H36	1.32848300	1.16181900	-5.00408100
H37	0.88989400	1.65696100	-2.61166300
H38	-2.80254600	-1.46859400	-0.35878600

H39	-5.07970500	-0.91195700	-1.17796300
H40	-5.55944800	1.45319700	-1.90118500
H41	-3.75580500	3.14239900	-1.73749800
H42	-2.10596600	4.44263800	-1.65903100
H43	-0.08925800	5.85740700	-1.41459500
H44	1.99976100	4.84783800	-0.42925600
H45	1.95702500	2.44163200	0.23826900
N46	0.05148200	2.16210800	4.16008800
C47	-0.29305200	3.04716900	3.20084500
C48	-0.33339500	4.41507600	3.43530000
C49	-0.00190000	4.89077200	4.70709700
C50	0.34943300	3.97715100	5.69991400
C51	0.36620100	2.60943600	5.41222900
C52	0.69205700	1.56904800	6.40068100
C53	1.08616800	1.84367500	7.71059900
C54	1.38747200	0.79672800	8.58523300
C55	1.29096700	-0.51433500	8.12122400
C56	0.89365300	-0.73450200	6.80580300
N57	0.59178800	0.27629800	5.96295300
H58	-0.54451500	2.62016400	2.23895500
H59	-0.62399400	5.09486600	2.64188600
H60	-0.02357900	5.95416100	4.92810200
H61	0.59692400	4.33595700	6.69186000
H62	1.16870600	2.86694300	8.05743500
H63	1.69648000	1.00693700	9.60530400
H64	1.52247700	-1.36107700	8.75954600

H65	0.82314800	-1.73892400	6.41533700
N66	-1.94857200	-0.23535000	4.50363400
C67	-2.86109800	0.75404800	4.61617400
C68	-4.14130400	0.53438800	5.11393300
C69	-4.49445500	-0.75712800	5.50925100
C70	-3.55807200	-1.78567300	5.37950300
C71	-2.28657200	-1.50645100	4.87493300
C72	-1.22808700	-2.52072300	4.70654200
C73	-1.35798800	-3.85933500	5.09320900
C74	-0.28347300	-4.73666300	4.93345900
C75	0.90501000	-4.26108500	4.37218800
C76	0.97878400	-2.92224400	3.99981800
N77	-0.05834400	-2.07168900	4.16296500
H78	-2.54379900	1.74254500	4.30863500
H79	-4.83799600	1.36222500	5.19854100
H80	-5.48106200	-0.96477600	5.91391800
H81	-3.82693200	-2.79180600	5.67946000
H82	-2.27879800	-4.21782200	5.53870900
H83	-0.37163600	-5.77105900	5.25440200
H84	1.76743500	-4.90691800	4.23975200
H85	1.88436400	-2.49669900	3.58208100
O86	2.65332200	0.88771500	2.49534900
H87	2.44659800	0.40122600	1.58343500
H88	3.58734100	0.72878900	2.76265600
H89	2.54057200	-0.27249500	-0.46043600
O90	3.62684600	-0.65478700	-1.58846900

H91	4.12075700	-1.49112500	-1.52163300
H92	4.27220300	-0.01312900	-1.93445400

Coordinates for Llobet's ruthenium catalyst.

Ll_0^{3+}, 1 additional H_2O, ^1A

Ru1	-0.0264380536	-2.3662412655	0.0129495693
N2	0.3792568569	-3.2543906945	-1.8236113707
O3	-0.5311544733	-1.3018815688	1.9520254119
O4	0.6298793695	1.1512846403	1.9296641088
C5	0.6024750537	-4.5712886558	-2.0222893109
H6	0.6285289090	-5.1933307367	-1.1364989095
Ru7	0.0580919143	2.3475061047	0.1679770546
N8	0.0738402540	-0.6302982512	-1.2905328495
C9	0.7875926379	-5.1173729984	-3.2844729322
H10	0.9658018623	-6.1822427471	-3.3895618029
N11	-0.0370244505	0.7121184165	-1.2502760942
C12	0.7356861798	-4.2732852720	-4.3966298322
H13	0.8709381998	-4.6682418581	-5.3988495040
N14	-0.2839228158	3.3707070136	-1.6186830640
C15	0.5130640504	-2.9161492475	-4.1995850613
H16	0.4760885519	-2.2330348918	-5.0412396943
N17	2.0021656896	-2.5157344402	0.6138714017
C18	0.3421350550	-2.4203831591	-2.9022382470
N19	-0.0645803309	-4.0797452355	1.0533125724
C20	0.1461505910	-1.0106230647	-2.6020328543
N21	-2.0683151644	-2.9632782583	-0.2256408768
C22	0.0485581149	0.1104739570	-3.4279110370

H23	0.0674475551	0.1449026604	-4.5075149916
N24	-1.9820240087	2.5013752790	0.7113250921
C25	-0.0715848001	1.1770057104	-2.5357672426
N26	0.1001840043	3.9529732422	1.3653808964
C27	-0.2377014991	2.6074901550	-2.7482565994
N28	2.1147866074	2.9111376495	0.0428845754
C29	-0.3619855034	3.1887363125	-4.0146587021
H30	-0.3195324894	2.5603777579	-4.8977974610
C31	-0.5418514517	4.5619053107	-4.1283863106
H32	-0.6385926539	5.0239648233	-5.1060484946
C33	-0.5989158609	5.3344458877	-2.9656387990
H34	-0.7419495043	6.4089291742	-3.0068277643
C35	-0.4646750867	4.7029739046	-1.7369058850
H36	-0.4959375533	5.2662233693	-0.8121040502
C37	3.0206037990	-1.6976777909	0.3007094640
H38	2.7521751236	-0.8220391378	-0.2786559317
C39	4.3345345175	-1.9534413338	0.6861726342
H40	5.1255591621	-1.2673774659	0.4024411420
C41	4.6061489080	-3.1007423721	1.4283927557
H42	5.6190276226	-3.3349461830	1.7409880571
C43	3.5547261093	-3.9540691086	1.7609044994
H44	3.7489213092	-4.8556415374	2.3311811699
C45	2.2591959966	-3.6488701737	1.3427509871
C46	1.0876715015	-4.5149963639	1.6216311153
C47	1.0837922900	-5.6956452741	2.3697465152
H48	1.9903951016	-6.0646618357	2.8355723662

C	-0.1115742598	-6.4038582168	2.5100787014
H	-0.1293562338	-7.3227823894	3.0876229086
C	-1.2819300962	-5.9399368793	1.9063443948
H	-2.2050810260	-6.4978729454	2.0118176784
C	-1.2340582021	-4.7552616835	1.1652026096
C	-2.3559077606	-4.1373503197	0.4206705719
C	-3.6220320667	-4.7193723770	0.3330543769
H	-3.8353786773	-5.6495741062	0.8472539661
C	-4.6078845943	-4.1095248514	-0.4416507377
H	-5.5922317395	-4.5593901676	-0.5276941121
C	-4.3012520657	-2.9280068467	-1.1137252894
H	-5.0321661419	-2.4328634458	-1.7447788381
C	-3.0233926455	-2.3904043185	-0.9753340521
H	-2.7311514143	-1.4814508956	-1.4911022487
C	-3.0174658392	1.7735828314	0.2542818535
H	-2.7530399297	0.9707997729	-0.4260259328
C	-4.3400618448	2.0392838241	0.6024589056
H	-5.1433771602	1.4420906356	0.1816446481
C	-4.6062868863	3.1063092422	1.4640157582
H	-5.6246718504	3.3522447771	1.7487194861
C	-3.5414919470	3.8690595005	1.9367983067
H	-3.7289364350	4.7137574317	2.5902572823
C	-2.2363087836	3.5590737476	1.5452188752
C	-1.0542274613	4.3522649406	1.9558300549
C	-1.0449290819	5.4346271972	2.8398108744
H	-1.9539553915	5.7710956101	3.3247971361

C75	0.1657617400	6.0828356998	3.0943618684
H76	0.1946488958	6.9252146191	3.7782043210
C77	1.3396212355	5.6536093684	2.4728798349
H78	2.2759999843	6.1610354664	2.6746634935
C79	1.2852097993	4.5678339728	1.5937430880
C80	2.4160537869	3.9932853702	0.8271082037
C81	3.7068045175	4.5241136540	0.8606539567
H82	3.9330830720	5.3806274377	1.4853621126
C83	4.7049286192	3.9556025141	0.0696874236
H84	5.7105866272	4.3644578966	0.0801270366
C85	4.3851740698	2.8680127997	-0.7399937436
H86	5.1269519701	2.4079490689	-1.3848283976
C87	3.0804474865	2.3783169056	-0.7205429939
H88	2.7790644998	1.5419560509	-1.3426377418
H89	0.4190779882	1.5765279243	2.7768700298
H90	0.2028541221	0.2605926370	1.9414898901
H91	-0.1885441260	-1.8287726596	2.6954515838
H92	-1.5182125262	-1.2080305681	2.1082165123
O93	-3.1375935724	-0.9602749924	2.4105868562
H94	-3.5691484616	-0.1623370117	2.0632347167
H95	-3.5557212914	-1.1426233382	3.2679298592

LI_1^{4+}, 1 additional H_2O, ^2A

Ru1	-0.01362987	-2.37655314	0.08525601
N2	0.44312303	-3.21357208	-1.75979018

O3	-0.66355141	-1.35989617	2.01223951
O4	0.40175474	1.10569869	1.84553053
C5	0.75616681	-4.50638631	-1.97835380
H6	0.84016582	-5.13818789	-1.10404617
Ru7	-0.03040108	2.33839675	0.10018855
N8	-0.01643905	-0.58563785	-1.23367184
C9	0.96186952	-5.02611204	-3.25385329
H10	1.21461149	-6.07509766	-3.36987851
N11	-0.16767179	0.76708426	-1.23625110
C12	0.83334550	-4.18466970	-4.35899845
H13	0.98043017	-4.56168206	-5.36642849
N14	-0.33234546	3.40172255	-1.66418499
C15	0.51890943	-2.84630266	-4.14278800
H16	0.42209759	-2.16373778	-4.98006431
N17	2.02751012	-2.42015833	0.69047751
C18	0.33564857	-2.37941272	-2.83674346
N19	0.05824287	-4.12478966	1.06611313
C20	0.06966108	-0.98166484	-2.53232265
N21	-2.03431820	-3.09007634	-0.15330826
C22	-0.06223808	0.12423005	-3.40009691
H23	-0.03462722	0.12354117	-4.47968997
N24	-2.04548362	2.77620939	0.64695653
C25	-0.21167888	1.20365616	-2.55484005
N26	0.16946282	3.94030358	1.38167471
C27	-0.35810439	2.63144269	-2.78945435
N28	2.04315313	2.83127048	-0.05648936

C29	-0.50967664	3.20790719	-4.05311633
H30	-0.52938037	2.57713759	-4.93559681
C31	-0.63733182	4.58961737	-4.16319567
H32	-0.75507378	5.05343672	-5.13802443
C33	-0.61301783	5.36866614	-3.00308574
H34	-0.71109291	6.44836727	-3.04684271
C35	-0.45850563	4.74026463	-1.77337885
H36	-0.43122528	5.30761906	-0.85111829
C37	2.99971090	-1.53310342	0.41815384
H38	2.68757908	-0.65473267	-0.13459181
C39	4.32400123	-1.72154820	0.80573927
H40	5.07510710	-0.98056885	0.55319709
C41	4.66054582	-2.87748516	1.50778908
H42	5.68369785	-3.06290095	1.82029466
C43	3.65937308	-3.80349628	1.79673412
H44	3.90496966	-4.71305932	2.33334364
C45	2.35014469	-3.56190391	1.37781686
C46	1.23720024	-4.51109868	1.61037818
C47	1.32031215	-5.73018815	2.28905634
H48	2.25358978	-6.06393817	2.72795655
C49	0.17893403	-6.52723915	2.39128874
H50	0.22718947	-7.47858507	2.91246026
C51	-1.02181662	-6.10932935	1.81584148
H52	-1.90310682	-6.73620754	1.88804090
C53	-1.05961640	-4.88567511	1.14091654
C54	-2.22824120	-4.31768157	0.43020562

C55	-3.44618233	-4.99031150	0.31223377
H56	-3.58580190	-5.96081267	0.77450145
C57	-4.48259084	-4.41776802	-0.42538515
H58	-5.42986191	-4.93762458	-0.53342944
C59	-4.27467904	-3.17894015	-1.02955900
H60	-5.04871177	-2.70676848	-1.62572731
C61	-3.04073298	-2.55318673	-0.86613385
H62	-2.82892158	-1.59501155	-1.32961474
C63	-3.14210273	2.20197424	0.11952775
H64	-2.96535229	1.42615047	-0.61692579
C65	-4.43055223	2.58269749	0.48554926
H66	-5.28686912	2.09803178	0.02797232
C67	-4.59128703	3.59627438	1.43007841
H68	-5.58252385	3.92084127	1.73269295
C69	-3.45747579	4.20436553	1.97126650
H70	-3.56408171	5.00862189	2.69042769
C71	-2.19115301	3.78711247	1.55956450
C72	-0.93266702	4.41686283	2.00787984
C73	-0.80861148	5.43872014	2.95267149
H74	-1.67796983	5.83633249	3.46390005
C75	0.46056452	5.95084808	3.22906846
H76	0.57637806	6.74547075	3.96019905
C77	1.57980909	5.45227976	2.56021216
H78	2.56232661	5.86083135	2.76726629
C79	1.40747619	4.43100136	1.62184320
C80	2.46364852	3.82139255	0.78931100

C81	3.79417414	4.24132993	0.79800526
H82	4.11858326	5.02682683	1.47103363
C83	4.70431926	3.65937539	-0.08541972
H84	5.74001073	3.98617360	-0.09702564
C85	4.25836522	2.67045102	-0.96147670
H86	4.92856047	2.20895617	-1.67979049
C87	2.92060469	2.28358619	-0.91591083
H88	2.52967970	1.52501645	-1.58468053
H89	0.26405596	1.53908812	2.70416135
H90	-0.02929140	0.21030889	1.89578212
H91	-0.37139252	-1.82986080	2.85857270
H92	-1.63639997	-1.39830724	2.01574164
O93	0.02295261	-2.60126356	4.25194319
H94	-0.64345262	-2.99185409	4.84219782
H95	0.74798827	-2.32068944	4.83450242

LI_1^{3+}, 1 additional H_2O, ^2A

Ru1	-0.02723076	-2.33909092	0.00144435
N2	0.47163701	-3.23348962	-1.83067535
O3	-0.69655052	-1.23358707	1.74228673
O4	0.57428401	1.08599395	1.63249759
C5	0.74316074	-4.54014723	-2.02387948
H6	0.76251932	-5.16142223	-1.13657502
Ru7	0.07665448	2.30321687	0.16314683
N8	0.10076779	-0.61590761	-1.30839101

C9	0.98381772	-5.07969825	-3.28136510
H10	1.19914078	-6.13832565	-3.38089993
N11	-0.06380805	0.71816730	-1.27450603
C12	0.93923990	-4.23854347	-4.39443641
H13	1.11823751	-4.62798640	-5.39186111
N14	-0.36393404	3.37107870	-1.63933247
C15	0.66684836	-2.88796109	-4.20372494
H16	0.63488846	-2.20628848	-5.04703845
N17	1.95942285	-2.47279841	0.70891735
C18	0.44070035	-2.40358752	-2.91236060
N19	-0.11549229	-4.03941393	1.04900461
C20	0.19212913	-0.99547479	-2.61759565
N21	-2.06000355	-2.92814740	-0.31548633
C22	0.04763762	0.11962732	-3.44873955
H23	0.06141750	0.14915505	-4.52861228
N24	-1.94095501	2.50115668	0.75983313
C25	-0.11812621	1.18456482	-2.56259964
N26	0.18650527	3.88548561	1.41356753
C27	-0.33574768	2.60613377	-2.76909737
N28	2.09717586	2.94575311	-0.11655296
C29	-0.52204019	3.18920841	-4.02918203
H30	-0.49620581	2.56794262	-4.91746490
C31	-0.74615468	4.55619499	-4.12668378
H32	-0.89330313	5.01784907	-5.09846967
C33	-0.78394517	5.32921006	-2.96003964
H34	-0.96161454	6.39858959	-2.99611844

C35	-0.58576221	4.69907081	-1.74169971
H36	-0.60021142	5.25638730	-0.81165030
C37	2.98649607	-1.64296121	0.46074125
H38	2.74412039	-0.77164908	-0.13618653
C39	4.27563650	-1.88033459	0.92910980
H40	5.07518905	-1.18585888	0.69329377
C41	4.51397474	-3.02253613	1.69162493
H42	5.50786388	-3.24390113	2.06806490
C43	3.45376034	-3.88588648	1.95954993
H44	3.62030090	-4.78311777	2.54526093
C45	2.18266233	-3.59777785	1.45945062
C46	1.00564296	-4.47011660	1.67497033
C47	0.97044623	-5.65003987	2.42228436
H48	1.85677573	-6.01766166	2.92667753
C49	-0.22885452	-6.35810038	2.51305036
H50	-0.27146413	-7.27756829	3.08839099
C51	-1.37222450	-5.89047808	1.86359536
H52	-2.30126110	-6.44416450	1.93273164
C53	-1.29022805	-4.70866583	1.12130292
C54	-2.38193767	-4.08692806	0.33890294
C55	-3.65680437	-4.64735703	0.23298257
H56	-3.89739449	-5.56581863	0.75596761
C57	-4.61690776	-4.02760194	-0.56453263
H58	-5.60844910	-4.45867242	-0.66231797
C59	-4.27653080	-2.85767726	-1.24084419
H60	-4.98804503	-2.35275475	-1.88605362

