Electronic Supplementary Information

Selective conversion of methane to methanol facilitated by metal-methoxy molecular complexes via a self-correcting chemical cycle

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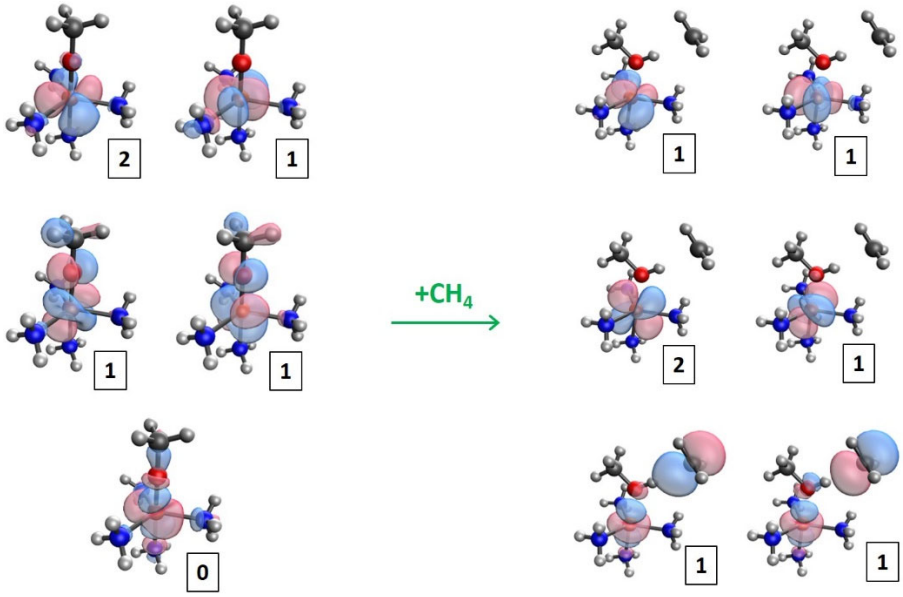

Figure S1. Molecular orbitals before and after the PCET process occurring during the $(NH_3)_4FeOCH_3^{2+}$ (S=3/2) + CH_4 reaction. The numbers in the boxes indicate the occupancy of each orbital. An electron pair of oxygen captures a H^+ from methane, and the two electrons of the cleaved CH bond populate the two bottom right orbitals. These orbitals are a linear combination of the $3d_{z^2}$ orbital of iron and the orbital of the methyl radical.

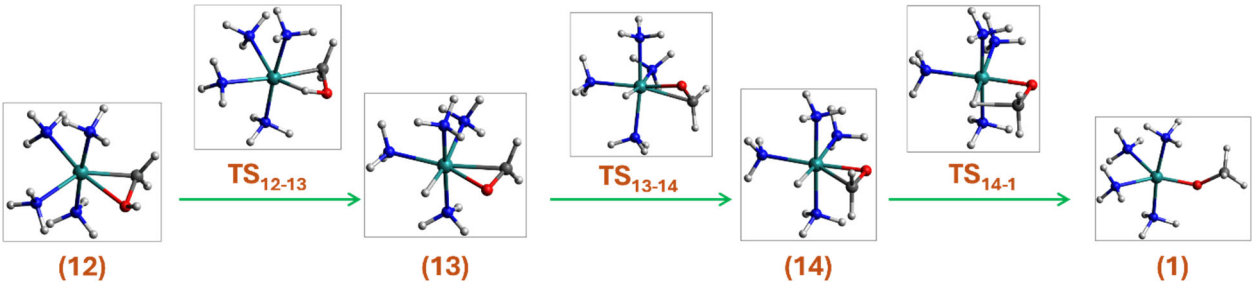

Figure S2. Isomerization mechanism from $(NH_3)_4RuCH_2OH^{2+}$ $(NH_3)_4RuOCH_3^{2+}$ (S=1/2): The hydrogen atom of the OH group migrates first to Ru ($TS_{12\text{-}13}$, rate determining step; see Figure S3), the CH_2O group rotates to bring the hydrogen close to carbon ($TS_{13\text{-}14}$), and finally the hydrogen is transferred to carbon ($TS_{14\text{-}1}$) to form (1).

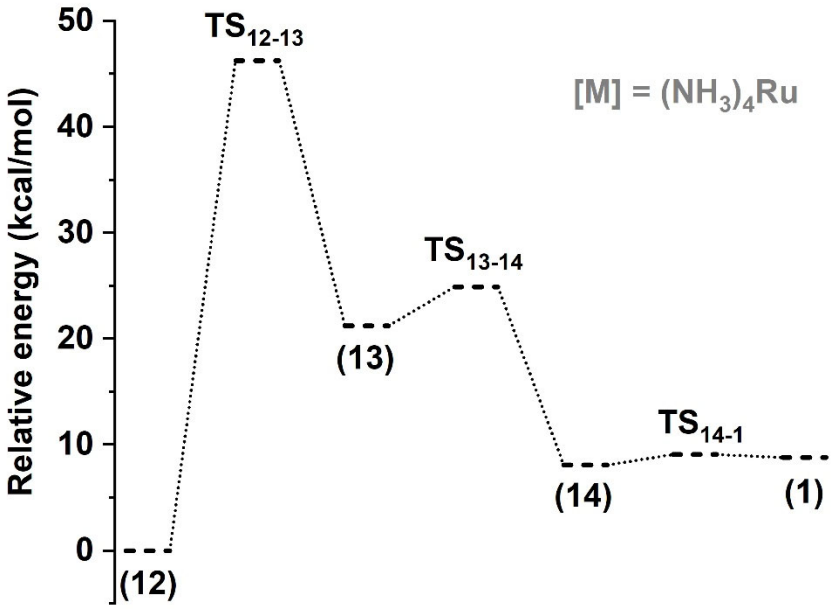

Figure S3. MN15 electronic energy diagram for the isomerization mechanism from $(NH_3)_4RuCH_2OH^{2+}$ to $(NH_3)_4RuOCH_3^{2+}$ (S=1/2); see Figure S2 for structures and more details of the mechanism.

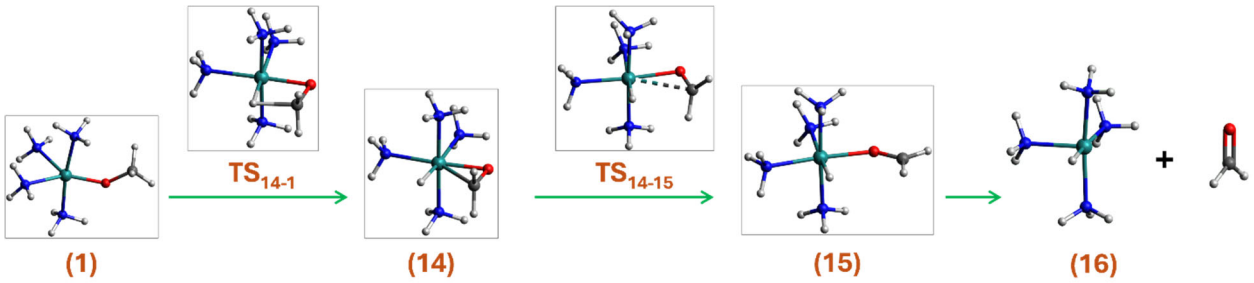

Figure S4. Mechanism for the β-hydrogen elimination from $(NH_3)_4RuOCH_3^{2+}$ (S=1/2): The hydrogen atom of the methyl group migrates first to Ru ($TS_{14\text{-}1}$) and the formed CH_2O group gradually detaches (via $TS_{14\text{-}15}$). Structures (1) and (14) are in a fast equilibrium, while the detachment of formaldehyde is not a favorable process; see Figure S5 for the energy diagram.

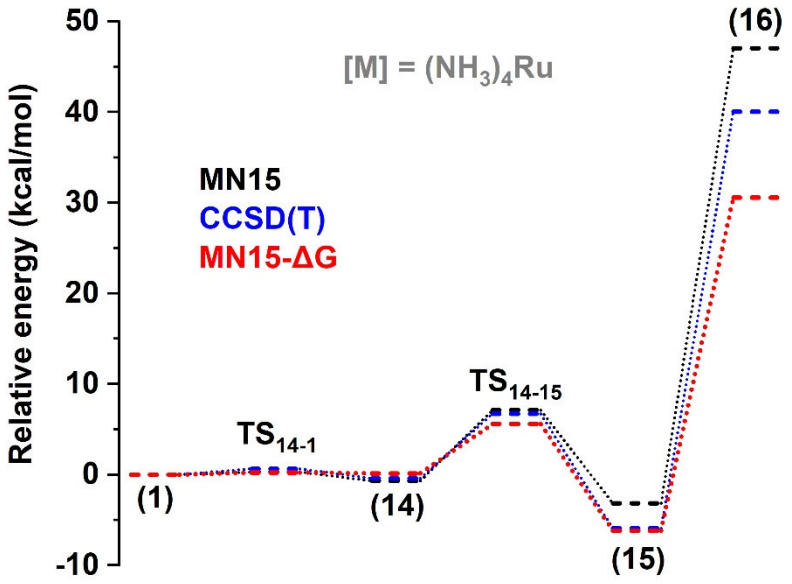

Figure S5. MN15 Electronic energy diagram for the β-hydrogen elimination from $(NH_3)_4RuOCH_3^{2+}$ (S=1/2); see Figure S4 for structures and more details of the mechanism. The CCSD(T) energies are obtained with the MN15 optimized structures.

Table S1. Energy values (kcal/mol) for the diagrams of Figures 3, 5, 6, 7, 8, S3 and S5.

Species	PCET			2+2		
	S = 1/2	**S = 3/2**	**S = 5/2**	**S = 1/2**	**S = 3/2**	**S = 5/2**
	Figure 3					
(1)+CH_4	11.72	1.52	0.00	11.72	1.52	
(2)	6.13	-6.08	-6.68	3.93	-5.90	
TS_{2-3}/TS_{2-6}	31.89	19.89	21.94	26.68	31.08	
(3)/(6)	15.82	4.55	4.67	-3.77	-9.90	
[M]CH_3+CH_3OH				34.63	16.06	
	Figure 5					
(1)+CH_3OH	11.72	1.52	0.00	11.72	1.52	
(7)/(10)	-21.63	-26.83	-29.06	-11.12	-21.54	
TS_{7-8}/TS_{10-11}	12.79	3.78	5.15	17.43	24.38	
(8)/(11)	-5.13	-16.94	-15.64	-16.90	-22.29	
TS_{8-9}	33.10	21.97	24.05			
(9)	-22.69	-26.55	-28.80			
(1)+CH_3OH	11.72	1.52	0.00			
	Figure 6					
(1)+CH_4	0.00	12.76	54.84	0.00	12.76	
(2)	-14.92	9.10	48.73	-14.92	6.29	
TS_{2-3}/TS_{2-6}	30.21	43.45	80.21	8.83	54.63	
(3)/(6)	17.84	30.19	63.08	-20.67	19.16	
[M]CH_3+CH_3OH				8.32	35.89	
	Figure 7					
(1)+CH_3OH	0.00	12.76		0.00		
(7)/(10)	-43.72	-6.79		-27.89		
TS_{7-8}/TS_{10-11}	-3.45	25.48		0.58		
(8)/(11)	-17.83	10.31		-34.24		
TS_{8-9}	20.30	43.11		12.01		
(9)	-43.62	10.97		-25.45		
(1)+CH_3OH	0.00	12.76		0.00		
	Figure 8					
	[M] = $(NH_3)_4Fe$			[M] = $(NH_3)_4Ru$		
	S = 1/2 (O_3)	**S = 3/2** (O_3)	**S = 5/2** (O_3)	**S = 1/2** (O_3)	**S = 3/2** (O_3)	**S = 1/2** (N_2O)
[M]CH_3+O_3	18.56	0.00	18.18	0.00	27.57	0.00
(4)	17.29	-12.48	-5.63	-34.67	-22.80	-8.41
TS_{4-5}	-7.76	-10.25	-5.51	-34.52	-22.68	15.71
(5)	-8.34	-19.51	-26.83	-62.96	-62.90	-37.12
[M](O)CH_3+O_2	-22.67	-22.67	-22.67	-58.06	-58.06	-31.47
TS_{5-1}+O_2	-19.32	-19.32	-19.32	-39.17	-39.17	-12.57
(1)+O_2	-89.49	-89.49	-89.49	-83.27	-83.27	-56.68
	Figure S3					
(12)	0.00					

TS_{12-13}	46.25					
(13)	21.24					
TS_{13-14}	24.89					
(14)	8.09					
TS_{14-1}	9.07					
(1)	8.78					
	Figure S5					
	MN15	CCSD(T)	MN15 (ΔG)			
(1)	0.00	0.00	0.00			
TS_{14-1}	0.29	0.64	0.23			
(14)	-0.69	-0.43	0.13			
TS_{14-15}	7.11	6.70	5.59			
(15)	-3.16	-5.92	-6.19			
(16)	47.02	40.03	30.56			

Table S2. MN15 Cartesian coordinates (in Å) and equilibrium energies (E/a.u.) of the optimized geometries for all iron structures shown in Figure 2 for three different multiplicities.

