

Supporting Information For:

Forming a ruthenium isomerisation catalyst from Grubbs II: A DFT study

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Figure S1. LUMO of A3

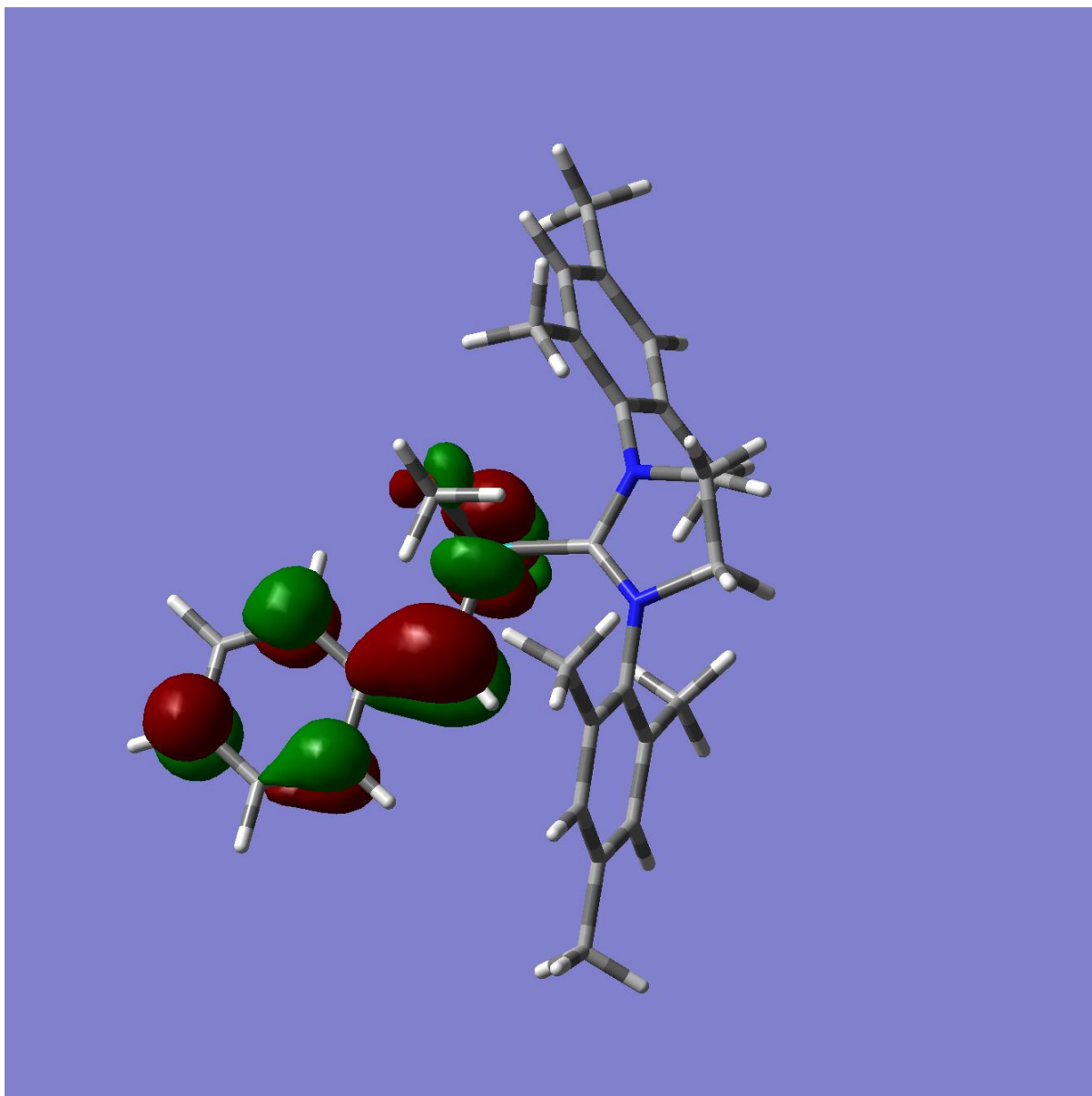


Table S1. Energetic and Thermochemical data for gas-phase optimised geometries. Electronic energies, enthalpies and free energies in Hartrees; zero point energy in kcal/mol; entropy in cal/mol.K; dipole moments in Debye and frequencies in cm^{-1} .

Species	Energy	Zero Point Energy	Enthalpy	Entropy	Gibbs Free Energy	Dipole	Minimum Frequency
A1/B1	-3258.2258	641.97	-3257.1468	301.74	-3257.2901	1.571	18.41
A2	-2211.0711	335.53	-2210.5007	217.96	-2210.6042	4.832	22.01
TSA2→A3	-2326.7623	366.32	-2326.1402	224.83	-2326.2470	5.536	-96.95
A3	-1865.9700	360.13	-1865.3585	225.87	-1865.4658	5.409	22.89
TSA3→A4	-1865.9266	357.55	-1865.3198	222.75	-1865.4257	8.359	-652.51
A4	-1865.9644	360.67	-1865.3529	218.30	-1865.4567	6.410	22.84
TSA4→A5	-1865.9578	359.30	-1865.3487	218.59	-1865.4526	6.183	-205.75
A5	-1865.9836	357.73	-1865.3759	226.76	-1865.4837	6.661	26.61
TSA5→A6	-1865.9667	357.04	-1865.3604	224.55	-1865.4671	5.340	-475.36
A6	-1594.4313	278.06	-1593.9575	195.63	-1594.0504	5.424	16.45
TSA6→A7	-1594.4335	275.80	-1593.9668	173.69	-1594.0493	7.289	-151.36
A7	-1594.4865	276.74	-1594.0143	201.06	-1594.1098	6.600	15.80
A8/B5	-2641.5852	584.68	-2640.6027	279.86	-2640.7357	2.170	13.06
TSA8→A9 (TSB5→B6)	-2641.5609	582.83	-2640.5816	279.34	-2640.7143	4.041	-536.56
A9/B6	-2641.6477	584.34	-2640.6658	282.07	-2640.7998	2.140	13.22
TSB1→B2	-3373.8666	673.86	-3372.7352	301.63	-3372.8785	5.008	-98.57
B2	-2913.1091	667.24	-2911.9889	303.56	-2912.1331	3.028	11.77
TSB2→B3	-2913.0582	664.48	-2911.9440	297.05	-2912.0852	4.827	-869.58
B3	-2913.0863	668.66	-2911.9642	305.60	-2912.1094	5.163	3.71
TSB3→B4	-2913.0717	667.27	-2911.9520	300.70	-2912.0949	4.160	-502.50
B4	-2913.1063	667.49	-2911.9864	297.20	-2912.1276	6.084	22.22
TSB4→B5	-2913.0889	665.36	-2911.9721	301.16	-2912.1152	3.719	-435.39
C2	-1980.0218	283.18	-1979.5390	197.33	-1979.6328	6.195	23.75
TSC2→C3^a	-2095.7164	313.94	-2095.1825	203.60	-2095.2792	5.691	-135.03
C3	-1634.9221	308.80	-1634.3974	200.44	-1634.4927	6.205	26.95
TSC3→C4	-1634.8787	306.15	-1634.3586	198.14	-1634.4528	9.183	-734.45
C4	-1634.9167	308.56	-1634.3929	194.30	-1634.4852	7.191	32.07
TSC4→C5	-1634.9104	307.36	-1634.3881	199.03	-1634.4827	6.884	-255.05
C5	-1634.9442	306.62	-1634.4228	201.39	-1634.5185	7.188	29.59

^aThe optimised geometry of this structure contains two imaginary frequencies. The dominant frequency (-135 cm^{-1}) corresponds to the sigma bond metathesis reaction involving the replacement of the chloride ligand for the methoxide ligand and the formation of HCl. The secondary imaginary frequency (-10.6 cm^{-1}) corresponds to spurious methyl group rotations in the structure that could not be removed.

In order to determine whether the inclusion of solvent via a polarisable continuum model would affect the calculated energetics of the reaction mechanisms. The structures of the methylene analogs (**C2** – **C5**) were reoptimised in the solvent phase using the CPCM solvation method as implemented in G09, with dichloromethane ($\epsilon=8.9$) as the solvent.

The inclusion of solvent via the polarisable continuum model does not significantly affect the calculated energetics for the reaction pathway for the methylene analogs (Figure S1). The largest effect is seen in the transition state from **C2** to **C3**, where the inclusion of solvent stabilises the transition state by $\sim 7 \text{ kcal/mol}$ relative to the gas phase results (Figure S2). Nonetheless, the rate-determining step in the reaction remains the abstraction of the hydride atom from the methoxide in **C3** to the alkylidene carbon (Figure S2). Raw data for optimised solvent phase structures is provided in Table S2 and the coordinates are also available below.

Figure S2. Relative free energy pathways for the conversion of **C2** to **C5** with the inclusion of solvent (bold line) and in the gas phase (normal line, values in parentheses).

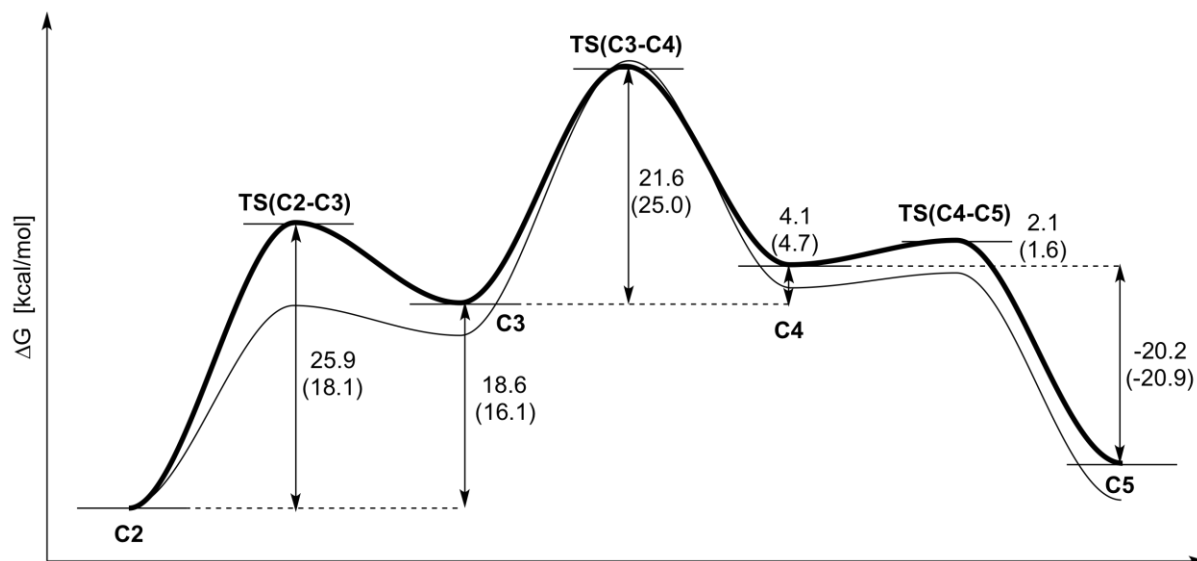


Table S2. Energetic and Thermochemical data for solvent-phase optimised geometries. Electronic energies, enthalpies and free energies in Hartrees; zero point energy in kcal/mol; entropy in cal/mol.K; dipole moments in Debye and frequencies in cm^{-1} .

C2	-1980.0438	282.63	-1979.5616	198.15	-1979.6558	7.827	27.12
TSC2→C3	-2095.7288	313.63	-2095.1945	210.11	-2095.2943	8.120	-194.45
C3	-1634.9421	308.37	-1634.4179	199.78	-1634.5128	8.733	31.83
TSC3→C4	-1634.9041	306.13	-1634.3840	198.38	-1634.4783	13.551	-704.43
C4	-1634.9381	308.87	-1634.4139	194.14	-1634.5062	11.123	26.73
TSC4→C5	-1634.9304	307.19	-1634.4084	198.79	-1634.5029	9.974	-380.88
C5	-1634.9618	305.9391	-1634.4410	204.82	-1634.5384	10.648	34.27

Coordinates for the gas phase optimised geometries of all species mentioned in the text in XYZ format.

A1/B1 (2)

Ru	-0.169719	-0.391429	-0.049821
Cl	0.087661	-0.543840	-2.485393
Cl	-0.054221	-0.344186	2.378132
P	1.366383	1.569120	-0.194793
C	-1.730557	0.526707	-0.364506
H	-1.989637	0.540965	-1.439149
C	-2.697481	1.323480	0.389666
C	-3.680968	1.980247	-0.375082
C	-2.700722	1.525410	1.781954
C	-4.619428	2.816669	0.215546
H	-3.692186	1.830709	-1.454413
C	-3.649350	2.347664	2.371446
H	-1.938971	1.035601	2.383293
C	-4.608558	2.998171	1.594802
H	-5.361265	3.321408	-0.400244
H	-3.636195	2.492164	3.449551
H	-5.340475	3.651497	2.065500
C	-0.961865	-2.306493	-0.110683
C	-2.386678	-4.164559	-0.329004
C	-0.950292	-4.632938	-0.467610
H	-2.850876	-4.494656	0.613703
H	-3.032771	-4.484327	-1.154187
H	-0.691668	-5.466168	0.195903
H	-0.705595	-4.924825	-1.499870
N	-2.237402	-2.703460	-0.325774
N	-0.201005	-3.426685	-0.097028
C	0.510011	2.932899	-1.160130
C	-0.436710	3.759219	-0.281270
C	1.353735	3.857509	-2.041920
H	-0.110321	2.326083	-1.843250
C	-1.336737	4.644688	-1.138089
H	0.147211	4.405185	0.390912
H	-1.043488	3.113203	0.362909
C	0.450914	4.748400	-2.893581
H	2.001711	4.495641	-1.418802
H	2.011227	3.276491	-2.701462
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H	-1.982358	4.004381	-1.762555
H	1.063682	5.409574	-3.520308
H	-0.128287	4.112198	-3.581719
H	-1.158651	6.181735	-2.661372
H	0.071828	6.250794	-1.400140
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C	4.050523	2.066244	-1.199116

C	3.335016	-0.321385	-0.951188
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C	5.079536	1.661732	-2.251119
H	4.526570	2.026526	-0.206971
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H	3.780398	-0.390583	0.055109
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H	4.622438	1.749015	-3.250755
H	4.715994	-1.755271	-1.792695
H	3.879336	-0.754392	-2.983200
H	6.266312	-0.066707	-2.808430
H	6.087390	0.172664	-1.070281
C	1.971200	2.279785	1.420137
C	2.896494	1.302565	2.162199
C	2.618027	3.671681	1.423715
H	1.035266	2.333383	2.006147
C	3.096587	1.759946	3.603450
H	3.876645	1.277570	1.657500
H	2.492150	0.283784	2.144547
C	2.813749	4.149473	2.861726
H	3.597596	3.628805	0.923375
H	2.020425	4.404089	0.868746
C	3.668134	3.172431	3.661684
H	3.754029	1.058309	4.133261
H	2.124142	1.727452	4.119943
H	3.266341	5.150025	2.867397
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H	3.765258	3.509767	4.701933
H	4.686819	3.163808	3.239880
C	1.204850	-3.507401	0.138705
C	1.650071	-3.596773	1.467879
C	2.090830	-3.643875	-0.941232
C	3.023770	-3.667770	1.696324
C	3.449367	-3.769318	-0.657197
C	3.938497	-3.734387	0.646786
H	3.384198	-3.704494	2.724852
H	4.148239	-3.885152	-1.487244
C	-3.424452	-1.914495	-0.276636
C	-3.995211	-1.617604	0.970991
C	-4.043835	-1.553617	-1.479093
C	-5.193710	-0.911517	0.988785
C	-5.243834	-0.845160	-1.408428
C	-5.826321	-0.509646	-0.188132
H	-5.635882	-0.644024	1.950150
H	-5.733317	-0.543397	-2.335516
C	-3.320390	-2.017543	2.246131