C61	-2.99089752	-2.34461663	-1.08559273
H62	-2.67457734	-1.44429961	-1.60217581
C63	-2.97627870	1.75631094	0.34466568
H64	-2.74194162	0.99283641	-0.38747213
C65	-4.26744987	1.94860385	0.82913235
H66	-5.07932108	1.32770461	0.46610436
C67	-4.48592607	2.94694634	1.77611807
H68	-5.48058285	3.12725712	2.17228430
C69	-3.40956508	3.72095246	2.21172166
H70	-3.56589032	4.50270296	2.94648345
C71	-2.13846098	3.48520572	1.69144794
C72	-0.93670761	4.26509236	2.06538032
C73	-0.88103717	5.32861717	2.96978616
H74	-1.76547946	5.65517712	3.50455624
C75	0.33941690	5.97591123	3.17352834
H76	0.40092654	6.80342753	3.87341454
C77	1.47775273	5.57473749	2.47261260
H78	2.41852843	6.09185904	2.62218476
C79	1.37563308	4.50764769	1.57540701
C80	2.45323129	3.97689713	0.71044933
C81	3.74878080	4.49455554	0.68825805
H82	4.02677062	5.31057083	1.34538173
C83	4.68545008	3.96008753	-0.19707556
H84	5.69508158	4.35847538	-0.22819105
C85	4.30554571	2.91939025	-1.04308874
H86	5.00246490	2.48568038	-1.75267595

C87	2.99986120	2.43945191	-0.97055147
H88	2.65066678	1.63540369	-1.60919827
H89	0.74803415	1.53879083	2.47629138
H90	-0.19938368	-0.37072888	1.75875787
H91	-0.51864759	-1.67996130	2.60537047
O92	-0.26519440	-2.48565527	4.14762533
H93	0.42470905	-2.24803932	4.78693919
H94	-1.04804748	-2.68343536	4.68627288

LI_2^{4+}, 1 additional H_2O, ^3A

Ru1	0.03450987	-2.35353448	-0.02016073
N2	0.35508442	-3.25236389	-1.88668408
O3	-0.43568034	-1.29832828	1.70070214
O4	0.33277378	1.11805701	1.75137975
C5	0.52711763	-4.57569869	-2.09610883
H6	0.53811232	-5.20772527	-1.21635787
Ru7	0.01771660	2.33959345	0.22440841
N8	0.08823569	-0.63191350	-1.30186999
C9	0.68065722	-5.10947112	-3.36755862
H10	0.81776134	-6.17865889	-3.49144740
N11	-0.03756775	0.71648041	-1.23722296
C12	0.65198420	-4.24702821	-4.46810248
H13	0.76617921	-4.63421285	-5.47634020
N14	-0.23968556	3.40611035	-1.60496281
C15	0.47685790	-2.88308029	-4.25576853

H16	0.45541073	-2.19380280	-5.09267432
N17	2.09688839	-2.63555046	0.37479818
C18	0.33138074	-2.40011203	-2.95171353
N19	0.02985497	-4.04506285	1.11915843
C20	0.15948325	-0.99057360	-2.62488005
N21	-1.97621953	-3.03602567	-0.20934125
C22	0.05683932	0.14304322	-3.42601605
H23	0.07447250	0.19727859	-4.50448941
N24	-2.05388880	2.63282795	0.59585487
C25	-0.06857767	1.19643151	-2.51491766
N26	0.05078396	3.90905057	1.49649610
C27	-0.21470212	2.63502790	-2.72902238
N28	2.06627915	2.95166397	0.12580886
C29	-0.33019242	3.21175118	-3.99677419
H30	-0.31015182	2.58510934	-4.88186767
C31	-0.47553743	4.59205798	-4.11275735
H32	-0.56689107	5.05284345	-5.09197247
C33	-0.50366514	5.37290016	-2.95423477
H34	-0.61676862	6.45101254	-3.00230211
C35	-0.38149347	4.74267040	-1.72241846
H36	-0.39449989	5.30954358	-0.79860008
C37	3.10904466	-1.91313970	-0.13664343
H38	2.82554352	-1.11834668	-0.81629072
C39	4.43878005	-2.16965385	0.18279710
H40	5.22755484	-1.56905901	-0.25758738
C41	4.72950003	-3.21292866	1.06141922

H42	5.75659697	-3.44508153	1.32720984
C43	3.68202894	-3.97106587	1.58627199
H44	3.89448832	-4.79666803	2.25643824
C45	2.36854552	-3.67433191	1.22621069
C46	1.19642923	-4.45980326	1.66294643
C47	1.21144238	-5.57178562	2.50948633
H48	2.13496337	-5.92821748	2.95119239
C49	0.00906856	-6.23339156	2.76895936
H50	-0.00056410	-7.10195015	3.42075174
C51	-1.17756160	-5.79615030	2.17804030
H52	-2.10415368	-6.32767891	2.36302114
C53	-1.14253638	-4.67968423	1.33789138
C54	-2.27692271	-4.11518158	0.57923699
C55	-3.56439744	-4.65170612	0.59294737
H56	-3.79793630	-5.50671827	1.21719969
C57	-4.55029792	-4.09227941	-0.22170783
H58	-5.55353809	-4.50825454	-0.22809918
C59	-4.22481449	-3.00740941	-1.03556683
H60	-4.95987973	-2.55761586	-1.69504332
C61	-2.92562813	-2.50812605	-1.00055584
H62	-2.62049076	-1.67127216	-1.61881632
C63	-3.08218599	1.99345982	0.01425422
H64	-2.81487936	1.24380271	-0.72136574
C65	-4.40841194	2.27775616	0.32611538
H66	-5.21023115	1.74655444	-0.17562961
C67	-4.67770100	3.25931111	1.27927424

H68	-5.70041976	3.51106549	1.54404401
C69	-3.61326272	3.92944946	1.88315344
H70	-3.80788000	4.70525423	2.61528855
C71	-2.30463166	3.60974190	1.52380957
C72	-1.11579268	4.31150059	2.05276865
C73	-1.11007668	5.33669862	3.00236456
H74	-2.02984472	5.67791687	3.46360044
C75	0.10663677	5.92772489	3.34996051
H76	0.12961758	6.72433945	4.08757618
C77	1.29165676	5.51005881	2.74169497
H78	2.23099747	5.98546605	3.00034226
C79	1.23931435	4.48191913	1.79553324
C80	2.37330191	3.95441521	1.00798097
C81	3.67074275	4.46119198	1.09243785
H82	3.90823901	5.25361466	1.79312338
C83	4.66119844	3.95567515	0.24963399
H84	5.67170197	4.35094330	0.29687983
C85	4.33049474	2.95229968	-0.66121424
H86	5.06882554	2.54945267	-1.34688646
C87	3.02253196	2.47591818	-0.68819949
H88	2.71298934	1.70196094	-1.38185903
H89	0.42466917	1.55101617	2.61751338
H90	-0.12081249	-0.32502938	1.75398641
H91	-0.39804259	-1.71801568	2.60553061
O92	-0.40791205	-2.42350328	4.13163362
H93	0.28817018	-2.26861771	4.79135207

H94 -1.23861902 -2.41570999 4.63594005

LI_2^{3+}, ^1A

Ru1 -0.0316332139 -2.2921025284 -0.0193739448
N2 0.4239715939 -3.2583772718 -1.8863019390
O3 -0.5575594549 -1.1475717890 1.4773290397
O4 0.7542730241 1.2166432285 1.6170606089
C5 0.6369998248 -4.5783622852 -2.0651296704
H6 0.6467151675 -5.1884268402 -1.1685804525
Ru7 0.1242276153 2.2933452013 0.1497886195
N8 0.1312569155 -0.6298331836 -1.3717374033
C9 0.8301833287 -5.1389247232 -3.3193077816
H10 0.9997648245 -6.2058214875 -3.4170864477
N11 -0.0144523955 0.7059875154 -1.3270252675
C12 0.7964991088 -4.3005225259 -4.4383556580
H13 0.9388211315 -4.7064868864 -5.4353820501
N14 -0.3093668191 3.3669242248 -1.6976341518
C15 0.5825357391 -2.9381264698 -4.2612639287
H16 0.5596631882 -2.2659826184 -5.1123003065
N17 1.9777243670 -2.5027039366 0.5872119767
C18 0.4013897393 -2.4301094885 -2.9701094721
N19 -0.1532844931 -3.9179997775 1.1661620594
C20 0.1957019549 -1.0158803845 -2.6814151114
N21 -2.0533420377 -2.9293961597 -0.3476735375
C22 0.0564773354 0.1043247248 -3.5042401020

H23	0.0573496298	0.1402363697	-4.5839771477
N24	-1.9123687858	2.3344827237	0.7728411304
C25	-0.0800322801	1.1700963632	-2.6098122937
N26	0.1504033449	3.8516389121	1.4204071044
C27	-0.2812910871	2.6020799598	-2.8230317861
N28	2.1319248226	2.9820397529	-0.0572712581
C29	-0.4483352544	3.1743085133	-4.0876347732
H30	-0.4207378694	2.5490363779	-4.9734290822
C31	-0.6550602963	4.5459251183	-4.1963189189
H32	-0.7878077174	5.0034327202	-5.1720074479
C33	-0.6898810481	5.3225969627	-3.0360089364
H34	-0.8501436201	6.3946105093	-3.0776596393
C35	-0.5074202130	4.6942874139	-1.8104587850
H36	-0.5155144438	5.2579009644	-0.8837528814
C37	3.0181627270	-1.7461451021	0.2033310683
H38	2.7908358270	-0.9590194229	-0.5052719958
C39	4.3049016410	-1.9593313989	0.6902225348
H40	5.1222139603	-1.3306300050	0.3539476478
C41	4.5138306669	-2.9881776501	1.6067913665
H42	5.5049779120	-3.1831175122	2.0048003035
C43	3.4333061250	-3.7737865396	2.0089699208
H44	3.5826366356	-4.5794614982	2.7189593747
C45	2.1666827697	-3.5186005151	1.4868472093
C46	0.9614957174	-4.3090658027	1.8258625321
C47	0.8921925477	-5.3876316044	2.7118774107
H48	1.7676701525	-5.7235245819	3.2549241628

C49	-0.3315744969	-6.0348958526	2.8916094681
H50	-0.4030184781	-6.8720579307	3.5789679990
C51	-1.4618013219	-5.6177881567	2.1866902735
H52	-2.4068020584	-6.1312805241	2.3216788311
C53	-1.3470266950	-4.5362224040	1.3089377244
C54	-2.4172189137	-3.9798518974	0.4505112755
C55	-3.7150191068	-4.4910076338	0.4090413235
H56	-4.0006391159	-5.3209495395	1.0446053652
C57	-4.6451001728	-3.9317397719	-0.4672530582
H58	-5.6563401690	-4.3247397920	-0.5117916957
C59	-4.2560903196	-2.8738693608	-1.2877122770
H60	-4.9468205073	-2.4226195690	-1.9923791401
C61	-2.9493653996	-2.4011523301	-1.1951043831
H62	-2.5932719823	-1.5846174753	-1.8140441235
C63	-2.9175902648	1.5496123084	0.3593298562
H64	-2.6514522114	0.7997391142	-0.3757131436
C65	-4.2168163130	1.6893732191	0.8407715154
H66	-5.0051547578	1.0404195989	0.4748496884
C67	-4.4769092458	2.6784009839	1.7868819785
H68	-5.4783622550	2.8207154334	2.1812362342
C69	-3.4328476978	3.4944965740	2.2215114995
H70	-3.6208505451	4.2713646044	2.9538193273
C71	-2.1526859472	3.3086013130	1.7024985966
C72	-0.9853786646	4.1356257628	2.0967274163
C73	-0.9737058035	5.1349860872	3.0712182554
H74	-1.8675676749	5.3852832064	3.6302451816

C75	0.2250391695	5.8066801258	3.3284528570
H76	0.2555149809	6.5837297685	4.0857998385
C77	1.3836604149	5.4809803364	2.6244198347
H78	2.3118536543	5.9993979323	2.8351258906
C79	1.3231468204	4.4743348758	1.6551446892
C80	2.4354430964	4.0006398613	0.8037958113
C81	3.7139081661	4.5615702794	0.8302604371
H82	3.9451669936	5.3687229202	1.5157137010
C83	4.6913518475	4.0839767417	-0.0410387745
H84	5.6879269332	4.5147372996	-0.0334598810
C85	4.3662193319	3.0563131655	-0.9249627541
H86	5.0942661315	2.6661439226	-1.6286475579
C87	3.0757451961	2.5335104886	-0.8975003359
H88	2.7714505880	1.7365274935	-1.5678897333
H89	0.2807464252	0.3480192692	1.6050647568
H90	-0.6892257623	-1.6086315041	2.3253480479

LI_3^{4+}, 1 additional H_2O, ^4A

Ru1	0.03762572	-2.33820162	-0.00327435
N2	0.45516382	-3.23990772	-1.84483861
O3	-0.48976085	-1.29511586	1.74423594
O4	0.37518621	1.17701894	1.58593031
C5	0.66867209	-4.55991543	-2.03396695
H6	0.65715312	-5.18458782	-1.14931035
Ru7	0.02954247	2.32201474	0.25161444

N8	0.14833008	-0.62188792	-1.29087966
C9	0.89130926	-5.09939476	-3.29315820
H10	1.06104419	-6.16557162	-3.40094944
N11	-0.03774371	0.72173337	-1.24769184
C12	0.88987722	-4.24744284	-4.40183421
H13	1.05883428	-4.63975880	-5.40032078
N14	-0.35952730	3.40239783	-1.65056389
C15	0.67190400	-2.88664548	-4.20986476
H16	0.67240517	-2.20416975	-5.05257430
N17	2.05830012	-2.69847302	0.54016275
C18	0.45790854	-2.39785130	-2.91805851
N19	-0.09976227	-4.03288130	1.12818604
C20	0.23832785	-0.99086532	-2.61051940
N21	-1.97965042	-2.94765429	-0.32066889
C22	0.08977904	0.12784219	-3.42436257
H23	0.10568478	0.17014086	-4.50362781
N24	-2.03988466	2.51261699	0.74367687
C25	-0.08463289	1.18758797	-2.52658446
N26	0.05425007	3.95985386	1.43314443
C27	-0.30206727	2.61741151	-2.76102954
N28	2.07622577	2.96328142	0.06190526
C29	-0.46087095	3.16091348	-4.03818244
H30	-0.41281746	2.52108471	-4.91272864
C31	-0.68794253	4.52895211	-4.17683073
H32	-0.81458212	4.96585710	-5.16298482
C33	-0.75380620	5.32582139	-3.03250561

H34	-0.93297070	6.39400984	-3.09706519
C35	-0.58279465	4.72348928	-1.79071535
H36	-0.62273460	5.30734822	-0.87743293
C37	3.12738663	-2.00420579	0.11177938
H38	2.92185276	-1.19828265	-0.58307220
C39	4.42030468	-2.30004638	0.53359548
H40	5.25732025	-1.71888330	0.16092733
C41	4.61286290	-3.35443954	1.42640219
H42	5.60993171	-3.61433914	1.76986502
C43	3.50754500	-4.08550429	1.86465849
H44	3.64298235	-4.91805209	2.54561331
C45	2.23540336	-3.74756266	1.40440263
C46	1.01024840	-4.49437107	1.74631164
C47	0.92608728	-5.61076506	2.58156758
H48	1.80476838	-6.00314354	3.08045098
C49	-0.31316762	-6.22708398	2.75983687
H50	-0.39769895	-7.09749193	3.40372740
C51	-1.44182356	-5.73862597	2.09902560
H52	-2.39928287	-6.23190944	2.22270477
C53	-1.30842488	-4.62198919	1.26941268
C54	-2.37104441	-4.01229238	0.44659165
C55	-3.67778203	-4.49599371	0.38457865
H56	-3.98208057	-5.33906206	0.99451651
C57	-4.59028642	-3.89906634	-0.48651898
H58	-5.60764605	-4.27381268	-0.55189147
C59	-4.17238944	-2.83099886	-1.28046251

H60	-4.84732012	-2.35407777	-1.98389521
C61	-2.85841483	-2.38446530	-1.16868163
H62	-2.48511096	-1.56330637	-1.77032909
C63	-3.06434982	1.77897588	0.28488678
H64	-2.80428332	0.98932770	-0.41056070
C65	-4.38165220	2.01552220	0.67020024
H66	-5.18300185	1.40485760	0.26818576
C67	-4.64242636	3.04914474	1.56747001
H68	-5.65723944	3.26471706	1.88816767
C69	-3.57939801	3.81667692	2.04509166
H70	-3.76843358	4.63154198	2.73476472
C71	-2.28192678	3.53808039	1.61869186
C72	-1.10131515	4.32850495	2.03243845
C73	-1.09072498	5.39403291	2.93488209
H74	-1.99721883	5.71526184	3.43460747
C75	0.11739876	6.04668585	3.19240326
H76	0.14331733	6.87442243	3.89499699
C77	1.29080321	5.64701593	2.54956112
H78	2.22224262	6.16305014	2.75172274
C79	1.23685480	4.57745040	1.65255389
C80	2.36408392	4.03901898	0.85942734
C81	3.64080284	4.60035521	0.86962269
H82	3.86342925	5.45278579	1.50113930
C83	4.63200738	4.06795262	0.04324013
H84	5.62693703	4.50311068	0.03538397
C85	4.32120546	2.98477608	-0.77677981

H	86	5.05972827	2.55530782 -1.44574766
C	87	3.03102738	2.46037893 -0.73429277
H	88	2.73697049	1.62315842 -1.35789254
H	89	-0.18141721	-0.34414297 1.74738722
H	90	-0.29511298	-1.68533608 2.64742895
O	91	0.03030792	-2.33210681 4.14787080
H	92	0.71924839	-1.92373111 4.69882585
H	93	-0.72673408	-2.44871093 4.74700815