S=1/2				S=3/2				S=5/2			
Structure (1)											
E = −1604.49193963				E = −1604.50817972				E = −1604.51060978			
Fe	0.187139	0.009471	-0.090302	Fe	0.256890	0.037359	-0.053652	Fe	0.205509	-0.000705	0.001823
O	-1.381401	0.708816	-0.087077	O	-1.311595	0.793963	-0.171501	O	-1.543774	0.002763	-0.018966
C	-2.724695	0.270842	-0.154783	C	-2.535863	0.106643	-0.010200	C	-2.952118	0.005556	-0.035702
H	-3.349327	1.139459	-0.356585	H	-3.268686	0.814082	0.377196	H	-3.308543	0.195540	-1.048355
H	-3.031533	-0.146795	0.807462	H	-2.455577	-0.726321	0.697769	H	-3.326552	0.785097	0.628109
H	-2.875637	-0.460630	-0.950182	H	-2.902537	-0.266588	-0.968884	H	-3.326005	-0.961829	0.300262
N	0.855340	1.924176	-0.297389	N	0.928437	1.914925	-0.508139	N	0.376209	0.380499	-2.105574
H	0.827988	2.217223	-1.275462	H	1.468782	2.014424	-1.368910	H	0.961069	-0.269188	-2.632063
H	1.770016	2.195458	0.062886	H	1.467447	2.386359	0.219795	H	0.720372	1.313256	-2.337959
H	0.159441	2.505024	0.174446	H	0.063679	2.447858	-0.631996	H	-0.556469	0.318598	-2.514799
N	1.914637	-0.697653	-1.014121	N	2.187648	-0.677701	-0.028648	N	2.439021	-0.009592	0.041784
H	2.674770	-0.017307	-1.035039	H	2.808930	-0.127542	0.567029	H	2.853081	0.862902	-0.288982
H	1.739148	-0.928191	-1.995196	H	2.627064	-0.665905	-0.951699	H	2.855010	-0.740419	-0.536916
H	2.314397	-1.542290	-0.603429	H	2.265678	-1.640323	0.302856	H	2.823811	-0.153974	0.976407
N	-0.614707	-1.848359	-0.120159	N	-0.378268	-1.558794	-1.216270	N	0.277749	-2.020889	0.726220
H	-1.031610	-2.052677	-1.031485	H	-0.893847	-1.189567	-2.018531	H	-0.121486	-2.651319	0.028748
H	-1.386783	-1.904283	0.546680	H	-1.051227	-2.136744	-0.709158	H	-0.336941	-2.103000	1.537445
H	0.005540	-2.631508	0.088260	H	0.320891	-2.199502	-1.592449	H	1.171235	-2.427710	1.000592
N	0.930189	-0.153951	1.841431	N	-0.032275	-0.421854	2.002970	N	0.278112	1.643864	1.380479
H	1.884226	0.178404	1.983330	H	0.775783	-0.328946	2.619565	H	1.177735	2.046866	1.640154
H	0.895596	-1.089100	2.247547	H	-0.396670	-1.360672	2.171738	H	-0.179117	1.379542	2.254673
H	0.339316	0.425907	2.441607	H	-0.739709	0.220467	2.364446	H	-0.285172	2.411359	1.010863
Structure (2)											
E = −1644.9728937				E = −1644.98856556				E = −1644.98980371			
Fe	-0.304429	-0.049525	0.007328	Fe	0.076470	-0.275724	0.003428	H	-2.065994	1.664019	0.025144
H	2.803886	2.771623	0.444624	H	-3.448008	2.215291	0.234196	Fe	-0.014839	-0.366722	0.006330
O	0.854680	-1.118293	0.709836	O	1.013075	0.967419	0.807877	O	1.507455	0.493814	-0.004690
C	1.875854	2.288794	0.150115	C	-2.803005	1.353823	0.083637	C	-1.563534	2.634037	-0.037479
C	1.979077	-1.829985	0.237065	C	1.990981	1.789443	0.204837	C	2.732750	1.186448	-0.013450
H	1.068334	2.718815	0.743281	H	-3.253830	0.502388	0.593194	H	-1.921654	3.163057	-0.917216
H	1.981948	1.219208	0.351154	H	-1.823495	1.593603	0.508017	H	-0.479529	2.519551	-0.098890
H	1.715645	2.482600	-0.911001	H	-2.741191	1.162134	-0.988052	H	-1.816203	3.217535	0.844133
H	2.677306	-1.173881	-0.289196	H	1.538989	2.639032	-0.312279	H	2.818608	1.774041	-0.927790
H	1.674992	-2.653851	-0.414650	H	2.625553	1.229844	-0.491727	H	3.558058	0.475788	0.034084
H	2.489528	-2.259434	1.097616	H	2.625334	2.183369	0.998027	H	2.785822	1.856002	0.845435
N	-1.919191	-1.307297	-0.337851	N	1.786286	-1.576332	-0.240642	N	-0.476489	0.307993	2.003395
H	-2.823574	-0.978977	0.000280	H	1.634718	-2.578763	-0.126425	H	-1.440750	0.255535	2.329766
H	-1.720533	-2.170282	0.172469	H	2.469362	-1.309588	0.470181	H	-0.216675	1.294626	2.044112
H	-2.063962	-1.586212	-1.308112	H	2.267894	-1.477424	-1.135064	H	0.093523	-0.155120	2.712398
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H	-0.536227	-0.448056	2.469316	H	-0.203507	0.142296	2.431072	H	-0.863910	1.100918	-2.068073
N	0.508826	-0.286071	-1.832471	N	0.034475	0.803798	-1.735247	N	0.883160	-2.310027	0.062357
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H	1.384773	0.239755	-1.886146	H	-0.277074	1.750932	-1.507152	H	0.282794	-3.124274	0.187863
N	-1.305479	1.647126	-0.643309	N	-1.263490	-1.634582	-0.761723	N	-2.043739	-1.305777	0.012430
H	-0.631989	2.368414	-0.912184	H	-2.189775	-1.209096	-0.852911	H	-2.192448	-1.963232	-0.753566
H	-1.893900	2.080735	0.068266	H	-1.396432	-2.456344	-0.171071	H	-2.796380	-0.620480	-0.069920

H -1.909880 1.507741 -1.453781	H -1.022113 -1.992009 -1.686758	H -2.244869 -1.831816 0.863459
Structure (3)		
E = −1644.98516138	E = −1644.99494275	Not available
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H -0.271057 0.069589 -2.554270	H 0.063642 -0.062180 -2.511594	
O 1.557436 0.423993 -0.670059	O -1.800894 -0.505625 -0.491908	
C -0.850645 -0.506456 -1.830962	C 0.934836 0.200351 -1.910198	
C 2.828878 0.012292 -0.113428	C -2.985003 0.118716 0.049629	
H -1.906101 -0.280082 -1.976960	H 1.757736 -0.483423 -2.105407	
H 1.650862 0.605906 -1.615580	H -2.047865 -1.026617 -1.267078	
H -0.688549 -1.569210 -2.009444	H 1.231733 1.227681 -2.106203	
H 3.195049 -0.878971 -0.618647	H -3.404647 0.829304 -0.659587	
H 2.664847 -0.199094 0.939577	H -2.687810 0.642794 0.955650	
H 3.550240 0.818303 -0.213531	H -3.728769 -0.632589 0.302123	
N 0.266399 0.693520 1.970586	N -0.209892 -0.285613 2.036845	
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H 0.997932 1.400632 1.893270	H -1.069502 -0.833086 2.088938	
H 0.628953 -0.006045 2.617509	H -0.386344 0.560299 2.577549	
N -0.850328 1.888859 -0.498830	N 0.677519 -2.050464 -0.293708	
H -1.335611 2.408283 0.233233	H 1.653849 -2.314592 -0.159432	
H -1.457360 1.915988 -1.318321	H 0.450120 -2.347222 -1.242941	
H -0.030603 2.449294 -0.734153	H 0.130218 -2.640946 0.332020	
N 0.333073 -1.938327 0.355290	N -0.290900 1.979303 -0.151938	
H -0.407692 -2.635125 0.276994	H 0.480057 2.630571 -0.300288	
H 0.782702 -2.103860 1.255483	H -0.821818 2.339587 0.640177	
H 1.018758 -2.198864 -0.354873	H -0.891847 2.075594 -0.971357	
N -2.184129 -0.508665 0.593530	N 2.413070 0.532209 0.642867	
H -2.507061 -1.334325 0.088365	H 2.948956 0.924255 -0.131552	
H -2.875245 0.211324 0.381310	H 2.974962 -0.244566 0.990770	
H -2.286651 -0.720954 1.586191	H 2.441198 1.232891 1.383395	
Structure (4)		
Not available	E = −1754.61423504	E = −1754.60331735
	Fe 0.626208 -0.038520 -0.034402	Fe 0.427486 -0.023442 0.034583
	O -1.641194 0.864168 0.385009	O -1.080996 0.679554 0.704064
	O -2.991784 -0.727316 -0.039002	O -2.927699 -0.345525 -0.042486
	O -2.757114 0.486491 -0.096820	O -2.480903 0.772658 0.248001
	C -0.158428 -0.704159 -1.720663	C -0.452949 0.339378 -1.911078
	H -0.768684 0.074838 -2.173902	H -0.903894 1.313547 -1.776923
	H -0.736661 -1.613635 -1.584624	H -1.153863 -0.486296 -1.955077
	H 0.716705 -0.897167 -2.344565	H 0.394031 0.287870 -2.582361
	N 2.722347 -0.673773 -0.234749	N 2.125894 -0.883204 -1.020681
	H 2.794231 -1.507825 -0.819506	H 1.860759 -1.536423 -1.758757
	H 3.183326 -0.918299 0.642096	H 2.726872 -1.414981 -0.389019
	H 3.333678 0.012550 -0.678008	H 2.733299 -0.195096 -1.467080
	N 0.011797 -1.787548 0.833934	N -0.358596 -2.074420 0.111637
	H -1.009221 -1.780244 0.895719	H -1.329924 -1.969337 0.415028
	H 0.363594 -1.966656 1.774540	H 0.085963 -2.709268 0.775266
	H 0.246211 -2.608527 0.274727	H -0.396873 -2.585321 -0.770695
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	H -0.049844 2.253283 -1.023938	H 0.652819 2.615889 0.209354
	H 1.098228 1.630975 -1.995693	H 1.465229 2.289534 -1.163871
	H 1.524402 2.391557 -0.608946	H 2.213403 2.136692 0.273422
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Structure (5)									
Not available	E = −1754.62543825						E = −1754.63711083		
	Fe	-0.532703	-0.012004	0.045124			Fe	-0.652174	-0.002685	-0.068923
	O	0.768243	-0.068400	1.003766			O	0.282647	-0.136174	-1.360952
	O	3.905335	0.031201	0.458834			O	3.253461	0.041487	0.014233
	O	2.956746	-0.008962	-0.257738			O	4.394188	-0.128026	-0.298629
	C	0.243460	-1.206197	-1.363972			C	0.528734	1.532451	0.840212
	H	1.064156	-1.733287	-0.891211			H	1.197176	1.816982	0.038798
	H	0.585073	-0.582798	-2.184586			H	1.008460	1.025064	1.668150
	H	-0.552704	-1.878563	-1.669394			H	-0.204472	2.273483	1.133290
	N	-2.215094	0.112755	-1.226073			N	-1.880922	0.117160	1.651644
	H	-1.966861	-0.023069	-2.207420			H	-1.424542	0.552216	2.454762
	H	-2.695556	1.011871	-1.176545			H	-2.183781	-0.804342	1.969666
	H	-2.932359	-0.587414	-1.032203			H	-2.743761	0.644001	1.511416
	N	0.241079	1.585442	-0.896542			N	0.539230	-1.370727	0.862471
	H	1.244149	1.411620	-0.998710			H	1.511379	-1.122490	0.654193
	H	0.161487	2.440049	-0.344334			H	0.400886	-2.292109	0.443372
	H	-0.121673	1.788286	-1.828075			H	0.458569	-1.480814	1.873239
	N	-1.192753	-1.731818	0.893754			N	-1.603630	1.563851	-0.984759
	H	-0.351877	-2.271724	1.108529			H	-0.891056	2.140973	-1.435966
	H	-1.780871	-2.332945	0.316121			H	-2.179962	2.186359	-0.418358
	H	-1.677870	-1.602369	1.782222			H	-2.189941	1.216904	-1.746103
	N	-1.691386	1.185472	1.426482			N	-2.109595	-1.485435	-0.840685
	H	-1.144462	1.274058	2.284635			H	-1.817532	-1.693454	-1.796897
	H	-2.594254	0.801101	1.704740			H	-3.085841	-1.194664	-0.896852
	H	-1.882365	2.140810	1.124591			H	-2.129405	-2.385250	-0.359906
Structure (6)									
E = −1644.95395593				E = −1644.97190833			E = −1644.9717126		
Fe	0.644597	-0.109431	0.015708	Fe	0.702282	0.078165	0.000700	H	3.746398	1.723059	0.959757
H	-3.692582	-1.600816	1.014052	H	-3.774602	1.729143	-0.919571	Fe	-0.696604	0.081588	0.001138
O	-1.202922	0.593962	-0.178779	O	-1.337440	-0.557549	-0.000638	O	1.329983	-0.600640	-0.001705
C	-3.774250	-1.069030	0.079432	C	-3.866999	1.185513	0.007003	C	3.835315	1.217665	0.011459
C	-1.577761	1.980001	-0.064316	C	-1.806641	-1.919908	-0.005743	C	1.781057	-1.968878	-0.008621
H	-3.718289	-1.615653	-0.848576	H	-3.774884	1.712709	0.943046	H	3.739227	1.782450	-0.901984
H	-1.991981	0.017326	-0.074420	H	-2.107250	0.053597	0.002578	H	2.103757	0.003175	0.002380
H	-4.243374	-0.096814	0.079529	H	-4.370945	0.231136	-0.001667	H	4.341200	0.264714	-0.021387
H	-2.438489	2.181842	-0.696794	H	-2.403260	-2.122627	0.881265	H	2.367382	-2.174134	-0.901849
H	-0.736103	2.576871	-0.409973	H	-0.929646	-2.565091	-0.004687	H	0.895421	-2.602014	-0.005685
H	-1.812262	2.234267	0.968044	H	-2.397959	-2.117876	-0.897381	H	2.376837	-2.179906	0.876936
N	0.858572	0.984217	1.806866	N	0.935781	-0.939168	-1.883957	N	-0.947278	-0.927983	1.888635
H	1.648020	0.752041	2.408215	H	1.456172	-0.428740	-2.597468	H	-1.449136	-0.402990	2.604868
H	0.026399	0.874609	2.386668	H	0.021088	-1.134246	-2.291277	H	-0.035472	-1.146871	2.290271
H	0.933912	1.987040	1.633011	H	1.402946	-1.842450	-1.803072	H	-1.438874	-1.818583	1.812007
N	-0.207188	-2.040182	-0.069111	N	-0.133563	2.074073	-0.009675	N	0.189051	2.054783	-0.020356
H	0.424960	-2.833631	0.028813	H	0.533183	2.844726	-0.018913	H	-0.455970	2.843714	-0.032565
H	-0.691696	-2.180220	-0.956631	H	-0.730368	2.233464	0.802687	H	0.797864	2.180459	-0.829858
H	-0.922002	-2.167696	0.648611	H	-0.738994	2.221253	-0.817941	H	0.791992	2.201057	0.790109
N	1.114069	0.828840	-1.825683	N	0.932456	-0.938787	1.886127	N	-0.956101	-0.935330	-1.880985
H	1.630213	1.703951	-1.733589	H	1.406084	-1.838971	1.808408	H	-1.438440	-1.830185	-1.795506
H	0.251017	1.064271	-2.315553	H	0.016661	-1.139596	2.288141	H	-0.046723	-1.147555	-2.291624
H	1.659005	0.265450	-2.477803	H	1.445208	-0.424562	2.602456	H	-1.470608	-0.418097	-2.593857
N	2.516779	-0.850274	0.179462	N	2.813538	0.765253	0.005328	N	-2.790995	0.814955	0.009066
H	2.779350	-1.463097	-0.593188	H	3.043501	1.343828	0.813184	H	-3.014873	1.390359	-0.802756
H	2.658743	-1.404291	1.024954	H	3.048378	1.338465	-0.804950	H	-3.005718	1.401503	0.815355
H	3.235452	-0.125969	0.205022	H	3.499242	0.010720	0.009738	H	-3.493389	0.075968	0.017892
Structure (7)									