H	-3.084352	-3.090090	2.271091
H	-2.366140	-1.487476	2.381880
H	-3.957809	-1.795003	3.107847
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H	-2.413270	-1.497003	-2.896227
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H	-4.038079	-1.517248	-3.624560
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H	-7.901094	-0.294949	0.363246
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H	-7.451106	0.558027	-1.123722
C	1.619659	-3.694430	-2.362677
H	0.720178	-3.090277	-2.521566
H	2.391895	-3.308830	-3.037745
H	1.412170	-4.729084	-2.670366
C	5.414837	-3.762334	0.901417
H	5.923999	-4.478582	0.246287
H	5.860213	-2.776936	0.704783
H	5.643494	-4.024054	1.939781
C	0.682140	-3.675935	2.606811
H	0.188720	-2.711430	2.778082
H	-0.106825	-4.414661	2.409696
H	1.196657	-3.965724	3.528432

A2

Ru	0.240908	0.848671	0.120241
C	-1.547503	0.963655	-0.214543
H	-2.156292	0.105482	-0.515451
C	-2.258823	2.225309	-0.159406
C	-3.626712	2.251767	-0.481825
C	-1.628230	3.430508	0.204156
C	-4.340424	3.440954	-0.446489
H	-4.117440	1.318283	-0.757789
C	-2.342805	4.616295	0.235892
H	-0.570759	3.432711	0.472554
C	-3.699036	4.624139	-0.089265
H	-5.398370	3.448126	-0.697984
H	-1.844710	5.540598	0.517454
H	-4.257050	5.557272	-0.061836
Cl	1.059656	1.508655	-1.965561
Cl	0.241423	1.082216	2.452866
C	0.526866	-1.061639	0.201936
C	1.811923	-2.962649	0.704756
C	0.383609	-3.394300	0.411706
H	2.563165	-3.514783	0.128122
H	2.064568	-3.052539	1.772366
H	0.293457	-3.930449	-0.546808
H	-0.050914	-4.027349	1.193316
N	1.790394	-1.555405	0.307254

N	-0.326134	-2.111012	0.339046
C	-1.730071	-2.123099	0.087292
C	-2.183590	-2.202853	-1.236454
C	-2.614230	-2.055967	1.170179
C	-3.559070	-2.212024	-1.458917
C	-3.981647	-2.065718	0.897573
C	-4.471933	-2.147829	-0.405198
H	-3.927148	-2.260117	-2.484510
H	-4.684470	-2.001181	1.729000
C	2.996999	-0.821882	0.084168
C	3.691521	-0.250619	1.159435
C	3.486223	-0.753101	-1.230458
C	4.841051	0.486049	0.872464
C	4.647615	-0.023570	-1.460747
C	5.325979	0.619883	-0.425842
H	5.378189	0.958830	1.696142
H	5.027439	0.055767	-2.479695
C	2.771039	-1.430807	-2.358601
H	2.516859	-2.471981	-2.118161
H	1.836002	-0.903972	-2.593040
H	3.388785	-1.433191	-3.261993
C	3.284825	-0.468703	2.584763
H	2.219022	-0.688513	2.690337
H	3.858024	-1.300134	3.018408
H	3.490120	0.420320	3.190145
C	6.576330	1.401448	-0.696062
H	6.617428	2.310813	-0.086543
H	7.471586	0.812701	-0.457685
H	6.646106	1.694743	-1.748422
C	-2.106169	-1.911078	2.570550
H	-1.379548	-2.691510	2.828462
H	-1.589940	-0.949681	2.700803
H	-2.928083	-1.962609	3.291027
C	-1.224825	-2.172104	-2.388281
H	-0.755721	-1.181488	-2.482764
H	-0.408602	-2.896132	-2.275531
H	-1.738714	-2.389194	-3.329643
C	-5.947283	-2.186767	-0.668409
H	-6.196321	-1.729648	-1.632242
H	-6.315854	-3.220215	-0.696468
H	-6.508675	-1.664146	0.113304

TSA2→A3

C	-1.192440	-1.028701	-0.831834
H	-1.262580	-0.779989	-1.910976
Ru	0.553682	-0.837921	-0.258514
C	-2.456746	-1.567887	-0.354742
C	-3.512936	-1.652569	-1.287618
C	-2.719744	-1.969754	0.970433

C	-4.772661	-2.103343	-0.917140
H	-3.325933	-1.342791	-2.314871
C	-3.981552	-2.413647	1.338427
H	-1.914703	-1.921575	1.696374
C	-5.014380	-2.480533	0.402088
H	-5.568432	-2.157690	-1.656104
H	-4.163730	-2.712519	2.368006
H	-6.000307	-2.830037	0.698579
Cl	0.448927	-1.612398	1.976476
C	0.417721	1.031774	0.450485
C	-0.119012	3.180679	1.236035
C	1.363916	2.918473	1.503801
H	-0.289938	4.009299	0.534778
H	-0.684047	3.401426	2.148901
H	2.022017	3.641353	1.007267
H	1.610433	2.927130	2.573022
N	1.560282	1.576207	0.949043
N	-0.581044	1.918744	0.642496
Cl	1.375719	-0.595602	-2.863149
O	1.817841	-2.321271	-0.781712
H	1.877889	-1.684232	-2.217494
C	2.209853	-3.437472	-0.030377
H	1.344381	-4.016061	0.319289
H	2.840094	-4.090398	-0.648828
H	2.785573	-3.136857	0.856959
C	-1.946712	1.749019	0.274749
C	-2.328317	1.986066	-1.054721
C	-2.869836	1.352921	1.249499
C	-3.667153	1.808284	-1.393968
C	-4.200202	1.187725	0.861798
C	-4.617224	1.407343	-0.450265
H	-3.973892	1.968182	-2.427312
H	-4.922287	0.840531	1.599523
C	2.846443	1.067638	0.575261
C	3.592392	0.288309	1.469550
C	3.325707	1.369203	-0.717062
C	4.800760	-0.250238	1.010737
C	4.527979	0.804013	-1.124192
C	5.273472	-0.025082	-0.277606
H	5.381396	-0.875008	1.688327
H	4.892181	1.012203	-2.129604
C	-2.418039	1.042649	2.641672
H	-1.574049	0.341016	2.636543
H	-2.080563	1.939847	3.176206
H	-3.227342	0.600194	3.227944
C	-6.046710	1.205093	-0.849102
H	-6.122415	0.686972	-1.810626
H	-6.590337	0.613048	-0.107817
H	-6.573862	2.159899	-0.960267

C	-1.311389	2.366380	-2.084470
H	-0.719758	3.238638	-1.782035
H	-0.594614	1.550153	-2.249788
H	-1.783205	2.596486	-3.042795
C	2.573405	2.300636	-1.617598
H	1.523159	2.011893	-1.720083
H	2.587743	3.330946	-1.237836
H	3.010236	2.313610	-2.618623
C	3.163524	0.054894	2.883309
H	3.188836	-1.010336	3.128482
H	3.841160	0.567729	3.576633
H	2.143822	0.395299	3.065550
C	6.555307	-0.638079	-0.752101
H	7.294774	0.125551	-1.016716
H	7.000043	-1.282125	0.010007
H	6.397327	-1.244495	-1.649932

A3

C	0.505934	-0.964929	0.329589
N	-0.338285	-2.024533	0.507142
C	0.390749	-3.269721	0.775372
C	1.760473	-2.758438	1.187211
N	1.766045	-1.412070	0.618154
C	5.386399	0.487808	-0.453228
C	4.863553	0.648377	0.823342
C	3.671808	0.035127	1.220894
C	2.987468	-0.744512	0.281199
C	3.521141	-0.973601	-1.002930
C	4.708760	-0.343597	-1.348394
C	-4.430484	-2.276742	-0.485647
C	-3.453508	-2.322990	-1.481264
C	-2.094361	-2.250565	-1.186377
C	-1.719549	-2.115740	0.160173
C	-2.671491	-2.087305	1.185711
C	-4.020654	-2.167586	0.840926
C	3.188850	0.236670	2.622763
C	2.827613	-1.866644	-1.984074
C	6.653743	1.171794	-0.866860
C	-1.082530	-2.238850	-2.290083
C	-2.269360	-1.881513	2.613193
C	-5.883755	-2.343376	-0.847558
Ru	0.253316	0.900270	-0.060726
C	-1.567504	0.993428	-0.117625
Cl	0.891389	1.032109	-2.330846
H	-6.113068	-3.254986	-1.412439
H	-6.521873	-2.329773	0.041754
H	-6.173273	-1.496070	-1.481103
H	-4.770732	-2.134690	1.631953
H	-1.989897	-0.832823	2.782753

H	-1.399182	-2.483445	2.900885
H	-3.093335	-2.123280	3.291705
H	-3.759740	-2.413088	-2.524462
H	-1.526990	-2.590419	-3.226298
H	-0.698497	-1.222336	-2.459503
H	-0.211417	-2.868831	-2.072031
H	0.425046	-3.892154	-0.133757
H	-0.111992	-3.848138	1.559065
H	1.868925	-2.708606	2.283454
H	2.589727	-3.353461	0.788598
H	1.923680	-1.376682	-2.367707
H	2.527057	-2.823996	-1.537571
H	3.478666	-2.083422	-2.836502
H	2.444865	-0.508227	2.920788
H	4.027348	0.194483	3.326882
H	2.703899	1.215483	2.714965
H	5.397911	1.265134	1.547378
H	6.458436	1.929770	-1.635246
H	7.136477	1.672202	-0.021226
H	7.370357	0.460672	-1.295121
H	5.122051	-0.505132	-2.344757
H	-2.224916	0.118258	-0.117932
C	-2.262179	2.269291	-0.146016
C	-3.673257	4.690253	-0.165171
C	-1.580655	3.497631	-0.235721
C	-3.665926	2.285339	-0.074767
C	-4.364627	3.484007	-0.083396
C	-2.281256	4.693423	-0.242652
H	-0.492608	3.512087	-0.311248
H	-4.195564	1.334177	-0.010466
H	-5.450812	3.480800	-0.027599
H	-1.742442	5.635057	-0.315294
H	-4.219387	5.630774	-0.175111
C	0.002671	1.075972	2.876324
O	0.592292	1.590182	1.732380
H	0.396824	1.594913	3.765460
H	0.200498	-0.007131	3.013334
H	-1.096567	1.211835	2.867031

TSA3→A4

C	0.572678	-0.909641	0.002725
N	-0.319363	-1.900720	-0.281668
C	0.296458	-3.230391	-0.301648
C	1.781918	-2.910122	-0.300380
N	1.813060	-1.479452	0.032070
C	5.540052	0.371557	-0.671113
C	5.191065	-0.054789	0.608434
C	3.955856	-0.647548	0.877694
C	3.059813	-0.800485	-0.183896

C	3.376175	-0.389671	-1.488593
C	4.623303	0.185630	-1.707810
C	-4.533924	-1.709689	-0.289454
C	-3.799469	-1.554211	-1.469609
C	-2.407690	-1.604120	-1.476770
C	-1.741825	-1.819679	-0.258433
C	-2.444225	-2.000656	0.940147
C	-3.839981	-1.932724	0.898380
C	3.601897	-1.054033	2.273378
C	2.374900	-0.497548	-2.595214
C	6.854412	1.043105	-0.925830
C	-1.624309	-1.369664	-2.730496
C	-1.745462	-2.271966	2.238741
C	-6.028581	-1.607695	-0.299970
Ru	0.317973	0.942276	0.614970
C	-1.587440	0.771364	0.603527
Cl	1.890555	2.334125	-0.646559
H	-6.454368	-1.998879	-1.228154
H	-6.478126	-2.150439	0.535664
H	-6.354246	-0.564472	-0.216176
H	-4.398885	-2.061138	1.824629
H	-2.159427	-1.655548	3.042917
H	-0.673769	-2.062600	2.185944
H	-1.870451	-3.317480	2.545252
H	-4.324643	-1.379211	-2.408134
H	-2.283669	-1.253458	-3.594041
H	-1.012392	-0.462314	-2.645517
H	-0.927391	-2.188141	-2.942617
H	-0.030486	-3.795763	-1.181659
H	-0.014374	-3.795308	0.589078
H	2.351724	-3.485483	0.437289
H	2.252830	-3.071149	-1.279460
H	1.558885	0.216543	-2.424590
H	1.924235	-1.494589	-2.676780
H	2.829125	-0.257623	-3.559422
H	2.898333	-1.892262	2.299399
H	4.491847	-1.333154	2.843953
H	3.125482	-0.214622	2.792668
H	5.896144	0.080183	1.427680
H	6.753851	2.132811	-0.865696
H	7.610525	0.749493	-0.192371
H	7.240729	0.814742	-1.923475
H	4.874142	0.525404	-2.711658
H	-2.061149	-0.109560	1.046629
C	-2.619130	1.705899	0.199592
C	-4.764118	3.314820	-0.658527
C	-2.429513	3.076842	-0.078986
C	-3.929343	1.183049	0.076763
C	-4.980866	1.967109	-0.369685

C	-3.493298	3.864261	-0.496074
H	-1.443810	3.511082	0.039152
H	-4.093025	0.134137	0.323825
H	-5.972742	1.536662	-0.479416
H	-3.328303	4.918344	-0.701221
H	-5.588397	3.938435	-0.994766
C	0.534834	0.624263	2.723088
O	1.305360	1.404970	2.109454
H	-0.311017	0.990558	3.323937
H	0.834715	-0.416105	2.944014
H	-0.656034	0.232471	1.787621

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C	3.540960	4.112135	-1.670395
C	4.135310	4.628977	-0.540578
C	3.996382	3.960153	0.694391
C	3.304337	2.774286	0.783325
C	2.676613	2.201875	-0.360343
C	2.812052	2.905450	-1.594269
C	2.051601	0.904391	-0.415077
Ru	0.021782	0.983813	0.227823
C	-0.637553	-0.855821	0.145374
N	0.097138	-2.005654	0.313793
C	-0.740219	-3.171431	0.610199
C	-2.109178	-2.700114	0.179386
N	-1.953671	-1.241673	0.177365
C	1.473704	-2.230536	0.019000
C	2.435077	-2.310508	1.033973
C	3.767703	-2.509883	0.652328
C	4.148453	-2.672588	-0.676769
C	3.144886	-2.696403	-1.651891
C	1.806995	-2.501047	-1.322335
C	-3.146391	-0.513195	-0.125000
C	-3.438958	-0.193824	-1.455212
C	-4.669703	0.407695	-1.737360
C	-5.600963	0.672963	-0.736601
C	-5.277927	0.325450	0.579946
C	-4.064058	-0.269697	0.909255
C	-6.915636	1.318688	-1.053190
C	-2.446743	-0.467977	-2.541164
C	-3.712685	-0.597934	2.324326
C	5.587984	-2.836352	-1.057013
C	2.087925	-2.255085	2.487899
C	0.731484	-2.629767	-2.359143
Cl	0.711076	0.679860	2.469815
H	6.208268	-3.088448	-0.193211
H	5.722452	-3.619038	-1.810110
H	5.991924	-1.912880	-1.487317
H	3.410558	-2.887752	-2.691670