LI_3^{3+}, ^4A

Ru	1	-0.06449700	-2.28599441 -0.03562734
N	2	0.38385551	-3.24163208 -1.93927636
O	3	-0.70329175	-1.29834304 1.49639962
O	4	0.67657404	1.08354399 1.44113453
C	5	0.54691181	-4.56448717 -2.13457754
H	6	0.51359026	-5.18763303 -1.24743516
Ru	7	0.15072497	2.23024105 0.17626082
N	8	0.16026835	-0.60918104 -1.39867062
C	9	0.74499809	-5.11579838 -3.39408537
H	10	0.87532331	-6.18720219 -3.50277945
N	11	0.03120964	0.72860448 -1.35644500
C	12	0.76487421	-4.26375100 -4.50073458
H	13	0.91093189	-4.66056915 -5.50080562
N	14	-0.31738112	3.38423305 -1.68836280
C	15	0.59589313	-2.89608773 -4.30675029

H16	0.61122228	-2.21219437	-5.14866374
N17	1.95271497	-2.45418757	0.62834418
C18	0.41016337	-2.40323595	-3.01176164
N19	-0.18834514	-3.91707107	1.13449000
C20	0.24001386	-0.98321667	-2.70796732
N21	-2.08924072	-2.88494641	-0.34360210
C22	0.13466062	0.14571750	-3.52761853
H23	0.14537131	0.18459317	-4.60710886
N24	-1.87128600	2.23995552	0.81592927
C25	-0.00490475	1.20903092	-2.63222331
N26	0.15527955	3.81778538	1.43215640
C27	-0.21584104	2.64225254	-2.82589113
N28	2.16508200	2.97317892	-0.06247211
C29	-0.33655556	3.23630687	-4.08593491
H30	-0.25059102	2.62862849	-4.98034549
C31	-0.57177735	4.60469561	-4.17722615
H32	-0.66824149	5.07911627	-5.14917243
C33	-0.68592373	5.35702177	-3.00540591
H34	-0.87529785	6.42466961	-3.03485821
C35	-0.54895266	4.70744467	-1.78538476
H36	-0.62409297	5.25271336	-0.85013720
C37	3.00382100	-1.69948892	0.27592388
H38	2.79089520	-0.89830303	-0.42165286
C39	4.28467832	-1.93012964	0.77120688
H40	5.11096334	-1.30211949	0.45580640
C41	4.47649322	-2.98115556	1.66539925

H42	5.46177358	-3.19413476	2.06872105
C43	3.38519671	-3.76754366	2.03510210
H44	3.52120674	-4.59274301	2.72482285
C45	2.12650025	-3.49034023	1.50486995
C46	0.91365323	-4.28260706	1.82554703
C47	0.82839165	-5.32592060	2.74846318
H48	1.69363035	-5.64118574	3.31985823
C49	-0.40378549	-5.95645655	2.94099963
H50	-0.48826704	-6.76640387	3.65882592
C51	-1.52622419	-5.54642223	2.22336073
H52	-2.48180372	-6.03197055	2.38379200
C53	-1.39297808	-4.49741259	1.30782284
C54	-2.45926095	-3.93238963	0.45443483
C55	-3.76019890	-4.43860740	0.41766053
H56	-4.04408049	-5.26842619	1.05460088
C57	-4.69099644	-3.87698266	-0.45436956
H58	-5.70440348	-4.26446488	-0.49533210
C59	-4.29712264	-2.82294186	-1.27780906
H60	-4.98657924	-2.36933676	-1.98236224
C61	-2.98756118	-2.35759946	-1.18875028
H62	-2.63105328	-1.54464866	-1.81283849
C63	-2.84632999	1.39989677	0.44238083
H64	-2.56504093	0.64306779	-0.27884950
C65	-4.13761588	1.49122467	0.95758374
H66	-4.90081022	0.79409039	0.62943637
C67	-4.41903102	2.48436090	1.89198245

H68	-5.41465784	2.58520341	2.31297665
C69	-3.40251079	3.35493915	2.28723572
H70	-3.60646829	4.13113321	3.01601525
C71	-2.12907275	3.21739267	1.73983112
C72	-0.98752225	4.09158433	2.09935334
C73	-0.99843721	5.13046627	3.03385905
H74	-1.89527737	5.37858645	3.58892473
C75	0.18119679	5.84607832	3.25153368
H76	0.19443652	6.65289196	3.97798806
C77	1.34575410	5.53419451	2.54627971
H78	2.25550782	6.09511008	2.72592496
C79	1.31077597	4.49009285	1.61871486
C80	2.43526929	4.02353358	0.77185628
C81	3.69859867	4.61511987	0.78725522
H82	3.91006679	5.44571425	1.45069759
C83	4.69283107	4.13327904	-0.06564103
H84	5.67909106	4.58748428	-0.06445310
C85	4.39992236	3.07195902	-0.91905361
H86	5.14248003	2.67671042	-1.60442220
C87	3.12101089	2.51905019	-0.88382932
H88	2.83899044	1.69503671	-1.53060218
H89	-0.20443032	-0.45543792	1.58510053

LI_4^{4+}, 1 additional H_2O, ^5A

Ru1	-0.12654287	-2.31544615	0.01126302

N2	0.49418324	-3.25164610	-1.84756098
O3	-0.82935342	-1.31328145	1.40869736
O4	0.76206073	1.19296018	1.55081081
C5	0.76673380	-4.56224161	-2.02858598
H6	0.77734025	-5.18386020	-1.14073382
Ru7	0.17837634	2.27758336	0.25056437
N8	0.11994380	-0.64305070	-1.31447030
C9	1.02186221	-5.10007794	-3.28219171
H10	1.24165355	-6.15787058	-3.38284359
N11	-0.05259466	0.69499280	-1.25245967
C12	0.98739492	-4.25450437	-4.39593516
H13	1.17752917	-4.64528057	-5.39134994
N14	-0.39692154	3.36595156	-1.61194671
C15	0.71272775	-2.90194120	-4.21413039
H16	0.69192098	-2.22530927	-5.06135001
N17	1.84713344	-2.46086408	0.73177138
C18	0.47221804	-2.41456152	-2.92703209
N19	-0.22081467	-4.04718337	1.05844670
C20	0.21463535	-1.01003347	-2.62849576
N21	-2.08759267	-3.02841683	-0.48980156
C22	0.06652639	0.11787000	-3.43452384
H23	0.08669514	0.16956167	-4.51351732
N24	-1.81813185	2.39326326	0.97166083
C25	-0.10767224	1.17077656	-2.52772115
N26	0.28487819	3.93004969	1.40359525
C27	-0.35013888	2.60145592	-2.73726836

N28	2.18557041	2.97485987	-0.16182693
C29	-0.55490365	3.15951853	-4.00077634
H30	-0.51433481	2.53437041	-4.88639206
C31	-0.82126335	4.52353935	-4.11120707
H32	-0.98434031	4.97263711	-5.08645157
C33	-0.88120491	5.29904085	-2.95236310
H34	-1.09345709	6.36233679	-2.99425525
C35	-0.65952166	4.68170098	-1.72543050
H36	-0.68967858	5.25063447	-0.80236143
C37	2.86030257	-1.61793194	0.46561068
H38	2.62574780	-0.78991072	-0.19122504
C39	4.12786700	-1.80089511	1.01058451
H40	4.92469845	-1.10464342	0.77177892
C41	4.34867479	-2.88871214	1.85428639
H42	5.32834405	-3.06281146	2.28974303
C43	3.29531837	-3.76319104	2.13253386
H44	3.45658888	-4.61558002	2.78324533
C45	2.04637136	-3.53611536	1.56211443
C46	0.87327273	-4.41263502	1.76777089
C47	0.80458601	-5.54263994	2.58430558
H48	1.65955193	-5.86780327	3.16625403
C49	-0.39681723	-6.25603385	2.64630504
H50	-0.46810957	-7.13486139	3.28068248
C51	-1.50509152	-5.85280147	1.89718069
H52	-2.42961030	-6.41647396	1.94960861
C53	-1.39474299	-4.71876014	1.08860717

C54	-2.44146424	-4.15276142	0.21158977
C55	-3.70667512	-4.71749631	0.05767430
H56	-3.98584430	-5.60575712	0.61317218
C57	-4.61506443	-4.13562793	-0.83022154
H58	-5.60224275	-4.56925510	-0.96165172
C59	-4.23479088	-3.00274412	-1.54847405
H60	-4.90999708	-2.52935820	-2.25398672
C61	-2.95923273	-2.47799493	-1.34987331
H62	-2.61649844	-1.59958252	-1.88556510
C63	-2.84920070	1.59460827	0.65812713
H64	-2.62717056	0.78856659	-0.02996192
C65	-4.12402121	1.78978218	1.18484108
H66	-4.93571806	1.12841643	0.90147993
C67	-4.33142477	2.84681377	2.06868036
H68	-5.31320839	3.03107928	2.49467054
C69	-3.25895937	3.67669048	2.39980362
H70	-3.40774077	4.50641229	3.08183378
C71	-2.00559649	3.43675364	1.83967756
C72	-0.81764631	4.27989251	2.10630152
C73	-0.75260688	5.37126379	2.97523118
H74	-1.61504069	5.67963654	3.55489496
C75	0.45324493	6.06710347	3.09344545
H76	0.52214593	6.91502254	3.76857846
C77	1.56948106	5.68496767	2.34633145
H78	2.49840569	6.23547996	2.44034288
C79	1.46193530	4.58961334	1.48542794

C80	2.52192528	4.06570878	0.59444063
C81	3.78273398	4.65302778	0.48309137
H82	4.04404833	5.51680191	1.08367983
C83	4.70752392	4.12916997	-0.42180642
H84	5.68940292	4.58223132	-0.52259262
C85	4.34741636	3.02917352	-1.19822705
H86	5.03267738	2.60276678	-1.92364553
C87	3.07630604	2.48164109	-1.03475635
H88	2.74708813	1.63101941	-1.62215568
H89	-0.26485180	-1.11639051	2.26837626
O90	0.70091290	-0.81916508	3.37095204
H91	0.96413276	0.07526054	3.06308293
H92	0.33360467	-0.71874578	4.26682692

LI_4^{3+}, ^1A

Ru1	-2.1495558446	0.3242288010	-0.5802612192
Ru2	2.1193054373	0.0225584281	0.7451487674
N3	-3.1606893820	-1.6578266945	-0.9899884212
O4	-1.0597508856	1.7250784894	-0.4177639059
O5	0.8151460777	0.7688567549	1.7036775363
C6	-4.4815488342	-1.9114143804	-1.0177382232
H7	-5.1330774136	-1.1050574655	-0.6959887372
N8	-0.5520400036	-1.1204784419	-0.6405034228
C9	-5.0035034807	-3.1317827438	-1.4315602659
H10	-6.0763184787	-3.2925388370	-1.4315547821

N11	0.7829423195	-1.0144544197	-0.5887036862
C12	-4.1179625822	-4.1299288129	-1.8432716110
H13	-4.4894803936	-5.0938114625	-2.1779924585
N14	3.4626397078	-1.2262526666	-0.5717191912
C15	-2.7488713279	-3.8786467674	-1.8114564548
H16	-2.0386948871	-4.6415274833	-2.1126812074
N17	-2.7080726290	0.3351460772	1.4736692367
C18	-2.2912858855	-2.6331116220	-1.3731514370
N19	-3.8282266616	1.4505744801	-0.6363918294
C20	-0.8721039390	-2.2934030244	-1.2538748280
N21	-2.3567233037	0.6777960254	-2.6967139113
C22	0.3043015814	-2.9520299834	-1.6326029114
H23	0.3993907597	-3.8995534384	-2.1423775136
N24	2.5680270113	1.8133168245	-0.3068818025
C25	1.3297958815	-2.1047926242	-1.1952940620
N26	3.5957314848	0.7877090090	1.8935246674
C27	2.7903989061	-2.1805990802	-1.2721582650
N28	2.3648945053	-1.5370063294	2.2110057332
C29	3.4740566724	-3.1374766390	-2.0271053416
H30	2.9210955244	-3.8898584469	-2.5788021905
C31	4.8652579340	-3.1051301346	-2.0722343059
H32	5.4105707663	-3.8404503147	-2.6562221605
C33	5.5473553824	-2.1127229131	-1.3654470085
H34	6.6300715915	-2.0480238773	-1.3835726326
C35	4.8065098075	-1.1974599890	-0.6267065088
H36	5.2949289251	-0.4131370492	-0.0570672612

C37	-2.0776692070	-0.2627997928	2.4919606200
H38	-1.1956153876	-0.8321039740	2.2302522659
C39	-2.5173316071	-0.1441737525	3.8094672507
H40	-1.9790939284	-0.6468448496	4.6056952948
C41	-3.6441822328	0.6281894536	4.0740859027
H42	-4.0136398356	0.7441307656	5.0883521870
C43	-4.2982908860	1.2594822424	3.0151962874
H44	-5.1748836310	1.8681920071	3.2054301208
C45	-3.8147529508	1.1028082436	1.7184038710
C46	-4.4435238248	1.7308608202	0.5334586036
C47	-5.5773334072	2.5480916461	0.5300724556
H48	-6.0952186379	2.7939734282	1.4495006071
C49	-6.0344685747	3.0521121730	-0.6890974716
H50	-6.9114463077	3.6918073148	-0.7119032280
C51	-5.3757462467	2.7411112749	-1.8808467557
H52	-5.7402790524	3.1377716788	-2.8211758004
C53	-4.2466643712	1.9197916202	-1.8316105834
C54	-3.4274836788	1.4779005938	-2.9866925471
C55	-3.7145207528	1.8297391161	-4.3054298819
H56	-4.5658052850	2.4613893646	-4.5323571453
C57	-2.9013030073	1.3614743353	-5.3378080176
H58	-3.1195668312	1.6284978120	-6.3673474494
C59	-1.8136102813	0.5490982008	-5.0275948401
H60	-1.1578339000	0.1623337605	-5.8005651728
C61	-1.5769543369	0.2317073653	-3.6913318238
H62	-0.7463794637	-0.4007177697	-3.3976631042

C63	1.9915659041	2.2621939118	-1.4285947648
H64	1.2150602979	1.6325912921	-1.8434693245
C65	2.3551688593	3.4733448534	-2.0151506599
H66	1.8666157775	3.8001572879	-2.9267182322
C67	3.3435544864	4.2425149780	-1.4084749822
H68	3.6518024439	5.1906443418	-1.8382654584
C69	3.9369798929	3.7821524777	-0.2319043992
H70	4.7043143691	4.3731954880	0.2550275413
C71	3.5347481584	2.5627773358	0.3080278495
C72	4.1067502295	1.9902984364	1.5497393678
C73	5.0940450709	2.5656392485	2.3545953357
H74	5.5258701443	3.5292821804	2.1113616337
C75	5.5154810891	1.8745780585	3.4927119459
H76	6.2782283128	2.3083091344	4.1321511768
C77	4.9681827880	0.6305974446	3.8176440359
H78	5.3059411964	0.1051955723	4.7026772433
C79	3.9843500851	0.0918106668	2.9839531366
C80	3.2991970434	-1.2136264110	3.1565347320
C81	3.5812077557	-2.0902352682	4.2040728633
H82	4.3229808276	-1.8325349890	4.9514820492
C83	2.9049913841	-3.3077248639	4.2857543361
H84	3.1201922052	-3.9966192325	5.0969200610
C85	1.9578919959	-3.6243488488	3.3147716455
H86	1.4135460997	-4.5624650638	3.3414091145
C87	1.7172095234	-2.7087373099	2.2921249056
H88	0.9935313794	-2.9077167535	1.5094841484

$LI_{TS4\text{-}5}^{3+}$, ^{1}A

Ru1	0.00728300	2.04251200	-0.11894800
N2	0.36904700	3.24750000	1.74801500
O3	-0.53143900	0.74872000	-1.31516700
O4	0.53292600	-0.72667400	-1.31153600
C5	0.57332000	4.57543900	1.81595100
H6	0.60284900	5.10518700	0.86919300
Ru7	-0.02831500	-2.03136100	-0.13792900
N8	0.06535500	0.65510300	1.44916600
C9	0.74260300	5.25232800	3.01921300
H10	0.90848700	6.32407800	3.01929500
N11	-0.11509000	-0.65880200	1.44143500
C12	0.69271000	4.52213700	4.20853400
H13	0.81835800	5.01686000	5.16662500
N14	-0.42624400	-3.25343400	1.71001900
C15	0.48221100	3.14652400	4.15119200
H16	0.44413300	2.55326200	5.05859500
N17	2.05573300	2.12139900	-0.74079100
C18	0.32435800	2.52676300	2.90874100
N19	-0.04867900	3.51708200	-1.51609300
C20	0.11556600	1.09024400	2.73514900
N21	-2.02866700	2.71265100	0.03231900
C22	-0.04774000	-0.01147300	3.59072100
H23	-0.05919700	-0.01629000	4.67097500

N24	-2.06469400	-2.10092700	-0.79969400
C25	-0.19272400	-1.10547600	2.72203500
N26	0.05176200	-3.49370500	-1.54674800
C27	-0.40537800	-2.54346600	2.87804500
N28	2.00364800	-2.70557900	0.04511300
C29	-0.58886100	-3.17466600	4.11116800
H30	-0.56944900	-2.58982300	5.02460700
C31	-0.80041200	-4.55073700	4.15147200
H32	-0.94584000	-5.05422000	5.10216900
C33	-0.82534600	-5.26994600	2.95470800
H34	-0.99077300	-6.34168400	2.94146700
C35	-0.63132400	-4.58197200	1.76150500
H36	-0.64087800	-5.10313100	0.80955800
C37	3.08740400	1.41152900	-0.26470600
H38	2.85353000	0.72423900	0.53848600
C39	4.38173600	1.54394000	-0.76336100
H40	5.18826900	0.95545900	-0.34007300
C41	4.60962200	2.44462600	-1.80084300
H42	5.60427200	2.57659300	-2.21490100
C43	3.53889100	3.18703300	-2.30086100
H44	3.70165200	3.89615200	-3.10408700
C45	2.26697800	3.01576600	-1.75571100
C46	1.08157600	3.78562600	-2.20553900
C47	1.04768700	4.73170800	-3.23256100
H48	1.93457900	4.97037000	-3.80740300
C49	-0.16204300	5.36958100	-3.51864500