E = −1720.18348454				E = −1720.1917661				E = −1720.19531651			
H	2.401633	-0.660216	-0.875539	H	-2.580790	-0.012103	0.925832	H	-2.740225	-0.551400	-0.016257
Fe	-0.393036	-0.025458	0.012793	Fe	0.385910	-0.116003	-0.018179	Fe	0.342348	0.046172	-0.001386
O	0.649546	1.149997	-0.812289	O	-0.414276	1.241298	0.778860	O	-0.942257	1.241499	-0.012557
C	2.429781	-1.279442	0.015561	C	-2.822529	-0.702720	0.123678	C	-2.445026	-1.594169	-0.000460
C	1.656679	1.917655	-0.195809	C	-1.070479	2.327690	0.164958	C	-2.007713	2.158735	-0.001448
O	1.176522	-1.055778	0.719096	O	-1.574746	-1.016861	-0.550969	O	-0.990928	-1.623247	0.008275
H	3.260819	-0.972427	0.644210	H	-3.514222	-0.231366	-0.569875	H	-2.816746	-2.099902	-0.887320
H	2.523187	-2.331391	-0.243501	H	-3.263628	-1.610135	0.528678	H	-2.827091	-2.076002	0.895261
H	2.412579	2.162992	-0.941711	H	-1.631245	2.853655	0.937285	H	-1.625189	3.179613	0.017173
H	2.147646	1.383231	0.624949	H	-1.780935	1.996920	-0.600255	H	-2.628421	2.000461	0.881796
H	1.261354	2.864323	0.185574	H	-0.367952	3.043086	-0.272657	H	-2.620427	2.030626	-0.895009
N	-1.634274	-1.485842	0.840350	N	1.223235	-1.856727	-0.769034	N	1.913361	-1.588635	0.017783
H	-1.657061	-1.514755	1.859727	H	1.144048	-1.984982	-1.777583	H	1.875209	-2.207225	-0.791908
H	-1.321421	-2.413054	0.550971	H	0.795755	-2.682402	-0.348700	H	1.866890	-2.197943	0.834039
H	-2.609882	-1.423955	0.549716	H	2.219479	-1.917736	-0.557886	H	2.858118	-1.205952	0.020490
H	1.203438	-1.472480	1.589331	H	-1.750815	-1.677051	-1.233564	H	-0.696139	-2.542516	0.018360
N	-0.420983	1.088573	1.689997	N	0.395861	0.813441	-1.838824	N	0.447287	-0.060655	-2.200612
H	-0.424981	2.078343	1.438676	H	0.630524	1.801509	-1.737508	H	0.207800	0.855650	-2.578093
H	0.443327	0.951224	2.215244	H	-0.554692	0.790658	-2.211629	H	-0.282463	-0.692561	-2.529146
H	-1.189929	0.953629	2.346416	H	1.009506	0.438586	-2.561470	H	1.306179	-0.349884	-2.665518
N	-0.289229	-1.072712	-1.712269	N	0.240944	-0.943494	1.854789	N	0.439878	-0.028421	2.200233
H	0.126031	-0.406506	-2.367489	H	0.158952	-0.133458	2.472362	H	0.188735	0.890197	2.564299
H	-1.146310	-1.429023	-2.133555	H	0.967361	-1.557029	2.221338	H	1.301658	-0.300228	2.670330
H	0.352409	-1.864339	-1.661144	H	-0.642486	-1.449301	1.934772	H	-0.282413	-0.664455	2.537180
N	-1.950007	0.978897	-0.749439	N	2.439318	0.712627	0.467530	N	1.980434	1.525720	-0.010903
H	-1.504897	1.679087	-1.347349	H	2.227464	1.596793	0.930863	H	1.540165	2.445518	-0.028670
H	-2.533866	1.485152	-0.083748	H	3.073271	0.939537	-0.297840	H	2.601189	1.495447	-0.818695
H	-2.590997	0.446624	-1.336834	H	3.001455	0.184635	1.134310	H	2.587309	1.520596	0.807925
Structure (8)											
E = −1720.15719017				E = −1720.17601048				E = −1720.17393956			
H	-1.150943	1.775318	0.405546	H	-2.084777	-0.834550	0.436372	H	-2.193002	-0.098668	0.481220
Fe	0.328474	-0.381533	-0.005868	Fe	0.391840	0.216121	-0.006070	Fe	0.459820	0.107063	-0.009053
O	-0.190018	1.617532	0.407043	O	-1.757306	0.029555	0.142635	O	-1.614343	0.640701	0.235345
C	-2.923634	0.510419	-0.079563	C	-0.752576	-2.817072	0.041198	C	-1.730877	-2.387323	0.030578
C	0.524314	2.813756	0.041042	C	-2.861994	0.936454	-0.065865	C	-2.401977	1.830862	0.012423
O	-2.115827	-0.497403	0.388745	O	0.275605	-2.004512	0.467889	O	-0.473101	-2.028660	0.464461
H	-2.796226	0.747933	-1.122294	H	-1.142983	-2.578676	-0.932399	H	-2.000771	-2.003780	-0.937974
H	-3.843539	0.714564	0.441373	H	-0.861423	-3.784498	0.498553	H	-2.183336	-3.268642	0.450256
H	0.012701	3.685603	0.438152	H	-2.513016	1.735035	-0.714437	H	-1.719366	2.625456	-0.272907
H	0.605816	2.902917	-1.042800	H	-3.200600	1.347776	0.882060	H	-2.921590	2.113897	0.923958
H	1.514912	2.761591	0.483694	H	-3.682054	0.420632	-0.557724	H	-3.118752	1.666715	-0.788307
N	0.185831	-2.459510	-0.249658	N	2.601647	0.099236	-0.170119	N	2.453428	-0.851679	-0.172725
H	-0.795333	-2.707944	-0.380465	H	2.923125	-0.851957	-0.346879	H	2.366198	-1.866670	-0.212235
H	0.515994	-3.024151	0.531640	H	3.094419	0.406870	0.667009	H	3.101666	-0.659304	0.589874
H	0.671854	-2.820029	-1.070217	H	2.984705	0.661197	-0.929425	H	2.950567	-0.588133	-1.022348
H	-2.492013	-0.867524	1.199278	H	0.749722	-2.419661	1.201414	H	-0.207136	-2.588084	1.206772
N	-0.167487	-0.131323	-1.962299	N	0.247147	-0.388465	-2.131534	N	0.036341	-0.450569	-2.112319
H	-0.319797	0.852364	-2.186404	H	-0.734500	-0.406450	-2.405346	H	-0.880652	-0.130875	-2.422311
H	-1.035136	-0.610178	-2.206277	H	0.604662	-1.328756	-2.298475	H	0.036614	-1.463097	-2.232846
H	0.527002	-0.462617	-2.631588	H	0.714903	0.208239	-2.812394	H	0.699409	-0.089934	-2.796720
N	0.705817	-0.561617	1.979170	N	0.420006	0.558774	2.196013	N	0.723165	0.403490	2.164081
H	0.629660	0.365673	2.398765	H	-0.422308	0.163592	2.612387	H	-0.172258	0.736209	2.519958
H	1.634178	-0.910121	2.216214	H	0.420202	1.542077	2.463063	H	1.409811	1.108254	2.429762
H	0.055802	-1.152954	2.495875	H	1.201030	0.143472	2.701315	H	0.952797	-0.419746	2.718552
N	2.433687	0.155735	-0.409463	N	0.252650	2.396633	-0.411038	N	1.060644	2.175139	-0.511690
H	2.548155	0.831887	-1.163629	H	-0.453536	2.842023	0.174339	H	0.783161	2.863997	0.186189

H	2.993757	-0.651418	-0.683215	H	-0.009956	2.625948	-1.368587	H	0.655541	2.498058	-1.389730
H	2.920583	0.559871	0.389480	H	1.115426	2.908662	-0.232477	H	2.067417	2.288492	-0.623672
Structure (9)												
E = −1720.18516172				E = −1720.1913156				E = −1720.19490029				
Fe	-0.335401	-0.132997	-0.024932	Fe	0.230650	0.251105	-0.001516	Fe	-0.152183	0.243162	-0.008414
C	0.612042	2.533849	0.174316	C	1.252941	-2.414515	0.186002	C	-2.471714	-1.907352	0.003456
O	-0.362578	1.571096	0.502406	O	0.900355	-1.186276	0.782277	O	-1.446342	-0.944704	-0.024210
H	0.361284	3.061886	-0.750970	H	2.123496	-2.317847	-0.471109	H	-3.414811	-1.459093	-0.309490
H	1.616420	2.103889	0.060950	H	0.422431	-2.858178	-0.372738	H	-2.586860	-2.303046	1.013294
H	0.654076	3.276955	0.970130	H	1.522961	-3.103639	0.985468	H	-2.230392	-2.728944	-0.671867
N	-0.379109	-2.152465	-0.524751	N	-0.741102	1.946675	-0.676956	N	1.601657	1.651801	0.137859
H	0.069253	-2.403172	-1.405674	H	-1.217821	1.840025	-1.572193	H	2.279450	1.326618	0.827204
H	-1.313003	-2.559549	-0.567630	H	-0.107170	2.738358	-0.788291	H	1.328226	2.585860	0.441084
H	0.119766	-2.678853	0.194377	H	-1.457324	2.248604	-0.015640	H	2.129380	1.786594	-0.723679
N	0.385616	0.392420	-1.847609	N	0.292737	-0.578531	-1.868475	N	-0.224038	0.453717	2.190702
H	0.011476	1.313384	-2.083119	H	1.137275	-1.136130	-2.000403	H	-1.166418	0.221723	2.503008
H	0.169079	-0.218113	-2.635294	H	0.230796	0.054952	-2.664878	H	0.015819	1.341960	2.627995
H	1.399483	0.508473	-1.840616	H	-0.489608	-1.230727	-1.945235	H	0.386415	-0.244497	2.614507
N	-1.026278	-0.556368	1.843828	N	0.182514	0.942648	1.929818	N	0.186692	0.191732	-2.186713
H	-1.868254	-1.120474	1.950415	H	0.392285	1.916050	2.146315	H	0.386373	1.055293	-2.688739
H	-1.224691	0.368529	2.231688	H	0.861330	0.349967	2.412043	H	-0.648493	-0.204618	-2.617095
H	-0.321491	-0.984186	2.444998	H	-0.723983	0.733580	2.349317	H	0.943003	-0.454018	-2.411920
N	-2.252775	0.136838	-0.618658	N	2.268942	1.182142	-0.321836	N	-1.472342	1.981241	-0.287300
H	-2.951792	-0.488721	-0.219893	H	2.474993	2.026862	0.210573	H	-1.116034	2.760397	-0.838840
H	-2.420519	0.138105	-1.624429	H	2.568900	1.385351	-1.274642	H	-1.808941	2.385499	0.586017
H	-2.462895	1.079119	-0.280772	H	2.914723	0.475568	0.032206	H	-2.306134	1.645758	-0.769628
O	1.498025	-0.405079	0.725025	O	-1.773080	-0.645186	0.262498	O	1.330016	-1.288138	0.182808
C	2.717655	-0.795537	0.052581	C	-3.166239	-0.413876	-0.049145	C	2.763201	-1.384718	0.018997
H	1.687959	0.268243	1.395533	H	-1.680430	-1.441232	0.804457	H	0.945210	-2.158485	0.349250
H	2.452978	-1.540040	-0.693698	H	-3.213335	0.430122	-0.731952	H	3.073407	-0.608654	-0.676600
H	3.401502	-1.235287	0.772885	H	-3.723656	-0.182043	0.854781	H	3.024393	-2.352967	-0.397843
H	3.185857	0.066754	-0.421156	H	-3.592808	-1.286854	-0.535851	H	3.261059	-1.251888	0.976768
Structure (10)												
E = −1720.16673164				E = −1720.18333709				Not available				
Fe	-0.601546	-0.201605	-0.005910	Fe	-0.561325	-0.192697	-0.027149					
H	4.494799	1.599656	-0.285000	H	4.591072	1.470024	-0.436500					
O	-1.328681	1.280373	-0.501845	O	-1.590486	1.046751	-0.712904					
C	3.919530	1.062410	0.464994	C	4.019641	0.939739	0.321394					
C	-2.310223	2.167241	-0.006596	C	-2.801644	1.474876	-0.128588					
O	3.283368	-0.093907	-0.118193	O	3.284504	-0.151827	-0.270200					
H	3.132299	1.710168	0.840363	H	3.294497	1.620341	0.758756					
H	4.566209	0.768439	1.288229	H	4.685539	0.575326	1.099956					
H	-2.134246	2.429071	1.038525	H	-2.636952	2.327113	0.534998					
H	-3.307071	1.733193	-0.121152	H	-3.301818	0.675933	0.431897					
H	-2.273625	3.078063	-0.601729	H	-3.468681	1.798736	-0.927095					
N	-1.600342	-1.765701	-0.944272	N	-2.073340	-1.681871	-0.245155					
H	-2.258818	-2.282261	-0.361791	H	-2.628009	-1.837651	0.597137					
H	-1.014610	-2.467043	-1.396995	H	-1.771333	-2.608570	-0.546286					
H	-2.159475	-1.341924	-1.687650	H	-2.727519	-1.349918	-0.955586					
N	0.682336	0.051788	-1.547465	N	0.634676	0.223108	-1.599538					
H	0.674372	-0.651397	-2.284799	H	0.518448	-0.424836	-2.379518					
H	1.659087	0.139816	-1.231045	H	1.638615	0.251433	-1.372161					
H	0.409594	0.935705	-1.979189	H	0.330239	1.136999	-1.939805					
N	-1.764927	-0.254316	1.652535	N	-0.778259	0.611175	1.876513					
H	-1.818534	-1.147956	2.141860	H	-0.103924	0.342714	2.592606					
H	-2.723043	0.011520	1.419315	H	-1.702431	0.407810	2.260510					
H	-1.454524	0.432624	2.342971	H	-0.736196	1.629337	1.801624					

N	0.847154	-1.350352	0.911086	N	0.848120	-1.522345	0.609145	
H	0.799210	-1.381612	1.929392	H	0.735064	-1.889021	1.553440	
H	1.780635	-0.967713	0.676403	H	1.784945	-1.086081	0.544585	
H	0.856411	-2.324749	0.610073	H	0.896798	-2.339302	-0.000956	
H	3.968630	-0.671438	-0.477388	H	3.917589	-0.747814	-0.690476	
Structure (11)								
E = −1720.17593467				E = −1720.18452233				Not available
Fe	-0.049230	0.193890	0.040736	Fe	-0.109157	0.224825	0.028585	
H	-0.777006	-2.239063	0.082508	H	-0.634260	-2.136680	0.170566	
O	1.425298	-1.055313	-0.524174	O	1.665412	-1.083577	-0.416372	
C	-1.234692	-1.328939	0.481994	C	-1.302657	-1.380364	0.587445	
C	2.816728	-1.034364	-0.127928	C	3.028351	-0.852580	-0.002016	
O	-2.504323	-1.099457	-0.074402	O	-2.498349	-1.326308	-0.063855	
H	1.182015	-1.938083	-0.834476	H	1.597180	-1.970132	-0.794302	
H	-1.287488	-1.399349	1.572264	H	-1.372323	-1.421370	1.671557	
H	2.995088	-1.744322	0.677011	H	3.325148	-1.567965	0.762160	
H	3.037962	-0.026349	0.211329	H	3.071571	0.153617	0.408743	
H	3.444647	-1.276135	-0.980917	H	3.702705	-0.921907	-0.852000	
N	1.221074	1.851093	-0.566372	N	1.151007	1.888933	-0.681045	
H	1.880881	2.204620	0.125440	H	1.671559	2.409129	0.023849	
H	0.705575	2.672343	-0.881136	H	0.644860	2.592763	-1.216817	
H	1.790292	1.566062	-1.364099	H	1.851406	1.512130	-1.319790	
N	-0.816637	0.089102	-1.832751	N	-0.731107	-0.193261	-1.992747	
H	-0.959048	0.979042	-2.308628	H	-1.006898	0.641580	-2.508181	
H	-1.733103	-0.364000	-1.751360	H	-1.543632	-0.811614	-2.001919	
H	-0.255959	-0.478110	-2.468067	H	-0.012225	-0.637551	-2.562622	
N	0.703473	0.177625	1.945840	N	0.676974	0.241712	2.033420	
H	-0.025128	0.238627	2.657609	H	-0.024129	0.355890	2.764688	
H	1.368017	0.919176	2.165331	H	1.381476	0.955137	2.216060	
H	1.184504	-0.703161	2.131385	H	1.127764	-0.654287	2.219367	
N	-1.580570	1.431156	0.537891	N	-1.806069	1.553377	0.438992	
H	-1.576953	1.799268	1.488316	H	-2.202715	1.444317	1.371660	
H	-2.439345	0.881017	0.429031	H	-2.555734	1.300838	-0.204730	
H	-1.670375	2.246070	-0.067553	H	-1.646302	2.553381	0.325342	
H	-3.136000	-1.803637	0.128821	H	-3.263668	-1.401320	0.522062	
Structure ($TS_{2\text{-}3}$)								
E = −1644.9366386				E = −1644.92962817				Not available
Fe	-0.261947	0.016502	0.009623	Fe	-0.245457	0.047123	-0.005910	
H	0.742891	-2.653519	0.896809	H	0.357387	-0.292710	2.922689	
O	1.418032	-0.427596	-0.661084	O	1.274208	-0.938572	0.368638	
C	-0.110320	-1.966227	0.791677	C	-0.288373	0.120330	2.132469	
C	2.678401	0.035383	-0.193272	C	2.606087	-0.587116	0.000476	
H	-0.888538	-2.532324	0.289928	H	-1.260283	-0.344387	2.273521	
H	0.816740	-1.339412	0.061423	H	0.681278	-0.441107	1.433231	
H	-0.405024	-1.735367	1.812877	H	-0.330859	1.193726	2.296358	
H	2.907015	-0.350424	0.802994	H	3.003198	0.195247	0.647799	
H	2.716374	1.128410	-0.181956	H	2.653478	-0.264089	-1.042183	
H	3.441903	-0.324288	-0.879582	H	3.218857	-1.478541	0.120710	
N	-0.260082	1.913322	-0.825415	N	-0.047834	-0.160724	-2.074390	
H	-0.079361	2.688250	-0.187334	H	-0.912395	-0.295151	-2.598621	
H	-1.092748	2.181152	-1.350515	H	0.521762	-0.993454	-2.236232	
H	0.511693	1.915987	-1.496394	H	0.440017	0.610309	-2.530627	
N	-0.932082	-0.765081	-1.742286	N	-1.366679	-1.935099	-0.027035	
H	-1.468228	-0.153683	-2.357863	H	-1.880835	-2.228007	-0.857196	
H	-1.478517	-1.620252	-1.641487	H	-2.004761	-2.088756	0.753492	
H	-0.083669	-1.026147	-2.251386	H	-0.619589	-2.620113	0.096652	
N	0.515529	0.779911	1.733252	N	0.886486	2.028902	-0.121893	