H	0.046285	-1.776619	-2.356631
H	0.122263	-3.527085	-2.186822
H	1.157781	-2.716337	-3.362673
H	4.528894	-2.547815	1.430860
H	2.364296	-3.199407	2.972181
H	2.629040	-1.452903	2.996150
H	1.028625	-2.063198	2.655463
H	-0.692920	-3.399669	1.684933
H	-0.386564	-4.050324	0.062067
H	-2.383285	-3.047612	-0.829826
H	-2.910290	-2.997397	0.862559
H	-2.773473	-0.108872	2.599805
H	-3.574699	-1.675246	2.480569
H	-4.495152	-0.266940	3.011366
H	-2.252914	-1.541795	-2.660297
H	-2.793855	-0.086458	-3.504917
H	-1.479789	0.002779	-2.320478
H	-4.901815	0.670026	-2.769034
H	-7.757919	0.705773	-0.714543
H	-7.035814	1.484857	-2.126902
H	-7.016603	2.289110	-0.555034
H	-5.990196	0.535061	1.376995
H	2.153682	2.636292	-2.424166
H	3.174837	2.274981	1.739008
H	4.443599	4.388342	1.588770
H	3.609377	4.633497	-2.621587
H	4.696512	5.557559	-0.593130
H	2.400746	0.144718	0.279717
H	2.118869	0.714416	-1.490289
C	-1.742594	2.202227	0.046173
H	-2.345023	1.911428	-0.833786
H	-1.436343	3.269621	0.047297
O	-1.853188	1.577557	1.160014

TSA4→A5

C	3.241167	2.789526	0.964343
C	3.195987	3.634610	-0.150795
C	1.969124	3.937902	-0.727829
C	0.785408	3.398932	-0.216936
C	0.806043	2.553698	0.927214
C	2.077028	2.257731	1.495331
C	-0.402785	1.843292	1.312778
Ru	0.213451	0.782684	-0.398847
C	-0.414299	-1.009157	0.161228
N	-1.609341	-1.461171	0.607802
C	-1.556567	-2.855590	1.070202
C	-0.124528	-3.281526	0.755990
N	0.470155	-2.043641	0.245303
C	-2.891510	-0.861321	0.411297

C	-3.515532	-1.036514	-0.835670
C	-4.783844	-0.497136	-1.012579
C	-5.430742	0.210488	0.006254
C	-4.786819	0.347701	1.232643
C	-3.518157	-0.193343	1.465233
C	1.881686	-1.841780	0.220951
C	2.486028	-1.251424	1.346061
C	3.851741	-0.977272	1.294942
C	4.619590	-1.302517	0.174927
C	4.000019	-1.968618	-0.885160
C	2.634821	-2.261424	-0.884222
C	6.067450	-0.926071	0.107352
C	1.691901	-1.000228	2.593869
C	2.005505	-3.009224	-2.016210
C	-6.779921	0.818213	-0.229782
C	-2.798860	-1.733645	-1.949130
C	-2.881365	-0.062282	2.815489
Cl	-1.709795	1.520679	-1.507573
H	-7.474723	0.100965	-0.678523
H	-7.227077	1.184289	0.698190
H	-6.715660	1.666733	-0.919844
H	-5.284032	0.886831	2.038220
H	-1.841375	-0.398033	2.809775
H	-3.421035	-0.649868	3.567680
H	-2.892216	0.976910	3.159147
H	-5.272824	-0.610076	-1.979258
H	-2.404357	-2.712053	-1.645903
H	-3.458779	-1.890134	-2.805681
H	-1.944107	-1.133575	-2.286027
H	-2.306837	-3.452743	0.539730
H	-1.795393	-2.902767	2.141620
H	0.420355	-3.632365	1.640481
H	-0.070143	-4.073269	-0.003056
H	0.961846	-2.720386	-2.149351
H	2.050341	-4.092102	-1.841203
H	2.527127	-2.811397	-2.955717
H	1.339819	-1.941538	3.035137
H	2.295942	-0.494949	3.351890
H	0.801677	-0.391658	2.406273
H	4.327010	-0.500917	2.152337
H	6.622651	-1.563772	-0.585648
H	6.550412	-0.986668	1.087013
H	6.185987	0.107043	-0.241683
H	4.595132	-2.257686	-1.750296
H	2.116746	1.621681	2.376616
H	-0.174233	3.657419	-0.657239
H	1.921958	4.596344	-1.591445
H	4.198122	2.546898	1.421753
H	4.112840	4.051252	-0.557274

H	-1.353552	2.349808	1.135661
H	-0.360744	1.337898	2.280423
C	1.738432	0.700762	-1.885201
H	1.868011	0.493192	-0.628808
H	2.377931	1.055880	-2.713423
O	0.921269	-0.214478	-2.252589

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C	-0.410776	-1.342426	-0.074981
N	0.494368	-2.325334	-0.180538
C	-0.131628	-3.657595	-0.178247
C	-1.602797	-3.326181	-0.406148
N	-1.636867	-1.893127	-0.099211
C	-5.144350	0.444718	-0.113862
C	-4.413479	0.268600	-1.283608
C	-3.258825	-0.516246	-1.319342
C	-2.836492	-1.114081	-0.123978
C	-3.574203	-0.993496	1.067873
C	-4.719322	-0.207298	1.046709
C	4.684968	-1.906049	-0.175811
C	3.987433	-2.066467	1.021387
C	2.601425	-2.208268	1.054848
C	1.914908	-2.178067	-0.165425
C	2.579695	-2.033919	-1.387911
C	3.966504	-1.901482	-1.370488
C	-2.542133	-0.698505	-2.625147
C	-3.124577	-1.668593	2.325275
C	-6.362982	1.316382	-0.087578
C	1.875491	-2.353316	2.357287
C	1.816203	-1.971487	-2.676016
C	6.172120	-1.719529	-0.173728
Ru	-0.319915	0.712611	0.034188
Cl	-0.434387	0.605158	2.466297
H	6.649086	-2.294280	0.627594
H	6.617818	-2.025943	-1.125928
H	6.433881	-0.665888	-0.014649
H	4.498296	-1.783632	-2.315362
H	1.244753	-1.034431	-2.745432
H	1.087268	-2.787116	-2.768885
H	2.491333	-2.019422	-3.535805
H	4.539323	-2.078369	1.961984
H	2.579534	-2.335589	3.194598
H	1.148753	-1.542098	2.511129
H	1.321896	-3.299600	2.416649
H	0.040600	-4.150361	0.789182
H	0.304062	-4.286850	-0.962502
H	-1.918202	-3.488869	-1.448944
H	-2.281977	-3.885784	0.246039
H	-2.189189	-1.216081	2.685959

H	-2.937423	-2.739492	2.173723
H	-3.880432	-1.567045	3.109877
H	-1.666706	-1.350882	-2.542374
H	-3.219847	-1.127639	-3.373482
H	-2.197562	0.267671	-3.014058
H	-4.746030	0.753697	-2.202331
H	-6.154690	2.263810	0.424648
H	-6.708535	1.557256	-1.097953
H	-7.187665	0.835396	0.450960
H	-5.296716	-0.093799	1.964846
C	2.061712	2.523650	0.069184
C	2.565892	5.279341	0.214735
C	2.031758	3.192128	1.302163
C	2.347580	3.263841	-1.086079
C	2.596302	4.628104	-1.016360
C	2.284500	4.556047	1.371899
H	1.784181	2.625270	2.199428
H	2.362456	2.750357	-2.048229
H	2.816060	5.187042	-1.923500
H	2.258075	5.060495	2.335482
H	2.759677	6.348063	0.272245
C	1.756673	1.084728	-0.028230
H	2.203076	0.632399	-0.919463
H	2.054447	0.524612	0.867448
H	0.017716	0.335212	-1.475754
C	-0.959174	2.060871	-1.039006
H	-0.517948	2.540304	0.025870
O	-1.478203	2.680726	-1.901574

TSA5→A6

C	-0.501855	-1.313983	-0.068493
N	0.365125	-2.329695	-0.183434
C	-0.311968	-3.636585	-0.202878
C	-1.767956	-3.245255	-0.433249
N	-1.748193	-1.816341	-0.106403
C	-5.162435	0.655727	-0.105284
C	-4.432626	0.467600	-1.273823
C	-3.309037	-0.360858	-1.314957
C	-2.916616	-0.991097	-0.126063
C	-3.655529	-0.858497	1.063766
C	-4.769230	-0.028271	1.048074
C	4.568726	-2.073321	-0.152470
C	3.859055	-2.223117	1.038957
C	2.468436	-2.311518	1.063692
C	1.790198	-2.237843	-0.159357
C	2.466654	-2.102683	-1.376456
C	3.857436	-2.024373	-1.350441
C	-2.592899	-0.552688	-2.619695
C	-3.239162	-1.567850	2.313740

C	-6.346542	1.573541	-0.072691
C	1.730414	-2.446312	2.360426
C	1.713114	-1.992882	-2.667252
C	6.061951	-1.944652	-0.140547
Ru	-0.332116	0.734278	0.069941
Cl	-0.499761	0.595938	2.433643
H	6.511982	-2.548495	0.654938
H	6.500588	-2.254916	-1.094777
H	6.363433	-0.904255	0.034570
H	4.398482	-1.914173	-2.290974
H	1.178742	-1.033502	-2.726287
H	0.953669	-2.778270	-2.775096
H	2.390513	-2.055060	-3.524339
H	4.404986	-2.269420	1.981964
H	2.430086	-2.467482	3.201314
H	1.034797	-1.609731	2.522105
H	1.140296	-3.371149	2.403815
H	-0.164165	-4.148994	0.758366
H	0.103268	-4.271352	-0.993760
H	-2.083789	-3.381150	-1.479745
H	-2.471796	-3.787070	0.207715
H	-2.288921	-1.156981	2.685277
H	-3.092780	-2.643001	2.148087
H	-3.994743	-1.447933	3.096009
H	-1.743837	-1.239602	-2.541833
H	-3.282665	-0.944828	-3.377261
H	-2.209098	0.404688	-2.993332
H	-4.741189	0.977889	-2.187253
H	-6.104504	2.505003	0.453784
H	-6.677055	1.841586	-1.081253
H	-7.192117	1.117490	0.455033
H	-5.346746	0.094820	1.964898
C	2.206332	2.458270	0.121485
C	2.815996	5.190063	0.308136
C	2.195619	3.110287	1.363562
C	2.526865	3.202730	-1.021876
C	2.827822	4.555228	-0.931814
C	2.500580	4.462285	1.453657
H	1.921449	2.541097	2.251572
H	2.527049	2.702414	-1.991053
H	3.073941	5.117720	-1.829943
H	2.488498	4.954001	2.424083
H	3.050686	6.249568	0.381577
C	1.846360	1.033743	0.002409
H	2.279726	0.576818	-0.892905
H	2.117394	0.450166	0.891575
H	0.815903	0.552092	-1.197836
C	-0.582742	1.954212	-1.284514
H	0.308990	2.363813	-0.532709

O -0.861539 2.481232 -2.305375

A6

C	2.868791	1.462260	-0.027224
C	2.432819	0.381310	0.753705
C	3.293611	-0.667251	1.106351
C	4.598483	-0.633650	0.621870
C	5.057556	0.407527	-0.184487
C	4.184007	1.450038	-0.487639
N	1.090222	0.379437	1.233159
C	0.002418	0.189789	0.439966
N	-1.091949	0.568091	1.150844
C	-0.747699	1.130701	2.460072
C	0.737604	0.797202	2.590815
C	-2.445804	0.352924	0.768632
C	-2.997044	-0.927307	0.929052
C	-4.319827	-1.122704	0.539329
C	-5.095104	-0.085062	0.018630
C	-4.518318	1.177253	-0.111271
C	-3.196669	1.422016	0.261128
C	-2.176725	-2.058078	1.467076
C	-2.587328	2.779047	0.084298
C	-6.525724	-0.320590	-0.361982
C	2.825918	-1.788613	1.980099
C	6.456414	0.395085	-0.722883
C	1.956603	2.602505	-0.368760
H	-0.936160	2.214975	2.475665
H	-1.360437	0.670025	3.244206
H	1.345808	1.659106	2.892230
H	0.920056	-0.017807	3.307383
H	4.536682	2.283219	-1.096875
H	5.275338	-1.449498	0.878353
H	-4.759656	-2.114944	0.648886
H	-5.110078	1.996368	-0.521377
H	-2.371415	3.258812	1.048078
H	-3.264154	3.439989	-0.465516
H	-1.644917	2.719021	-0.474775
H	-1.453755	-2.413466	0.718406
H	-2.813141	-2.900889	1.753724
H	-1.588926	-1.759232	2.345640
H	2.533077	3.479764	-0.679387
H	1.322291	2.893650	0.479693
H	1.279136	2.337649	-1.192433
H	1.853628	-2.168756	1.643313
H	2.721960	-1.468090	3.025988
H	3.538536	-2.618673	1.962041
H	-6.663353	-1.308466	-0.815179
H	-7.180103	-0.276721	0.518078
H	-6.882799	0.432723	-1.071847

H	6.794669	1.402328	-0.988256
H	6.522567	-0.220628	-1.628769
H	7.163674	-0.022918	0.002120
Ru	0.178581	-0.512919	-1.333803
Cl	0.756825	-2.686789	-0.826566
C	-1.461271	0.108232	-1.936448
H	-2.517280	-0.205886	-2.028469
O	-1.003625	1.181715	-2.356494

TSA6→A7

Ru	0.789602	-0.536502	-0.735192
C	-0.415425	0.198327	-1.924937
O	-1.141807	0.848412	-2.601726
Cl	1.939818	-2.632368	-0.333602
C	-0.191309	0.236417	0.724808
C	-1.251419	1.376468	2.419320
C	0.254774	1.655093	2.508531
H	-1.861138	2.284052	2.454588
H	-1.594112	0.704808	3.218614
H	0.512356	2.658814	2.141974
H	0.642097	1.544494	3.525005
N	0.771268	0.617952	1.604467
N	-1.388770	0.709107	1.107637
C	-2.641044	0.250163	0.596470
C	-3.460694	1.175256	-0.066328
C	-3.012926	-1.092738	0.756188
C	-4.684979	0.731922	-0.559591
C	-4.246689	-1.488965	0.233807
C	-5.094145	-0.597011	-0.422282
H	-5.328772	1.439527	-1.079900
H	-4.554463	-2.526858	0.351759
C	1.985819	0.532359	0.810567
C	2.001902	1.288891	-0.431171
C	3.153557	-0.105231	1.339023
C	3.199245	1.117604	-1.209104
C	4.271925	-0.154031	0.547312
C	4.288921	0.408650	-0.760128
H	3.246243	1.618968	-2.175145
H	5.150214	-0.689217	0.902020
C	3.074191	-0.785620	2.661627
H	2.842118	-0.089257	3.476275
H	2.274089	-1.534855	2.640947
H	4.010163	-1.293936	2.902100
C	5.495138	0.208726	-1.619777
H	6.414803	0.494710	-1.097833
H	5.604272	-0.848922	-1.886669
H	5.435935	0.782378	-2.547923
C	1.236036	2.575003	-0.626793
H	0.224777	2.549190	-0.210977