H	-0.20719100	6.10349100	-4.31703000
C	-1.31253400	5.07137000	-2.78683500
H	-2.24605300	5.57079100	-3.01735800
C	-1.23168300	4.11969200	-1.76572300
C	-2.33338000	3.69329900	-0.87216800
C	-3.60477800	4.27015300	-0.89741700
H	-3.83964500	5.04846400	-1.61417600
C	-4.57111900	3.85273500	0.01738700
H	-5.55972100	4.30089000	0.00922400
C	-4.24180100	2.86649300	0.94553900
H	-4.95744800	2.52587100	1.68627500
C	-2.95906500	2.32278300	0.91640100
H	-2.65125300	1.56082800	1.62408600
C	-3.10369600	-1.39199200	-0.33840800
H	-2.88369800	-0.71116100	0.47414000
C	-4.38837300	-1.51717700	-0.86323400
H	-5.20153200	-0.92975000	-0.45131500
C	-4.59821900	-2.40937500	-1.91181200
H	-5.58493400	-2.53563100	-2.34614900
C	-3.51971000	-3.15051300	-2.39672400
H	-3.66845900	-3.85282400	-3.20861500
C	-2.25822500	-2.98659400	-1.82567500
C	-1.06588000	-3.75502600	-2.25919500
C	-1.01442400	-4.69306800	-3.29283400
H	-1.89087500	-4.92567800	-3.88586700
C	0.19945900	-5.33065600	-3.56143700

H76	0.25835600	-6.05837100	-4.36458400
C77	1.33660200	-5.03999800	-2.80610300
H78	2.27349200	-5.53912300	-3.02321500
C79	1.23829000	-4.09626600	-1.77917300
C80	2.32390000	-3.67880100	-0.86202500
C81	3.59504300	-4.25673200	-0.86907700
H82	3.84227100	-5.02912200	-1.58808400
C83	4.54497000	-3.84799900	0.06660600
H84	5.53319900	-4.29701100	0.07255200
C85	4.19966500	-2.86938400	0.99699900
H86	4.90203600	-2.53579600	1.75346900
C87	2.91812600	-2.32420600	0.94928000
H88	2.59813200	-1.56814700	1.65788500

LI_5^{3+}, ^1A

Ru1	0.02127649	2.02051241	-0.04473639
N2	0.04750238	3.24648007	1.76532582
O3	-0.44250662	0.53058895	-1.22824906
O4	0.44475152	-0.53457648	-1.22745086
C5	0.06597127	4.59188185	1.78973215
H6	0.09186444	5.08830567	0.82526978
Ru7	-0.01971641	-2.02294293	-0.04298983
N8	-0.01515167	0.66123075	1.53020370
C9	0.05601075	5.32186088	2.97241791
H10	0.07584261	6.40593623	2.93878166

N11	0.02162670	-0.66091045	1.53126047
C12	0.01886948	4.63085203	4.18513372
H13	0.00811454	5.16911844	5.12802470
N14	-0.04613117	-3.24535324	1.77194793
C15	-0.00647540	3.23927819	4.17134213
H16	-0.03807990	2.67604064	5.09781675
N17	2.14393523	2.14415610	-0.24431829
C18	0.00814094	2.56212499	2.95015385
N19	0.20143022	3.38179971	-1.54080526
C20	-0.01342026	1.10901360	2.81326767
N21	-2.01401658	2.63230536	-0.35407102
C22	-0.00101907	0.00245251	3.67777188
H23	-0.00293158	0.00332066	4.75819922
N24	-2.14257330	-2.13529738	-0.24547786
C25	0.01477722	-1.10569791	2.81519520
N26	-0.20631322	-3.38370652	-1.54006086
C27	-0.00713229	-2.55818195	2.95527030
N28	2.01333967	-2.64128666	-0.35404857
C29	0.00722369	-3.23129218	4.17872931
H30	0.03851353	-2.66414067	5.10326880
C31	-0.01712648	-4.62284852	4.19621601
H32	-0.00631169	-5.15870296	5.14046809
C33	-0.05292782	-5.31712412	2.98524153
H34	-0.07142129	-6.40129906	2.95468804
C35	-0.06334535	-4.59068811	1.80025787
H36	-0.08811667	-5.09003446	0.83726453

C37	3.07486922	1.56968805	0.53281492
H38	2.69790576	0.93767226	1.32841721
C39	4.43831395	1.78169667	0.34615119
H40	5.15667868	1.31115255	1.00915598
C41	4.84987876	2.61785754	-0.68951755
H42	5.90426413	2.81045248	-0.86281117
C43	3.88582178	3.22364642	-1.49533264
H44	4.18967046	3.89123170	-2.29355589
C45	2.53390554	2.98294823	-1.25250185
C46	1.44164252	3.63612103	-2.01622651
C47	1.59199106	4.46864016	-3.12603740
H48	2.57188387	4.68930320	-3.53299013
C49	0.45015315	5.01386789	-3.72008391
H50	0.55159015	5.65986241	-4.58672003
C51	-0.81711213	4.73298138	-3.20944841
H52	-1.69846245	5.15591618	-3.67683744
C53	-0.91858403	3.89517315	-2.09396509
C54	-2.16385393	3.50142767	-1.40072312
C55	-3.41930507	4.00737539	-1.74278787
H56	-3.52588702	4.69526667	-2.57359767
C57	-4.53576398	3.63669381	-0.99497041
H58	-5.51645815	4.02930896	-1.24548149
C59	-4.36865579	2.76883785	0.08247704
H60	-5.20885943	2.47015286	0.70054866
C61	-3.09211283	2.28804606	0.36455759
H62	-2.90996458	1.61292339	1.19304721

C63	-3.07167755	-1.55474370	0.52933162
H64	-2.69232043	-0.92807933	1.32806601
C65	-4.43626457	-1.75375296	0.33588667
H66	-5.15331373	-1.27842943	0.99693615
C67	-4.85078781	-2.58305234	-0.70429886
H68	-5.90604544	-2.76491580	-0.88364069
C69	-3.88867086	-3.19602985	-1.50676846
H70	-4.19468639	-3.85854781	-2.30838813
C71	-2.53596845	-2.96864641	-1.25688413
C72	-1.44742098	-3.63009547	-2.01823465
C73	-1.60318712	-4.46174842	-3.12883012
H74	-2.58357715	-4.67605559	-3.53757921
C75	-0.46256421	-5.01354460	-3.72007812
H76	-0.56518110	-5.65896368	-4.58701032
C77	0.80580352	-4.73986398	-3.20753218
H78	1.68527703	-5.16758122	-3.67421078
C79	0.91164624	-3.90273414	-2.09203697
C80	2.15887220	-3.51372413	-1.39886026
C81	3.41228838	-4.02564369	-1.73998175
H82	3.51615003	-4.71629811	-2.56888639
C83	4.53071122	-3.65701336	-0.99392854
H84	5.50972951	-4.05420512	-1.24388733
C85	4.36790241	-2.78506063	0.08080615
H86	5.20975871	-2.48751561	0.69713432
C87	3.09339359	-2.29861885	0.36239598
H88	2.91450590	-1.62036583	1.18904700

$LI_{TS5\text{-}6}^{3+}$, 1 additional H_2O, ^1A

Ru1	2.03614500	0.00085600	0.01229900
Ru2	-2.21361500	-0.01351700	-0.04441500
N3	3.08799900	0.13037900	1.84191200
O4	0.27276700	0.96249700	-1.00620400
O5	-0.75257100	0.10645200	-1.33753400
C6	4.41884200	0.33754000	1.93018000
H7	4.94696700	0.48617200	0.99719800
N8	0.51827100	-0.13946800	1.49364900
C9	5.09136900	0.35732500	3.14409500
H10	6.16212600	0.52819200	3.16155300
N11	-0.80011400	-0.28422000	1.46987500
C12	4.36472100	0.15363300	4.32089700
H13	4.86189500	0.15978800	5.28581200
N14	-3.41373100	-0.48507000	1.72378800
C15	2.99223800	-0.05222300	4.23909800
H16	2.39798200	-0.20580200	5.13329800
N17	2.50174300	-2.10370700	0.05528100
C18	2.36500000	-0.05686600	2.98897100
N19	3.68330100	-0.08030300	-1.18181900
C20	0.93865000	-0.22583500	2.78710600
N21	2.51282500	2.06439500	-0.28660300
C22	-0.16672400	-0.43924000	3.62232100
H23	-0.17787100	-0.54551400	4.69731200

N24	-2.57225700	2.08296700	0.23501900
C25	-1.25537800	-0.46781300	2.73909600
N26	-3.67188500	0.33382300	-1.41040700
C27	-2.70130800	-0.61849100	2.88297300
N28	-2.56877100	-1.97500200	-0.81921000
C29	-3.33951800	-0.88781800	4.09649800
H30	-2.75253400	-0.99035700	5.00294900
C31	-4.72483700	-1.02632600	4.12690200
H32	-5.23376500	-1.23537100	5.06263100
C33	-5.44569600	-0.89673400	2.93805900
H34	-6.52499300	-1.00068600	2.91634900
C35	-4.75127200	-0.62835100	1.76329200
H36	-5.27278100	-0.51933800	0.81824600
C37	1.91370700	-3.06481300	0.78194500
H38	1.12011400	-2.74062400	1.44558800
C39	2.29832900	-4.40212000	0.70714800
H40	1.79913800	-5.14440600	1.32068700
C41	3.33551200	-4.75025400	-0.15498400
H42	3.66569600	-5.78070800	-0.24077300
C43	3.96011700	-3.75022500	-0.90088000
H44	4.77834200	-4.00424700	-1.56433200
C45	3.53230400	-2.42845600	-0.78053400
C46	4.17986100	-1.30063700	-1.48953400
C47	5.24955300	-1.39897900	-2.38062600
H48	5.66504300	-2.36187300	-2.65232200
C49	5.78536100	-0.22995600	-2.92770700

H50	6.61254500	-0.29270900	-3.62753600
C51	5.27233200	1.01550200	-2.56903700
H52	5.69803400	1.92119500	-2.98432400
C53	4.20056100	1.06592800	-1.67310900
C54	3.55295400	2.28230200	-1.14491000
C55	3.96991700	3.57924200	-1.44736200
H56	4.79528100	3.74379900	-2.13021000
C57	3.32015300	4.66395500	-0.86103300
H58	3.63953900	5.67699000	-1.08447100
C59	2.26170800	4.42654600	0.01511100
H60	1.73403900	5.24323200	0.49543200
C61	1.88524800	3.11063400	0.27115900
H62	1.05977000	2.86880000	0.92835800
C63	-2.03165300	2.89756200	1.15352600
H64	-1.30858000	2.44040600	1.81946000
C65	-2.38238100	4.24119300	1.26771600
H66	-1.92989700	4.85633500	2.03821100
C67	-3.32936800	4.76134300	0.38757100
H68	-3.63133900	5.80229400	0.44630200
C69	-3.90071200	3.91871800	-0.56620200
H70	-4.64975000	4.30474600	-1.24783600
C71	-3.51632700	2.57827300	-0.62342400
C72	-4.11281000	1.60300000	-1.56920800
C73	-5.06521100	1.88181600	-2.55192200
H74	-5.43581200	2.88842900	-2.70524200
C75	-5.53923200	0.83567700	-3.34777300

H76 -6.27846200 1.03605800 -4.11671300
C77 -5.06942300 -0.46433200 -3.15926600
H78 -5.44147600 -1.27083200 -3.78000500
C79 -4.11490400 -0.69763400 -2.16392000
C80 -3.51200600 -2.00235200 -1.81202500
C81 -3.88004600 -3.20522700 -2.41777300
H82 -4.62921600 -3.21774300 -3.20100100
C83 -3.28628400 -4.39707300 -2.00436500
H84 -3.56942800 -5.33740700 -2.46647600
C85 -2.33298100 -4.35825400 -0.98866100
H86 -1.85178300 -5.26258500 -0.63250400
C87 -2.00373900 -3.12692300 -0.42614900
H88 -1.26865400 -3.04208400 0.36558100
O89 1.40440200 -1.19474600 -2.32128600
H90 1.55562800 -0.44260800 -2.94556200
H91 0.44236300 -1.15342300 -2.16481900
H92 0.96650100 1.47094800 -2.74904200
O93 1.60461600 1.27147800 -3.46481700
H94 1.19401300 1.55374700 -4.29730800

Ll_6^{3+}, 1 additional H_2O, ^3A

Ru1 2.30828131 -0.15139024 -0.02633680
Ru2 -2.32476347 0.11374983 -0.01093362
N3 3.21138570 0.04354569 1.84245390
O4 -0.91066034 1.90189746 -1.76461769

O5	-1.11065987	0.60894492	-1.58678184
C6	4.53511193	0.19698835	2.04820313
H7	5.15178755	0.26820094	1.16086610
N8	0.56113805	-0.06455017	1.33915237
C9	5.09597123	0.25703302	3.31867387
H10	6.16823139	0.38179593	3.42647248
N11	-0.79323656	-0.16567269	1.33742589
C12	4.26205498	0.15143916	4.43349217
H13	4.66972600	0.19021199	5.43871479
N14	-3.42664001	-0.45112718	1.73746744
C15	2.89485419	0.00102309	4.23218573
H16	2.21855281	-0.07218680	5.07670049
N17	2.62629053	-2.25453056	0.03485669
C18	2.38909595	-0.04517926	2.92870393
N19	3.98639802	-0.31106619	-1.09935274
C20	0.96928383	-0.16184916	2.63139934
N21	2.70399143	1.89168380	-0.48819525
C22	-0.13683941	-0.36227533	3.48565118
H23	-0.12747444	-0.48728498	4.55834109
N24	-2.94524409	2.11276507	0.37197645
C25	-1.22799110	-0.37285903	2.63812778
N26	-3.88987035	0.37017285	-1.31662129
C27	-2.65760250	-0.56566203	2.85473438
N28	-2.56189449	-1.82436470	-0.84243088
C29	-3.23108283	-0.86276077	4.09479427
H30	-2.60417253	-0.95093283	4.97532732

C31	-4.60774153	-1.04810385	4.18271323
H32	-5.06815176	-1.28029109	5.13818780
C33	-5.38670348	-0.93484336	3.02847927
H34	-6.46209809	-1.07590754	3.05617775
C35	-4.75726110	-0.63319803	1.82672614
H36	-5.32015291	-0.53046850	0.90542589
C37	1.94259001	-3.19039982	0.71178335
H38	1.11556326	-2.82473214	1.31125369
C39	2.26999042	-4.54311025	0.67840404
H40	1.69145913	-5.25691948	1.25587038
C41	3.35514345	-4.94796668	-0.09627333
H42	3.64264573	-5.99340805	-0.15039768
C43	4.08092838	-3.98315881	-0.79146859
H44	4.93918912	-4.27651248	-1.38500863
C45	3.70903773	-2.64027101	-0.70781317
C46	4.46225074	-1.54948185	-1.36762411
C47	5.58411700	-1.69690905	-2.18777135
H48	5.98364726	-2.67745503	-2.41814051
C49	6.18663760	-0.55396636	-2.71714397
H50	7.05841744	-0.65038009	-3.35657840
C51	5.66913691	0.71100505	-2.43522989
H52	6.13037553	1.59500311	-2.85973590
C53	4.54327949	0.81133616	-1.61249877
C54	3.84612159	2.05729022	-1.22479996
C55	4.30435814	3.32772471	-1.57373984
H56	5.21506443	3.44373192	-2.14995153

C57	3.58475526	4.45109452	-1.17130497
H58	3.93255099	5.44588277	-1.43180944
C59	2.41742517	4.27401898	-0.43170336
H60	1.82743805	5.12176554	-0.09966893
C61	2.01364843	2.97956996	-0.11465980
H62	1.11168749	2.78830383	0.45554129
C63	-2.43699811	2.92057490	1.31549777
H64	-1.65959525	2.49721484	1.94106165
C65	-2.87674348	4.23036148	1.48768072
H66	-2.44013173	4.84774783	2.26558581
C67	-3.88014694	4.71660918	0.65264418
H68	-4.24974785	5.73164774	0.76076497
C69	-4.41401359	3.87636051	-0.32340749
H70	-5.20297560	4.23382950	-0.97524913
C71	-3.93401756	2.57356249	-0.44801011
C72	-4.45312328	1.59291084	-1.42252980
C73	-5.44503000	1.82020726	-2.38147462
H74	-5.91148260	2.79312658	-2.48281898
C75	-5.82766563	0.76776115	-3.21396584
H76	-6.59593154	0.92497654	-3.96473680
C77	-5.22842162	-0.48722150	-3.08593017
H78	-5.52800275	-1.30295364	-3.73349612
C79	-4.24021663	-0.66321477	-2.11408652
C80	-3.50720553	-1.91376946	-1.82572692
C81	-3.75305559	-3.12770818	-2.46569200
H82	-4.50672850	-3.19496511	-3.24168671