H	-0.133721	1.306002	2.319136	H	0.376590	2.841805	-0.467545				
H	1.294053	1.409506	1.533232	H	1.723323	1.964703	-0.702010				
H	0.906801	0.051185	2.332088	H	1.229268	2.298920	0.800772				
N	-2.179484	0.207785	0.715225	N	-2.018528	1.092113	-0.095443				
H	-2.279974	-0.224179	1.635551	H	-2.068350	1.804614	0.634415				
H	-2.867242	-0.263403	0.127177	H	-2.814574	0.474806	0.069880				
H	-2.509726	1.167731	0.817923	H	-2.205683	1.569922	-0.976903				
Structure (TS_{4-5})											
Not available				E = −1754.61069361				E = −1754.60312771			
				Fe	0.415929	0.015152	-0.029756	Fe	0.425983	0.012473	-0.021445
				O	-0.987964	0.172822	0.970451	O	-1.041677	-0.505989	-0.833028
				O	-2.979430	-0.419204	-0.069475	O	-2.980677	0.299357	0.135652
				O	-2.440875	0.536878	0.430690	O	-2.562977	-0.683186	-0.429095
				C	-0.444308	0.932076	-1.576493	C	-0.437463	-0.745857	1.791824
				H	-0.901536	1.835299	-1.185689	H	-0.964814	-1.629413	1.458467
				H	-1.187955	0.269133	-2.007330	H	-1.074266	0.085709	2.072296
				H	0.359981	1.152771	-2.274605	H	0.415488	-0.918180	2.434794
				N	2.189495	-0.247208	-1.084682	N	2.050513	0.677033	1.248451
				H	2.047744	-0.665398	-2.005516	H	1.729394	1.187105	2.072313
				H	2.845185	-0.855341	-0.592521	H	2.682383	1.311409	0.758092
				H	2.691149	0.624305	-1.261436	H	2.635937	-0.080533	1.601943
				N	-0.222301	-1.748777	-0.755140	N	-0.364949	2.083536	0.166632
				H	-1.184866	-1.872797	-0.430599	H	-0.953643	2.227253	-0.655397
				H	0.303633	-2.556873	-0.421175	H	0.272374	2.878435	0.212771
				H	-0.253559	-1.812342	-1.773432	H	-1.000058	2.188267	0.958929
				N	1.048974	1.834102	0.558729	N	1.352794	-1.980496	-0.201900
				H	0.310147	2.199888	1.163532	H	0.723160	-2.502516	-0.814347
				H	1.168369	2.511443	-0.195996	H	1.409457	-2.522167	0.660597
				H	1.908684	1.842889	1.108298	H	2.278158	-2.036605	-0.626698
				N	1.356093	-0.936613	1.736666	N	1.439076	0.537035	-1.871856
				H	0.649325	-0.836979	2.467957	H	0.954888	0.025855	-2.612986
				H	2.206774	-0.520200	2.114767	H	2.429212	0.313064	-1.968034
				H	1.548951	-1.936716	1.684019	H	1.352159	1.521956	-2.123636
Structure (TS_{5-1})											
E = −1604.39077871				E = −1604.39635073				E = −1604.37202456			
H	1.315402	2.201251	0.563395	H	-0.623507	-2.590717	0.071386	H	2.712841	-0.777306	0.301088
H	1.549837	1.867238	-1.023840	H	0.688295	-2.344402	-0.875364	H	2.526348	0.377569	-0.836275
N	0.860096	1.831432	-0.271435	N	0.246478	-2.060591	0.001035	N	2.205073	0.081593	0.086548
H	0.142638	2.505349	-0.543911	H	0.845234	-2.398333	0.755556	H	2.556611	0.778719	0.743959
O	-0.821895	0.349042	-1.445868	O	0.744087	0.059885	-1.492811	O	0.000149	0.533146	-1.575144
H	1.917472	-1.817807	-0.012955	H	-2.879821	0.188218	-0.281898	H	0.808400	-2.134027	-1.440857
H	2.620948	-0.351931	-0.145242	H	-2.287810	-0.917728	-1.317294	H	-0.808748	-2.134000	-1.440824
N	1.812880	-0.898907	-0.444801	N	-2.077226	-0.022609	-0.874140	N	-0.000160	-2.019053	-0.827659
Fe	0.001549	-0.004800	-0.172181	Fe	-0.025727	-0.005869	-0.076004	Fe	-0.000035	-0.053526	-0.063514
H	-2.588339	0.908683	-0.215995	H	2.698732	-0.789657	-0.229397	H	0.922362	2.671029	-0.485768
C	-1.814092	0.838288	0.535329	C	2.311802	0.104142	0.234792	C	0.000464	2.429497	0.019792
H	-2.039149	0.124937	1.320589	H	2.622200	1.033975	-0.215735	H	-0.921072	2.671392	-0.486253
H	1.932240	-1.044323	-1.450246	H	-2.104806	0.647842	-1.643918	H	-0.000163	-2.808484	-0.181779
H	0.124522	0.717969	2.380101	H	-1.315737	0.726270	2.152727	H	-0.000704	0.255906	2.627504
N	0.466876	-0.112078	1.893410	N	-0.778672	-0.100026	1.887360	N	-0.000274	-0.555075	2.005845
H	0.012454	-0.893245	2.368579	H	-1.414896	-0.885724	2.028187	H	-0.814266	-1.104763	2.283029
H	-1.485543	1.806568	0.894523	H	2.172007	0.091245	1.309078	H	0.000170	2.348268	1.101569
H	-1.908970	-1.716093	-0.143688	H	0.517420	2.424741	-0.738978	H	-2.526176	0.378288	-0.836587
N	-0.893838	-1.826102	-0.155067	N	0.070890	2.060617	0.104599	N	-2.205076	0.082264	0.086281
H	-0.690872	-2.294768	-1.039895	H	-0.847271	2.504519	0.158151	H	-2.713108	-0.776482	0.300810
H	1.455076	-0.185890	2.137853	H	-0.061343	-0.198342	2.607469	H	0.813965	-1.104206	2.283401
H	-0.660363	-2.485621	0.587665	H	0.606404	2.415038	0.897901	H	-2.556483	0.779518	0.743625

Structure (TS_{2-6})									
E = −1644.92833637				E = −1644.94746904				E = −1644.94420408		
Fe	0.573802	0.040141	-0.023510	Fe	0.676480	0.049332	-0.001253	H	2.825525	2.100557	0.703940
H	-2.500826	2.116619	-0.127389	H	-3.355123	2.063560	-0.227561	Fe	-0.637815	0.038809	0.015677
O	-1.201999	-0.602429	0.441854	O	-1.359753	-0.305551	0.020403	O	1.360048	-0.486570	-0.142085
C	-2.995013	1.178591	0.107357	C	-3.541010	1.014141	-0.020973	C	3.185606	1.282122	0.088911
C	-1.823534	-1.725936	-0.179882	C	-1.910039	-1.621051	0.025671	C	2.148218	-1.662422	0.012162
H	-3.537404	1.181331	1.047177	H	-3.937117	0.820512	0.970083	H	3.437885	1.558651	-0.929587
H	-2.059490	0.337654	0.333382	H	-2.406933	0.479284	-0.006096	H	2.215954	0.484886	-0.029849
H	-3.549651	0.745953	-0.719632	H	-4.063896	0.496088	-0.817918	H	3.942826	0.674976	0.574678
H	-2.844124	-1.829288	0.181721	H	-2.595463	-1.755164	0.861482	H	2.961169	-1.677224	-0.711135
H	-1.269599	-2.615469	0.124097	H	-1.079987	-2.324036	0.145180	H	1.492302	-2.514513	-0.182694
H	-1.816063	-1.648145	-1.268080	H	-2.423571	-1.839502	-0.910034	H	2.544397	-1.749042	1.023316
N	-0.033987	0.474197	-1.987693	N	0.773442	-1.050943	-1.841062	N	-0.555567	-0.360904	2.138949
H	0.412214	1.276623	-2.431306	H	1.406461	-0.672094	-2.545528	H	-0.916412	0.382602	2.736787
H	-1.037322	0.657249	-2.026903	H	-0.148256	-1.079320	-2.277611	H	0.414282	-0.500901	2.421194
H	0.126036	-0.307879	-2.624101	H	1.054139	-2.024154	-1.718353	H	-1.052500	-1.204887	2.424627
N	0.294837	1.464942	1.522689	N	0.098979	2.124437	-0.056388	N	-0.116212	1.933887	-0.851544
H	1.109237	1.679686	2.096895	H	0.837753	2.825898	-0.053201	H	-0.842709	2.393816	-1.399387
H	-0.416360	1.113297	2.164496	H	-0.504100	2.346130	0.735942	H	0.684667	1.828682	-1.475184
H	-0.049296	2.367696	1.195258	H	-0.465733	2.314487	-0.884415	H	0.170032	2.617250	-0.150113
N	1.325896	-1.805194	0.674638	N	0.797725	-0.905573	1.915750	N	-1.006923	-1.452782	-1.510704
H	1.247608	-2.554585	-0.013538	H	1.130909	-1.869045	1.876080	H	-1.184453	-2.378759	-1.121001
H	0.786369	-2.116817	1.482885	H	-0.129720	-0.946310	2.338956	H	-0.183834	-1.556329	-2.104272
H	2.301015	-1.812513	0.971208	H	1.396894	-0.439166	2.597007	H	-1.787412	-1.270626	-2.140895
N	2.447739	0.712584	-0.411696	N	2.840342	0.495616	-0.035170	N	-2.808259	0.488321	0.196474
H	3.070266	0.655310	0.394753	H	3.140180	1.065552	0.755888	H	-3.233434	0.748335	-0.693453
H	2.475233	1.691330	-0.699677	H	3.123439	1.022851	-0.861256	H	-3.015742	1.263781	0.825414
H	2.919195	0.196079	-1.155254	H	3.442533	-0.327086	-0.019361	H	-3.363969	-0.295588	0.538017
Structure (TS_{7-8})											
E = −1720.12863356				E = −1720.14297835				E = −1720.14080223		
H	2.112097	0.220193	-0.297222	H	-2.134545	-0.441672	0.209358	H	-2.069576	-0.351013	0.286948
Fe	-0.513497	-0.095678	0.001594	Fe	0.495962	0.046216	-0.008869	Fe	0.497168	0.023667	-0.000024
O	1.077959	1.015469	-0.453689	O	-1.439765	0.682320	0.239537	O	-1.379214	0.708790	0.470886
C	2.564132	-0.925987	-0.050569	C	-2.083808	-1.687255	0.122340	C	-2.141518	-1.590639	-0.027094
C	1.403558	2.318457	0.004259	C	-2.240040	1.806710	-0.085580	C	-2.166755	1.826285	0.082355
O	1.418487	-1.693880	-0.192456	O	-0.730187	-1.914195	0.360302	O	-0.806279	-1.948317	0.167055
H	2.893132	-0.876232	0.984489	H	-2.354251	-1.897188	-0.909130	H	-2.417230	-1.582676	-1.078637
H	3.348228	-1.133750	-0.771475	H	-2.751314	-2.108130	0.866784	H	-2.847290	-2.094670	0.623809
H	2.426203	2.567225	-0.275117	H	-1.708023	2.700735	0.250959	H	-1.703575	2.716536	0.513177
H	1.285646	2.423219	1.085337	H	-3.181449	1.772028	0.460747	H	-3.171912	1.747671	0.491575
H	0.750192	3.030908	-0.503878	H	-2.428073	1.875245	-1.156520	H	-2.216092	1.934043	-1.002841
N	-1.670926	-1.806494	0.308882	N	2.340799	-1.123966	-0.205528	N	2.429330	-0.993544	-0.383612
H	-1.057869	-2.592132	0.529639	H	2.137265	-2.107807	-0.380636	H	2.328624	-2.006313	-0.444151
H	-2.240355	-2.109043	-0.480242	H	2.923480	-1.104662	0.630193	H	3.138901	-0.828565	0.329136
H	-2.314852	-1.733425	1.096268	H	2.949977	-0.830175	-0.968288	H	2.861528	-0.712144	-1.262726
H	1.477861	-2.248219	-0.982824	H	-0.602176	-2.398415	1.187399	H	-0.721051	-2.619638	0.857867
N	0.018578	-0.148853	1.961668	N	0.080571	-0.406407	-2.154800	N	-0.046888	-0.195316	-2.137682
H	0.708656	0.567147	2.189455	H	-0.810133	0.008707	-2.425292	H	-0.932374	0.251269	-2.374971
H	0.457809	-1.040796	2.193395	H	-0.014991	-1.408138	-2.318917	H	-0.157270	-1.182734	-2.368306
H	-0.737906	-0.026958	2.634523	H	0.757776	-0.077652	-2.841746	H	0.631383	0.171728	-2.804206
N	-0.895373	-0.103309	-1.991743	N	0.758170	0.276231	2.200752	N	0.837198	-0.133059	2.173093
H	-0.225666	0.531715	-2.428052	H	-0.136394	0.576439	2.587365	H	-0.054484	0.099102	2.610523
H	-1.822936	0.220183	-2.264944	H	1.434844	0.984888	2.480177	H	1.513571	0.532585	2.545461
H	-0.774475	-1.000722	-2.460062	H	1.018960	-0.560864	2.719342	H	1.116268	-1.038184	2.548668
N	-1.816432	1.621223	0.304327	N	1.266460	2.060914	-0.387925	N	1.224949	2.094893	-0.235796
H	-1.526966	2.211654	1.083241	H	0.964508	2.716800	0.331994	H	1.135285	2.623074	0.631459