H	1.772976	3.415147	-0.166200
H	1.132704	2.794912	-1.693652
C	-2.117572	-2.078968	1.440890
H	-1.351773	-2.473016	0.760526
H	-1.573547	-1.638021	2.282722
H	-2.689203	-2.930378	1.818191
C	-2.991860	2.576033	-0.303021
H	-2.728152	3.098797	0.623848
H	-2.096215	2.572537	-0.933916
H	-3.757338	3.167575	-0.810066
C	-6.398654	-1.058786	-0.996258
H	-6.781208	-1.940838	-0.475616
H	-7.162597	-0.278098	-0.947046
H	-6.290091	-1.331754	-2.052270
H	-0.485314	-1.088472	-1.887495

A7

C	-0.071530	0.260881	0.457895
N	0.980185	0.510632	1.270193
N	-1.198762	0.620151	1.110479
C	0.588732	1.211632	2.493544
H	1.092543	0.786977	3.369391
H	0.865895	2.275053	2.422315
C	-0.921960	1.000989	2.501822
H	-1.225776	0.187158	3.177734
H	-1.487283	1.898057	2.778317
C	-2.534532	0.309956	0.707997
C	-5.158035	-0.246711	-0.039118
C	-3.335775	1.346208	0.214686
C	-3.015327	-0.998934	0.845919
C	-4.330795	-1.251015	0.461641
C	-4.644373	1.044240	-0.154396
H	-4.719184	-2.266018	0.555352
H	-5.278911	1.839035	-0.548058
C	2.338260	0.399416	0.841459
C	4.986432	0.138639	0.016056
C	3.049155	-0.764781	1.181836
C	2.934437	1.445822	0.126762
C	4.260737	1.287537	-0.280447
C	4.367093	-0.872241	0.755543
H	4.737053	2.091961	-0.842850
H	4.929921	-1.772581	1.004621
C	2.396509	-1.867131	1.956622
H	1.841483	-1.489397	2.824500
H	3.141748	-2.584136	2.314094
H	1.681906	-2.410593	1.322447
C	2.215046	2.724429	-0.189468
H	1.156449	2.700131	0.089719
H	2.259985	2.945568	-1.262066

H	2.682221	3.569101	0.332763
C	-2.145031	-2.114803	1.337551
H	-1.467794	-1.803484	2.142988
H	-1.508162	-2.499700	0.528421
H	-2.752496	-2.945809	1.709452
C	-2.790195	2.733363	0.059785
H	-1.974641	2.761977	-0.673958
H	-2.384276	3.125126	1.001719
H	-3.569369	3.422886	-0.278980
C	6.402598	-0.023522	-0.446552
H	6.475034	-0.786278	-1.231441
H	7.055562	-0.346037	0.372848
H	6.803597	0.910353	-0.853268
C	-6.578093	-0.545438	-0.415086
H	-6.672509	-1.537713	-0.869480
H	-6.969425	0.191469	-1.124147
H	-7.232166	-0.530992	0.466292
Ru	0.184906	-0.525612	-1.306494
Cl	0.728819	-2.794228	-1.126771
H	-1.347347	-0.691144	-1.476548
C	-0.108209	1.143432	-2.004441
O	-0.320083	2.187571	-2.481712

A8 (B5)

Ru	0.594001	0.027705	-0.188821
P	-1.405472	1.420085	-0.143065
C	0.506121	-0.173747	1.653928
H	0.032256	-0.753721	2.459584
O	1.327909	0.742478	1.872326
Cl	-0.554631	-1.174290	-1.912211
C	1.965517	-1.468864	-0.259248
C	2.661752	-3.723203	-0.323076
C	3.885710	-2.822786	-0.436059
H	2.618715	-4.253059	0.640716
H	2.603189	-4.474688	-1.117506
H	4.662725	-3.049529	0.302663
H	4.349430	-2.867635	-1.431769
N	3.318577	-1.489212	-0.205695
N	1.556431	-2.760743	-0.419323
C	-2.696533	0.618340	-1.210538
C	-3.035755	-0.790872	-0.714778
C	-3.959910	1.402171	-1.580086
H	-2.121006	0.488723	-2.141803
C	-3.859632	-1.547155	-1.751031
H	-3.603604	-0.728740	0.227967
H	-2.109432	-1.338901	-0.482773
C	-4.773371	0.630451	-2.617860
H	-4.583072	1.580057	-0.693119
H	-3.695493	2.388073	-1.981645

C	-5.116481	-0.771556	-2.129301
H	-4.121605	-2.543387	-1.374646
H	-3.236362	-1.708401	-2.644224
H	-5.684346	1.185515	-2.871676
H	-4.187340	0.554458	-3.545111
H	-5.690493	-1.313346	-2.890196
H	-5.769252	-0.695642	-1.245992
C	-1.279978	3.138829	-0.880107
C	-2.255696	4.187988	-0.337392
C	0.159471	3.660921	-0.811037
H	-1.512554	2.967286	-1.944575
C	-2.092264	5.530058	-1.046430
H	-2.076166	4.323929	0.740429
H	-3.290991	3.845949	-0.437198
C	0.311675	5.010046	-1.504742
H	0.457207	3.754070	0.246522
H	0.832338	2.920628	-1.257615
C	-0.661749	6.042420	-0.952584
H	-2.796679	6.259953	-0.630262
H	-2.364319	5.407916	-2.105750
H	1.345838	5.362683	-1.413923
H	0.124785	4.878446	-2.580832
H	-0.558136	6.996705	-1.481810
H	-0.418933	6.244792	0.101410
C	-2.057920	1.594232	1.602852
C	-3.546302	1.912393	1.787028
C	-1.702877	0.344958	2.427367
H	-1.467993	2.432011	2.015962
C	-3.886681	2.116565	3.261277
H	-4.137239	1.067724	1.402056
H	-3.847672	2.788551	1.207161
C	-2.058015	0.524870	3.899461
H	-2.244075	-0.523813	2.020071
H	-0.636161	0.123996	2.324392
C	-3.525116	0.889153	4.087621
H	-4.950827	2.357668	3.370726
H	-3.331926	2.988219	3.640087
H	-1.809529	-0.388039	4.456002
H	-1.427958	1.322310	4.320339
H	-3.751892	1.055291	5.147254
H	-4.151741	0.043892	3.765135
C	0.219618	-3.176693	-0.129011
C	-0.257429	-3.103879	1.195210
C	-0.563923	-3.712636	-1.160791
C	-1.553969	-3.544775	1.452323
C	-1.847641	-4.164166	-0.845137
C	-2.365704	-4.076769	0.446313
H	-1.936646	-3.477508	2.470993
H	-2.467959	-4.574962	-1.641120

C	4.168016	-0.350156	-0.082829
C	4.634231	-0.006977	1.194394
C	4.526009	0.386223	-1.222502
C	5.467674	1.105383	1.315530
C	5.359361	1.491646	-1.049977
C	5.840814	1.866469	0.206904
H	5.826118	1.388737	2.304271
H	5.639262	2.076670	-1.925309
C	3.990161	0.023135	-2.569309
H	4.097692	-1.046495	-2.781351
H	2.915602	0.235105	-2.638436
H	4.501324	0.577057	-3.360474
C	6.759221	3.041242	0.354212
H	7.790279	2.776544	0.092094
H	6.469621	3.866653	-0.302856
H	6.774147	3.415949	1.381061
C	4.194705	-0.777570	2.399266
H	3.135727	-0.581669	2.606699
H	4.300669	-1.859914	2.263445
H	4.768731	-0.489111	3.283076
C	-0.051397	-3.758022	-2.564048
H	0.181281	-2.745147	-2.915241
H	0.872199	-4.342221	-2.648833
H	-0.788822	-4.201504	-3.237794
C	0.602555	-2.583367	2.307001
H	1.580908	-3.078325	2.333824
H	0.805765	-1.509551	2.198987
H	0.121788	-2.736163	3.277100
C	-3.766899	-4.511286	0.749926
H	-4.215950	-5.046943	-0.090854
H	-3.810297	-5.163867	1.627918
H	-4.408921	-3.648887	0.968543

TSA8→A9 (TSB5→B6)

Ru	0.540826	-0.120566	-0.105020
P	-1.322765	1.410521	-0.156981
C	1.240965	0.693145	1.414634
H	0.259035	-0.728077	1.751593
O	1.899851	1.561686	1.938809
Cl	-0.727625	-1.736547	-1.608521
C	1.901280	-1.647087	-0.225106
C	2.458295	-3.939102	-0.261226
C	3.736767	-3.105624	-0.159051
H	2.362346	-4.682283	0.538035
H	2.375712	-4.466996	-1.221476
H	4.224362	-3.209114	0.821374
H	4.475173	-3.352883	-0.928061
N	3.246276	-1.729666	-0.332345
N	1.423458	-2.907979	-0.147015

C	-2.562718	0.903643	-1.441655
C	-3.177300	-0.454930	-1.100666
C	-3.641713	1.900413	-1.871477
H	-1.897418	0.748985	-2.307471
C	-3.962272	-1.013551	-2.280869
H	-3.857551	-0.349659	-0.240687
H	-2.386532	-1.152071	-0.791227
C	-4.438341	1.336379	-3.048183
H	-4.323606	2.115159	-1.035769
H	-3.190659	2.856537	-2.162937
C	-5.037006	-0.029053	-2.728502
H	-4.411305	-1.979587	-2.015436
H	-3.266225	-1.210484	-3.110769
H	-5.224628	2.041330	-3.343400
H	-3.766956	1.240191	-3.913597
H	-5.583876	-0.419143	-3.594706
H	-5.776877	0.081729	-1.920809
C	-0.891048	3.159842	-0.659744
C	-1.812705	4.258386	-0.118711
C	0.574074	3.493115	-0.355643
H	-0.990290	3.124888	-1.757545
C	-1.419940	5.633537	-0.651162
H	-1.753545	4.267549	0.980941
H	-2.858576	4.052254	-0.369577
C	0.955419	4.876004	-0.872342
H	0.740788	3.445479	0.732620
H	1.221285	2.733365	-0.809367
C	0.032148	5.959169	-0.330451
H	-2.091354	6.398096	-0.242521
H	-1.563007	5.647411	-1.742133
H	1.999946	5.092390	-0.619187
H	0.899990	4.870051	-1.970850
H	0.305808	6.940858	-0.734424
H	0.153279	6.027967	0.760935
C	-2.152859	1.460015	1.516382
C	-3.588158	1.985965	1.628079
C	-2.073239	0.070015	2.169729
H	-1.491935	2.124992	2.100658
C	-4.033647	2.038219	3.088793
H	-4.259749	1.313055	1.074529
H	-3.695703	2.971571	1.167574
C	-2.510507	0.115145	3.627804
H	-2.717317	-0.631028	1.618696
H	-1.050509	-0.320428	2.093425
C	-3.922556	0.673739	3.757810
H	-5.060029	2.418195	3.155128
H	-3.401454	2.759074	3.628450
H	-2.446362	-0.886869	4.071592
H	-1.807346	0.747424	4.189376

H	-4.221699	0.735607	4.810515
H	-4.628065	-0.020113	3.274979
C	0.035377	-3.158227	0.063433
C	-0.468849	-3.134420	1.378124
C	-0.786137	-3.451099	-1.039294
C	-1.825898	-3.407837	1.560546
C	-2.126460	-3.748132	-0.797077
C	-2.667216	-3.718475	0.490663
H	-2.234550	-3.383478	2.570616
H	-2.774227	-3.974776	-1.642988
C	4.121683	-0.608213	-0.200475
C	4.494417	-0.172326	1.079031
C	4.575909	0.033748	-1.363654
C	5.314263	0.954502	1.175061
C	5.391571	1.154002	-1.213840
C	5.763887	1.634811	0.044344
H	5.598762	1.313259	2.163397
H	5.744352	1.666704	-2.107883
C	4.176752	-0.460916	-2.716268
H	4.328785	-1.541518	-2.814243
H	3.111057	-0.273480	-2.900561
H	4.752774	0.035926	-3.500827
C	6.620742	2.857784	0.168690
H	6.923068	3.036374	1.203783
H	7.529073	2.778535	-0.437500
H	6.090789	3.751725	-0.178216
C	4.039887	-0.882676	2.318331
H	3.049528	-1.331825	2.197108
H	4.734164	-1.686159	2.597253
H	3.981526	-0.195716	3.165534
C	-0.245820	-3.366476	-2.430707
H	0.068208	-2.336491	-2.654740
H	0.632099	-4.004991	-2.579383
H	-1.000705	-3.659748	-3.164441
C	0.417432	-2.842065	2.553974
H	1.373341	-3.373646	2.486777
H	0.660064	-1.774388	2.632617
H	-0.067245	-3.136195	3.488644
C	-4.125517	-3.972074	0.720821
H	-4.292825	-4.650099	1.563417
H	-4.654125	-3.040433	0.959017
H	-4.606985	-4.402362	-0.161212

A9/B6 (4)

Ru	-0.321307	0.317995	0.112104
P	1.206179	-1.505663	-0.120024
O	-1.528545	-0.960164	2.530229
Cl	0.343679	0.915888	-2.203764
C	-1.552624	1.998709	0.167618

C	-3.495060	3.326648	0.255168
C	-2.272176	4.219759	0.421394
H	-3.996390	3.474089	-0.712923
H	-4.242241	3.461726	1.044061
H	-2.262068	5.077000	-0.259444
H	-2.170694	4.604602	1.447198
N	-1.167873	3.295217	0.130108
N	-2.900085	1.986646	0.313885
C	2.798639	-0.988204	-0.907005
C	3.611521	-0.085823	0.027639
C	3.692524	-2.037901	-1.573552
H	2.415022	-0.341842	-1.711170
C	4.735312	0.601795	-0.738856
H	4.044943	-0.689704	0.840440
H	2.954198	0.659119	0.497159
C	4.822547	-1.344204	-2.334911
H	4.121830	-2.719638	-0.826106
H	3.110607	-2.656994	-2.267832
C	5.631301	-0.419743	-1.431384
H	5.324050	1.234456	-0.062585
H	4.288331	1.275053	-1.485628
H	5.474739	-2.090607	-2.804067
H	4.385672	-0.754639	-3.153688
H	6.418881	0.081821	-2.005698
H	6.144244	-1.022873	-0.666612
C	0.384112	-2.650152	-1.347011
C	0.773338	-4.130733	-1.347437
C	-1.144886	-2.511003	-1.228910
H	0.673674	-2.205409	-2.314233
C	0.045181	-4.897134	-2.449799
H	0.516353	-4.571262	-0.371139
H	1.856059	-4.250011	-1.465156
C	-1.869666	-3.281978	-2.325192
H	-1.478059	-2.866266	-0.239803
H	-1.439929	-1.450751	-1.281201
C	-1.466885	-4.750657	-2.331699
H	0.334943	-5.954321	-2.425119
H	0.371134	-4.509737	-3.426344
H	-2.953834	-3.176677	-2.199472
H	-1.623660	-2.827953	-3.297175
H	-1.970098	-5.287094	-3.144419
H	-1.804325	-5.220025	-1.395283
C	1.556793	-2.482295	1.425597
C	2.680361	-3.526568	1.378422
C	1.792458	-1.584949	2.653023
H	0.601990	-3.013277	1.593105
C	2.664331	-4.382007	2.643618
H	3.644214	-2.999457	1.312294
H	2.616439	-4.161196	0.490406