C83 -3.02969193 -4.26092323 -2.09645089
H84 -3.21762860 -5.21103841 -2.58709655
C85 -2.07313106 -4.15564648 -1.08829505
H86 -1.49332219 -5.01485786 -0.76887948
C87 -1.86949852 -2.91936008 -0.48301539
H88 -1.13839311 -2.78072851 0.30381329
O89 1.34032885 -0.47869941 -1.94617972
H90 1.55854419 0.26088674 -2.58672950
H91 0.37396949 -0.34354994 -1.83175965
H92 0.54665258 2.00380978 -2.97717780
O93 1.40521358 1.74148291 -3.38122696
H94 1.27019026 1.75769836 -4.34239296

$LI_{TS\text{-}O2\text{-}release}$, 1 additional H_2O, ^3A

Ru1 2.279861 -0.094686 -0.000994
Ru2 -2.323574 0.054253 -0.058545
N3 3.242234 0.031899 1.856167
O4 -0.908651 3.250140 -2.101592
O5 -0.893598 2.046497 -2.262452
C6 4.568056 0.192263 2.044273
H7 5.169381 0.296564 1.149317
N8 0.613294 -0.115493 1.362278
C9 5.151657 0.222302 3.304551
H10 6.223985 0.354575 3.397949
N11 -0.720059 -0.251400 1.321233

C12	4.333807	0.078263	4.427637
H13	4.756295	0.093847	5.427278
N14	-3.346261	-0.531943	1.614090
C15	2.964517	-0.080335	4.244501
H16	2.300886	-0.185227	5.095833
N17	2.683411	-2.191051	-0.028799
C18	2.434467	-0.097901	2.949888
N19	3.932024	-0.163837	-1.137575
C20	1.012798	-0.231835	2.665048
N21	2.608351	1.975984	-0.386108
C22	-0.096583	-0.466916	3.482824
H23	-0.116675	-0.611449	4.553094
N24	-2.800839	2.083171	0.415983
C25	-1.172284	-0.475571	2.590485
N26	-3.898848	0.388766	-1.275421
C27	-2.600364	-0.678450	2.752241
N28	-2.528534	-1.840076	-1.013719
C29	-3.213325	-1.024132	3.962236
H30	-2.603781	-1.134186	4.852424
C31	-4.586763	-1.230286	4.010155
H32	-5.068914	-1.500247	4.944303
C33	-5.333833	-1.089701	2.836974
H34	-6.406710	-1.246972	2.825179
C35	-4.679977	-0.738268	1.664475
H36	-5.221389	-0.612924	0.735723
C37	2.048538	-3.168873	0.639089

H38	1.193110	-2.855376	1.227487
C39	2.462401	-4.498912	0.607843
H40	1.921477	-5.247918	1.176487
C41	3.584109	-4.833516	-0.149165
H42	3.940416	-5.857747	-0.194659
C43	4.256702	-3.824610	-0.837368
H44	5.142204	-4.062808	-1.415479
C45	3.798303	-2.507531	-0.759936
C46	4.483625	-1.369553	-1.414437
C47	5.612203	-1.442830	-2.235792
H48	6.072980	-2.395604	-2.468981
C49	6.146986	-0.264142	-2.757824
H50	7.024129	-0.303815	-3.395559
C51	5.559850	0.966771	-2.458655
H52	5.979914	1.880058	-2.863822
C53	4.434720	0.995216	-1.629527
C54	3.707209	2.203054	-1.176165
C55	4.112863	3.502931	-1.487208
H56	4.985443	3.669776	-2.108380
C57	3.402980	4.590527	-0.980883
H58	3.717115	5.603634	-1.210819
C59	2.296098	4.351295	-0.167712
H60	1.723693	5.167821	0.259153
C61	1.935341	3.033277	0.101738
H62	1.087652	2.794446	0.734270
C63	-2.246593	2.869099	1.354742

H64	-1.415467	2.435997	1.900637
C65	-2.709942	4.153530	1.635065
H66	-2.232706	4.743382	2.410377
C67	-3.794809	4.646508	0.913166
H68	-4.187447	5.639817	1.106104
C69	-4.382084	3.836022	-0.058892
H70	-5.236249	4.198009	-0.619514
C71	-3.876970	2.555924	-0.291062
C72	-4.464219	1.619476	-1.279797
C73	-5.510793	1.894388	-2.164742
H74	-5.979364	2.871141	-2.193339
C75	-5.949051	0.885393	-3.024809
H76	-6.760625	1.082432	-3.717822
C77	-5.347859	-0.375020	-3.000189
H78	-5.690629	-1.151706	-3.673736
C79	-4.304260	-0.606479	-2.099989
C80	-3.555795	-1.874533	-1.922409
C81	-3.866654	-3.048076	-2.610051
H82	-4.683987	-3.066482	-3.321841
C83	-3.130138	-4.207785	-2.366238
H84	-3.372864	-5.128091	-2.888013
C85	-2.090605	-4.163378	-1.439718
H86	-1.499102	-5.044011	-1.213669
C87	-1.823080	-2.960330	-0.789041
H88	-1.026272	-2.870632	-0.060373
O89	1.000270	-0.272283	-1.808671

H90 1.422119 -0.716105 -2.593444
H91 0.743149 0.612182 -2.115312
H92 2.355396 -0.949644 -4.779238
O93 2.170295 -1.446597 -3.965931
H94 1.865838 -2.317850 -4.266391

$LI^{*3+}_{TS4\text{-}5}$, 1 additional H_2O, ^3A

Ru1 0.72173900 -2.20168500 -0.24594100
Ru2 0.58627900 2.38598500 -0.00913800
N3 2.15137400 -3.02666400 -1.73814000
O4 -0.54151900 -1.38409400 0.77981200
O5 0.95355300 1.23256600 1.63267900
C6 2.64930400 -4.27827100 -1.78395700
H7 2.40906900 -4.92428200 -0.94643900
N8 1.31781600 -0.49142200 -1.40473200
C9 3.42919000 -4.73852400 -2.83607300
H10 3.81116300 -5.75337000 -2.82492100
N11 0.95121400 0.80209100 -1.44350900
C12 3.70114000 -3.86761400 -3.89620700
H13 4.30258900 -4.19463100 -4.73871400
N14 0.51661800 3.41428900 -1.89222900
C15 3.19885000 -2.57175300 -3.85430200
H16 3.40647900 -1.87095000 -4.65540400
N17 2.19638300 -2.25348600 1.28857300
C18 2.42930900 -2.16573100 -2.75717700

N19	0.34859500	-4.00635100	0.58846100
C20	1.90457000	-0.81772300	-2.59699500
N21	-0.82013100	-2.95338700	-1.53669500
C22	1.88941100	0.29531700	-3.43953100
H23	2.27787000	0.37351700	-4.44441000
N24	-1.52746100	2.41265400	0.18395700
C25	1.27236000	1.29230800	-2.67464900
N26	0.33271500	3.97478700	1.16867600
C27	0.95404300	2.68926500	-2.95938000
N28	2.60783900	3.05075600	0.22939200
C29	1.05546100	3.25731100	-4.23271200
H30	1.40588100	2.65707200	-5.06542400
C31	0.69355300	4.58839200	-4.41980900
H32	0.76517400	5.04395000	-5.40238900
C33	0.23182400	5.32208200	-3.32558600
H34	-0.06764700	6.35963200	-3.42592300
C35	0.16216000	4.69875500	-2.08436300
H36	-0.18223800	5.23636000	-1.20817500
C37	3.11449400	-1.31739500	1.56682000
H38	3.07064600	-0.42012600	0.96284500
C39	4.05263700	-1.48351200	2.58538200
H40	4.78617000	-0.70721000	2.77360300
C41	4.02652500	-2.65383800	3.33952100
H42	4.74665500	-2.81859900	4.13492500
C43	3.05816700	-3.62136500	3.06260900
H44	3.02303200	-4.53531300	3.64426000

C45	2.14642200	-3.40404700	2.03126400
C46	1.09056800	-4.37605100	1.65585600
C47	0.81795200	-5.59476300	2.28191300
H48	1.38840900	-5.92605100	3.14165000
C49	-0.21668000	-6.38932600	1.78068600
H50	-0.44414100	-7.33772200	2.25714600
C51	-0.95844800	-5.97895100	0.67088900
H52	-1.75451400	-6.60686100	0.28889000
C53	-0.65210400	-4.75274200	0.07313700
C54	-1.30696000	-4.16251900	-1.11878700
C55	-2.34587100	-4.78623100	-1.80904000
H56	-2.73078500	-5.74356300	-1.47712500
C57	-2.89046100	-4.17159700	-2.93813400
H58	-3.69831300	-4.65061200	-3.48230900
C59	-2.38066900	-2.94389500	-3.35411800
H60	-2.77269300	-2.43562600	-4.22841600
C61	-1.34343600	-2.36666800	-2.62225000
H62	-0.91064400	-1.41331300	-2.90300800
C63	-2.42510500	1.59661800	-0.39059200
H64	-2.01154800	0.81103400	-1.01214300
C65	-3.79844500	1.73671700	-0.20471100
H66	-4.48358200	1.05369200	-0.69509900
C67	-4.26337200	2.76535900	0.61273300
H68	-5.32643100	2.90820900	0.77828700
C69	-3.33850000	3.61782500	1.21364500
H70	-3.68114200	4.42807300	1.84698800

C71	-1.97385200	3.42755700	0.98746900
C72	-0.92381900	4.29452300	1.56567800
C73	-1.12126500	5.37100800	2.43480900
H74	-2.11604800	5.64757900	2.76406100
C75	-0.01259400	6.09220000	2.88091600
H76	-0.14885100	6.93161600	3.55494300
C77	1.27120700	5.73645900	2.46374500
H78	2.12916300	6.29707000	2.81588300
C79	1.42551100	4.65415300	1.59334300
C80	2.70257500	4.14936400	1.04061200
C81	3.93758200	4.75097800	1.29343100
H82	4.00058000	5.62435800	1.93226800
C83	5.09250200	4.23229700	0.71024300
H84	6.05516100	4.69801100	0.89581900
C85	4.98518500	3.11742100	-0.11934700
H86	5.85563400	2.68758500	-0.60344300
C87	3.72570500	2.56051000	-0.33091000
H88	3.59144900	1.69985300	-0.97726600
O89	-0.27145600	0.60043900	2.18813900
H90	-0.39624400	-0.28808100	1.57185500
H91	0.02561100	0.31965100	3.12052400
O92	0.47206000	-0.16418500	4.58554900
H93	1.08569500	0.44553200	5.02786600
H94	-0.25071800	-0.30664400	5.22006000

LI*$_5^{3+}$, 1 additional H_2O, ^3A

Ru1	-0.03622861	-0.07709607	0.02454914
Ru2	-0.00898910	0.01044590	4.71311341
O3	1.66252962	-0.34783240	0.95437696
O4	1.13960217	-1.01825530	3.53577141
O5	1.86719556	-2.09895455	4.04986781
N6	-1.33130465	0.43984576	1.71695995
N7	-1.25567993	0.62404196	3.05054103
N8	-0.37149108	-2.16192467	-0.20064616
C9	-1.16229225	-2.94997294	0.54384330
C10	-1.28428989	-4.31555589	0.30296418
C11	-0.55857514	-4.87979548	-0.74496627
C12	0.26576755	-4.06496397	-1.52063648
C13	0.34754133	-2.70304568	-1.23293206
C14	1.17383380	-1.75202612	-2.01029317
C15	2.01808290	-2.06319062	-3.07974930
C16	2.72018759	-1.03132804	-3.70445088
C17	2.57586644	0.28644344	-3.26773813
N18	1.05212341	-0.46757230	-1.61335943
C19	1.71963237	0.55094752	-2.19560444
C20	1.42001131	1.87882684	-1.61380336
C21	1.94590218	3.07323474	-2.10615118
C22	1.56890611	4.28378689	-1.52625452
C23	0.66606532	4.27614235	-0.46392895
C24	0.18152167	3.05282017	-0.00969563
N25	0.54895902	1.88543712	-0.55951222

H26	-1.69827875	-2.45469544	1.34512640
H27	-1.93722614	-4.91954919	0.92370874
H28	-0.63366578	-5.94103624	-0.96145072
H29	0.83239843	-4.48884992	-2.34165741
H30	2.13485213	-3.08502030	-3.42183852
H31	3.38209025	-1.25468416	-4.53535190
H32	3.12397687	1.08272066	-3.75718337
H33	2.63726530	3.06472113	-2.94110980
H34	1.96901374	5.21841588	-1.90750030
H35	0.33549937	5.19820411	0.00294877
H36	-0.52738781	2.98753477	0.80851827
N37	-1.91893118	0.32276486	-0.93603516
C38	-2.16836620	0.18419292	-2.25464519
C39	-3.38424324	0.53255450	-2.82402896
C40	-4.38458606	1.05063340	-1.99563604
C41	-4.13495957	1.19199216	-0.63525414
C42	-2.88907970	0.81771966	-0.11941226
C43	-2.54226174	0.91773696	1.29374682
C44	-3.25000486	1.43900547	2.37877203
C45	-2.40074134	1.23935795	3.46889048
C46	-2.54070427	1.57125930	4.88473796
C47	-3.63051023	2.27582823	5.40591230
C48	-3.67584430	2.56118187	6.76673597
C49	-2.62719628	2.13746477	7.58686911
C50	-1.57548627	1.43738439	7.01133612
H51	-1.35966130	-0.21636926	-2.85553912

H52	-3.54235213	0.40355968	-3.88938995
H53	-5.34754360	1.33799046	-2.40695350
H54	-4.89791185	1.58534641	0.02706163
H55	-4.23037779	1.89172266	2.37570652
H56	-4.42984310	2.59760338	4.74713324
H57	-4.51619588	3.10793114	7.18364889
H58	-2.62343756	2.34213833	8.65217400
H59	-0.74219634	1.08321127	7.60786370
N60	1.34925316	1.65824572	4.81915670
C61	1.38474034	2.75339855	4.04488930
C62	2.32104030	3.76752968	4.22884021
C63	3.25581402	3.63678908	5.25382253
C64	3.22176722	2.50144905	6.06262509
C65	2.25736878	1.52061439	5.83341008
C66	2.12647767	0.29751498	6.66162389
C67	2.96186004	-0.08352137	7.71374447
C68	2.68836778	-1.27206312	8.39367668
C69	1.59797103	-2.06056225	8.02636413
C70	0.78980689	-1.64040535	6.96671567
C71	-0.40098341	-2.33780097	6.43385019
C72	-0.91620557	-3.51115831	6.98530919
C73	-2.06730699	-4.08053237	6.44410790
C74	-2.68390158	-3.45937108	5.35953600
N75	-1.00749841	-1.74560478	5.35947113
C76	-2.11950829	-2.29454196	4.84749819
H77	0.63356888	2.79976690	3.26494483

H78	3.99972657	4.40792208	5.42930489
H79	3.93773367	2.38906038	6.86889477
H80	3.81369846	0.52197227	8.00068240
H81	3.32956282	-1.58555015	9.21152873
H82	1.39415055	-2.98421250	8.55488869
H83	-0.43047863	-3.97522137	7.83622397
H84	-2.47830290	-4.99044238	6.87048775
H85	-3.58935006	-3.86251252	4.91825115
H86	-2.56211948	-1.76782667	4.00897856
H87	2.31116961	4.64014613	3.58460253
N88	1.07640499	-0.48509627	6.33043503
N89	-1.52624214	1.15703333	5.69382040
H90	1.49388097	-0.33809691	1.91950294
H91	2.26229646	-2.46633114	3.19192652
O92	2.75152443	-2.76042270	1.64532507
H93	3.70830692	-2.90556998	1.56767503
H94	2.55864976	-1.90348114	1.19524863

$LI^*_{TS5\text{-}6}{}^{3+}$, 1 additional H_2O, ^1A

Ru1	-0.12847700	-0.01960100	-0.23247900
Ru2	0.14300500	0.15574200	4.59802800
O3	2.03097500	0.30570700	2.51033800
O4	1.45203400	1.07364400	3.44635000
N5	-0.99397000	-0.89883700	1.58607900
N6	-1.03706200	-0.72432800	2.92683400

C7	-2.02494600	-1.52991900	3.42382700
C8	-2.62054600	-2.25609800	2.39142100
C9	-1.94409000	-1.83576000	1.25093600
C10	-2.10246900	-2.22724700	-0.13527800
N11	-1.33989200	-1.54783000	-1.03688700
C12	-1.42588600	-1.86442400	-2.34814200
C13	-2.26485500	-2.86022200	-2.82145300
C14	-3.05692800	-3.56229600	-1.90436900
C15	-2.97375800	-3.24257700	-0.55628200
C16	-2.31699200	-1.53034300	4.85447800
C17	-3.39143300	-2.23693800	5.40790300
C18	-3.62233900	-2.17202000	6.77806600
C19	-2.77391500	-1.39441700	7.56929300
C20	-1.72442700	-0.71967900	6.95672900
N21	-1.48960100	-0.78405200	5.63221900
H22	-1.04058900	-0.10805800	7.53426800
H23	-2.91867800	-1.31029100	8.64085600
H24	-4.45130800	-2.71462700	7.22135300
H25	-4.04025000	-2.82522900	4.76867700
H26	-3.41996700	-2.97824200	2.46229400
H27	-3.57115800	-3.77418700	0.17558800
H28	-3.72581000	-4.34817700	-2.24105800
H29	-2.29764000	-3.08061300	-3.88272000
H30	-0.79901500	-1.29436700	-3.02312000
C31	2.04810200	-2.20405700	0.22173300
C32	3.21503700	-2.90532400	-0.07386800