H	-2.786477	1.372044	0.496806	H	0.937485	2.455152	-1.268168	H	0.666879	2.607848	-0.918157
H	-1.850044	2.239090	-0.505703	H	2.282750	2.133957	-0.411807	H	2.193513	2.208243	-0.531129
Structure (TS_{8-9})												
E = −1720.0962587				E = −1720.11399294				E = −1720.11068579				
Fe	0.083826	-0.408203	-0.028703	Fe	0.014584	0.352787	-0.002142	Fe	0.034537	0.367853	-0.002608
C	-2.723768	1.490051	-0.048849	C	2.755122	-1.576921	0.015439	C	-2.895935	-1.624099	0.115739
O	-1.839913	0.598332	0.552832	O	1.475248	-1.220448	0.422427	O	-1.844221	-0.791589	-0.264916
H	-3.508758	1.077427	-0.670399	H	3.585703	-0.990323	0.387215	H	-3.842513	-1.469414	-0.383997
H	-2.405638	2.519128	-0.157953	H	2.849582	-2.173833	-0.883378	H	-2.842954	-2.090390	1.090470
H	-2.763777	1.071174	1.166359	H	2.060312	-2.142785	0.939940	H	-1.951423	-1.908975	-0.704714
N	2.122882	-1.224186	-0.399224	N	-1.616339	1.743447	-0.572505	N	1.896212	1.536196	0.335655
H	2.542929	-1.022973	-1.305255	H	-2.223859	1.312063	-1.268767	H	2.507676	1.047623	0.989140
H	2.178288	-2.237026	-0.300435	H	-1.302657	2.618900	-0.988806	H	1.740786	2.458270	0.740123
H	2.771140	-0.849162	0.292532	H	-2.229899	2.010068	0.196060	H	2.461045	1.695877	-0.497214
N	-0.052971	0.376875	-1.899349	N	0.562475	0.085514	-2.129628	N	-0.410473	0.455643	2.170976
H	-1.012823	0.603988	-2.161565	H	1.473174	-0.345583	-2.280931	H	-1.302873	0.022766	2.403187
H	0.293842	-0.238899	-2.634459	H	0.565643	0.940034	-2.684360	H	-0.460184	1.402718	2.543351
H	0.469415	1.247198	-1.998828	H	-0.114651	-0.532675	-2.575567	H	0.290123	-0.023182	2.735247
N	0.139778	-1.091728	1.879778	N	-0.483851	0.312047	2.146641	N	0.355322	-0.021864	-2.153466
H	0.315136	-2.088111	2.002504	H	-0.693255	1.193771	2.611964	H	0.924406	0.644545	-2.672983
H	-0.738899	-0.900553	2.361460	H	0.273259	-0.114392	2.678858	H	-0.536605	-0.068862	-2.644838
H	0.865480	-0.615681	2.415658	H	-1.296261	-0.284291	2.298016	H	0.794831	-0.931146	-2.289946
N	-1.109305	-2.039421	-0.583773	N	1.538567	1.909275	0.369910	N	-1.198296	2.129176	-0.521069
H	-0.730347	-2.947480	-0.317850	H	1.168876	2.791135	0.722840	H	-0.766471	2.819687	-1.133366
H	-1.341682	-2.121034	-1.572317	H	2.080016	2.151989	-0.458395	H	-1.532128	2.651131	0.287614
H	-1.998802	-1.950515	-0.092680	H	2.218461	1.599435	1.063249	H	-2.037364	1.807339	-1.002450
O	0.968305	1.350129	0.683181	O	-1.324204	-1.338604	-0.255860	O	1.148172	-1.472553	0.403947
C	1.920179	2.215014	0.032394	C	-2.730098	-1.483826	0.029376	C	2.479705	-1.781797	-0.058056
H	0.473891	1.840534	1.352052	H	-0.907003	-2.207129	-0.318680	H	0.783775	-2.232401	0.874251
H	2.488038	1.601025	-0.662507	H	-3.116693	-0.493306	0.256100	H	2.802697	-0.948731	-0.678054
H	2.600716	2.640707	0.764819	H	-2.880014	-2.131763	0.890322	H	2.475634	-2.691585	-0.653826
H	1.414093	3.014678	-0.506250	H	-3.254385	-1.888875	-0.832330	H	3.159993	-1.895004	0.782806
Structure (TS_{10-11})												
E = −1720.1212291				E = −1720.1101627				Not available				
Fe	0.043072	0.303868	0.015420	Fe	0.051332	0.318916	0.025912					
H	-0.890342	-2.448576	0.761719	H	-0.709013	-2.539237	0.703255					
O	1.070730	-1.057358	-0.735746	O	1.013458	-0.986961	-0.927646					
C	-1.157725	-1.386378	0.654213	C	-1.010167	-1.480668	0.701082					
C	2.283426	-1.602169	-0.234401	C	2.142298	-1.723655	-0.459383					
O	-2.367013	-1.217634	-0.033385	O	-2.299772	-1.277330	0.222022					
H	-0.036274	-1.402896	-0.110701	H	-0.045570	-1.406394	-0.226103					
H	-1.210877	-0.994651	1.674337	H	-0.872924	-1.122317	1.725852					
H	2.137830	-2.103402	0.726118	H	1.922465	-2.246905	0.475930					
H	3.048760	-0.827884	-0.130662	H	2.999758	-1.065783	-0.316389					
H	2.641456	-2.338575	-0.950600	H	2.386522	-2.463667	-1.219362					
N	1.249093	1.841397	-0.643117	N	1.170817	1.903563	-0.755072					
H	1.778596	2.343457	0.069195	H	1.846375	2.337262	-0.126293					
H	0.790149	2.560621	-1.202004	H	0.629736	2.667215	-1.158840					
H	1.938873	1.405619	-1.259535	H	1.710633	1.494107	-1.520053					
N	-0.909788	0.272771	-1.748640	N	-1.198188	0.388644	-1.831226					
H	-1.182914	1.154520	-2.179536	H	-1.566129	1.265644	-2.194994					
H	-1.757482	-0.292993	-1.625962	H	-2.002165	-0.221887	-1.677538					
H	-0.310071	-0.222644	-2.411035	H	-0.656938	-0.033893	-2.585491					
N	1.085402	0.281299	1.773804	N	1.393497	0.335301	1.858125					
H	0.962328	1.108728	2.358293	H	2.362736	0.195662	1.570938					
H	2.086576	0.213854	1.584117	H	1.212507	-0.402070	2.539670					
H	0.872939	-0.517509	2.373229	H	1.390372	1.202966	2.394957					

N	-1.440247	1.513292	0.734973	N	-1.421492	1.449335	0.937282	
H	-1.442482	1.670163	1.742991	H	-1.331205	1.559435	1.947725	
H	-2.321635	1.037200	0.520299	H	-2.293449	0.935687	0.779546	
H	-1.492686	2.439696	0.312326	H	-1.550372	2.387022	0.559700	
H	-3.007785	-1.915382	0.161513	H	-2.882688	-2.032304	0.384794	

Table S3. MN15 Cartesian coordinates (in Å) and equilibrium energies (E/a.u.) of the optimized geometries for all ruthenium structures shown in Figure 2 for three different multiplicities.

S=1/2				S=3/2				S=5/2			
Structure (1)											
E = −435.043047938				E = −435.022713106				E = −434.955651165			
Ru	0.142535	0.065665	-0.006731	Ru	0.169426	0.000663	-0.149363	Ru	0.184217	0.000231	0.000004
O	-1.560292	0.675461	-0.014207	O	-1.621547	-0.000800	0.191775	O	-1.702777	-0.000843	-0.000328
C	-2.889743	0.173642	0.001039	C	-2.938802	-0.006705	-0.337920	C	-3.113750	-0.001691	-0.000337
H	-3.562976	1.016604	0.142545	H	-3.642697	0.008530	0.490742	H	-3.476025	0.509687	-0.892886
H	-3.027942	-0.527338	0.825034	H	-3.089641	-0.905094	-0.937375	H	-3.476032	0.515247	0.888984
H	-3.120032	-0.300468	-0.953754	H	-3.085953	0.870917	-0.968208	H	-3.475048	-1.030683	0.002886
N	0.730760	2.121402	-0.004972	N	0.146717	2.142222	-0.238421	N	0.274711	-0.973867	-2.111061
H	1.172740	2.469268	-0.855967	H	0.134845	2.511323	-1.190259	H	0.924764	-1.752587	-2.213442
H	1.301206	2.455688	0.771467	H	0.901494	2.623121	0.250881	H	0.497526	-0.310891	-2.853738
H	-0.162874	2.615209	0.067327	H	-0.718497	2.464068	0.198193	H	-0.653398	-1.338883	-2.323750
N	1.632885	-0.561855	-1.412901	N	2.199947	-0.005071	-0.918180	N	2.540672	0.001030	0.000649
H	2.464497	0.031345	-1.429318	H	2.692972	0.881752	-0.806290	H	2.940430	0.443101	-0.827113
H	1.234724	-0.490721	-2.351826	H	2.214128	-0.201628	-1.921352	H	2.941964	-0.936288	0.031985
H	1.975446	-1.519536	-1.326170	H	2.803716	-0.706952	-0.487582	H	2.940439	0.497486	0.797025
N	-0.698448	-1.914087	-0.019658	N	0.153006	-2.141769	-0.225784	N	0.273731	-1.341544	1.898729
H	-1.413649	-1.992573	-0.744483	H	0.081321	-2.512900	-1.174159	H	0.474192	-2.320013	1.690927
H	-1.178172	-2.124151	0.856925	H	-0.680125	-2.467237	0.266876	H	-0.648562	-1.326024	2.333482
H	-0.056510	-2.690284	-0.180927	H	0.941286	-2.618419	0.211979	H	0.939245	-1.055743	2.616272
N	1.552973	-0.550677	1.474681	N	0.701108	0.009370	2.163665	N	0.270495	2.315690	0.212126
H	2.447735	-0.058902	1.436034	H	1.230655	0.807350	2.510416	H	0.938706	2.795597	-0.390074
H	1.780721	-1.545559	1.489760	H	1.169779	-0.818084	2.528478	H	0.464823	2.624755	1.164736
H	1.167129	-0.336887	2.396881	H	-0.208297	0.047460	2.623975	H	-0.651121	2.682795	-0.023941
Structure (2)											
E = −475.535372054				E = −475.501572924				E = −475.433940078			
Ru	-0.142825	-0.073782	-0.012603	Ru	0.255330	-0.066484	0.012012	Ru	0.240188	-0.267337	0.000637
H	-1.567393	2.944283	1.144742	H	-3.750593	-1.775030	0.525261	H	-2.876139	-0.088332	0.059698
O	1.412640	0.542275	0.852651	O	-0.490433	1.599590	-0.043897	O	0.855466	1.517840	-0.012641
C	-1.623336	1.983282	0.634057	C	-2.738699	-1.482725	0.257643	C	-3.084629	0.983741	-0.000373
C	2.713322	0.591442	0.315973	C	-1.718575	2.304939	0.040584	C	1.246316	2.873044	-0.019069
H	-2.431011	1.402147	1.067555	H	-2.132024	-1.479992	1.165895	H	-3.714420	1.177364	-0.864976
H	-0.612670	1.576205	0.888783	H	-2.768390	-0.484041	-0.180195	H	-2.160514	1.559526	-0.090188
H	-1.781586	2.173746	-0.422993	H	-2.352634	-2.205848	-0.461904	H	-3.618514	1.291867	0.894928
H	3.033084	1.633555	0.239385	H	-2.281866	1.972894	0.913368	H	0.361695	3.506918	-0.093891
H	2.781341	0.127048	-0.674764	H	-2.308220	2.117263	-0.859245	H	1.900311	3.056927	-0.872151
H	3.405697	0.091850	0.995922	H	-1.502807	3.368290	0.114052	H	1.780982	3.100362	0.903779
N	0.837961	-1.807604	-0.639695	N	2.424955	0.768294	-0.530330	N	-0.748655	0.019160	2.094169
H	0.290631	-2.665290	-0.553476	H	3.161103	0.629580	0.159538	H	-1.597716	-0.518553	2.263328
H	1.669773	-1.938934	-0.059596	H	2.285915	1.776152	-0.601460	H	-1.011114	1.002321	2.162485
H	1.169221	-1.784041	-1.604945	H	2.816963	0.471536	-1.422110	H	-0.117347	-0.167237	2.873300
N	-0.616129	-0.934361	1.884133	N	0.613096	0.166642	2.115717	N	-0.730861	-0.040158	-2.109006
H	-0.650813	-1.949744	1.972173	H	1.531002	-0.122235	2.453382	H	-0.310080	-0.597313	-2.852098
H	-1.485725	-0.586538	2.289145	H	-0.075882	-0.305707	2.702299	H	-0.626592	0.936375	-2.383158
H	0.133993	-0.615646	2.502563	H	0.533522	1.161093	2.333424	H	-1.731389	-0.236805	-2.117376
N	0.402139	0.948228	-1.815237	N	-0.264831	-0.353895	-2.046549	N	2.383993	-1.153358	0.026902
H	0.943405	0.415640	-2.496969	H	0.412489	-0.842988	-2.631351	H	2.555064	-1.870788	0.730841
H	0.990251	1.744594	-1.560517	H	-0.395361	0.563544	-2.475307	H	3.032558	-0.391142	0.222783
H	-0.383122	1.341917	-2.335501	H	-1.153608	-0.846927	-2.149276	H	2.672822	-1.551850	-0.866477
N	-2.035050	-0.755684	-0.891710	N	0.777944	-2.170207	0.158712	N	-0.676949	-2.441613	0.013132
H	-2.710936	0.007840	-0.950637	H	-0.073617	-2.723829	0.279602	H	-0.361279	-3.019493	-0.765643
H	-2.501818	-1.473005	-0.335685	H	1.379993	-2.405324	0.948619	H	-1.695372	-2.427924	-0.048639

H	-1.971533	-1.139839	-1.834483	H	1.248469	-2.548959	-0.664132	H	-0.457755	-2.971045	0.856820
Structure (3)											
E = −475.544534188				E = −475.481066068				Not available			
Ru	0.243074	-0.010150	0.010773	Ru	0.291540	0.055801	-0.052101				
H	-0.348556	-1.579542	2.003447	H	0.297258	-1.262701	-2.351126				
O	-1.667847	0.402245	0.719578	O	-1.654249	-0.539326	-0.664385				
C	0.603120	-1.363422	1.507085	C	0.889784	-0.443937	-1.938582				
C	-2.920950	-0.036911	0.137179	C	-2.948670	-0.294157	-0.064653				
H	1.308798	-1.018103	2.265344	H	1.947204	-0.698419	-2.011303				
H	-1.767614	0.525520	1.674052	H	-1.746721	-0.865816	-1.571206				
H	0.967450	-2.316943	1.113550	H	0.708823	0.458769	-2.535624				
H	-3.131448	-1.064485	0.426422	H	-3.507493	0.417996	-0.666865				
H	-2.816457	0.047371	-0.940725	H	-2.768186	0.117683	0.924285				
H	-3.719345	0.617634	0.474284	H	-3.497893	-1.227759	0.020061				
N	-0.149977	1.511022	-1.705445	N	-0.192526	0.073160	2.207965				
H	0.581416	2.207086	-1.845053	H	0.616141	-0.085317	2.807846				
H	-0.987960	2.047663	-1.480335	H	-0.871609	-0.641044	2.467716				
H	-0.319352	1.111462	-2.627303	H	-0.589466	0.961962	2.511640				
N	0.950836	1.549785	1.292945	N	0.660854	-2.335252	0.437819				
H	1.753225	2.078385	0.950579	H	1.106871	-2.609337	1.311654				
H	1.234957	1.166344	2.195855	H	1.225887	-2.737643	-0.308447				
H	0.238709	2.253579	1.491881	H	-0.232174	-2.824463	0.407166				
N	-0.483780	-1.672418	-1.136077	N	-0.671958	2.337487	-0.199734				
H	-0.994218	-1.444083	-1.988644	H	-0.174808	3.082193	0.286209				
H	-1.117783	-2.231193	-0.563117	H	-1.639861	2.394537	0.113204				
H	0.251146	-2.322432	-1.416455	H	-0.683795	2.607092	-1.183090				
N	2.209189	-0.390088	-0.667316	N	2.288035	0.831070	0.221016				
H	2.586868	-1.189325	-0.154513	H	2.599026	1.325137	-0.616790				
H	2.867510	0.372313	-0.505264	H	2.952894	0.065641	0.344323				
H	2.283285	-0.618712	-1.658983	H	2.426628	1.464171	1.007815				
Structure (4)											
E = −585.194381095				E = −585.175469858				Not available			
Ru	-0.301759	0.048173	0.075738	Ru	-0.348535	-0.011913	0.020949				
O	1.162275	1.046163	0.510186	O	1.129190	-0.078552	1.167566				
O	2.812615	-0.151283	-0.468336	O	2.810274	0.268257	-0.279260				
O	2.511828	0.381348	0.611788	O	2.441871	-0.496993	0.629407				
C	-1.372311	-0.404018	1.715310	C	-1.158163	-1.847061	0.510209				
H	-1.378987	-1.438637	2.046917	H	-1.517379	-2.366235	-0.377045				
H	-2.348551	0.063586	1.812580	H	-1.976095	-1.714367	1.217711				
H	-0.613023	0.171014	2.285837	H	-0.360412	-2.421894	0.980696				
N	-2.169317	-0.889022	-0.716929	N	-2.179913	0.223016	-1.132981				
H	-2.338555	-1.820268	-0.335134	H	-2.055779	0.132125	-2.142772				
H	-2.235464	-0.992197	-1.729678	H	-2.629767	1.130449	-0.999823				
H	-2.988037	-0.344328	-0.444607	H	-2.875595	-0.478546	-0.873687				
N	0.665106	-1.836022	0.387827	N	0.634270	-1.099747	-1.522761				
H	1.161324	-1.811324	1.282025	H	1.174992	-1.851633	-1.085298				
H	1.383356	-2.057275	-0.304036	H	1.316767	-0.546635	-2.045302				
H	0.046943	-2.646239	0.438984	H	0.021263	-1.558471	-2.198044				
N	-1.194542	1.988676	-0.065311	N	-1.236409	0.823209	1.766612				
H	-0.446701	2.681072	0.031207	H	-0.820715	0.320811	2.556958				
H	-1.843020	2.174106	0.702153	H	-2.248413	0.738362	1.866514				
H	-1.696912	2.226267	-0.920526	H	-0.995478	1.804530	1.918640				
N	0.138832	-0.093084	-1.988496	N	0.317652	2.023537	-0.834959				
H	1.113415	0.224633	-2.042710	H	1.253965	2.162397	-0.449291				
H	-0.404149	0.504586	-2.612776	H	-0.227945	2.846281	-0.577253				
H	0.125311	-1.034164	-2.383318	H	0.425229	2.077578	-1.848105				