C	1.761968	-2.414716	3.931438
H	2.775867	-1.103040	2.556173
H	1.059532	-0.777221	2.701921
C	2.803704	-3.527219	3.898205
H	3.460292	-5.134800	2.600569
H	1.715204	-4.937897	2.682211
H	1.919243	-1.769677	4.803921
H	0.757143	-2.847446	4.045841
H	2.736115	-4.150477	4.797398
H	3.807419	-3.076400	3.910292
C	-1.056973	-0.419924	1.593363
H	0.672300	1.052091	1.057850
C	0.191496	3.735037	0.137193
C	0.723026	4.249206	-1.057277
C	0.962909	3.638738	1.302915
C	2.067873	4.606250	-1.078442
C	2.311584	3.999798	1.226795
C	2.884588	4.470456	0.047962
H	2.494977	4.982646	-2.007084
H	2.930021	3.903875	2.119054
C	-3.681978	0.799772	0.174541
C	-3.847994	0.226325	-1.097040
C	-4.253627	0.226274	1.320422
C	-4.557746	-0.972030	-1.185051
C	-4.939695	-0.979236	1.181114
C	-5.085491	-1.603964	-0.058784
H	-4.693794	-1.426927	-2.165899
H	-5.356578	-1.450355	2.070267
C	0.395086	3.182228	2.614878
H	0.279491	4.027494	3.304457
H	-0.576910	2.695561	2.510143
H	1.062370	2.463197	3.101175
C	-0.127642	4.374009	-2.281459
H	-0.459337	3.385618	-2.617471
H	-1.024299	4.979418	-2.101082
H	0.428166	4.842056	-3.097534
C	4.334768	4.843376	-0.012279
H	4.821556	4.419295	-0.896473
H	4.469635	5.929637	-0.070993
H	4.878393	4.493524	0.869434
C	-3.270839	0.853252	-2.327877
H	-3.271830	1.947168	-2.278553
H	-2.221752	0.566739	-2.483497
H	-3.831412	0.550822	-3.216591
C	-4.116820	0.877967	2.661666
H	-3.127533	1.324535	2.794800
H	-4.856110	1.677480	2.798071
H	-4.266487	0.153467	3.465051
C	-5.759148	-2.936919	-0.176062

H	-6.206889	-3.080395	-1.163535
H	-5.039044	-3.752113	-0.030874
H	-6.542443	-3.068100	0.575705

TSB1→B2

C	0.834376	1.387550	-0.689330
H	0.833842	1.651734	-1.764324
Ru	-0.429548	0.068068	-0.148253
Cl	-0.865931	-0.340833	-2.453754
Cl	-0.810632	0.340231	2.819907
P	1.454070	-1.631847	-0.060553
O	-1.610981	-1.559166	0.522398
H	-1.913239	0.142885	2.143463
C	-2.246433	-2.471340	-0.306313
H	-3.070460	-2.040958	-0.900416
H	-1.568090	-2.925235	-1.049654
H	-2.676031	-3.302220	0.286548
C	1.992728	1.996990	-0.049337
C	2.975770	2.628446	-0.838292
C	2.204056	1.962476	1.344278
C	4.127021	3.163143	-0.272491
H	2.815691	2.680090	-1.915118
C	3.345900	2.505884	1.914647
H	1.432408	1.520171	1.971335
C	4.317709	3.101866	1.106921
H	4.875391	3.634185	-0.905839
H	3.482186	2.472178	2.993199
H	5.215758	3.520883	1.553314
C	-2.003508	1.414377	0.147170
C	-3.156396	3.395802	0.748115
C	-3.912352	2.215373	1.312393
H	-2.918364	4.156179	1.496847
H	-3.675702	3.896582	-0.083099
H	-3.836495	2.163742	2.407586
H	-4.970753	2.205001	1.043810
N	-3.221067	1.046293	0.711108
N	-1.923581	2.766970	0.251746
C	1.049377	-3.396190	-0.478221
C	0.780387	-3.587455	-1.978177
C	1.977347	-4.523377	0.005354
H	0.089613	-3.518281	0.048244
C	0.119902	-4.940215	-2.230361
H	1.739791	-3.547195	-2.518532
H	0.163463	-2.771864	-2.372840
C	1.292917	-5.872369	-0.207328
H	2.912236	-4.513289	-0.566941
H	2.259287	-4.405310	1.056136
C	0.957521	-6.088207	-1.678824
H	-0.063546	-5.077325	-3.302488

H	-0.867002	-4.940791	-1.743930
H	1.930341	-6.683230	0.165681
H	0.368729	-5.902500	0.389393
H	0.443275	-7.046075	-1.820887
H	1.896485	-6.154671	-2.249073
C	1.911469	-1.649228	1.756268
C	0.924105	-2.500412	2.572529
C	3.362354	-1.936250	2.157948
H	1.728836	-0.600695	2.040459
C	1.143249	-2.302292	4.069532
H	1.072673	-3.563119	2.340755
H	-0.105773	-2.267857	2.275456
C	3.550256	-1.733093	3.659378
H	3.636090	-2.969689	1.902498
H	4.050767	-1.283799	1.605950
C	2.585407	-2.595847	4.463367
H	0.449218	-2.934743	4.635987
H	0.901117	-1.263935	4.339812
H	4.589360	-1.943903	3.939399
H	3.373218	-0.673542	3.901722
H	2.733991	-2.440083	5.538328
H	2.806256	-3.656856	4.270795
C	3.020598	-1.174880	-0.972017
C	4.123814	-2.240346	-1.056281
C	2.756108	-0.655022	-2.393525
H	3.413614	-0.328379	-0.381336
C	5.407427	-1.640057	-1.624127
H	3.784247	-3.041429	-1.728734
H	4.318259	-2.711864	-0.089749
C	4.025993	-0.062359	-2.998537
H	2.401739	-1.486329	-3.019691
H	1.946375	0.078730	-2.406331
C	5.173272	-1.064249	-3.014803
H	6.199387	-2.398125	-1.646914
H	5.758495	-0.843276	-0.949510
H	3.820411	0.307617	-4.010409
H	4.324716	0.812852	-2.401700
H	6.088387	-0.600703	-3.401770
H	4.927801	-1.886705	-3.703493
C	-4.103185	0.018355	0.210990
C	-4.576208	0.106333	-1.106521
C	-4.602120	-0.952035	1.094259
C	-5.519845	-0.829569	-1.538407
C	-5.552017	-1.853416	0.619567
C	-6.018454	-1.818939	-0.696105
H	-5.879834	-0.769061	-2.564526
H	-5.928872	-2.616512	1.300028
C	-0.847160	3.648363	-0.090463
C	-0.603536	3.954392	-1.442254

C	-0.123541	4.272156	0.937205
C	0.426319	4.843379	-1.738970
C	0.896618	5.157963	0.585699
C	1.195938	5.448809	-0.742225
H	0.638434	5.061601	-2.785103
H	1.496150	5.604858	1.378175
C	-4.104581	1.172998	-2.040989
H	-4.725256	1.206924	-2.939652
H	-4.136882	2.167146	-1.577674
H	-3.070279	0.990871	-2.355545
C	-4.088127	-1.090585	2.491503
H	-3.081943	-1.528470	2.462177
H	-4.026441	-0.134713	3.025583
H	-4.726650	-1.752649	3.081959
C	-7.027561	-2.815677	-1.178418
H	-6.647148	-3.839532	-1.096638
H	-7.950134	-2.777062	-0.589089
H	-7.293391	-2.644776	-2.224577
C	-0.391067	3.984797	2.382176
H	-1.139729	4.668727	2.803252
H	-0.754022	2.965336	2.536792
H	0.518906	4.111687	2.975950
C	-1.405138	3.324965	-2.533320
H	-1.281629	2.234491	-2.545998
H	-2.476680	3.520956	-2.411613
H	-1.103243	3.709799	-3.510429
C	2.318033	6.374094	-1.098878
H	1.947483	7.330240	-1.485869
H	2.950354	6.590847	-0.233685
H	2.955398	5.943270	-1.878538

B2

Ru	-0.241728	0.493062	0.116949
Cl	-0.859086	-0.041328	2.443906
P	1.547020	-1.285439	0.083579
C	-1.480194	-0.475127	-0.823029
H	-1.923013	0.054548	-1.684044
C	-1.909326	-1.866649	-0.773216
C	-1.917883	-2.628808	0.406364
C	-2.345452	-2.472130	-1.965390
C	-2.294425	-3.966234	0.376057
H	-1.653264	-2.136231	1.340790
C	-2.689906	-3.816577	-1.998058
H	-2.379525	-1.872042	-2.876093
C	-2.657218	-4.570501	-0.826005
H	-2.304147	-4.543569	1.298301
H	-2.991828	-4.277169	-2.936577
H	-2.931677	-5.622869	-0.847449
C	-1.451234	2.131314	0.418796

C	-3.206810	3.551905	1.090700
C	-1.879620	4.208343	1.433844
H	-3.737637	4.061530	0.269316
H	-3.888270	3.488819	1.946483
H	-1.804598	5.245200	1.089959
H	-1.673255	4.187645	2.515077
N	-2.783013	2.213348	0.666355
N	-0.919559	3.345822	0.735438
C	1.362110	-2.444055	1.553381
C	1.675757	-3.934147	1.395481
C	1.997265	-1.890375	2.836101
H	0.278480	-2.378670	1.725828
C	1.178973	-4.704707	2.617529
H	2.761477	-4.094299	1.290344
H	1.200302	-4.342024	0.492183
C	1.502766	-2.669179	4.051334
H	3.095228	-1.967352	2.787705
H	1.742719	-0.830181	2.958339
C	1.783525	-4.159752	3.905289
H	1.401744	-5.774174	2.505269
H	0.081364	-4.614827	2.667389
H	1.969256	-2.276674	4.964406
H	0.419297	-2.501232	4.154965
H	1.403579	-4.712873	4.774188
H	2.874031	-4.322701	3.883993
C	3.283790	-0.592628	0.259849
C	4.445409	-1.584167	0.421424
C	3.658559	0.458830	-0.790835
H	3.191974	-0.053688	1.221693
C	5.707519	-0.852116	0.871446
H	4.651579	-2.065190	-0.544110
H	4.203880	-2.391213	1.123452
C	4.934176	1.185452	-0.374748
H	3.821613	-0.044217	-1.760332
H	2.839830	1.170201	-0.950003
C	6.093719	0.228325	-0.132344
H	6.530320	-1.567071	1.004401
H	5.528463	-0.394040	1.858767
H	5.202155	1.936232	-1.131290
H	4.727710	1.742719	0.556148
H	6.984275	0.772883	0.208489
H	6.367480	-0.253724	-1.085134
C	1.460485	-2.377421	-1.442934
C	1.118377	-1.605210	-2.722870
C	2.652844	-3.295610	-1.733039
H	0.585590	-3.017076	-1.215564
C	0.797982	-2.567510	-3.864102
H	1.968481	-0.960569	-2.999538
H	0.280043	-0.923972	-2.547401

C	2.311011	-4.284541	-2.844647
H	3.500530	-2.675549	-2.067400
H	2.988049	-3.831620	-0.839195
C	1.934007	-3.548367	-4.123747
H	0.560290	-2.000558	-4.774279
H	-0.111042	-3.134074	-3.600405
H	3.155981	-4.963185	-3.020554
H	1.464796	-4.912680	-2.518152
H	1.659686	-4.258243	-4.915056
H	2.814603	-2.995641	-4.489718
C	0.364716	3.842125	0.346087
C	0.432009	4.721626	-0.744167
C	1.523938	3.473239	1.044181
C	1.682463	5.183535	-1.153930
C	2.747790	3.968897	0.604818
C	2.852032	4.811848	-0.500012
H	1.740168	5.848965	-2.016503
H	3.652620	3.686790	1.145660
C	-3.761628	1.224868	0.343024
C	-4.157610	1.083586	-0.996735
C	-4.350312	0.456342	1.354749
C	-5.039960	0.059344	-1.324130
C	-5.243165	-0.549812	0.978993
C	-5.568950	-0.790999	-0.351504
H	-5.322831	-0.081533	-2.368552
H	-5.684243	-1.172117	1.758903
C	-3.654438	2.018514	-2.054611
H	-3.978940	3.050521	-1.862138
H	-2.559408	2.038625	-2.108366
H	-4.037064	1.732216	-3.039754
C	-4.102274	0.718416	2.808610
H	-3.154749	1.235939	2.976808
H	-4.921149	1.317756	3.231830
H	-4.059649	-0.220360	3.371023
C	-6.443238	-1.944782	-0.736445
H	-7.111993	-2.237327	0.080114
H	-7.054770	-1.713725	-1.616118
H	-5.832262	-2.822130	-0.987314
C	1.476075	2.541139	2.212099
H	0.616289	2.723325	2.865932
H	1.379738	1.489686	1.897994
H	2.394896	2.612855	2.804893
C	4.189835	5.318174	-0.946771
H	4.584440	6.071209	-0.252583
H	4.926721	4.506816	-0.989496
H	4.134337	5.778241	-1.938970
C	-0.793341	5.183475	-1.477096
H	-1.611254	4.456189	-1.417361
H	-1.167019	6.136486	-1.076641

H	-0.568473	5.349470	-2.536412
O	0.785449	1.217444	-1.456524
C	0.182787	1.850673	-2.516012
H	-0.494034	2.678840	-2.222509
H	0.948085	2.288856	-3.181791
H	-0.424018	1.158140	-3.142736

TSB2→B3

Ru	0.471902	-0.025730	-0.179176
Cl	0.669505	0.110007	2.347768
P	-1.933444	-1.048863	-0.037903
C	-0.076312	1.744124	-0.799582
H	0.449857	2.306378	-1.582458
C	-1.176883	2.587298	-0.310750
C	-1.751188	2.379014	0.956314
C	-1.572340	3.721817	-1.043323
C	-2.693066	3.266352	1.461657
H	-1.392362	1.542419	1.555042
C	-2.524859	4.602135	-0.544754
H	-1.112051	3.903702	-2.014179
C	-3.088703	4.374261	0.710178
H	-3.114416	3.099257	2.449929
H	-2.825273	5.468347	-1.128920
H	-3.828508	5.064845	1.106846
C	2.462333	0.638208	0.086159
C	4.122384	1.987492	1.124561
C	4.646710	0.569920	1.008989
H	4.758343	2.728067	0.623145
H	3.990428	2.309661	2.165314
H	5.543547	0.487219	0.379317
H	4.883048	0.113260	1.977334
N	2.817476	1.906925	0.457578
N	3.529505	-0.151145	0.383608
C	-2.239247	-1.355949	1.775604
C	-3.666093	-1.475720	2.319262
C	-1.342175	-2.496106	2.285885
H	-1.819467	-0.441317	2.221026
C	-3.640617	-1.530528	3.846832
H	-4.163762	-2.376340	1.930663
H	-4.272119	-0.618152	1.998936
C	-1.336704	-2.527090	3.808323
H	-1.703058	-3.462605	1.908236
H	-0.328486	-2.367292	1.898679
C	-2.750250	-2.654876	4.362608
H	-4.662099	-1.633265	4.233535
H	-3.259501	-0.570391	4.225856
H	-0.706185	-3.351970	4.162609
H	-0.871227	-1.599647	4.170952
H	-2.741911	-2.660259	5.458983