N33	1.58380300	-1.22464700	-0.57026800
C34	3.92167300	-2.57707800	-1.22899300
C35	3.44517200	-1.55422300	-2.05107500
C36	2.27237000	-0.88456900	-1.70542200
C37	1.68028900	0.20754500	-2.50976000
C38	2.18134500	0.72747600	-3.70620800
C39	1.47882400	1.75303400	-4.34105500
C40	0.29074600	2.24012200	-3.79363500
C41	-0.17622900	1.68797200	-2.59732700
N42	0.53136500	0.70382000	-1.99875800
C43	-1.42736800	2.04346100	-1.89124500
N44	-1.67778600	1.34384700	-0.74095600
C45	-2.81232800	1.57023300	-0.05943700
C46	-3.75476800	2.50801400	-0.47542000
H47	-4.22181400	3.97243900	-1.99389200
C48	-3.50837300	3.23538800	-1.63885100
C49	-2.33272900	2.99894900	-2.35258200
H50	-2.13276600	3.55067200	-3.26394600
H51	-4.66153000	2.65543400	0.10115500
H52	-2.95208800	0.97520200	0.83559000
H53	-0.25679200	3.02768100	-4.29799300
H54	1.85446900	2.16874400	-5.27057800
H55	3.09686500	0.34577100	-4.14296000
H56	3.98599700	-1.28619400	-2.95146100
H57	4.83260700	-3.10589000	-1.49132000
H58	3.55687300	-3.68967800	0.59220700

H59	1.46693400	-2.40422700	1.11305900
N60	-0.74838700	2.07164600	4.88671700
C61	-1.74460800	2.63608100	4.18804700
C62	-2.25774000	3.89558900	4.48923900
C63	-1.71169100	4.60348500	5.55831900
C64	-0.67463000	4.02607000	6.28868400
C65	-0.20630600	2.75787000	5.93940200
C66	0.87509800	2.06104400	6.66999900
C67	1.61178800	2.56972400	7.74349400
C68	2.60613700	1.77613100	8.31615700
C69	2.85799600	0.49654800	7.81829500
C70	2.09746900	0.02600000	6.74477900
N71	1.13232400	0.81281400	6.21361300
C72	2.22602800	-1.29808200	6.09441300
C73	3.10962700	-2.28462000	6.53634100
C74	3.14475500	-3.51925100	5.89001800
C75	2.29061000	-3.73895000	4.81090000
C76	1.43979100	-2.71088400	4.41173800
N77	1.40073000	-1.51919100	5.02617800
H78	0.75061100	-2.83325100	3.58379900
H79	2.27315600	-4.69087800	4.29092800
H80	3.82159400	-4.29569500	6.23206600
H81	3.75942200	-2.09934200	7.38368700
H82	3.63768700	-0.11255800	8.25996100
H83	3.18936200	2.15679800	9.14828500
H84	1.42515600	3.56602100	8.12650900

H85	-0.24100500	4.55913900	7.12686600
H86	-2.08628500	5.58661400	5.82485900
H87	-3.06944800	4.30620500	3.89857400
H88	-2.13127000	2.04471300	3.36594400
O89	0.98965700	1.43348900	0.67273400
H90	1.60689200	0.98494100	1.48203000
H91	1.56450900	2.00575700	0.09970500
O92	2.64423100	3.04105500	-0.81560300
H93	3.57969400	2.96141500	-0.56502600
H94	2.44943700	3.98815300	-0.72039700

$LI^{H+}_{TS4\text{-}5}{}^{4+}$, 1 additional H_2O, ^3A

Ru1	0.05882000	0.04470800	-0.01919600
Ru2	0.05148700	0.01192300	4.17012500
O3	1.51216900	0.12196300	1.42558100
O4	0.97149500	1.00831700	2.98475000
N5	0.73955300	-1.85755500	-0.72574300
C6	0.24161700	-3.05633800	-0.37106500
C7	0.74946900	-4.25150900	-0.87310000
C8	1.81125400	-4.20261400	-1.77700100
C9	2.32069200	-2.96056200	-2.15791700
C10	1.76603000	-1.79416000	-1.62941100
C11	2.16920000	-0.43299000	-2.03575900
C12	3.16500400	-0.10435000	-2.96036400
C13	3.36636100	1.23903900	-3.28513600

C14	2.57054400	2.22887500	-2.70588300
C15	1.59017200	1.85106700	-1.78394900
N16	1.43132800	0.54719400	-1.46723100
C17	0.61737200	2.74238000	-1.12352000
C18	0.52742000	4.11337700	-1.36395900
C19	-0.48614700	4.85654600	-0.75752500
C20	-1.39524300	4.20788100	0.07874300
C21	-1.25362300	2.83975300	0.29062500
N22	-0.26941200	2.12218400	-0.28166000
H23	-1.93690000	2.28882800	0.92542300
H24	-2.20893200	4.74707100	0.55158500
H25	-0.57087000	5.92182700	-0.94967000
H26	1.22838400	4.59946900	-2.03296700
H27	2.71199500	3.26784200	-2.98019400
H28	4.13272500	1.51244200	-4.00389100
H29	3.76750300	-0.87197000	-3.43215300
H30	3.13163700	-2.90615500	-2.87526300
H31	2.22882500	-5.11439600	-2.19328400
H32	0.31041900	-5.19557100	-0.56790400
H33	-0.58974900	-3.04431900	0.32431500
N34	-1.68043000	-0.32847100	-1.20950900
C35	-1.78638300	-0.14210400	-2.53973400
C36	-2.94161700	-0.45634600	-3.24781700
C37	-4.03271400	-0.98854300	-2.55619100
C38	-3.93319600	-1.18180800	-1.17936100
C39	-2.74876800	-0.84382000	-0.52155100

C40	-2.54079800	-0.98049500	0.91706300
N41	-1.33595400	-0.52818100	1.38040800
N42	-1.29372800	-0.69394800	2.70485900
C43	-2.45578700	-1.26247700	3.11292800
C44	-3.28661300	-1.46579500	1.99498400
C45	-2.58216400	-1.52592400	4.54547400
C46	-3.67140000	-2.18635600	5.11677600
C47	-3.69219200	-2.41005300	6.49328000
C48	-2.61789800	-1.96781700	7.26757300
C49	-1.56438200	-1.31132500	6.63750000
N50	-1.53460000	-1.08917500	5.31007800
H51	-0.71468800	-0.95158000	7.20738300
H52	-2.59167300	-2.12590800	8.34047600
H53	-4.53159200	-2.92326200	6.95245300
H54	-4.48986200	-2.52497600	4.49044900
H55	-4.27722300	-1.89689200	1.97722500
H56	-4.76668900	-1.58794800	-0.61605600
H57	-4.94753500	-1.24662000	-3.08087700
H58	-2.97996900	-0.28646800	-4.31856000
H59	-0.91734700	0.26988700	-3.04010900
N60	-0.98779900	1.78321700	4.84818100
C61	-2.13707400	2.29399900	4.38130000
C62	-2.73032200	3.42848400	4.93285800
C63	-2.10197700	4.05791600	6.00599300
C64	-0.90982900	3.52549400	6.50051100
C65	-0.36857600	2.38053700	5.91449300

C66	0.85227900	1.71050000	6.41807900
C67	1.65258700	2.13368000	7.48354500
C68	2.74678200	1.34954900	7.85685700
C69	3.03066200	0.15605900	7.18582300
C70	2.20898400	-0.22897900	6.12433800
N71	1.16672300	0.56120100	5.77614100
C72	2.32704400	-1.46714800	5.31991000
N73	1.39793200	-1.62846100	4.32279000
C74	1.41081000	-2.74625800	3.57999400
C75	2.34212100	-3.76282600	3.77966400
C76	3.29726600	-3.61001000	4.78305300
C77	3.28800900	-2.44820300	5.55844200
H78	0.64750400	-2.81335400	2.81475400
H79	2.30921800	-4.65617500	3.16565900
H80	4.03566800	-4.38361200	4.97061700
H81	4.01908800	-2.32149600	6.34876000
H82	3.87457900	-0.44990400	7.49447300
H83	3.37798500	1.66537800	8.68201100
H84	1.43696800	3.05056800	8.01961400
H85	-0.41945000	3.99573800	7.34522100
H86	-2.53425000	4.94327400	6.46219500
H87	-3.66700900	3.80003900	4.53091600
H88	-2.59212800	1.76457200	3.55173700
H89	2.27629400	0.75765700	1.27977200
O90	3.54216300	1.83633400	0.94681300
H91	4.45378100	1.49984000	0.92087400

H92	3.58743400	2.63945800	1.49160900

LI$^{H+_5\ 4+}$, 1 additional H_2O, ^{1}A

Ru1	0.01727909	0.05648914	-0.00483205
Ru2	0.03058227	-0.02380886	4.10277241
O3	1.48468236	0.01746234	1.60726865
O4	1.17870674	0.84872441	2.79222084
N5	0.53845014	-1.92096990	-0.62600885
C6	-0.09434463	-3.04878136	-0.25291790
C7	0.27972645	-4.30406309	-0.72351904
C8	1.34806879	-4.39703275	-1.61491350
C9	1.99774337	-3.22956017	-2.01414789
C10	1.57313880	-1.99681525	-1.51789852
C11	2.13597660	-0.70084867	-1.94502088
C12	3.19300139	-0.51491372	-2.84119342
C13	3.56060235	0.78844324	-3.18196912
C14	2.87309401	1.87580702	-2.64059649
C15	1.82664841	1.63767166	-1.74657948
N16	1.49691933	0.36917811	-1.41950590
C17	0.96103259	2.65538191	-1.11787592
C18	1.05994389	4.02338144	-1.36826563
C19	0.14448098	4.89858811	-0.78205256
C20	-0.85474152	4.38293764	0.04292166
C21	-0.90113718	3.00944825	0.26526708
N22	-0.01252469	2.16423503	-0.28875601

H23	-1.66056234	2.55994131	0.89402176
H24	-1.59574535	5.03001748	0.50082912
H25	0.20470336	5.96489780	-0.97949577
H26	1.83038049	4.40609959	-2.02769945
H27	3.14906356	2.88479351	-2.92329279
H28	4.37506421	0.95675554	-3.88031496
H29	3.71487529	-1.35928431	-3.27692862
H30	2.81577215	-3.28094449	-2.72402316
H31	1.66348161	-5.35917213	-2.00752924
H32	-0.26709064	-5.18528588	-0.40410198
H33	-0.92655588	-2.92822444	0.43123988
N34	-1.69145345	-0.13037352	-1.23281318
C35	-1.72789618	0.05714105	-2.56601218
C36	-2.89096554	-0.12061511	-3.30870044
C37	-4.05963511	-0.51038178	-2.65177872
C38	-4.03014212	-0.70373319	-1.27135351
C39	-2.83736297	-0.50702452	-0.57583763
C40	-2.68124523	-0.65789974	0.86785539
C41	-3.47755739	-1.03317618	1.94716346
H42	1.38359968	-5.08624881	3.27507516
N43	-1.40323873	-0.50743127	2.66212143
N44	-1.42550291	-0.34910598	1.33712812
C45	-2.62500979	-0.91976521	3.07222836
C46	-2.76518851	-1.12832154	4.51248589
C47	-3.91483919	-1.62851287	5.12381013
C48	-3.93679895	-1.79773298	6.50857198

C49	-2.80601248	-1.45767344	7.25087190
C50	-1.69039722	-0.95592402	6.58415383
N51	-1.65790233	-0.79464937	5.24908366
H52	-0.79389055	-0.67617595	7.12665201
H53	-2.78187888	-1.57525811	8.32930359
H54	-4.82325540	-2.18943593	6.99827395
H55	-4.78068663	-1.88690911	4.52318205
H56	-4.51455517	-1.33738949	1.93528469
H57	-4.92516613	-1.00109473	-0.73437667
H58	-4.98168659	-0.65912851	-3.20569403
H59	-2.87430930	0.04412815	-4.38103834
H60	-0.79911178	0.35669141	-3.03750787
N61	-0.61351036	1.91953950	4.71413701
C62	-1.69101706	2.59681842	4.28672843
C63	-2.05143146	3.83840192	4.80490054
C64	-1.25868275	4.40379330	5.80241892
C65	-0.14191627	3.70254021	6.25593809
C66	0.16181206	2.45587812	5.70795323
C67	1.27823431	1.60990786	6.18109454
C68	2.22057992	1.94577421	7.15797805
C69	3.18736761	1.00358914	7.50928281
C70	3.20739745	-0.25456261	6.89902143
C71	2.25005388	-0.54656952	5.92670465
N72	1.33028640	0.38992151	5.60146240
C73	2.09718947	-1.82967153	5.19671616
C74	2.89148088	-2.94783718	5.44427723

C75	2.64947555	-4.13486260	4.75064929
C76	1.61313355	-4.17661263	3.81983989
C77	0.85749579	-3.02634353	3.60868106
N78	1.08954188	-1.87983101	4.26862355
H79	0.03622081	-3.00522803	2.90220529
H80	3.25660728	-5.01366276	4.94672539
H81	3.68554608	-2.90603795	6.18137970
H82	3.95770488	-0.98120798	7.18750496
H83	3.92662378	1.24597641	8.26688450
H84	2.20768704	2.91618345	7.64074133
H85	0.47424446	4.11984374	7.04448040
H86	-1.50909108	5.36909693	6.23207640
H87	-2.93987434	4.34207985	4.43806190
H88	-2.28155988	2.11330431	3.51612345
H89	2.40379952	0.38357778	1.38997980
O90	3.83624682	1.02646129	1.00191883
H91	4.64224594	0.48559686	1.05837113
H92	4.05861422	1.85901307	1.45174812

$LI^{H+}_{TS5\text{-}6}{}^{4+}$, 3A

Ru1	0.05457300	-2.02199500	-0.18495400
Ru2	-0.81659400	1.96900600	1.42409400
N3	1.40529600	-2.32090300	-1.71497900
O4	-1.86898200	-0.53472500	0.55903300
O5	-1.78630700	0.30168200	1.76618400

C6	1.60528100	-3.50570300	-2.33023400
H7	0.99459400	-4.33520700	-1.99714100
N8	0.79562900	-0.10674700	-0.46339300
C9	2.54863600	-3.66002000	-3.33847100
H10	2.67659300	-4.63015300	-3.80688400
N11	0.61836300	1.09022200	0.11546600
C12	3.31610100	-2.55695700	-3.72447300
H13	4.06225400	-2.65004700	-4.50770700
N14	0.53358000	3.59978600	1.01568800
C15	3.10991400	-1.33367100	-3.09178100
H16	3.68687600	-0.45911800	-3.37286600
N17	1.56580800	-2.80320800	1.09386800
C18	2.14504100	-1.22891100	-2.08668100
N19	-0.57795300	-3.95394500	0.14701100
C20	1.82414000	-0.00745400	-1.36776600
N21	-1.50129300	-2.30194900	-1.63334800
C22	2.32132400	1.29281300	-1.36053900
H23	3.12781300	1.70112200	-1.95231600
N24	-2.16872000	2.75496600	-0.04449000
C25	1.52905500	1.95570400	-0.40509900
N26	-2.15823400	2.94492200	2.59074600
C27	1.50940700	3.32747700	0.09605800
N28	0.07941400	1.80617400	3.35331300
C29	2.42161500	4.30724400	-0.30166900
H30	3.18807000	4.07084700	-1.03184100
C31	2.34092500	5.58488600	0.25126600

H32	3.04305500	6.35706600	-0.04790700
C33	1.34829900	5.85219700	1.19629700
H34	1.25288600	6.83119300	1.65384200
C35	0.46799000	4.83416400	1.55084300
H36	-0.31679800	5.00366700	2.27924200
C37	2.70303000	-2.17720100	1.44362000
H38	2.87029400	-1.19988200	1.00639000
C39	3.62868500	-2.74801000	2.31384300
H40	4.53864500	-2.21151000	2.56107000
C41	3.36799000	-4.01410900	2.83592200
H42	4.07109600	-4.49326400	3.51042900
C43	2.19390900	-4.67141800	2.46325200
H44	1.98700800	-5.66497000	2.84434500
C45	1.30504900	-4.05270100	1.58548400
C46	0.07751900	-4.69109300	1.07253600
C47	-0.40552700	-5.95581100	1.41964600
H48	0.10368800	-6.56702900	2.15581800
C49	-1.56037100	-6.43375000	0.79577200
H50	-1.95041800	-7.41291100	1.05642800
C51	-2.20327900	-5.66463400	-0.17623500
H52	-3.08680300	-6.04635500	-0.67468600
C53	-1.67968900	-4.40815000	-0.49404200
C54	-2.18142100	-3.48639000	-1.53172900
C55	-3.22697400	-3.78424800	-2.40632500
H56	-3.76252600	-4.72320500	-2.32263200
C57	-3.56748000	-2.87399800	-3.40839300

H	-4.37192700	-3.10171600	-4.10122900
C	-2.85023100	-1.68183400	-3.51474700
H	-3.07337400	-0.95800900	-4.29121700
C	-1.82432000	-1.43167100	-2.60723700
H	-1.23904000	-0.52083200	-2.64678900
C	-2.05828300	2.70362700	-1.38264600
H	-1.18260100	2.19279000	-1.76612500
C	-2.99575900	3.28144400	-2.23496700
H	-2.85739900	3.23064800	-3.30968700
C	-4.09432400	3.93371500	-1.67641500
H	-4.84421100	4.40042600	-2.30791000
C	-4.21254200	3.99543300	-0.28644000
H	-5.05395800	4.51293400	0.15975700
C	-3.23561300	3.40848200	0.51721000
C	-3.24726000	3.48494500	1.99771200
C	-4.23628400	4.07377800	2.78867000
H	-5.12240100	4.51406300	2.34661400
C	-4.07013300	4.08947500	4.17709600
H	-4.83169300	4.54101400	4.80543200
C	-2.92963900	3.53472400	4.75933700
H	-2.80499200	3.55677500	5.83571500
C	-1.96430600	2.95508000	3.92888800
C	-0.68630600	2.34711200	4.35492500
C	-0.23632400	2.34639200	5.67603100
H	-0.84396700	2.77853700	6.46290000
C	1.01173800	1.80219000	5.98069700