Structure (5)									
E = −585.23946055				E = −585.239364912				Not available	
Ru	-0.493145	-0.026843	-0.143170	Ru	0.500324	0.025178	-0.146529		
O	0.408747	-0.382022	-1.491902	O	-0.364773	0.363109	-1.523540		
O	3.175198	-0.008382	0.084245	O	-3.197395	0.018414	0.089793		
O	4.329445	-0.158404	-0.187866	O	-4.352010	0.147895	-0.191530		
C	-2.002259	1.150324	-0.952711	C	2.020860	-1.175897	-0.897643		
H	-2.068718	2.105537	-0.436703	H	2.067345	-2.122800	-0.364432		
H	-2.958196	0.631987	-0.921304	H	2.979392	-0.663583	-0.850265		
H	-1.696871	1.309944	-1.985737	H	1.740628	-1.350421	-1.935383		
N	-1.810913	0.488906	1.685853	N	1.767876	-0.471607	1.723057		
H	-1.586795	1.409846	2.065935	H	1.532167	-1.388477	2.105925		
H	-1.794854	-0.144039	2.485941	H	1.731614	0.169163	2.516212		
H	-2.791129	0.557084	1.409913	H	2.754941	-0.544015	1.473915		
N	0.658700	1.759167	0.105512	N	-0.670029	-1.748846	0.104454		
H	1.290475	1.800398	-0.698319	H	-1.292920	-1.793311	-0.706021		
H	1.257688	1.817756	0.929320	H	-1.278327	-1.795640	0.922173		
H	0.103079	2.615001	0.075887	H	-0.119996	-2.608666	0.088820		
N	-1.697399	-1.744991	-0.576797	N	1.727648	1.727106	-0.579543		
H	-2.149689	-1.602546	-1.482094	H	2.196900	1.567415	-1.473271		
H	-2.442299	-1.964101	0.084652	H	2.460917	1.949638	0.093671		
H	-1.134675	-2.590720	-0.682355	H	1.174675	2.575943	-0.708951		
N	0.563773	-1.024437	1.466865	N	-0.585288	1.059632	1.419976		
H	1.444193	-1.346027	1.052973	H	-1.446983	1.392552	0.976918		
H	0.106328	-1.848814	1.856945	H	-0.124164	1.879581	1.814953		
H	0.827130	-0.432227	2.254822	H	-0.883617	0.480818	2.205457		
Structure (6)									
E = −475.483168465				E = −475.46349305				E = −475.411077982	
Ru	-0.550254	-0.006858	-0.164870	Ru	0.569909	0.023822	0.109527	Ru	0.665082	-0.097350	-0.031438
H	3.168283	-2.091935	0.906565	H	-3.309635	-2.101710	-0.300139	H	-3.798482	-1.972434	0.954499
O	1.320153	0.991295	-0.018839	O	-1.286982	0.993412	-0.216681	O	-1.571446	0.684143	0.074783
C	3.562577	-1.130239	0.616347	C	-3.608941	-1.077383	-0.459491	C	-3.965267	-1.391256	0.061867
C	1.652487	2.083527	-0.905429	C	-1.775319	1.954606	0.745207	C	-2.017197	2.051681	0.049138
H	3.813584	-0.420429	1.389679	H	-3.788971	-0.738638	-1.468356	H	-3.914358	-1.869468	-0.903402
H	2.100254	0.418793	0.120430	H	-2.018641	0.404322	-0.489041	H	-2.340159	0.081283	0.112993
H	4.021160	-1.027222	-0.354924	H	-4.051088	-0.531521	0.360049	H	-4.501838	-0.458378	0.144668
H	2.529498	2.603477	-0.529692	H	-2.633462	2.478137	0.332071	H	-2.580364	2.258845	-0.859198
H	0.806171	2.765732	-0.907182	H	-0.972333	2.663141	0.929029	H	-1.129065	2.680740	0.077564
H	1.833239	1.719016	-1.914649	H	-2.049460	1.460618	1.677273	H	-2.634824	2.272196	0.917432
N	0.384107	-1.651761	-1.192615	N	-0.332561	-1.174411	1.660953	N	0.751224	0.826407	2.066316
H	-0.003992	-2.577317	-1.010256	H	0.029429	-2.120358	1.779283	H	1.092430	0.208792	2.802182
H	1.377885	-1.717947	-0.961542	H	-1.339061	-1.266814	1.511317	H	-0.204830	1.075649	2.318629
H	0.350891	-1.545127	-2.207644	H	-0.223967	-0.719405	2.569032	H	1.303729	1.680421	2.132799
N	-0.067627	-0.802423	1.686587	N	-0.016171	-1.373871	-1.723867	N	-0.402854	-2.097554	-0.297018
H	-0.847275	-0.854720	2.342748	H	0.623424	-2.138496	-1.931360	H	-0.137968	-2.596985	-1.145396
H	0.645051	-0.222089	2.134616	H	-0.090984	-0.828790	-2.581791	H	-1.418778	-1.989665	-0.329299
H	0.322798	-1.744351	1.642079	H	-0.933098	-1.799723	-1.590408	H	-0.207767	-2.734341	0.474846
N	-1.376948	1.738351	0.781280	N	1.434061	1.683427	-0.945689	N	0.721266	1.263167	-1.860770
H	-1.876589	2.354072	0.138148	H	1.944596	2.313669	-0.325707	H	1.121196	2.177883	-1.654248
H	-0.622798	2.304608	1.172936	H	0.691841	2.239403	-1.373016	H	-0.229653	1.431423	-2.188269
H	-2.026531	1.576295	1.550705	H	2.084857	1.444288	-1.693977	H	1.243217	0.900478	-2.657789
N	-2.470393	-0.936300	-0.317874	N	2.487538	-0.848300	0.464334	N	2.892472	-0.786929	0.055241
H	-3.149459	-0.607926	0.368522	H	3.151964	-0.697343	-0.294314	H	3.165551	-1.258993	-0.806100
H	-2.457589	-1.951157	-0.218030	H	2.463991	-1.858524	0.600765	H	3.083091	-1.451351	0.803939
H	-2.909008	-0.765189	-1.224673	H	2.935963	-0.468967	1.299132	H	3.556853	-0.024031	0.176736
Structure (7)									

E = −550.75112222				E = −550.692273377				Not available
H	-2.796702	-0.764599	0.962050	H	-3.624317	1.048182	0.894280	
Ru	0.328144	-0.049307	0.007156	Ru	0.359575	-0.279659	0.086317	
O	-0.923469	1.170092	0.728256	O	0.623179	1.491947	0.664026	
C	-2.483409	-1.342094	0.096830	C	-2.977231	1.059833	0.018595	
C	-1.605470	2.171199	0.011882	C	1.239448	2.519423	-0.078796	
O	-1.058885	-1.625358	0.182026	O	-2.588696	-0.274424	-0.357757	
H	-2.641153	-0.762675	-0.807993	H	-2.063251	1.604197	0.258714	
H	-3.024036	-2.281157	0.027086	H	-3.489712	1.564998	-0.797882	
H	-2.002335	2.905367	0.710775	H	1.806591	3.153720	0.601629	
H	-2.453655	1.750322	-0.541184	H	0.476377	3.144390	-0.552777	
H	-0.947088	2.689195	-0.696941	H	1.914098	2.126231	-0.846961	
N	1.794632	-1.541301	-0.654269	N	-0.123266	-2.340068	-0.417167	
H	1.307242	-2.381014	-0.970807	H	-1.136522	-2.387308	-0.537542	
H	2.435065	-1.856332	0.073774	H	0.103508	-3.020445	0.308273	
H	2.384847	-1.261406	-1.437310	H	0.286998	-2.702706	-1.277031	
H	-0.911568	-2.303307	0.854638	H	-3.384754	-0.772237	-0.585454	
N	-0.351790	0.151292	-2.016597	N	-0.097642	0.340691	-1.957393	
H	-1.101727	0.840863	-2.084991	H	0.077390	1.333199	-2.115503	
H	-0.743191	-0.726658	-2.361569	H	-1.107290	0.194588	-2.047261	
H	0.345953	0.428893	-2.706998	H	0.351986	-0.165139	-2.719611	
N	0.824891	-0.210936	2.075456	N	-0.546151	-0.440310	2.004032	
H	0.116657	0.385160	2.513920	H	-0.425355	0.479893	2.434983	
H	1.732319	0.145503	2.373465	H	-0.190440	-1.138696	2.656564	
H	0.741740	-1.132492	2.502928	H	-1.548183	-0.606311	1.893247	
N	1.694367	1.541458	-0.241959	N	2.648394	-0.563498	-0.081657	
H	1.365326	2.314954	0.339672	H	3.005401	-1.480823	0.183482	
H	1.758710	1.912881	-1.189853	H	3.092346	0.111495	0.541337	
H	2.652674	1.349913	0.051532	H	3.015315	-0.375664	-1.014103	
Structure (8)								
E = −550.709279477				E = −550.673711202				Not available
Ru	0.035212	0.226745	-0.008743	Ru	0.756810	-0.436772	0.118376	
C	2.637126	-1.543827	0.028607	C	-3.617874	-0.414399	-0.493740	
O	1.401136	-1.343309	0.610826	O	-3.097845	0.531535	0.352419	
H	3.133777	-0.643752	-0.286999	H	-4.587459	-0.825949	-0.270537	
H	3.156670	-2.456779	0.259768	H	-3.239854	-0.373686	-1.502583	
H	1.072165	-2.155369	1.018774	H	-3.755554	0.836565	0.993063	
N	-1.311372	1.733810	-0.650589	N	2.086756	-0.296139	-1.563296	
H	-2.032891	1.318435	-1.241902	H	1.703076	0.341128	-2.263594	
H	-0.884946	2.469567	-1.213254	H	2.228026	-1.186771	-2.041263	
H	-1.811065	2.219428	0.094150	H	3.022561	0.047382	-1.349404	
N	0.730611	0.001386	-2.029826	N	-0.515964	-1.753639	-1.004692	
H	1.436029	-0.735816	-2.097473	H	-1.481176	-1.748446	-0.661372	
H	1.153946	0.824613	-2.457626	H	-0.210607	-2.727120	-0.983619	
H	-0.022672	-0.272588	-2.661385	H	-0.586266	-1.503553	-1.990924	
N	-0.648859	0.361442	2.035861	N	2.047029	0.819447	1.293564	
H	-0.839716	1.307203	2.366537	H	2.451984	0.336172	2.096055	
H	0.044748	-0.013152	2.683706	H	1.546685	1.626122	1.668082	
H	-1.503273	-0.164204	2.218281	H	2.842241	1.206862	0.786605	
N	1.583672	1.602791	0.486152	N	-0.486986	-0.803892	1.828925	
H	1.257765	2.455531	0.940743	H	-0.580670	-1.798040	2.037796	
H	2.139642	1.920392	-0.307824	H	-1.425650	-0.459430	1.608117	
H	2.250946	1.184905	1.136626	H	-0.212005	-0.359498	2.703794	
O	-1.525652	-1.163914	-0.559998	O	-0.532411	1.392901	-0.444420	
C	-2.795996	-1.305342	0.105367	C	-0.117031	2.753188	-0.641585	
H	-1.276839	-2.000119	-0.972150	H	-1.491586	1.334743	-0.279715	
H	-3.127564	-0.307009	0.381282	H	0.956658	2.742328	-0.821000	

H -2.702360 -1.927096 0.994819 H -3.522700 -1.744203 -0.573025	H -0.331205 3.358800 0.237511 H -0.613202 3.181709 -1.509096	
Structure (9)		
E = −550.750952618	E = −550.663963547	Not available
Ru 0.068296 0.220597 0.011388 C 2.344318 -1.660434 0.047045 O 0.957255 -1.436462 0.157845 H 2.820191 -0.966814 -0.657298 H 2.517620 -2.678741 -0.296642 H 2.832387 -1.552349 1.020849 N -1.175814 2.010095 -0.246914 H -1.880939 1.853555 -0.968365 H -0.683600 2.859443 -0.523666 H -1.702434 2.262829 0.589606 N 0.546176 0.275843 -2.064449 H 1.329072 -0.352888 -2.251575 H 0.788596 1.172538 -2.484700 H -0.240256 -0.095498 -2.600603 N -0.488502 0.018264 2.065930 H -0.091894 0.672262 2.740330 H -0.154297 -0.909683 2.333945 H -1.495524 0.017937 2.227998 N 1.777472 1.366259 0.521635 H 1.598318 2.206199 1.072807 H 2.318535 1.676963 -0.285666 H 2.421262 0.798334 1.075229 O -1.499323 -1.083896 -0.551362 C -2.847223 -1.140251 -0.041152 H -1.085557 -1.964278 -0.542712 H -3.226857 -0.122331 -0.010774 H -2.867964 -1.580584 0.954432 H -3.463053 -1.729408 -0.714903	Ru 0.842531 -0.400766 0.078788 C -4.295624 -0.027973 -0.071145 O -2.933336 -0.097471 0.001059 H -4.774466 -1.008161 -0.049881 H -4.639242 0.610713 -0.889035 H -4.611527 0.495199 0.857105 N 2.168311 -0.116996 -1.588820 H 1.778857 0.581374 -2.224499 H 2.303422 -0.961606 -2.145089 H 3.105960 0.205338 -1.351633 N -0.420555 -1.642034 -1.135871 H -1.376473 -1.648248 -0.776289 H -0.123457 -2.616174 -1.189539 H -0.498037 -1.316226 -2.098955 N 2.105821 0.802506 1.338764 H 2.571804 0.259770 2.066564 H 1.581690 1.533257 1.820555 H 2.854197 1.289886 0.847018 N -0.346756 -0.972310 1.775019 H -0.209445 -1.952585 2.023502 H -1.335301 -0.868641 1.532921 H -0.200871 -0.442699 2.633239 O -0.551332 1.349733 -0.410928 C -0.344697 2.769617 -0.350109 H -1.499365 1.122221 -0.420809 H 0.728816 2.943472 -0.380479 H -0.754504 3.183648 0.569339 H -0.801893 3.257056 -1.207864	
Structure (10)		
E = −550.725896404	Not available	Not available
Ru -0.218933 -0.224595 -0.006318 H 2.258394 1.916198 1.322110 O -1.505565 1.146720 -0.157155 C 1.987389 0.938739 0.920420 C -1.245648 2.516621 0.073533 O 2.786379 0.545586 -0.160252 H 0.939738 1.168630 0.552382 H 1.989386 0.212944 1.734393 H -0.432537 2.874056 -0.568079 H -0.964927 2.690953 1.116741 H -2.143109 3.090007 -0.147692 N -1.805931 -1.313617 -0.784967 H -1.660463 -1.712003 -1.712366 H -2.548700 -0.611278 -0.872052 H -2.165506 -2.071144 -0.204726 N 0.527150 0.222941 -1.939982 H 0.484673 -0.514353 -2.642959 H 1.510266 0.499001 -1.855297 H 0.016617 1.017748 -2.327955 N -0.929670 -0.626923 1.978592 H -1.189962 -1.592172 2.181331 H -1.775852 -0.067730 2.103433 H -0.295902 -0.345272 2.727018		