H	-3.176851	-3.621807	4.052773
C	-2.037029	-2.706328	-0.887825
C	-3.101270	-3.716998	-0.430325
C	-2.127810	-2.587657	-2.418177
H	-1.053986	-3.135504	-0.637446
C	-2.817180	-5.080690	-1.058406
H	-4.099437	-3.379316	-0.737600
H	-3.129555	-3.811238	0.658165
C	-1.815220	-3.932141	-3.067399
H	-3.150956	-2.292164	-2.695424
H	-1.469093	-1.800577	-2.805699
C	-2.784330	-5.004605	-2.581076
H	-3.566277	-5.810966	-0.729598
H	-1.846878	-5.443404	-0.688755
H	-1.851909	-3.848531	-4.160205
H	-0.784906	-4.218489	-2.809202
H	-2.527995	-5.980304	-3.009948
H	-3.793266	-4.762616	-2.947924
C	-3.412939	-0.075363	-0.650813
C	-3.187319	0.628170	-1.998429
C	-4.768714	-0.799086	-0.731466
H	-3.511284	0.713741	0.112316
C	-4.285660	1.655958	-2.254397
H	-3.200422	-0.121238	-2.801287
H	-2.206405	1.105363	-2.045809
C	-5.891669	0.209177	-0.970871
H	-4.746988	-1.508920	-1.570321
H	-4.973276	-1.390614	0.163516
C	-5.662768	1.003838	-2.250514
H	-4.106110	2.174432	-3.204742
H	-4.239342	2.425243	-1.469394
H	-6.858670	-0.306542	-1.007060
H	-5.939060	0.897867	-0.113291
H	-6.448605	1.756606	-2.382536
H	-5.740646	0.322703	-3.111177
C	3.839366	-1.496505	0.001508
C	4.416232	-1.699776	-1.264590
C	3.714445	-2.541844	0.922192
C	4.823428	-2.984358	-1.614490
C	4.140679	-3.813085	0.526386
C	4.687657	-4.058479	-0.730440
H	5.260933	-3.148506	-2.598788
H	4.037860	-4.637363	1.231149
C	2.203418	3.152240	0.128928
C	2.350365	3.639381	-1.185955
C	1.590804	3.934051	1.120372
C	1.806852	4.878882	-1.507828
C	1.055436	5.170531	0.745375
C	1.142681	5.658117	-0.554662

H	1.895815	5.243028	-2.531236
H	0.537484	5.760778	1.500971
C	3.027507	2.806310	-2.228734
H	4.046873	2.530440	-1.932765
H	2.495541	1.859918	-2.392443
H	3.084369	3.335265	-3.183249
C	1.503305	3.490328	2.545298
H	1.495906	2.401711	2.637231
H	2.347320	3.882861	3.127513
H	0.591366	3.873756	3.013122
C	0.545957	6.980168	-0.928232
H	1.318563	7.740239	-1.091635
H	-0.028532	6.913948	-1.858520
H	-0.122662	7.353670	-0.147816
C	3.113664	-2.335125	2.272478
H	3.289625	-1.328544	2.659404
H	2.024324	-2.432476	2.214898
H	3.494093	-3.067284	2.990547
C	5.121007	-5.435477	-1.132658
H	4.463691	-5.853128	-1.903591
H	6.132613	-5.435776	-1.552667
H	5.109830	-6.125184	-0.284893
C	4.547517	-0.564144	-2.232657
H	3.563580	-0.210211	-2.566370
H	5.047042	0.306002	-1.788948
H	5.115041	-0.861882	-3.117833
O	0.950903	-2.137533	-0.041997
C	1.055725	-1.725847	-1.277940
H	2.054352	-1.641485	-1.728535
H	0.292202	-2.046831	-2.003502
H	-0.132598	0.606198	-1.620034

B3

Ru	0.224590	0.003429	0.161064
O	-0.384145	0.756284	-1.219370
C	-0.172148	-0.463218	-1.446182
H	-0.400364	-1.193630	-2.081762
H	0.410986	-0.603756	-2.204493
P	2.480617	0.033852	-0.230748
Cl	0.441946	1.736745	1.547164
C	0.372504	-1.872680	0.867066
H	-0.540139	-2.398085	0.677510
H	1.181242	-2.374872	0.378552
C	0.635377	-1.831123	2.383895
C	1.944982	-1.820768	2.864828
C	-0.435735	-1.803723	3.276933
C	2.183327	-1.783704	4.238523
H	2.789206	-1.843153	2.160536
C	-0.197486	-1.765651	4.651050

H	-1.467972	-1.811699	2.898050
C	1.111778	-1.755776	5.131954
H	3.215544	-1.776175	4.617692
H	-1.042207	-1.743639	5.354922
H	1.299950	-1.726495	6.215019
C	-1.755590	-0.023274	0.504969
C	-3.510898	0.991059	-0.891078
C	-3.486768	-0.503227	-1.179074
H	-4.498186	1.287032	-0.454844
H	-3.380144	1.575981	-1.835655
H	-4.488033	-0.958209	-0.973611
H	-3.256242	-0.688552	-2.258382
N	-2.421359	-1.134556	-0.294248
N	-2.386936	1.297246	0.088218
C	3.371804	-0.225970	1.334717
C	4.651909	-0.991962	1.069469
C	3.657720	1.112780	1.984749
H	2.706811	-0.831493	2.005013
C	5.467659	-1.158730	2.335283
H	5.261310	-0.444808	0.302908
H	4.405172	-2.000321	0.646424
C	4.472789	0.945920	3.251014
H	4.217483	1.765175	1.264061
H	2.691568	1.627753	2.225152
C	5.752429	0.178948	2.986977
H	6.434354	-1.672403	2.094192
H	4.908876	-1.812715	3.055314
H	4.719936	1.954236	3.673820
H	3.862453	0.399531	4.017447
H	6.299450	0.017563	3.952025
H	6.419255	0.784799	2.318671
C	2.911036	-1.291819	-1.401106
C	2.240158	-1.030156	-2.734232
C	4.417166	-1.368689	-1.550121
H	2.528898	-2.256071	-0.974074
C	2.638193	-2.066565	-3.765236
H	2.527074	-0.009839	-3.101652
H	1.126961	-1.039996	-2.602596
C	4.815211	-2.405691	-2.580554
H	4.812983	-0.365381	-1.858421
H	4.879988	-1.624434	-0.561773
C	4.143824	-2.145570	-3.913603
H	2.176375	-1.809630	-4.753767
H	2.240768	-3.069598	-3.458058
H	5.928323	-2.395556	-2.712556
H	4.528856	-3.425834	-2.212071
H	4.407791	-2.963723	-4.633007
H	4.527192	-1.182626	-4.342687
C	2.952012	1.643523	-0.937251

C	4.449049	1.837062	-0.806137
C	2.514701	1.709795	-2.386703
H	2.420343	2.438139	-0.350666
C	4.897523	3.129703	-1.456903
H	4.979748	0.973930	-1.287515
H	4.733023	1.844589	0.278268
C	2.962487	3.002818	-3.037227
H	2.948714	0.840402	-2.947180
H	1.398524	1.626132	-2.446642
C	4.459171	3.197815	-2.905485
H	6.013859	3.212258	-1.398062
H	4.465163	3.999244	-0.895349
H	2.678956	2.995131	-4.121707
H	2.430702	3.865433	-2.556010
H	4.748152	4.190394	-3.338929
H	4.991804	2.405040	-3.493834
C	-3.358859	-2.234488	-0.562848
C	-4.300349	-2.599340	0.399935
C	-3.307280	-2.913347	-1.780237
C	-5.189576	-3.643272	0.145566
C	-4.197356	-3.956972	-2.035229
C	-5.138335	-4.322104	-1.072538
H	-5.931283	-3.931322	0.904641
H	-4.156726	-4.491772	-2.995340
C	-3.267109	2.472289	0.162172
C	-4.041717	2.692979	1.301360
C	-3.327810	3.366669	-0.906448
C	-4.877317	3.807460	1.371550
C	-4.162872	4.482068	-0.835994
C	-4.937680	4.702515	0.302696
H	-5.488373	3.981139	2.269182
H	-4.210218	5.187297	-1.678540
C	-3.975192	1.704673	2.480523
H	-4.139879	0.710067	2.122003
H	-3.010949	1.762843	2.940688
H	-4.728525	1.954429	3.198166
C	-2.472692	3.123415	-2.163907
H	-1.436158	3.207764	-1.912150
H	-2.668682	2.142697	-2.544275
H	-2.719097	3.850770	-2.908984
C	-5.860367	5.933038	0.380551
H	-6.740779	5.684141	0.935371
H	-5.345877	6.734310	0.868572
H	-6.135531	6.235637	-0.608195
C	-2.268302	-2.510635	-2.843227
H	-2.300469	-1.451243	-2.990038
H	-1.291242	-2.795422	-2.512847
H	-2.491307	-3.005435	-3.765367
C	-4.356226	-1.850258	1.744314

H	-3.362166	-1.700864	2.110955
H	-4.831166	-0.901675	1.604592
H	-4.914171	-2.427769	2.451476
C	-6.120391	-5.474683	-1.353121
H	-6.461477	-5.414164	-2.365494
H	-5.625291	-6.410629	-1.198910
H	-6.956743	-5.400075	-0.689910

TSB3→B4

Ru	-0.382015	0.081786	-0.198794
O	0.255014	1.343122	-1.803442
C	-0.369883	0.401864	-2.236613
H	-1.098284	-0.801173	-2.185146
H	-1.412100	0.941222	-2.812438
P	1.979689	-0.854193	-0.112916
Cl	0.281563	0.975411	2.038714
C	-1.335435	-1.674502	-1.337410
H	-2.394019	-1.493731	-1.495777
H	-0.772974	-2.190608	-2.117838
C	-1.230369	-2.459332	-0.112008
C	-0.495280	-3.668611	-0.035535
C	-1.792455	-1.961412	1.082444
C	-0.403007	-4.366806	1.151402
H	-0.053597	-4.067833	-0.947872
C	-1.626004	-2.634523	2.298028
H	-2.408065	-1.075165	1.044336
C	-0.965087	-3.848607	2.330873
H	0.124860	-5.317746	1.180789
H	-2.047339	-2.207144	3.204387
H	-0.875585	-4.401710	3.262174
C	-2.134586	1.330010	-0.278330
C	-3.250804	3.364582	-0.791642
C	-4.287656	2.276942	-0.654223
H	-3.440096	4.233212	-0.153408
H	-3.141694	3.727382	-1.823959
H	-4.911076	2.387758	0.245761
H	-4.960803	2.195471	-1.514217
N	-3.456839	1.067872	-0.538650
N	-2.012907	2.686578	-0.373207
C	2.279945	-1.637586	1.606823
C	2.890413	-3.048551	1.682492
C	3.011493	-0.774439	2.646209
H	1.239315	-1.717645	1.958620
C	2.733919	-3.632103	3.088149
H	3.961469	-3.006039	1.441897
H	2.435265	-3.739189	0.964659
C	2.757465	-1.318028	4.048025
H	4.092605	-0.835922	2.459413
H	2.713066	0.272810	2.575721

C	3.313574	-2.730424	4.169949
H	3.195827	-4.627194	3.124099
H	1.665275	-3.778280	3.288935
H	3.212365	-0.657940	4.796014
H	1.674694	-1.313370	4.243225
H	3.114902	-3.152480	5.162570
H	4.408254	-2.690764	4.064737
C	2.608825	-2.183163	-1.276388
C	2.080449	-2.133765	-2.714145
C	4.131741	-2.375977	-1.316856
H	2.175825	-3.095455	-0.838937
C	2.421057	-3.429702	-3.446990
H	2.525390	-1.285255	-3.250787
H	0.999281	-1.970386	-2.721645
C	4.485075	-3.680561	-2.025441
H	4.579863	-1.538956	-1.869793
H	4.571756	-2.345380	-0.315500
C	3.920808	-3.702919	-3.442027
H	2.041033	-3.395310	-4.474971
H	1.899224	-4.264327	-2.953127
H	5.571996	-3.823726	-2.042720
H	4.070878	-4.523106	-1.450367
H	4.140236	-4.659107	-3.931343
H	4.426170	-2.928273	-4.037676
C	3.078083	0.644550	-0.399947
C	4.492814	0.752587	0.185550
C	3.182978	0.975686	-1.901616
H	2.466829	1.435337	0.064685
C	5.012763	2.180786	0.010012
H	5.167029	0.049347	-0.324575
H	4.521320	0.503679	1.243657
C	3.650159	2.415169	-2.085330
H	3.923786	0.304958	-2.363509
H	2.240646	0.813414	-2.422596
C	5.018025	2.621352	-1.447867
H	6.016823	2.269069	0.442954
H	4.364489	2.856345	0.588646
H	3.679344	2.672552	-3.151845
H	2.910019	3.081950	-1.618998
H	5.335040	3.668020	-1.532147
H	5.762298	2.027822	-2.000282
C	-4.198892	-0.148423	-0.432140
C	-4.668963	-0.577522	0.817492
C	-4.582990	-0.802785	-1.616326
C	-5.443594	-1.739498	0.866901
C	-5.362407	-1.952101	-1.518028
C	-5.789695	-2.447170	-0.282269
H	-5.787891	-2.097251	1.836483
H	-5.643288	-2.476733	-2.430455

C	-0.964685	3.558546	0.080039
C	-0.944607	3.896080	1.443046
C	-0.116408	4.191680	-0.836111
C	0.045411	4.764696	1.895694
C	0.867266	5.046530	-0.333579
C	0.986252	5.320354	1.027844
H	0.083488	5.008016	2.956537
H	1.552921	5.521894	-1.035565
C	-1.980965	3.362733	2.381539
H	-3.000015	3.606101	2.050251
H	-1.904003	2.274616	2.460975
H	-1.850448	3.779027	3.383422
C	-0.258380	4.030138	-2.318769
H	0.681253	3.698422	-2.771870
H	-1.016678	3.290211	-2.582048
H	-0.527406	4.985779	-2.785786
C	2.085136	6.197887	1.544368
H	1.766091	6.778908	2.414869
H	2.950038	5.603421	1.861685
H	2.439903	6.896907	0.781348
C	-4.142840	-0.278817	-2.948788
H	-4.543171	0.723291	-3.144828
H	-3.052217	-0.185544	-3.006894
H	-4.474064	-0.931805	-3.759579
C	-4.371267	0.183579	2.075019
H	-3.390282	0.669938	2.053759
H	-5.111379	0.975419	2.245731
H	-4.402689	-0.474191	2.947648
C	-6.589657	-3.710879	-0.200623
H	-7.350267	-3.760399	-0.985678
H	-5.950364	-4.592376	-0.324791
H	-7.092616	-3.809859	0.764670

B4

Ru	0.557771	-0.308539	-0.174518
O	-0.815691	-2.255721	-1.990039
C	-0.259805	-1.163268	-1.878005
H	0.849666	0.462163	-1.487270
H	0.013859	-0.613218	-2.812441
P	-1.721576	0.825452	-0.134065
Cl	0.350098	-0.789427	2.220842
C	1.881546	1.296040	0.335870
H	2.296036	0.916499	1.272941
H	2.663252	1.339387	-0.422092
C	1.287554	2.631432	0.524610
C	1.359886	3.600655	-0.489853
C	0.713800	3.010721	1.750798
C	0.866887	4.886794	-0.296799
H	1.822869	3.331258	-1.440088