H84	1.37345600	1.80587800	7.00434100
C85	1.78621400	1.26822900	4.95128900
H86	2.76716800	0.84819600	5.14542800
C87	1.28237400	1.28820000	3.65307900
H88	1.84599300	0.88664300	2.81905900
O89	-0.80496300	-2.10724200	2.65628200
H90	-1.17773400	-1.21088400	2.75310800
H91	-1.25507700	-2.65351700	3.32020800
H92	-2.67438400	-1.04608300	0.77111600

$LI^{H+}{}_{6}{}^{4+}$, 1 additional H_2O, ^1A

Ru1	0.07623359	0.36311579	-0.29176879
Ru2	0.10154021	-0.15091494	4.40176237
O3	2.86601137	0.62174875	3.98235384
O4	1.69459542	0.15151735	3.31305639
N5	1.25786863	-1.33462312	-0.76331315
C6	1.14198821	-2.54886180	-0.19730070
C7	1.94558670	-3.62159756	-0.57183496
C8	2.89886622	-3.43066051	-1.57116167
C9	3.01542759	-2.17391488	-2.16664882
C10	2.18099595	-1.13561698	-1.75506465
C11	2.17216107	0.21166566	-2.36105461
C12	3.00988210	0.67105875	-3.38029929
C13	2.82933732	1.96773250	-3.86665611
C14	1.81745531	2.77874850	-3.34990410

C15	1.00091072	2.27612827	-2.33254922
N16	1.21084268	1.02489922	-1.86452335
C17	-0.15057705	2.96030162	-1.70995188
C18	-0.60512793	4.22231284	-2.08796219
C19	-1.75030142	4.75154637	-1.49083412
C20	-2.41842050	4.00110487	-0.52483385
C21	-1.91495025	2.74936256	-0.18016356
N22	-0.80624758	2.24183287	-0.74698940
H23	-2.40262575	2.12802515	0.56204431
H24	-3.32046011	4.37007362	-0.04764383
H25	-2.11763638	5.72963843	-1.78715372
H26	-0.08458755	4.78763112	-2.85256896
H27	1.66873896	3.77704433	-3.74476011
H28	3.46983660	2.34208352	-4.65974378
H29	3.78288225	0.03610939	-3.79841762
H30	3.74082014	-2.01537880	-2.95664718
H31	3.53726189	-4.24789896	-1.89377626
H32	1.81694997	-4.58680919	-0.09365236
H33	0.38431271	-2.64327432	0.57134611
N34	-1.47508358	-0.49661126	-1.38766999
C35	-1.51290771	-0.61957293	-2.73119640
C36	-2.60863351	-1.15864365	-3.39200286
C37	-3.70854888	-1.58281412	-2.64050139
C38	-3.67123762	-1.45839760	-1.25488346
C39	-2.53931988	-0.91277862	-0.64291922
C40	-2.38429621	-0.75334926	0.79602243

C41	-3.24443642	-0.96938676	1.86098223
H42	-0.23199509	-5.38787352	3.55851844
N43	-1.23196077	-0.24522814	2.62568315
N44	-1.16907788	-0.30028697	1.26906945
C45	-2.48318195	-0.63759209	2.99347333
C46	-2.83755852	-0.67102996	4.41058216
C47	-4.13720308	-0.91369624	4.86200520
C48	-4.40198359	-0.90827746	6.22994576
C49	-3.35646341	-0.65597149	7.11916441
C50	-2.08382991	-0.42575000	6.60705804
N51	-1.82048239	-0.43445845	5.28647911
H52	-1.24461683	-0.23045229	7.26447431
H53	-3.51845973	-0.63800547	8.19190706
H54	-5.40783009	-1.09363684	6.59478131
H55	-4.93509110	-1.09670140	4.15102872
H56	-4.26531464	-1.32009572	1.82990069
H57	-4.50896076	-1.78548376	-0.64889130
H58	-4.58098155	-2.00611869	-3.12938023
H59	-2.59818078	-1.24172602	-4.47386340
H60	-0.64227938	-0.27370563	-3.27509615
N61	0.04330021	1.88579789	5.01049585
C62	-0.62831119	2.89604749	4.43368763
C63	-0.58449204	4.19816828	4.92313395
C64	0.18740639	4.46485641	6.05387197
C65	0.88360259	3.42048571	6.66161226
C66	0.79607740	2.13351215	6.12893148

C67	1.45536761	0.95745791	6.73180930
C68	2.28110887	0.95721261	7.85981014
C69	2.81430443	-0.25505064	8.30069937
C70	2.51634937	-1.44349734	7.62984116
C71	1.68239897	-1.39399921	6.50953428
N72	1.18662745	-0.20590938	6.09948893
C73	1.23435879	-2.55143644	5.70281696
C74	1.56071428	-3.87172653	6.01650954
C75	1.04289474	-4.91029821	5.24287894
C76	0.20658449	-4.60533979	4.16902657
C77	-0.07365776	-3.26933199	3.89779969
N78	0.42798261	-2.26274845	4.63379680
H79	-0.72683961	-2.98011697	3.08187509
H80	1.28022384	-5.94178205	5.48589508
H81	2.19859422	-4.09443405	6.86399918
H82	2.92930366	-2.38178038	7.98109303
H83	3.46054054	-0.27537985	9.17303092
H84	2.51035800	1.87574238	8.38736748
H85	1.47852226	3.60910002	7.54786337
H86	0.24180253	5.46880004	6.46424218
H87	-1.14903208	4.98257542	4.43016193
H88	-1.21431608	2.63431084	3.55971237
H89	3.45693440	0.81776451	3.21368047
O90	1.50752569	1.30706167	0.97608825
H91	1.50446559	0.90923683	1.89647637
H92	2.46278230	1.34791959	0.74857013

O93	4.21165374	1.35926600	1.60110159
H94	4.58586514	2.25049818	1.72525762
H95	4.97802477	0.80273160	1.37469886

$LI^{H+}*_{TS4\text{-}6}{}^{4+}$, 1 additional H_2O, ^1A

Ru1	0.31142200	-2.34718600	0.02784700
Ru2	0.56637000	2.34270800	0.09627500
N3	1.55247100	-3.29962500	-1.43195900
O4	-0.89174900	-1.27675600	1.21131600
O5	0.82968500	1.28457400	1.51202400
C6	1.85652500	-4.61382900	-1.46234400
H7	1.48341500	-5.21488300	-0.64149700
N8	1.06428400	-0.64984000	-1.15280000
C9	2.60708900	-5.18355800	-2.48278000
H10	2.83082200	-6.24472200	-2.46183400
N11	0.85110000	0.67945900	-1.27449500
C12	3.05670200	-4.36458000	-3.52241300
H13	3.64215600	-4.77773300	-4.33807000
N14	0.65523700	3.29896400	-1.88339500
C15	2.74719000	-3.00689000	-3.49620200
H16	3.09215000	-2.34839900	-4.28570600
N17	1.84612000	-2.63541400	1.46954500
C18	1.99515800	-2.49203600	-2.43629700
N19	-0.33069800	-4.01372100	0.97125500
C20	1.64447700	-1.08062200	-2.31150400

N21	-1.32665700	-2.94775000	-1.21027400
C22	1.78476400	-0.01469900	-3.20547200
H23	2.19295900	-0.03423300	-4.20536400
N24	-1.54136000	2.46898400	0.13636500
C25	1.26568700	1.07843100	-2.51132200
N26	0.30982700	4.06617200	1.11150600
C27	1.08924100	2.47939000	-2.88196700
N28	2.60820200	3.04057200	0.28463000
C29	1.30713000	2.96962600	-4.17230500
H30	1.65100600	2.30177400	-4.95449100
C31	1.06658800	4.31459300	-4.44491200
H32	1.22947600	4.70884000	-5.44336500
C33	0.60533400	5.14420800	-3.41901300
H34	0.39462300	6.19410900	-3.59192100
C35	0.41729300	4.59883800	-2.15508500
H36	0.06642200	5.21091500	-1.33208200
C37	2.97278100	-1.91753600	1.60974600
H38	3.10506700	-1.10635800	0.90390100
C39	3.91361300	-2.19684300	2.59790200
H40	4.81687900	-1.60080100	2.67045900
C41	3.67372400	-3.25615200	3.47265500
H42	4.38887700	-3.50712700	4.25010700
C43	2.50310500	-4.00394500	3.33134200
H44	2.30941500	-4.83585400	3.99877200
C45	1.59974800	-3.68328900	2.31857700
C46	0.36385000	-4.45115700	2.04841700

C47	-0.09501000	-5.56549200	2.75626000
H48	0.43944600	-5.93928000	3.62189300
C49	-1.26079000	-6.20536000	2.32625500
H50	-1.63152500	-7.07129600	2.86592300
C51	-1.94188900	-5.74741700	1.19678000
H52	-2.83383900	-6.26079600	0.85713500
C53	-1.44725500	-4.62931700	0.51668700
C54	-1.99968200	-4.03675100	-0.72065600
C55	-3.10602900	-4.55399400	-1.39595200
H56	-3.63471800	-5.41635300	-1.00623400
C57	-3.52336900	-3.96467100	-2.59041600
H58	-4.37742700	-4.36614200	-3.12728500
C59	-2.82132400	-2.86577300	-3.08515200
H60	-3.10602400	-2.38723900	-4.01618500
C61	-1.72916400	-2.38831700	-2.36426900
H62	-1.14776200	-1.54252300	-2.71298100
C63	-2.41624700	1.62975300	-0.43893200
H64	-1.98587800	0.80581700	-0.99444300
C65	-3.79400000	1.80675700	-0.32528000
H66	-4.47010100	1.11205800	-0.81150400
C67	-4.27557200	2.88709500	0.41139700
H68	-5.34282800	3.05641600	0.51667900
C69	-3.36582500	3.76257000	1.01010600
H70	-3.72747200	4.61160600	1.57885700
C71	-1.99875500	3.54087400	0.86015200
C72	-0.95817800	4.43044400	1.42159000

C73	-1.16456400	5.57913000	2.18821700
H74	-2.16260100	5.90440700	2.45782100
C75	-0.05229400	6.31503700	2.60782000
H76	-0.19541500	7.21037100	3.20538900
C77	1.24207100	5.91633100	2.26024800
H78	2.09357100	6.50159000	2.58723300
C79	1.40856800	4.76203500	1.49124300
C80	2.69182000	4.20287800	1.00458700
C81	3.92531400	4.81617300	1.22193800
H82	3.99039300	5.73918000	1.78678000
C83	5.08501600	4.24159300	0.69521200
H84	6.04868600	4.71555100	0.85510400
C85	4.98281700	3.06305800	-0.04057600
H86	5.85782800	2.58974200	-0.47324000
C87	3.72262300	2.49288200	-0.22203400
H88	3.59094000	1.58040200	-0.79265000
O89	-0.60267600	0.87970500	2.57905400
H90	-0.72312900	-0.01062100	2.07381800
H91	-0.13056200	0.67597300	3.45243500
H92	-1.51554400	-1.85112700	1.68981600
O93	0.44333300	0.18658500	4.91507800
H94	-0.21982900	0.10451000	5.62176200
H95	1.19377100	0.64478400	5.32799800

Energies and spin populations.

Table S1. The energies and spin populations for the ruthenium blue dimer.

		ZPE	Solvation (P-O)	E cc-pVTZ(-f)	vdW	Sum	Spins
BD_0^{4+}	^3A	0.728878	-0.692950	-2472.081935	-0.186079	-2472.232086	$Ru_1^{0.57}$ $Ru_2^{0.70}$ $O_5^{0.74}$
BD_1^{5+}	^2A	0.727386	-1.069763	-2471.484856	-0.182537	-2472.009770	$Ru_1^{1.12}$ $Ru_2^{-0.61}$ $O_5^{0.51}$
	^4A	0.726812	-1.066108	-2471.476832	-0.178472	-2471.994600	$Ru_1^{0.98}$ $Ru_2^{1.21}$ $O_5^{0.73}$
BD_1^{4+}	^2A	0.716535	-0.684717	-2471.452348	-0.183609	-2471.604139	$Ru_1^{1.10}$ $Ru_2^{-0.69}$ $O_4^{-0.15}$ $O_5^{0.71}$
	^4A	0.716627	-0.683949	-2471.453014	-0.182851	-2471.603187	$Ru_1^{1.08}$ $Ru_2^{1.00}$ $O_4^{0.18}$ $O_5^{0.73}$
BD_2^{5+}	^1A	0.715787	-1.060505	-2470.837986	-0.184920	-2471.367624	$Ru_1^{1.26}$ $Ru_2^{-1.32}$ $O_4^{-0.14}$ $O_5^{0.20}$
	^3A	0.714309	-1.060432	-2470.826814	-0.184011	-2471.356948	$Ru_1^{1.25}$ $Ru_2^{0.16}$ $O_4^{0.28}$ $O_5^{0.29}$
	^5A	0.715027	-1.061433	-2470.832154	-0.182570	-2471.361130	$Ru_1^{1.31}$ $Ru_2^{1.57}$ $O_4^{0.27}$ $O_5^{0.67}$
BD_2^{4+}	^1A	0.705646	-0.682731	-2470.802408	-0.178703	-2470.958196	$Ru_1^{1.08}$ $Ru_2^{-1.19}$ $O_3^{0.84}$ $O_5^{-0.73}$
	^3A	0.705601	-0.681120	-2470.793602	-0.177628	-2470.946749	$Ru_1^{0.13}$ $Ru_2^{1.18}$ $O_3^{-0.07}$ $O_5^{0.74}$
	^5A	0.705652	-0.682301	-2470.804997	-0.178619	-2470.960265	$Ru_1^{1.24}$ $Ru_2^{1.17}$ $O_3^{0.85}$ $O_5^{0.71}$

	^{2}A	0.703615	-1.054820	-2470.177719	-0.179311	-2470.708235	$Ru_1^{1.57}$ $Ru_2^{-1.28}$ $O_3^{0.95}$ $O_5^{-0.25}$
BD_3^{5+}	^{4}A	0.703868	-1.056249	-2470.172068	-0.179870	-2470.704319	$Ru_1^{1.51}$ $Ru_2^{0.13}$ $O_3^{0.97}$ $O_5^{0.31}$
	^{6}A	0.702582	-1.049313	-2470.166540	-0.175812	-2470.689083	$Ru_1^{1.20}$ $Ru_2^{1.20}$ $O_3^{0.89}$ $O_5^{0.74}$
	^{2}A	0.693517	-0.683527	-2470.138428	-0.174782	-2470.303220	$Ru_1^{-0.57}$ $Ru_2^{0.97}$ $O_4^{1.00}$ $O_5^{-0.42}$
BD_3^{4+}	^{4}A	0.693336	-0.681927	-2470.139896	-0.175115	-2470.303602	$Ru_1^{0.45}$ $Ru_2^{1.15}$ $O_3^{-0.10}$ $O_4^{1.00}$ $O_5^{0.48}$
	^{6}A	0.692512	-0.683426	-2470.141956	-0.176942	-2470.309812	$Ru_1^{1.50}$ $Ru_2^{1.31}$ $O_3^{0.44}$ $O_4^{1.02}$ $O_5^{0.69}$
	^{1}A	0.690500	-1.053728	-2469.510786	-0.176266	-2470.050280	$Ru_1^{-1.69}$ $Ru_2^{1.51}$ $O_3^{-0.51}$ $O_4^{1.08}$ $O_5^{-0.40}$
BD_4^{5+}	^{3}A	0.691749	-1.053257	-2469.503921	-0.171921	-2470.037350	$Ru_1^{0.65}$ $Ru_2^{0.56}$ $O_3^{-0.16}$ $O_4^{0.49}$ $O_5^{0.49}$
	^{5}A	0.690569	-1.057718	-2469.513073	-0.178781	-2470.059003	$Ru_1^{1.67}$ $Ru_2^{0.61}$ $O_3^{0.49}$ $O_4^{0.55}$ $O_5^{0.60}$
	^{1}A	0.657328	-0.688579	-2393.047078	-0.168743	-2393.247072	$Ru_1^{-0.64}$ $Ru_2^{0.65}$ $O_3^{-0.72}$ $O_4^{0.74}$
BD_4^{4+}	^{3}A	0.657310	-0.687365	-2393.046425	-0.168398	-2393.244878	$Ru_1^{0.45}$ $Ru_2^{0.47}$ $O_3^{0.81}$ $O_4^{0.81}$ $O_5^{-0.51}$
	^{5}A	0.657186	-0.686000	-2393.040592	-0.169369	-2393.238775	$Ru_1^{0.68}$ $Ru_2^{1.30}$ $O_3^{0.66}$ $O_4^{0.99}$ $O_5^{0.34}$
$BD_{TS4\text{-}5}^{4+}$	^{1}A	0.656520	-0.686214	-2393.032678	-0.172522	-2393.234894	$Ru_1^{-0.98}$ $Ru_2^{0.48}$ $O_3^{-0.56}$ $O_4^{0.59}$ $O_5^{0.46}$
	^{3}A	0.656817	-0.686299	-2393.038259	-0.172724	-2393.240465	$Ru_1^{0.03}$ $Ru_2^{1.40}$ $O_3^{-0.67}$ $O_4^{0.58}$ $O_5^{0.63}$
BD_5^{4+}	^{1}A	0.658554	-0.690019	-2393.057994	-0.174312	-2393.263771	$Ru_1^{1.05}$ $Ru_2^{-0.56}$ $O_3^{-0.44}$ $O_4^{-0.46}$ $O_5^{0.34}$