N 1.186633 -1.897978 0.071980 H 2.117311 -1.546165 -0.169838 H 0.988253 -2.670095 -0.563146 H 1.281000 -2.325948 0.993101 H 3.680139 0.907266 -0.092206		
Structure (11)		
E = −550.736006189	Not available	Not available
Ru -0.027115 0.170463 0.021971 H -0.745828 -2.297229 0.214050 O 1.523716 -1.012777 -0.722017 C -1.258346 -1.381294 0.538581 C 2.836072 -1.222377 -0.144583 O -2.503559 -1.223200 -0.115450 H 1.308351 -1.725462 -1.338996 H -1.400372 -1.442842 1.623622 H 2.808143 -2.043037 0.569064 H 3.118247 -0.295127 0.346417 H 3.546000 -1.441186 -0.936931 N 1.230079 2.046627 -0.490260 H 0.745421 2.750562 -1.045466 H 2.025459 1.759899 -1.061363 H 1.625788 2.553925 0.299835 N -0.926245 0.149778 -1.913712 H -1.258634 1.050808 -2.255329 H -1.749060 -0.456614 -1.829981 H -0.344590 -0.221050 -2.664587 N 0.802281 0.069456 2.005559 H 1.476797 0.797752 2.238658 H 1.281416 -0.818427 2.158669 H 0.087545 0.108799 2.732886 N -1.660249 1.324567 0.671381 H -2.490486 0.745490 0.491888 H -1.782925 2.195908 0.155695 H -1.677336 1.581789 1.657832 H -3.129537 -1.927489 0.102274		
Structure (12)		
E = −435.057043745		
Ru -0.071591 0.008709 0.071109 C 1.692937 -0.583935 0.844697 O 1.863323 -0.414228 -0.551697 H 2.125013 -1.219610 -1.024326 N 0.682603 2.005099 0.215017 H 0.810795 2.326287 1.175004 H 0.141618 2.732330 -0.252531 H 1.611123 2.034944 -0.212479 N -1.774003 0.475038 1.253870 H -2.064583 1.452216 1.208361 H -1.557021 0.300857 2.237825 H -2.609891 -0.075692 1.055142 N -0.703464 -2.050325 0.002850 H -0.705575 -2.477631 0.929953 H -0.099936 -2.646904 -0.564405 H -1.641455 -2.197505 -0.370871 N -0.906935 0.441047 -1.974203 H -1.581769 1.205511 -1.996618 H -1.365365 -0.343818 -2.435181 H -0.152835 0.724381 -2.600331		

H 2.280400 0.134238 1.407449 H 1.807870 -1.611369 1.176876		
Structure (13)		
E = −435.023190967		
Ru -0.082915 -0.000174 -0.199988 C 1.973024 0.001417 0.534878 O 1.833482 0.000784 -0.734409 H -0.109510 -0.001119 -1.755936 N 0.011522 2.120577 -0.348254 H 0.009981 2.656875 0.519828 H -0.701589 2.533058 -0.950554 H 0.900596 2.319852 -0.815820 N -0.436503 0.001170 2.123208 H -0.028367 0.809862 2.591707 H -0.026578 -0.805912 2.592922 H -1.418134 0.000262 2.399692 N 0.014648 -2.120935 -0.346425 H 0.903887 -2.319188 -0.814108 H -0.697997 -2.535065 -0.948144 H 0.014217 -2.656480 0.522125 N -2.204926 -0.001746 -0.383050 H -2.660679 0.811687 0.034266 H -2.659255 -0.816487 0.033270 H -2.471121 -0.001408 -1.369072 H 2.196365 0.936260 1.053074 H 2.197248 -0.932766 1.053886		
Structure (14)		
E = −435.044152159		
Ru 0.044864 0.000004 -0.145729 O -1.715735 0.000235 0.665499 C -2.034077 0.000369 -0.598059 H -2.380873 -0.925635 -1.053369 H -0.302439 0.000168 -1.687150 H -2.380607 0.926531 -1.053251 N -0.000333 -2.127996 -0.189882 H 0.801056 -2.605600 0.223702 H -0.116914 -2.511533 -1.128642 H -0.814720 -2.436076 0.347857 N 0.733320 -0.000285 2.008856 H 1.262167 -0.811388 2.327897 H -0.129456 -0.000136 2.556806 H 1.262393 0.810696 2.327837 N 0.000460 2.128035 -0.189674 H -0.813831 2.436361 0.348076 H -0.116060 2.511597 -1.128430 H 0.801979 2.605427 0.223891 N 2.064361 -0.000284 -0.858371 H 2.771156 -0.000691 -0.122379 H 2.264099 0.806866 -1.451196 H 2.263699 -0.807156 -1.451710		
Structure (15)		
E = −435.048083096		
Ru 0.175054 -0.000001 -0.148941 O -1.812631 -0.000662 0.206491 C -2.876923 -0.000365 -0.405778 H -3.810585 -0.001092 0.158591		

H -0.140744 -0.000351 -1.703991 H -2.895600 0.000660 -1.497717 N 0.138340 -2.142420 -0.201816 H 0.936944 -2.608182 0.228577 H 0.087563 -2.490386 -1.158845 H -0.683369 -2.517376 0.272637 N 0.522158 0.000312 2.129450 H 1.004147 -0.810961 2.514398 H -0.400560 -0.000700 2.566230 H 1.002518 0.812399 2.514713 N 0.136945 2.142378 -0.201875 H 0.933868 2.608791 0.230923 H -0.686485 2.516571 0.270195 H 0.088633 2.490449 -1.158998 N 2.191420 0.000556 -0.761589 H 2.851316 0.000345 0.018402 H 2.425204 0.812538 -1.333765 H 2.425318 -0.810936 -1.334407		
Structure (16)		
E = −320.550373933		
Ru 0.000071 -0.061929 -0.244647 H -0.000876 -1.476071 -0.930852 N -2.099733 -0.237018 -0.519826 H -2.653064 0.499989 -0.077815 H -2.495307 -1.124593 -0.207855 H -2.319363 -0.183893 -1.518388 N 0.003107 2.071793 0.641357 H -0.805952 2.285681 1.225345 H 0.008145 2.793638 -0.081295 H 0.808198 2.281300 1.232358 N 2.099550 -0.241894 -0.518732 H 2.321791 -0.178737 -1.516113 H 2.490413 -1.134578 -0.215514 H 2.655023 0.487759 -0.067295 N -0.003091 -1.202596 1.472716 H 0.812825 -1.032023 2.063742 H -0.008228 -2.201881 1.263439 H -0.815540 -1.023736 2.066128		
Structure (TS_{2-3})		
E = −475.497531446	E = −475.424535985	Not available
Ru 0.227744 -0.011677 -0.009835 H -1.017014 2.505643 1.166398 O -1.584538 0.472505 -0.575654 C -0.162662 1.807211 1.194805 C -2.800539 -0.189601 -0.231535 H 0.689297 2.437961 0.951502 H -1.064443 1.273047 0.291446 H -0.119390 1.478068 2.230964 H -3.147068 0.126968 0.755249 H -2.672019 -1.273257 -0.251966 H -3.555186 0.094219 -0.961001 N 0.507996 -1.790029 -1.257043 H 1.343162 -1.795351 -1.843183 H -0.281443 -1.832629 -1.904920 H 0.513585 -2.684873 -0.768106 N 0.804687 1.267750 -1.612678 H 1.452681 0.905993 -2.312037	Ru 0.227994 0.029579 -0.040087 H -0.631841 -0.498235 -2.926483 O -1.415243 -0.957802 -0.362626 C 0.093831 -0.034125 -2.235420 C -2.710420 -0.820012 0.218828 H 1.027000 -0.560857 -2.437542 H -0.914028 -0.528256 -1.471932 H 0.156130 1.008593 -2.540948 H -3.311173 -0.126673 -0.369509 H -2.631907 -0.465037 1.247915 H -3.191780 -1.795377 0.208040 N 0.172782 0.070111 2.177800 H 1.071414 0.141830 2.654559 H -0.271448 -0.778396 2.531185 H -0.392453 0.846546 2.521910 N 1.485101 -2.075745 0.219878 H 2.070810 -2.246363 1.035900	

H	1.190315	2.159423	-1.301085	H	2.069507	-2.273715	-0.591607		
H	-0.059898	1.493656	-2.111340	H	0.765992	-2.798933	0.224799		
N	-0.496072	-1.206183	1.615442	N	-1.107363	2.176423	0.108806		
H	-0.568377	-2.206153	1.427352	H	-0.737830	2.967610	0.634042		
H	-1.437204	-0.909173	1.878813	H	-2.038614	1.998037	0.483499		
H	0.059820	-1.120159	2.467395	H	-1.255988	2.520641	-0.839319		
N	2.228786	-0.153673	0.785250	N	2.034322	1.226255	-0.105680		
H	2.323871	0.482152	1.579845	H	2.145416	1.680018	-1.013625		
H	2.949002	0.140029	0.124494	H	2.868505	0.649413	0.014349		
H	2.517286	-1.072541	1.121747	H	2.098108	1.965635	0.593511		
Structure (TS_{4-5})									
E = −585.194132937				E = −585.175278882				Not available	
Ru	0.291790	0.057970	-0.060058	Ru	0.348441	-0.016925	-0.021638		
O	-1.106369	1.090279	-0.452654	O	-1.101772	-0.030617	-1.165340		
O	-2.837383	-0.188165	0.449799	O	-2.859990	0.272114	0.260945		
O	-2.586614	0.450291	-0.557510	O	-2.486372	-0.459826	-0.647290		
C	1.310680	-0.302323	-1.784308	C	1.172912	-1.814305	-0.623182		
H	1.337553	-1.339110	-2.109500	H	1.468406	-2.415288	0.236080		
H	2.295253	0.155657	-1.836609	H	2.035536	-1.638523	-1.264788		
H	0.599659	0.260698	-2.407676	H	0.401301	-2.337442	-1.187501		
N	2.184631	-0.963797	0.599260	N	2.179456	0.148799	1.150709		
H	2.339846	-1.846892	0.111761	H	2.038430	0.072339	2.159684		
H	2.285575	-1.177982	1.591511	H	2.668344	1.035864	1.018139		
H	2.995406	-0.392327	0.359879	H	2.847149	-0.583908	0.903959		
N	-0.693168	-1.797882	-0.467456	N	-0.642861	-1.186569	1.457017		
H	-1.235761	-1.699998	-1.328996	H	-1.159580	-1.925949	0.972005		
H	-1.367317	-2.094141	0.239686	H	-1.336105	-0.681898	2.012162		
H	-0.067983	-2.588287	-0.627464	H	-0.023163	-1.673421	2.106385		
N	1.249849	1.962476	0.157917	N	1.278222	0.945772	-1.681290		
H	0.525621	2.683716	0.109315	H	0.873501	0.511112	-2.515800		
H	1.886263	2.158195	-0.616859	H	2.289622	0.839513	-1.766276		
H	1.778482	2.142108	1.011302	H	1.066878	1.941364	-1.765113		
N	-0.066291	-0.213426	2.020840	N	-0.316283	1.986742	0.930582		
H	-1.019094	0.138949	2.159138	H	-1.186711	2.220455	0.449469		
H	0.534271	0.312826	2.656502	H	0.296932	2.794938	0.825112		
H	-0.072862	-1.180992	2.345423	H	-0.554063	1.954806	1.921993		
Structure (TS_{5-1})									
E = −434.972764143				E = −434.947149705				Not available	
Ru	0.014709	0.000008	-0.123584	Ru	0.008875	-0.000008	0.057385		
O	-1.391684	0.000036	-1.094071	O	-1.328088	0.002148	-1.122300		
C	-2.201710	-0.000035	0.726275	C	-2.226745	0.004989	0.579243		
H	-2.735863	0.905224	0.476693	H	-2.753129	0.914576	0.328601		
H	-1.788763	0.000296	1.731214	H	-1.818334	0.003948	1.596348		
H	-2.735451	-0.905642	0.477074	H	-2.757667	-0.901998	0.328731		
N	1.077408	-0.000047	1.828310	N	1.563963	-0.001333	1.648759		
H	1.672254	-0.812369	1.998096	H	2.514534	0.011710	1.275986		
H	0.401281	0.000036	2.593234	H	1.523032	-0.817636	2.260544		
H	1.672428	0.812153	1.998072	H	1.506872	0.801959	2.276320		
N	-0.070929	2.150747	-0.158483	N	-0.035249	2.147194	0.079836		
H	-0.762457	2.392603	-0.871719	H	-0.588329	2.451500	-0.723881		
H	0.779023	2.650255	-0.420199	H	0.869077	2.611605	-0.004992		
H	-0.398496	2.576727	0.708874	H	-0.486866	2.551985	0.901079		
N	-0.070938	-2.150728	-0.158547	N	-0.045061	-2.146944	0.083216		
H	-0.762939	-2.392500	-0.871354	H	-0.600128	-2.450037	-0.719590		
H	-0.397918	-2.576811	0.708981	H	-0.497837	-2.548419	0.905453		
H	0.778835	-2.650203	-0.420911	H	0.857101	-2.615533	-0.001727		
N	2.034959	-0.000001	-0.833811	N	1.483566	-0.005014	-1.712232		