C	0.209373	4.292868	1.941824
H	0.683822	2.276968	2.556060
C	0.275582	5.235839	0.916240
H	0.946908	5.622691	-1.093776
H	-0.228620	4.564221	2.899935
H	-0.114150	6.238892	1.067423
C	2.144689	-1.661265	-0.221960
C	2.991710	-3.879693	-0.339851
C	4.113849	-2.906749	-0.672384
H	3.185414	-4.473688	0.563609
H	2.771607	-4.578238	-1.156048
H	4.958913	-2.970760	0.022942
H	4.514171	-3.037195	-1.686191
N	3.463319	-1.586900	-0.554273
N	1.851396	-2.984536	-0.123635
C	-2.159751	1.286233	1.641484
C	-2.892150	2.601727	1.926132
C	-2.812748	0.143724	2.437874
H	-1.157664	1.393668	2.072613
C	-2.839895	2.906630	3.422666
H	-3.944991	2.535716	1.612954
H	-2.447465	3.434629	1.366980
C	-2.750739	0.449909	3.930602
H	-3.864780	0.021684	2.141640
H	-2.305020	-0.804625	2.238632
C	-3.432553	1.774130	4.252013
H	-3.351763	3.854121	3.633830
H	-1.787784	3.048568	3.712945
H	-3.208161	-0.367275	4.501816
H	-1.693525	0.488104	4.231529
H	-3.355713	2.001800	5.321934
H	-4.507714	1.690367	4.030825
C	-1.870420	2.423628	-1.110506
C	-1.134416	2.362887	-2.455298
C	-3.258631	3.035417	-1.351125
H	-1.308989	3.121781	-0.466511
C	-1.054710	3.727671	-3.132834
H	-1.634968	1.643665	-3.116406
H	-0.120977	1.977443	-2.314217
C	-3.128812	4.441754	-1.931006
H	-3.793728	2.417770	-2.085457
H	-3.869208	3.043764	-0.444518
C	-2.415550	4.393749	-3.275930
H	-0.570831	3.623355	-4.111954
H	-0.406256	4.380429	-2.533805
H	-4.120067	4.900041	-2.032164
H	-2.560780	5.073086	-1.229440
H	-2.310117	5.399023	-3.700779
H	-3.034339	3.821481	-3.983099

C	-3.142843	-0.328813	-0.567142
C	-4.556509	0.257734	-0.422042
C	-3.041545	-1.074721	-1.898964
H	-3.026947	-1.095047	0.218928
C	-5.606147	-0.847734	-0.452986
H	-4.758595	0.929614	-1.262921
H	-4.655286	0.864237	0.483753
C	-4.131071	-2.140890	-2.007362
H	-3.118547	-0.364618	-2.735252
H	-2.059430	-1.543486	-1.997345
C	-5.534346	-1.595148	-1.778712
H	-6.606125	-0.425456	-0.297342
H	-5.430091	-1.547800	0.378607
H	-4.062773	-2.642906	-2.981174
H	-3.933081	-2.913023	-1.250100
H	-6.271286	-2.406685	-1.812483
H	-5.798392	-0.902370	-2.591421
C	4.323962	-0.464761	-0.348084
C	4.727630	-0.168094	0.965016
C	4.770234	0.283848	-1.441210
C	5.575767	0.918466	1.161353
C	5.622725	1.363508	-1.194456
C	6.029184	1.701350	0.095011
H	5.883080	1.168084	2.176111
H	5.969690	1.961336	-2.036439
C	0.538148	-3.525018	0.047245
C	0.115271	-3.906681	1.334045
C	-0.270937	-3.743439	-1.080799
C	-1.193357	-4.357964	1.485609
C	-1.574244	-4.204923	-0.872958
C	-2.065000	-4.481142	0.401091
H	-1.542125	-4.621442	2.483391
H	-2.213471	-4.366445	-1.740229
C	1.045162	-3.894302	2.506751
H	1.460722	-4.897228	2.673156
H	1.870770	-3.195232	2.367790
H	0.522150	-3.597404	3.418446
C	0.236731	-3.616916	-2.486278
H	-0.401343	-2.972897	-3.097833
H	1.248582	-3.206838	-2.535295
H	0.255424	-4.604655	-2.961682
C	-3.486475	-4.906171	0.606920
H	-3.571756	-5.691880	1.363692
H	-4.100206	-4.065557	0.955513
H	-3.939130	-5.273066	-0.318690
C	4.288797	0.003193	-2.830709
H	4.119152	-1.062413	-3.010213
H	3.329182	0.502391	-3.019683
H	4.995276	0.372337	-3.578489

C	4.207464	-0.967049	2.120394
H	3.116344	-0.870884	2.223510
H	4.412651	-2.039713	2.009387
H	4.661440	-0.641072	3.059047
C	6.922241	2.878875	0.341174
H	6.393215	3.672557	0.879810
H	7.788834	2.608423	0.953037
H	7.292521	3.307340	-0.593627

TSB4→B5

Ru	0.561728	-0.270929	-0.199780
O	-0.414462	-1.344035	-2.338977
C	0.326333	-0.384725	-2.106584
H	1.383224	0.948233	-0.763046
H	0.704677	0.238935	-2.952109
P	-1.593730	0.985621	-0.128418
Cl	0.538575	-0.894940	2.367124
C	1.943324	1.330650	0.609896
H	2.270976	0.659118	1.402271
H	2.816477	1.600504	0.005938
C	1.328217	2.561348	1.164299
C	1.572821	3.806245	0.566283
C	0.563863	2.538081	2.343818
C	1.058933	4.981103	1.108677
H	2.183450	3.846798	-0.336553
C	0.039525	3.709742	2.878522
H	0.407075	1.579911	2.833760
C	0.275999	4.937739	2.260024
H	1.269866	5.934398	0.629181
H	-0.549610	3.666442	3.791848
H	-0.131046	5.853793	2.679995
C	2.038677	-1.799687	-0.250029
C	2.842791	-4.025348	-0.262026
C	3.994455	-3.087170	-0.589136
H	2.960609	-4.523048	0.710465
H	2.687113	-4.800865	-1.019712
H	4.859456	-3.210088	0.071464
H	4.348475	-3.189620	-1.624981
N	3.381657	-1.765458	-0.404301
N	1.690511	-3.115135	-0.218774
C	-2.300305	0.635232	1.560445
C	-3.357997	1.552808	2.177468
C	-2.681074	-0.852675	1.680507
H	-1.407068	0.742631	2.189224
C	-3.595604	1.153797	3.633743
H	-4.308941	1.500351	1.628256
H	-3.024315	2.597875	2.130603
C	-2.935383	-1.221499	3.136873
H	-3.582243	-1.076813	1.095187

H	-1.876252	-1.479313	1.274308
C	-3.990584	-0.313682	3.759124
H	-4.358653	1.801873	4.081924
H	-2.667803	1.323622	4.200892
H	-3.241145	-2.273746	3.204225
H	-1.987703	-1.133131	3.685644
H	-4.153294	-0.574877	4.811613
H	-4.954926	-0.470871	3.250342
C	-1.678853	2.821787	-0.455380
C	-0.808638	3.199213	-1.667175
C	-3.084083	3.407809	-0.641091
H	-1.226029	3.284157	0.436790
C	-0.783228	4.706950	-1.906768
H	-1.204385	2.706453	-2.565805
H	0.209909	2.815531	-1.529025
C	-3.023201	4.923120	-0.809264
H	-3.533598	2.979815	-1.547414
H	-3.745343	3.138444	0.187018
C	-2.184301	5.292535	-2.025446
H	-0.192881	4.929389	-2.804442
H	-0.269023	5.190596	-1.066660
H	-4.036327	5.333428	-0.897072
H	-2.580482	5.370888	0.093752
H	-2.134541	6.380545	-2.150195
H	-2.673724	4.898804	-2.929356
C	-2.815327	0.187269	-1.312445
C	-4.321327	0.279576	-1.003836
C	-2.653366	0.531683	-2.803241
H	-2.528920	-0.873317	-1.210289
C	-5.064095	-0.788403	-1.805463
H	-4.698046	1.270636	-1.288754
H	-4.541062	0.169457	0.059246
C	-3.359786	-0.526642	-3.646667
H	-3.109137	1.514848	-2.998136
H	-1.609083	0.614177	-3.106271
C	-4.843462	-0.608750	-3.303759
H	-6.135039	-0.765857	-1.570092
H	-4.695965	-1.779312	-1.494779
H	-3.227443	-0.313435	-4.714643
H	-2.873375	-1.494716	-3.456742
H	-5.325759	-1.417966	-3.864810
H	-5.335274	0.322251	-3.623172
C	4.182905	-0.589949	-0.433829
C	4.754203	-0.155682	0.773405
C	4.368062	0.105551	-1.633217
C	5.500969	1.019500	0.760634
C	5.110655	1.289712	-1.593135
C	5.676044	1.764901	-0.409776
H	5.930653	1.380650	1.693973

H	5.246613	1.857085	-2.513332
C	0.370508	-3.635873	-0.012326
C	-0.072392	-3.922870	1.292579
C	-0.429973	-3.932768	-1.128297
C	-1.409168	-4.284366	1.461646
C	-1.766344	-4.270601	-0.906056
C	-2.286048	-4.402540	0.381557
H	-1.773629	-4.469297	2.471677
H	-2.411846	-4.447634	-1.766389
C	0.862971	-3.974234	2.461160
H	1.185158	-5.012234	2.625470
H	1.746246	-3.349618	2.320319
H	0.374553	-3.627510	3.374144
C	0.137542	-4.012835	-2.512499
H	-0.585999	-3.689588	-3.262964
H	1.032600	-3.400470	-2.636082
H	0.406369	-5.053784	-2.736979
C	-3.740587	-4.680803	0.604962
H	-4.274332	-3.767071	0.895159
H	-4.225250	-5.064676	-0.297211
H	-3.898351	-5.404182	1.410960
C	3.796131	-0.394263	-2.924684
H	2.870744	-0.957414	-2.773456
H	3.582129	0.431581	-3.608794
H	4.500086	-1.059436	-3.440153
C	4.488016	-0.905047	2.042036
H	3.411296	-0.948139	2.262539
H	4.829992	-1.945959	1.986542
H	4.990243	-0.435366	2.890754
C	6.427520	3.060761	-0.380533
H	7.373537	2.969129	0.162203
H	6.650106	3.423291	-1.387381
H	5.848831	3.840461	0.127962

C2

Ru	0.101895	0.448487	-1.355487
C	-1.565345	0.334130	-2.028139
H	-2.504828	0.020762	-1.566686
Cl	1.090981	-1.502882	-2.170710
Cl	0.346518	2.742842	-0.991026
C	-0.098298	0.026574	0.522802
C	0.600451	-0.133118	2.763234
C	-0.891151	-0.417087	2.688303
H	1.165747	-0.908217	3.290445
H	0.822062	0.831615	3.242622
H	-1.130568	-1.473908	2.881189
H	-1.485805	0.191121	3.377176
N	0.978925	-0.088470	1.349957
N	-1.211171	-0.073233	1.298304

C -2.557722 -0.200039 0.850539
 C -3.016332 -1.444288 0.394749
 C -3.380915 0.932630 0.878129
 C -4.343210 -1.535415 -0.026037
 C -4.699877 0.792603 0.445320
 C -5.200449 -0.431890 -0.003096
 H -4.712970 -2.491149 -0.394727
 H -5.350299 1.665961 0.449394
 C 2.348373 -0.153799 0.944415
 C 3.136259 1.004068 0.892115
 C 2.889208 -1.428945 0.688802
 C 4.460219 0.868683 0.459115
 C 4.213715 -1.509594 0.277371
 C 5.008412 -0.367134 0.129386
 H 5.080545 1.761577 0.393886
 H 4.637624 -2.488745 0.059415
 C 2.058792 -2.659984 0.875791
 H 1.693256 -2.750143 1.906910
 H 1.183774 -2.652314 0.218750
 H 2.636579 -3.558691 0.648884
 C 2.640771 2.339349 1.354882
 H 1.559330 2.362080 1.496573
 H 3.122408 2.610359 2.302508
 H 2.879511 3.124451 0.632953
 C 6.417147 -0.481186 -0.365825
 H 6.977508 0.444389 -0.211100
 H 6.957194 -1.292147 0.132670
 H 6.440034 -0.701833 -1.438736
 C -2.827337 2.258371 1.295497
 H -2.349000 2.212872 2.280545
 H -2.052818 2.596679 0.595659
 H -3.609230 3.020134 1.335330
 C -2.081496 -2.607349 0.270981
 H -1.320026 -2.416583 -0.497967
 H -1.537354 -2.810920 1.200443
 H -2.617371 -3.517434 -0.007810
 C -6.629053 -0.564814 -0.434118
 H -6.750402 -1.333949 -1.201637
 H -7.271705 -0.849701 0.407060
 H -7.021298 0.375342 -0.830701
 H -1.630010 0.616971 -3.095221

TSC2→C3

C 1.26634800 -1.77515700 -0.39606800
 H 1.60299100 -2.42953800 0.42529100
 Ru -0.34770300 -0.94664500 -0.33962500
 Cl -0.09413200 -0.30168400 -2.60093600
 C 0.32694800 0.81728500 0.32375300
 C 1.44411900 2.73156100 1.06610400

C	-0.03894100	3.06190200	0.91320200
H	1.75839000	2.70020300	2.11985800
H	2.10111900	3.43346900	0.54329400
H	-0.47211500	3.51812100	1.80916500
H	-0.23391300	3.73015900	0.06113700
N	-0.60972600	1.73898000	0.66655300
N	1.54045500	1.38932700	0.47366100
Cl	-1.12219800	-2.32237800	1.82983600
O	-2.03244600	-1.99774700	-0.70774900
H	-1.90327900	-2.54579200	0.73474000
C	-2.64856900	-2.25816600	-1.93954400
H	-1.92355700	-2.57060200	-2.70215700
H	-3.39406200	-3.05562500	-1.81373700
H	-3.16700600	-1.36472300	-2.32125400
C	2.79881300	0.74111000	0.30782700
C	3.29271100	-0.08338900	1.32989400
C	3.50435300	0.95026100	-0.88375800
C	4.52197500	-0.70948000	1.12957900
C	4.73505600	0.30964600	-1.03374200
C	5.25807800	-0.52324000	-0.04353200
H	4.91168800	-1.36431700	1.90801400
H	5.29191400	0.45293900	-1.95869800
C	-1.99443600	1.41903700	0.50686100
C	-2.61093900	1.58352000	-0.74702900
C	-2.66616300	0.82910300	1.59082600
C	-3.88881500	1.05097200	-0.91434500
C	-3.93937700	0.30893200	1.36755800
C	-4.54955900	0.37823000	0.11409900
H	-4.36484300	1.13548500	-1.89059200
H	-4.45457300	-0.19036100	2.18672300
C	2.91633200	1.78160500	-1.97887000
H	2.01438200	1.30089700	-2.38121600
H	2.61163700	2.77481800	-1.62784200
H	3.62799800	1.91880100	-2.79625800
C	6.58677400	-1.19236900	-0.22345300
H	6.57524000	-2.21965400	0.15246800
H	6.88477800	-1.22156000	-1.27458500
H	7.37718300	-0.66507300	0.32324200
C	2.49250500	-0.31716200	2.57349800
H	2.22942000	0.61919700	3.07953600
H	1.54485400	-0.82116700	2.34257900
H	3.03981000	-0.93840700	3.28620600
C	-2.03314200	0.76096200	2.94687200
H	-0.96891000	0.51405700	2.89046700
H	-2.11234600	1.72438200	3.46624000
H	-2.51995900	0.00867500	3.57093000
C	-1.94697700	2.32800600	-1.86340900
H	-2.19949800	1.88747000	-2.83057700
H	-2.27403000	3.37573700	-1.87419300