	^{3}A	0.658885	-0.688512	-2393.060824	-0.173369	-2393.263820	$Ru_1^{1.15}$ $Ru_2^{-0.45}$ $O_3^{0.41}$ $O_4^{0.43}$ $O_5^{0.45}$
	^{5}A	0.657915	-0.688797	-2393.051873	-0.173270	-2393.256025	$Ru_1^{1.14}$ $Ru_2^{1.13}$ $O_3^{0.46}$ $O_4^{0.46}$ $O_5^{0.67}$
	^{1}A	0.707045	-0.679683	-2545.910730	-0.183164	-2546.066532	$Ru_1^{0.69}$ $Ru_2^{-1.11}$ $O_4^{0.51}$ $O_5^{0.59}$ $O_6^{-0.69}$
$BD_{TS5\text{-}6}^{4+}$	^{3}A	0.707691	-0.678817	-2545.912580	-0.183369	-2546.067075	$Ru_1^{0.90}$ $Ru_2^{1.13}$ $O_4^{-0.44}$ $O_5^{-0.34}$ $O_6^{0.66}$
	^{5}A	0.707100	-0.679590	-2545.914686	-0.183412	-2546.070588	$Ru_1^{0.93}$ $Ru_2^{1.18}$ $O_4^{0.49}$ $O_5^{0.60}$ $O_6^{0.69}$
	^{1}A	0.707171	-0.684021	-2545.940280	-0.181282	-2546.098412	$Ru_1^{-0.31}$ $Ru_2^{-0.77}$ $O_3^{0.79}$ $O_5^{-0.73}$ $O_{86}^{1.00}$
BD_6^{4+}	^{3}A	0.708781	-0.684616	-2545.939670	-0.183008	-2546.098513	$Ru_1^{-0.56}$ $Ru_2^{1.08}$ $O_3^{0.31}$ $O_5^{0.65}$ $O_{86}^{0.51}$
	^{5}A	0.707359	-0.684369	-2545.939436	-0.181613	-2546.098059	$Ru_1^{0.64}$ $Ru_2^{0.82}$ $O_3^{0.78}$ $O_5^{0.75}$ $O_{86}^{0.99}$
	^{1}A	0.706228	-0.678261	-2545.904853	-0.179207	-2546.056093	$Ru_1^{-1.12}$ $Ru_2^{1.00}$ $O_3^{-0.21}$ $O_4^{0.89}$ $O_5^{-0.67}$ $O_{86}^{0.13}$
$BD^*_{TS4\text{-}5}^{4+}$	^{3}A	0.706103	-0.678764	-2545.904163	-0.180943	-2546.057767	$Ru_1^{-0.66}$ $Ru_2^{1.44}$ $O_3^{-0.25}$ $O_4^{0.84}$ $O_5^{0.54}$ $O_{86}^{0.07}$
	^{5}A	0.706329	-0.678967	-2545.908367	-0.180831	-2546.061836	$Ru_1^{1.04}$ $Ru_2^{1.33}$ $O_3^{0.20}$ $O_4^{0.88}$ $O_5^{0.62}$ $O_{86}^{-0.09}$
	^{1}A	0.708562	-0.679123	-2545.924416	-0.181298	-2546.076275	$Ru_1^{0.93}$ $Ru_2^{-1.14}$ $O_3^{0.29}$ $O_4^{-0.37}$ $O_5^{0.23}$ $O_{86}^{0.08}$
$BD^*_5^{4+}$	^{3}A	0.707750	-0.680626	-2545.928239	-0.179858	-2546.080973	$Ru_1^{0.33}$ $Ru_2^{1.22}$ $O_3^{-0.45}$ $O_4^{0.33}$ $O_5^{0.74}$ $O_{86}^{-0.20}$
	^{5}A	0.707412	-0.680303	-2545.927688	-0.179509	-2546.080088	$Ru_1^{0.98}$ $Ru_2^{1.26}$ $O_3^{0.45}$ $O_4^{0.34}$ $O_5^{0.78}$ $O_{86}^{0.20}$
$BD^*_{TS5\text{-}6}^{4+}$	^{1}A	0.707569	-0.684059	-2545.911775	-0.184628	-2546.072893	$Ru_1^{1.24}$ $Ru_2^{-1.05}$ $O_3^{0.23}$ $O_4^{-0.37}$ $O_5^{0.08}$ $O_{86}^{-0.13}$

	^{3}A	0.707315	-0.683730	-2545.906205	-0.183807	-2546.066427	$Ru_1^{1.15}$ $Ru_2^{-0.26}$ $O_3^{0.20}$ $O_4^{0.50}$ $O_5^{0.16}$ $O_{86}^{0.23}$
	^{1}A	0.690166	-1.061567	-2469.493228	-0.180342	-2470.044971	$Ru_1^{1.30}$ $Ru_2^{-0.99}$ $O_3^{0.27}$ $O_4^{-0.40}$ $O_5^{-0.26}$
$BD^{H+}{}_{TS4\text{-}5}{}^{5+}$	^{3}A	0.689873	-1.062861	-2469.497565	-0.180594	-2470.051147	$Ru_1^{1.51}$ $Ru_2^{-0.09}$ $O_3^{0.24}$ $O_4^{-0.50}$ $O_5^{0.74}$
	^{5}A	0.689906	-1.062427	-2469.500528	-0.180897	-2470.053946	$Ru_1^{1.50}$ $Ru_2^{1.31}$ $O_3^{0.18}$ $O_4^{0.15}$ $O_5^{0.68}$
	^{1}A	0.693469	-1.064453	-2469.517056	-0.181038	-2470.069078	$Ru_1^{1.17}$ $Ru_2^{-1.15}$ $O_4^{-0.26}$ $O_5^{0.26}$
$BD^{H+}{}_{5}{}^{5+}$	^{3}A	0.691983	-1.064797	-2469.513485	-0.179120	-2470.065419	$Ru_1^{-0.29}$ $Ru_2^{1.30}$ $O_3^{0.14}$ $O_4^{0.38}$ $O_5^{0.47}$
	^{5}A	0.691357	-1.060377	-2469.506915	-0.177509	-2470.053444	$Ru_1^{1.24}$ $Ru_2^{1.36}$ $O_3^{0.12}$ $O_4^{0.36}$ $O_5^{0.66}$
$BD^{H+}{}_{TS5\text{-}6}{}^{5+}$	^{1}A	0.717759	-1.049557	-2545.941470	-0.180316	-2546.453584	$Ru_1^{1.17}$ $Ru_2^{-0.98}$ $O_3^{-0.24}$ $O_4^{-0.43}$ $O_5^{0.53}$
	^{3}A	0.717524	-1.050486	-2545.938398	-0.181010	-2546.452370	$Ru_1^{-0.58}$ $Ru_2^{1.17}$ $O_3^{0.37}$ $O_4^{0.53}$ $O_5^{0.45}$
	^{1}A	0.719801	-1.059975	-2545.970583	-0.183605	-2546.494362	$Ru_1^{1.17}$ $Ru_2^{-1.02}$ $O_4^{-0.37}$ $O_5^{-0.14}$ $O_6^{0.37}$
$BD^{H+}{}_{6}{}^{5+}$	^{3}A	0.718468	-1.062707	-2545.962736	-0.180031	-2546.487006	$Ru_1^{1.22}$ $Ru_2^{0.48}$ $O_4^{-0.27}$ $O_5^{-0.18}$ $O_6^{0.70}$
	^{5}A	0.718434	-1.059555	-2545.957357	-0.183244	-2546.481722	$Ru_1^{1.26}$ $Ru_2^{1.28}$ $O_4^{0.43}$ $O_5^{0.17}$ $O_6^{0.72}$
	^{1}A	0.716884	-1.057186	-2545.930762	-0.185758	-2546.456822	$Ru_1^{1.36}$ $Ru_2^{-1.23}$ $O_3^{0.30}$ $O_4^{-0.13}$ $O_5^{-0.42}$ $O_{86}^{0.09}$
$BD^{H+}{*}_{TS4\text{-}6}{}^{5+}$	^{3}A	0.716473	-1.058696	-2545.931659	-0.184281	-2546.458163	$Ru_1^{1.63}$ $Ru_2^{-0.62}$ $O_3^{0.29}$ $O_4^{-0.21}$ $O_5^{0.83}$
	^{5}A	0.716145	-1.058964	-2545.932482	-0.184572	-2546.459873	$Ru_1^{1.61}$ $Ru_2^{1.04}$ $O_3^{0.27}$ $O_4^{0.21}$ $O_5^{0.81}$

H_2O	0.021131	0.000000	-76.417655	0.000000	-76.396524
O_2	0.003775	0.000000	-150.304632	0.000000	-150.300857

Table S2. The energies and spin populations for Llobet's ruthenium catalyst.

		ZPE	Solvation (P-O)	E cc-pVTZ(-f)	vdW	Sum	Spins
Ll_0^{3+}	^1A	0.743036	-0.397585	-2620.520765	-0.188295	-2620.363609	$Ru_1^{0.00}$ $Ru_7^{0.00}$
Ll_1^{4+}	^2A	0.743230	-0.677518	-2620.050302	-0.186425	-2620.171015	$Ru_1^{0.03}$ $Ru_7^{0.72}$
Ll_1^{3+}	^2A	0.731016	-0.390100	-2619.906568	-0.184094	-2619.749746	$Ru_1^{0.00}$ $Ru_7^{0.81}$ $O_4^{0.15}$
Ll_2^{4+}	^1A	0.731267	-0.667886	-2619.439325	-0.183265	-2619.559209	$Ru_1^{-0.87}$ $Ru_7^{0.83}$ $O_4^{0.14}$
	^3A	0.731235	-0.668008	-2619.439355	-0.183254	-2619.559382	$Ru_1^{0.87}$ $Ru_7^{0.83}$ $O_4^{0.13}$
Ll_2^{3+}	^1A	0.695169	-0.391619	-2542.827027	-0.176211	-2542.699688	$Ru_1^{-0.80}$ $Ru_7^{0.69}$ $O_3^{-0.18}$ $O_4^{0.31}$
	^3A	0.695246	-0.391595	-2542.827652	-0.175572	-2542.699573	$Ru_1^{0.79}$ $Ru_7^{0.69}$ $O_3^{0.19}$ $O_4^{0.32}$
Ll_3^{4+}	^2A	0.720442	-0.666757	-2618.792802	-0.180017	-2618.919134	$Ru_1^{-0.87}$ $Ru_7^{1.12}$ $O_4^{0.84}$
	^4A	0.720468	-0.667304	-2618.792743	-0.180167	-2618.919746	$Ru_1^{0.87}$ $Ru_7^{1.12}$ $O_4^{0.84}$
Ll_3^{3+}	^2A	0.684007	-0.390896	-2542.183944	-0.173480	-2542.064313	$Ru_1^{-0.71}$ $Ru_7^{1.05}$ $O_3^{-0.28}$ $O_4^{0.92}$
	^4A	0.684000	-0.391177	-2542.184098	-0.173698	-2542.064973	$Ru_1^{0.72}$ $Ru_7^{1.04}$ $O_3^{0.32}$ $O_4^{0.91}$

Ll_4^{4+}	^1A	0.707483	-0.669631	-2618.123931	-0.179931	-2618.266010	$Ru_1^{-1.38}$ $Ru_7^{1.09}$ $O_3^{-0.49}$ $O_4^{0.88}$
	^3A	0.707399	-0.668783	-2618.113923	-0.179472	-2618.254779	$Ru_1^{1.37}$ $Ru_7^{0.01}$ $O_3^{0.50}$
	^5A	0.707513	-0.670014	-2618.123380	-0.180149	-2618.266030	$Ru_1^{1.38}$ $Ru_7^{1.09}$ $O_3^{0.49}$ $O_4^{0.90}$
Ll_4^{3+}	^1A	0.672607	-0.388875	-2541.539804	-0.171940	-2541.428012	$Ru_1^{-0.98}$ $Ru_2^{0.98}$ $O_4^{-0.99}$ $O_5^{0.99}$
	^3A	0.672565	-0.389246	-2541.528994	-0.172069	-2541.417744	$Ru_1^{0.99}$ $Ru_2^{-0.05}$ $O_4^{0.99}$
	^5A	0.672432	-0.388683	-2541.539933	-0.171102	-2541.427286	$Ru_1^{0.98}$ $Ru_2^{0.98}$ $O_4^{1.00}$ $O_5^{1.00}$
$Ll_{TS4\text{-}5}^{3+}$	^1A	0.671688	-0.390847	-2541.518852	-0.174624	-2541.412635	$Ru_1^{-0.75}$ $Ru_7^{0.75}$ $O_3^{-0.60}$ $O_4^{0.60}$
Ll_5^{3+}	^1A	0.673491	-0.390425	-2541.536098	-0.174150	-2541.427182	$Ru_1^{0.61}$ $Ru_7^{-0.61}$ $O_3^{0.20}$ $O_4^{-0.20}$
	^3A	0.673382	-0.391162	-2541.534063	-0.174949	-2541.426792	$Ru_1^{0.64}$ $Ru_7^{0.64}$ $O_3^{0.33}$ $O_4^{0.33}$
$Ll_{TS5\text{-}6}^{3+}$	^1A	0.724186	-0.390531	-2694.377595	-0.194331	-2694.238271	$Ru_1^{-0.65}$ $Ru_2^{0.51}$ $O_5^{0.24}$
	^3A	0.723881	-0.391227	-2694.373985	-0.193806	-2694.235137	$Ru_1^{0.69}$ $Ru_2^{0.62}$ $O_4^{0.26}$ $O_5^{0.31}$ $O_{89}^{0.05}$
Ll_6^{3+}	^1A	0.725038	-0.387684	-2694.384712	-0.194930	-2694.242288	$Ru_1^{-0.52}$ $Ru_2^{0.46}$ $O_4^{-0.11}$ $O_5^{0.18}$
	^3A	0.724410	-0.388959	-2694.392068	-0.188128	-2694.244745	$Ru_1^{0.09}$ $Ru_2^{0.77}$ $O_4^{0.58}$ $O_5^{0.39}$
$Ll_{TS\text{-}O2\text{-}release}^{3+}$	^3A	0.720784	-0.386894	-2694.372316	-0.181659	-2694.220085	$Ru_1^{0.00}$ $Ru_2^{0.02}$ $O_4^{1.04}$ $O_5^{0.93}$
$Ll^*_{TS4\text{-}5}^{3+}$	^1A	0.717045	-0.390274	-2694.347760	-0.182699	-2694.203688	$Ru_1^{-0.02}$ $Ru_2^{0.19}$ $O_4^{-0.18}$

	^{3}A	0.718685	-0.389818	-2694.359808	-0.183440	-2694.214381	$Ru_1^{1.06}$ $Ru_2^{0.17}$ $O_4^{0.68}$ $O_5^{0.06}$
$Ll^*_5{}^{3+}$	^{1}A	0.724796	-0.388730	-2694.399474	-0.186843	-2694.250251	$Ru_1^{-0.79}$ $Ru_2^{0.49}$ $O_3^{-0.20}$ $O_4^{0.36}$ $O_5^{0.15}$
	^{3}A	0.725061	-0.389721	-2694.403522	-0.184812	-2694.252994	$Ru_1^{0.77}$ $Ru_2^{0.52}$ $O_3^{0.22}$ $O_4^{0.34}$ $O_5^{0.14}$
$Ll^*_{TS5\text{-}6}{}^{3+}$	^{1}A	0.718267	-0.393161	-2694.380457	-0.183840	-2694.239191	$Ru_1^{-0.74}$ $Ru_2^{0.18}$ $O_3^{0.26}$ $O_4^{0.40}$ $O_{89}^{-0.05}$
$Ll^{H+}_{TS4\text{-}5}{}^{4+}$	^{1}A	0.707832	-0.672489	-2618.109771	-0.182175	-2618.256603	$Ru_1^{-0.86}$ $Ru_2^{0.77}$ $O_3^{-0.14}$ $O_4^{0.35}$
	^{3}A	0.707866	-0.672711	-2618.110122	-0.182123	-2618.257090	$Ru_1^{0.81}$ $Ru_2^{0.80}$ $O_3^{-0.13}$ $O_4^{0.34}$
$Ll^{H+}_5{}^{4+}$	^{1}A	0.709827	-0.676527	-2618.115376	-0.182387	-2618.264463	$Ru_1^{-0.80}$ $Ru_2^{0.78}$ $O_4^{0.19}$
	^{3}A	0.709837	-0.676282	-2618.115505	-0.182471	-2618.264421	$Ru_1^{0.80}$ $Ru_2^{0.78}$ $O_4^{0.19}$
$Ll^{H+}_{TS5\text{-}6}{}^{4+}$	^{1}A	0.709254	-0.674416	-2618.084851	-0.183898	-2618.233911	$Ru_1^{-0.82}$ $Ru_2^{0.76}$ $O_5^{0.19}$
	^{3}A	0.708488	-0.675606	-2618.086001	-0.184491	-2618.237610	$Ru_1^{0.83}$ $Ru_2^{0.80}$ $O_5^{0.18}$
$Ll^{H+}_6{}^{4+}$	^{1}A	0.736433	-0.668175	-2694.564359	-0.186354	-2694.682455	$Ru_1^{-0.83}$ $Ru_2^{0.66}$ $O_3^{0.08}$ $O_4^{0.24}$
$Ll^{H+*}_{TS4\text{-}6}{}^{4+}$	^{1}A	0.732886	-0.666056	-2694.545526	-0.184487	-2694.663183	$Ru_1^{-0.85}$ $Ru_2^{0.82}$ $O_4^{-0.12}$ $O_5^{0.30}$ $O_{89}^{-0.15}$
	^{3}A	0.732916	-0.666070	-2694.545527	-0.184486	-2694.663167	$Ru_1^{0.85}$ $Ru_2^{0.82}$ $O_4^{0.12}$ $O_5^{0.30}$ $O_{89}^{-0.15}$