H	1.984824	-0.000232	-1.854923	H	0.878002	-0.008446	-2.534884				
H	2.598213	-0.813380	-0.581203	H	2.089849	-0.819675	-1.800657				
H	2.598056	0.813600	-0.581575	H	2.087962	0.810401	-1.806380				
Structure ($TS_{2\text{-}6}$)											
E = −475.463449442				E = −475.442355738				E = −475.383771797			
Ru	-0.515212	-0.007142	-0.157375	Ru	-0.528882	0.039316	-0.115830	Ru	-0.591163	0.069070	-0.020333
H	2.971493	-1.630711	1.181354	H	2.749953	-1.903690	0.700351	H	2.978972	2.036467	0.804668
O	1.365060	0.753763	0.059207	O	1.376618	0.754471	0.099116	O	1.555030	-0.501783	-0.180030
C	3.326149	-0.808718	0.567227	C	3.215075	-0.924111	0.646429	C	3.376373	1.245998	0.176272
C	1.894300	1.516186	-1.036133	C	1.986474	1.484739	-0.973641	C	2.303082	-1.698043	0.018813
H	3.964898	-0.105239	1.090051	H	3.629285	-0.566462	1.582760	H	3.671240	1.561075	-0.819186
H	2.239593	-0.020944	0.342848	H	2.221388	-0.071419	0.434627	H	2.409771	0.443483	-0.015777
H	3.683407	-1.089424	-0.417850	H	3.862429	-0.779474	-0.211970	H	4.115459	0.625559	0.672650
H	2.920935	1.803989	-0.818733	H	2.976779	1.817599	-0.670775	H	3.144812	-1.744622	-0.669577
H	1.292719	2.419847	-1.131713	H	1.362847	2.357021	-1.168465	H	1.629404	-2.532444	-0.189284
H	1.858439	0.948219	-1.966914	H	2.056511	0.882072	-1.880422	H	2.658432	-1.781181	1.046041
N	0.268128	-1.871873	-0.870484	N	0.113794	-1.305452	-1.671703	N	-0.395544	-0.544257	2.208021
H	-0.118341	-2.718568	-0.452514	H	-0.367333	-2.202986	-1.729655	H	-0.693972	0.165424	2.876352
H	1.276431	-1.918048	-0.708630	H	1.109625	-1.516223	-1.587273	H	0.588442	-0.725686	2.402443
H	0.149528	-1.994553	-1.877446	H	-0.001861	-0.868358	-2.587811	H	-0.898913	-1.396217	2.452894
N	-0.304073	-0.568643	1.820171	N	-0.120610	-1.219174	1.844893	N	0.083465	2.106521	-0.797188
H	-1.084670	-0.304146	2.421647	H	-0.892843	-1.243866	2.508792	H	-0.564021	2.559925	-1.440775
H	0.524032	-0.106396	2.204005	H	0.674763	-0.823688	2.345199	H	0.971845	2.020448	-1.290904
H	-0.169307	-1.569488	1.966223	H	0.115884	-2.193856	1.664505	H	0.238552	2.770057	-0.038812
N	-1.188126	1.936896	0.469057	N	-1.119323	1.846292	0.897139	N	-0.853310	-1.477995	-1.709402
H	-1.507024	2.523841	-0.303228	H	-1.512132	2.536816	0.255609	H	-1.084194	-2.404439	-1.352370
H	-0.408841	2.441691	0.894076	H	-0.292275	2.278756	1.311201	H	0.025305	-1.575107	-2.217468
H	-1.944284	1.965115	1.153064	H	-1.802454	1.742474	1.647265	H	-1.566817	-1.256542	-2.402755
N	-2.549933	-0.670842	-0.407101	N	-2.580460	-0.549500	-0.368654	N	-2.880788	0.413700	0.329167
H	-3.219832	-0.221094	0.216561	H	-3.221347	-0.112241	0.292993	H	-3.343394	0.737135	-0.519774
H	-2.680548	-1.671753	-0.261604	H	-2.728572	-1.552636	-0.259564	H	-3.078350	1.121818	1.034729
H	-2.904447	-0.491783	-1.348422	H	-2.945869	-0.314422	-1.292213	H	-3.385116	-0.423498	0.617117
Structure ($TS_{7\text{-}8}$)											
E = −550.686947568				E = −550.640843071				Not available			
H	2.082038	-0.256771	-0.530185	H	-2.101637	0.521309	0.469432				
Ru	-0.368776	-0.033174	0.004053	Ru	0.570045	-0.182921	0.064994				
O	1.420790	0.696338	-0.643156	O	-0.948303	1.124978	0.445003				
C	2.182941	-1.557907	0.035670	C	-3.180138	-0.137208	0.241525				
C	2.156554	1.764080	-0.032462	C	-1.194205	2.266884	-0.368845				
O	0.797833	-1.792476	-0.068275	O	-2.796755	-1.444330	0.093795				
H	2.471314	-1.338577	1.059357	H	-3.501607	0.294289	-0.706527				
H	2.791864	-2.284875	-0.485631	H	-3.845944	0.065855	1.075961				
H	2.892676	2.146819	-0.734623	H	-0.445951	3.024598	-0.136338				
H	2.671297	1.420404	0.867628	H	-2.173037	2.682739	-0.134403				
H	1.463868	2.561752	0.232976	H	-1.150725	2.026386	-1.434809				
N	-2.238043	-0.955069	0.554834	N	2.162200	-1.609100	-0.187330				
H	-2.088029	-1.865194	0.990839	H	1.864905	-2.559245	0.036892				
H	-2.859966	-1.133189	-0.233166	H	2.971414	-1.431954	0.407315				
H	-2.795643	-0.426907	1.226096	H	2.529232	-1.651146	-1.137794				
H	0.610373	-2.489848	-0.712962	H	-3.045611	-1.992908	0.849837				
N	0.170410	0.126421	2.081544	N	-0.432776	-0.921187	-1.690586				
H	0.963005	0.750016	2.236065	H	-0.807055	-0.177115	-2.279463				
H	0.452550	-0.780522	2.456320	H	-1.246093	-1.446344	-1.350524				
H	-0.564097	0.457309	2.707121	H	0.085458	-1.543074	-2.309402				
N	-0.760129	-0.183659	-2.099475	N	1.005530	0.109924	2.146447				
H	0.086133	0.148737	-2.566766	H	0.306950	0.760704	2.509294				
H	-1.520150	0.396647	-2.453474	H	1.919631	0.514398	2.349812				

H	-0.945192	-1.115408	-2.469799	H	0.943715	-0.737574	2.710485	
N	-1.299658	1.878280	0.017091	N	1.906569	1.550842	-0.874118	
H	-0.874988	2.486600	-0.684124	H	2.851283	1.287138	-1.148238	
H	-1.206227	2.378802	0.901069	H	2.007997	2.333498	-0.229570	
H	-2.298692	1.874103	-0.190800	H	1.470976	1.940365	-1.709034	
Structure (TS_{8-9})								
E = −550.649102548				E = −550.612749067			Not available	
Ru	0.050546	0.237808	0.006434	Ru	0.834730	-0.403447	0.076096	
C	2.578117	-1.615620	0.108693	C	-4.288629	-0.083146	-0.197337	
O	1.208017	-1.442545	0.379771	O	-2.939136	-0.024275	0.149307	
H	3.123865	-0.760670	-0.269122	H	-4.802806	-1.019354	-0.026477	
H	2.891090	-2.630629	-0.092642	H	-4.646687	0.629911	-0.927485	
H	1.979691	-1.547607	1.268752	H	-3.801823	0.437527	0.862398	
N	-1.311463	1.803411	-0.518300	N	2.114813	-0.216116	-1.639542	
H	-1.969010	1.479439	-1.228604	H	1.718032	0.458305	-2.296146	
H	-0.874612	2.636109	-0.913383	H	2.219443	-1.088644	-2.158059	
H	-1.887431	2.143622	0.251822	H	3.064151	0.100728	-1.445483	
N	0.685877	0.134435	-2.041787	N	-0.506002	-1.647064	-1.048945	
H	1.503785	-0.459360	-2.185213	H	-1.462137	-1.525842	-0.708508	
H	0.904402	1.014910	-2.507085	H	-0.297693	-2.643825	-0.995874	
H	-0.060016	-0.292493	-2.593244	H	-0.541092	-1.419225	-2.041956	
N	-0.657173	0.192698	2.043001	N	2.169039	0.807112	1.253616	
H	-0.206207	0.835478	2.693615	H	2.646531	0.275329	1.982023	
H	-0.519375	-0.738169	2.437934	H	1.679621	1.565162	1.729601	
H	-1.657055	0.374628	2.131568	H	2.911456	1.260357	0.721877	
N	1.570474	1.649031	0.521557	N	-0.320168	-0.882146	1.823687	
H	1.212386	2.477257	0.997977	H	-0.214920	-1.859828	2.096274	
H	2.092538	2.005519	-0.278908	H	-1.310195	-0.744558	1.603503	
H	2.274991	1.263357	1.151515	H	-0.128015	-0.335328	2.661637	
O	-1.423618	-1.206776	-0.566675	O	-0.553393	1.349918	-0.414061	
C	-2.749248	-1.301011	-0.009601	C	-0.334023	2.768631	-0.383911	
H	-1.042415	-2.092330	-0.645299	H	-1.503259	1.129843	-0.375814	
H	-3.155729	-0.293714	0.031763	H	0.738643	2.933569	-0.458193	
H	-2.720784	-1.732027	0.990108	H	-0.705162	3.200773	0.543717	
H	-3.376559	-1.909546	-0.655270	H	-0.819832	3.246225	-1.231444	
Structure (TS_{10-11})								
E = −550.68052046				Not available			Not available	
Ru	0.046869	0.279940	-0.010481					
H	-0.833829	-2.542296	0.747739					
O	1.119567	-1.203282	-0.726682					
C	-1.131252	-1.480905	0.703540					
C	2.322219	-1.744353	-0.185443					
O	-2.365632	-1.324197	0.046783					
H	0.018639	-1.527087	-0.096253					
H	-1.181653	-1.172533	1.752099					
H	2.137650	-2.222589	0.780327					
H	3.078458	-0.965005	-0.075998					
H	2.693295	-2.498877	-0.874744					
N	1.180960	1.980319	-0.759462					
H	0.644372	2.678578	-1.274506					
H	1.863305	1.612691	-1.426127					
H	1.720468	2.499508	-0.067376					
N	-0.970503	0.093408	-1.855981					
H	-1.196042	0.932905	-2.387229					
H	-1.845196	-0.409697	-1.678961					
H	-0.404828	-0.499910	-2.466753					
N	1.139494	0.362243	1.848555					

H 1.315573 1.304866 2.196357 H 2.056302 -0.077943 1.760045 H 0.676422 -0.128198 2.614857 N -1.547445 1.468488 0.800085 H -2.383450 0.877628 0.746131 H -1.763009 2.310350 0.265330 H -1.458801 1.772807 1.769185 H -2.994738 -2.022352 0.275246		
Structure (TS_{12-13})		
E = −434.983342571		
Ru -0.047238 0.059666 -0.153606 C 1.890085 -0.516105 0.551972 O 1.954734 -0.239662 -0.722657 H 0.815669 -0.472613 -1.434746 N 0.543762 2.094636 0.024314 H 0.436605 2.525930 0.942920 H 0.080426 2.724033 -0.633391 H 1.540206 2.147005 -0.205486 N -0.819851 -0.245031 1.949564 H -0.612798 0.552985 2.550563 H -0.385073 -1.042052 2.414205 H -1.826596 -0.392704 2.020444 N -0.504517 -2.026225 -0.466217 H 0.331309 -2.579249 -0.669797 H -1.120197 -2.181756 -1.265031 H -0.950078 -2.487148 0.327642 N -2.087130 0.584672 -0.707087 H -2.493708 1.354179 -0.174076 H -2.764513 -0.176515 -0.658721 H -2.097527 0.891018 -1.682246 H 2.290467 0.229968 1.235091 H 1.930046 -1.560842 0.856721		
Structure (TS_{13-14})		
E = −435.017372957		
Ru -0.059191 -0.005078 -0.192115 C 2.119033 0.049228 0.297092 O 1.725518 -0.782495 -0.582277 H -0.172234 -0.017257 -1.751347 N 0.286934 2.109272 -0.391157 H 0.603136 2.598973 0.446126 H -0.531704 2.619656 -0.724746 H 0.995817 2.271633 -1.109247 N -0.329725 0.020611 2.122285 H 0.008668 0.869087 2.575538 H 0.176521 -0.743574 2.571111 H -1.294067 -0.084198 2.438091 N -0.564804 -2.070568 -0.301686 H 0.314709 -2.563952 -0.471771 H -1.156358 -2.287996 -1.104191 H -0.993231 -2.508577 0.513692 N -2.132660 0.468453 -0.324556 H -2.435312 1.232257 0.281638 H -2.732523 -0.325736 -0.095235 H -2.385913 0.732187 -1.278520 H 2.572439 0.990377 -0.015441 H 2.297908 -0.289238 1.318815		

Structure (TS_{14-1})		
E = −435.042584313		
Ru -0.029634 0.000039 -0.111517		
O 1.707619 0.000611 0.726173		
C 2.067268 0.000742 -0.541607		
H 2.475126 0.921595 -0.956390		
H 0.717860 0.000174 -1.543604		
H 2.475695 -0.919823 -0.956438		
N 0.021218 2.130628 -0.130526		
H -0.805757 2.605755 0.232123		
H 0.203120 2.530505 -1.051969		
H 0.797635 2.425774 0.467317		
N -1.019699 -0.000460 1.876773		
H -1.593773 0.810188 2.107244		
H -0.257434 0.000034 2.558064		
H -1.592733 -0.811858 2.107241		
N 0.023088 -2.130592 -0.130551		
H 0.801362 -2.425012 0.465219		
H 0.202877 -2.530420 -1.052418		
H -0.802431 -2.606436 0.234418		
N -1.951921 -0.000791 -1.096153		
H -2.762039 0.001533 -0.476151		
H -2.065269 -0.808568 -1.710132		
H -2.063707 0.804015 -1.714320		
Structure (TS_{14-15})		
E = −435.031721966		
Ru -0.121316 0.015766 -0.160728		
O 1.834728 -0.143544 0.522418		
C 2.486340 0.126082 -0.498400		
H 2.423252 1.109960 -0.969946		
H 0.272212 0.163971 -1.691129		
H 3.200030 -0.598367 -0.901561		
N -0.082511 2.145440 -0.055272		
H -0.914575 2.584166 0.340574		
H 0.063639 2.572531 -0.970162		
H 0.692654 2.459271 0.532990		
N -0.638427 -0.183288 2.068326		
H -1.209747 0.550832 2.484633		
H 0.247241 -0.166539 2.576375		
H -1.086419 -1.057623 2.339892		
N -0.067897 -2.109487 -0.343145		
H 0.798404 -2.443657 0.083977		
H -0.043966 -2.430726 -1.311493		
H -0.822125 -2.621337 0.114445		
N -2.125142 0.060116 -0.800711		
H -2.808578 -0.143694 -0.070950		
H -2.281159 -0.624052 -1.543526		
H -2.390984 0.953950 -1.215406		

Table S4. MN15 Spin contamination for the studied species.

	Fe-species			Ru-species	
Structure	S=1/2	S=3/2	S=5/2	S=1/2	S=3/2
1	0.3560	0.0055	0.0021	0.0101	0.0022
2	0.3980	0.0050	0.0021	0.0056	0.0017
3	0.1944	0.0229		0.0056	0.0013
4		0.0779	0.0631	0.0033	0.0047
5		0.1321	0.0582	0.4192 [a]	0.0038
6	0.4174	0.2381	0.0020	0.0021	0.0020
7	0.0603	0.0046	0.0018	0.0042	0.0016
8	0.4139	0.2361	0.0018	0.0021	0.0020
9				0.0038	0.0019
10	0.3554	0.0049		0.0024	
11	0.1704	0.0867		0.0054	
12				0.0101	
13				0.0030	
14				0.0040	
15				0.0040	
16				0.0074	
TS2-3	0.1434	0.0094		0.0059	0.0014
TS4-5		0.0464	0.0641	0.0154	0.0067
TS5-1	0.0299	0.1051	0.0078	0.0030	0.0048
TS2-6	0.4220	0.2137	0.0023	0.0037	0.0028
TS7-8	0.3707	0.2143	0.0022	0.0040	0.0024
TS8-9	0.1675	0.0045	0.0018	0.0041	0.0025
TS10-11	0.1363	0.0285		0.0050	
TS12-13				0.0028	
TS13-14				0.0091	
TS14-1				0.0076	
TS14-15				0.0091	

[a] This is the only structure with high spin contamination. See Table S5 and its footnote a.

Table S5. CASSCF leading coefficients and spin-orbit corrections for the studied Ru-species. The CASSCF active space was 11 electrons in 8 orbitals corresponding largely to the d-orbitals of the metal and the 2p orbitals of oxygen. The spin-orbit corrections (ΔE_{SO} in kcal/mol) were obtained by diagonalizing the Breit-Pauli Hamiltonian using four doublet and two quartet states as basis.

Structure	S=1/2	S=3/2	ΔE_{SO}
1	0.9532	0.9708	-0.46
2	0.9676	0.7718	-0.43
3	0.9695	0.9693	-1.21
4	0.9566	0.8758	-0.44
5	0.7684 [a]	0.9431	-0.02
6	0.9890	0.9297	-0.72
7	0.9720	0.8398	-0.43
8	0.9888	0.9115	-0.56
9	0.9736	0.9708	-0.46
10	0.9705	0.8828	-0.42
11	0.9719	0.9738	-0.83
12	0.9675	0.9624	-0.51
13	0.9510	0.9555	-0.32
14	0.9623	0.9679	-0.29
15	0.9767	0.9788	-1.66
16	0.9694	0.9713	-0.98
TS2-3	0.9800	0.9865	-0.58
TS4-5	0.9234	0.9310	-0.76
TS5-1	0.9226	0.9460	-0.12
TS2-6	0.9805	0.9434	-0.69
TS7-8	0.8995	0.8668	-0.44
TS8-9	0.9787	0.9212	-0.54
TS10-11	0.9792	0.9850	-0.55
TS12-13	0.9566	0.9346	-0.32
TS13-14	0.9478	0.9415	-0.35
TS14-1	0.9705	0.9757	-0.34
TS14-15	0.9736	0.9788	-1.39

[a] This is the only multi-reference case for the S=1/2 state and corresponds to $(NH_3)_4Ru(O)CH_3$ (S=1/2) and O_2 (S=1). The three involved electronic configurations are: $0.77\uparrow\downarrow\downarrow - 0.38\downarrow\uparrow\downarrow - 0.38\downarrow\downarrow\uparrow$ (the first electron is localized on Ru and the other two to O_2). The corresponding quartet is dominated by the corresponding $\uparrow\uparrow\uparrow$ and is quasi-degenerate with the doublet. Despite the high spin contamination (see Table S4), the MN15 energies for the two states are practically the same (see Figure 8 of the manuscript).