H	-0.85727300	2.30838200	-1.78839000
C	-5.87014700	-0.27988600	-0.14049700
H	-6.59022200	0.40955000	-0.59280300
H	-5.75275500	-1.11728000	-0.83837300
H	-6.31147900	-0.67495100	0.77790000
H	1.90774000	-1.76772800	-1.28938900

C3

C	-0.096217	0.225764	0.428214
N	-1.213357	0.149105	1.212050
C	-0.880515	0.039386	2.637472
C	0.565004	0.503328	2.674201
N	0.976361	0.378002	1.273293
C	4.969323	-0.642323	0.315570
C	4.569499	0.690157	0.334334
C	3.260891	1.072132	0.650524
C	2.332894	0.061261	0.932629
C	2.717361	-1.294249	0.974540
C	4.030694	-1.620635	0.658075
C	-5.204701	-0.637123	0.088449
C	-4.249256	-1.657089	0.084261
C	-2.922538	-1.427320	0.444864
C	-2.554355	-0.121602	0.808370
C	-3.484945	0.925098	0.827408
C	-4.803496	0.644433	0.464569
C	2.909503	2.525195	0.690256
C	1.734738	-2.358854	1.346912
C	6.367947	-1.026869	-0.057470
C	-1.910596	-2.526822	0.396584
C	-3.060118	2.319392	1.164262
C	-6.626153	-0.921765	-0.290580
Ru	0.175744	0.338600	-1.470909
C	-1.519323	0.395486	-2.104905
Cl	1.054605	-1.789187	-2.002250
H	-7.110372	-1.580306	0.439026
H	-7.219274	-0.005921	-0.350764
H	-6.691356	-1.427494	-1.259184
H	-5.533616	1.452739	0.468897
H	-2.425077	2.731752	0.371510
H	-2.467631	2.367468	2.084780
H	-3.922342	2.979902	1.282247
H	-4.544092	-2.663837	-0.208945
H	-2.388842	-3.496243	0.238675
H	-1.190384	-2.370547	-0.418019
H	-1.325865	-2.586285	1.321274
H	-1.003114	-1.002045	2.974588
H	-1.551919	0.663504	3.236264
H	0.657114	1.549811	3.002658
H	1.201335	-0.109107	3.320493

H 0.946441 -2.440879 0.591151
 H 1.248804 -2.158777 2.310753
 H 2.223739 -3.333115 1.419252
 H 1.978908 2.709771 1.231306
 H 3.708840 3.102457 1.164928
 H 2.765804 2.915046 -0.321707
 H 5.297673 1.467909 0.107006
 H 6.401441 -1.463418 -1.061912
 H 7.039982 -0.164785 -0.054235
 H 6.777132 -1.778159 0.625103
 H 4.329855 -2.667480 0.674818
 H -2.467973 0.152626 -1.617827
 C 0.074061 3.196060 -0.747961
 O 0.734573 2.204104 -1.466159
 H 0.666245 4.122944 -0.779403
 H -0.076171 2.935337 0.316182
 H -0.919721 3.413660 -1.177961
 H -1.602400 0.700454 -3.164294

TSC3→C4

C 0.171677 0.367637 0.337930
 N 1.290679 1.079033 0.653114
 C 1.025793 2.182017 1.580583
 C -0.493824 2.236829 1.610773
 N -0.884479 0.999523 0.925643
 C -4.970677 0.727845 -0.093916
 C -4.492192 0.149932 1.079614
 C -3.142433 0.204682 1.432648
 C -2.265484 0.860499 0.562571
 C -2.711378 1.467816 -0.622601
 C -4.066603 1.392275 -0.925621
 C 5.330649 0.229626 -0.217562
 C 4.584658 1.105574 -1.015296
 C 3.247559 1.379182 -0.745768
 C 2.646253 0.751888 0.360648
 C 3.363654 -0.120419 1.187385
 C 4.703498 -0.371307 0.870942
 C -2.663804 -0.465131 2.681472
 C -1.748875 2.111252 -1.571000
 C -6.414848 0.617175 -0.474935
 C 2.433673 2.262163 -1.639168
 C 2.732629 -0.800419 2.364232
 C 6.768831 -0.047783 -0.532429
 Ru -0.065322 -1.363890 -0.542195
 C 1.408886 -1.260172 -1.727507
 Cl -1.932056 -1.353063 -2.083219
 H 7.213508 -0.740331 0.186125
 H 6.883799 -0.485053 -1.529717
 H 7.365216 0.870520 -0.523400

H 5.272535 -1.052141 1.502829
 H 2.536390 -1.857032 2.147401
 H 1.774166 -0.353745 2.641295
 H 3.391440 -0.772210 3.237356
 H 5.056810 1.580037 -1.874611
 H 3.046613 2.698585 -2.431004
 H 1.621015 1.694079 -2.108608
 H 1.956629 3.082369 -1.090878
 H 1.489933 3.108655 1.222690
 H 1.463286 1.954529 2.563303
 H -0.908550 2.258462 2.624675
 H -0.898998 3.103713 1.071245
 H -1.193543 1.335205 -2.113630
 H -1.009970 2.747055 -1.068310
 H -2.272931 2.722862 -2.309622
 H -1.768961 0.010209 3.096106
 H -3.439532 -0.468550 3.451982
 H -2.404901 -1.507596 2.464370
 H -5.186109 -0.365877 1.742049
 H -6.561221 -0.172312 -1.220590
 H -7.044248 0.371777 0.384578
 H -6.790691 1.544355 -0.918272
 H -4.422596 1.842094 -1.851369
 H 2.405049 -0.802026 -1.729185
 C -0.130615 -2.393973 1.297820
 O -1.235066 -2.621471 0.634917
 H 0.618268 -3.199073 1.374952
 H -0.165095 -1.725807 2.175948
 H 1.532471 -1.530311 -0.226458
 H 1.294296 -1.980480 -2.555493

C4

C 1.004504 -1.932482 1.809982
 Ru -0.069290 -1.423071 0.121628
 C -0.042325 0.501247 0.308362
 N 1.028017 1.294388 0.584844
 C 0.643478 2.708961 0.671088
 C -0.861525 2.623693 0.839269
 N -1.154287 1.294417 0.288897
 C 2.386300 0.975248 0.260764
 C 2.763729 0.926106 -1.091388
 C 4.097117 0.652420 -1.382910
 C 5.042170 0.426460 -0.379591
 C 4.631280 0.505178 0.950364
 C 3.308660 0.789184 1.296154
 C -2.509007 0.865653 0.188925
 C -3.033659 -0.044524 1.113476
 C -4.387879 -0.375710 1.033637
 C -5.215327 0.166292 0.050954

C -4.644100 1.026595 -0.891561
 C -3.297620 1.381692 -0.850387
 C -6.674060 -0.168894 -0.005501
 C -2.131973 -0.728165 2.086356
 C -2.675241 2.204739 -1.932527
 C 6.456867 0.079529 -0.729743
 C 1.762560 1.136871 -2.185573
 C 2.902589 0.903445 2.733588
 Cl 1.684286 -2.153689 -1.171202
 H 6.821538 0.669284 -1.576176
 H 7.135234 0.240013 0.112542
 H 6.541949 -0.973983 -1.019197
 H 5.358115 0.339220 1.744490
 H 1.865107 0.593888 2.886697
 H 2.993590 1.935188 3.097083
 H 3.538413 0.284480 3.371958
 H 4.401845 0.595906 -2.426883
 H 1.213789 2.080169 -2.070116
 H 2.254919 1.160211 -3.160610
 H 1.017928 0.331895 -2.209782
 H 0.932785 3.233554 -0.251079
 H 1.149688 3.194501 1.510515
 H -1.166641 2.662225 1.895875
 H -1.407676 3.405115 0.303921
 H -1.819699 1.665119 -2.353089
 H -2.304185 3.174009 -1.578464
 H -3.389928 2.404605 -2.733978
 H -1.401064 -0.062535 2.553777
 H -2.692133 -1.238862 2.874764
 H -1.559063 -1.563417 1.612605
 H -4.799645 -1.083539 1.751573
 H -7.287812 0.655685 0.375249
 H -6.910474 -1.052071 0.593253
 H -7.004608 -0.358538 -1.031181
 H -5.261780 1.416549 -1.699591
 H 2.061170 -1.667456 1.695022
 H 0.623208 -1.514973 2.752750
 C -1.686809 -1.951632 -1.195912
 H -2.666241 -1.867110 -0.682121
 H -1.424528 -2.980451 -1.518888
 O -1.188591 -0.946560 -1.804306
 H 0.956350 -3.031443 1.869172

TSC4→C5

C -0.783717 -1.110130 -2.391967
 Ru 0.027955 -1.318724 -0.517598
 C 0.062727 0.550607 0.026787
 N -1.012288 1.365423 0.181186
 C -0.635338 2.758160 0.438333

C 0.855280 2.654860 0.730349
 N 1.175180 1.297321 0.276893
 C -2.386916 0.986302 0.190369
 C -2.913590 0.424879 1.363593
 C -4.264202 0.090101 1.375730
 C -5.083001 0.293402 0.261923
 C -4.526725 0.872984 -0.877538
 C -3.180425 1.238368 -0.934157
 C 2.534639 0.884969 0.168574
 C 3.126309 0.854393 -1.105685
 C 4.462265 0.471307 -1.205300
 C 5.211476 0.131041 -0.075699
 C 4.593142 0.186744 1.173122
 C 3.258215 0.567515 1.325587
 C 6.652572 -0.258551 -0.203117
 C 2.327106 1.191590 -2.326456
 C 2.634511 0.634571 2.683783
 C -6.520137 -0.128912 0.286061
 C -2.032157 0.170588 2.545955
 C -2.613939 1.894974 -2.156003
 Cl -1.884615 -2.385348 0.156807
 H -6.988794 0.082310 1.251991
 H -7.103843 0.371770 -0.491007
 H -6.614634 -1.207747 0.118341
 H -5.155278 1.045502 -1.750339
 H -1.551695 1.665162 -2.284823
 H -2.709778 2.987332 -2.106606
 H -3.139053 1.570784 -3.058437
 H -4.685166 -0.360230 2.273543
 H -1.476413 1.068025 2.846194
 H -2.615049 -0.167402 3.405765
 H -1.287779 -0.603964 2.322289
 H -1.214704 3.157772 1.276687
 H -0.850346 3.377338 -0.445044
 H 1.455520 3.389675 0.183703
 H 1.087048 2.759604 1.800247
 H 1.563538 0.426900 2.643954
 H 2.783060 1.621069 3.142222
 H 3.083857 -0.103327 3.352009
 H 1.747080 2.112963 -2.198179
 H 2.970883 1.309429 -3.201171
 H 1.596039 0.406324 -2.558234
 H 4.928305 0.434733 -2.189145
 H 6.831521 -0.863142 -1.096872
 H 6.994464 -0.828331 0.664682
 H 7.297399 0.624263 -0.284352
 H 5.162625 -0.085855 2.060406
 H -1.848793 -0.854229 -2.341850
 H -0.267153 -0.389781 -3.040630

C 1.697904 -2.228019 0.199842
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H 1.780124 -3.301980 -0.064456
O 1.430254 -1.853082 1.380612
H -0.711221 -2.112419 -2.841363

C5

C 0.167574 0.686024 0.286459
N 1.307741 1.262479 0.689322
C 1.079586 2.608345 1.241586
C -0.433178 2.626844 1.442228
N -0.862309 1.494205 0.612012
C -4.799260 0.005666 0.281765
C -3.948027 -0.466719 1.276096
C -2.652171 0.034367 1.442918
C -2.213160 1.021968 0.544257
C -3.061939 1.557550 -0.442141
C -4.345188 1.033623 -0.552680
C 5.186470 -0.250387 0.044070
C 4.534650 0.481930 -0.952137
C 3.251468 0.995233 -0.769814
C 2.622414 0.753709 0.459685
C 3.239713 0.025647 1.483168
C 4.524934 -0.465905 1.253702
C -1.825021 -0.459872 2.593396
C -2.581193 2.640717 -1.352436
C -6.168419 -0.572452 0.097401
C 2.537941 1.727575 -1.862399
C 2.517310 -0.259243 2.763454
C 6.556152 -0.808976 -0.194635
Ru -0.309716 -1.131967 -0.566341
Cl -0.711445 -0.011561 -2.705252
H 7.227550 -0.061596 -0.627580
H 7.008651 -1.176277 0.729854
H 6.524744 -1.646856 -0.900462
H 5.018055 -1.038446 2.037926
H 1.660262 -0.922124 2.588740
H 2.116084 0.648192 3.229948
H 3.173477 -0.745363 3.489081
H 5.036348 0.654011 -1.903527
H 3.201276 1.917979 -2.708853
H 1.674223 1.156169 -2.230592
H 2.140688 2.691847 -1.524503
H 1.418631 3.366878 0.523167
H 1.645835 2.745442 2.168091
H -0.721952 2.451509 2.489102
H -0.902474 3.558379 1.112700
H -1.708492 2.300862 -1.920639
H -2.288151 3.540738 -0.798170
H -3.359693 2.928779 -2.062196
H -0.813061 -0.048524 2.604202
H -2.305946 -0.197408 3.543084
H -1.733528 -1.549980 2.569845
H -4.294334 -1.249302 1.949711
H -6.207492 -1.211248 -0.791658

H -6.468625 -1.184271 0.951482
 H -6.921497 0.208857 -0.043418
 H -5.005907 1.427968 -1.323138
 C 1.525037 -1.952234 -1.141097
 H 2.241227 -2.052717 -0.323067
 H 1.888432 -1.232137 -1.881203
 H 0.350634 -1.484684 0.836892
 C -1.195756 -2.624093 0.026795
 H -0.941160 -2.696236 -1.197400
 O -1.817747 -3.438803 0.627321
 H 1.372598 -2.919642 -1.624871

Coordinates for the solvent-phase optimised geometries of methylidine species in XYZ format.

C2

Ru 0.123961 0.698176 -1.334749
 C -1.519195 0.505217 -2.046774
 H -2.432308 0.072010 -1.628538
 Cl 1.199807 -1.194617 -2.301184
 Cl 0.011393 2.968208 -0.618518
 C -0.084309 0.041759 0.489224
 C 0.605899 -0.311561 2.710450
 C -0.887935 -0.558364 2.613976
 H 1.153962 -1.133110 3.179912
 H 0.847319 0.612529 3.252740
 H -1.147468 -1.621995 2.711409
 H -1.469142 0.000308 3.351855
 N 0.988764 -0.172039 1.300167
 N -1.202242 -0.091447 1.251957
 C -2.538813 -0.278432 0.785494
 C -2.895539 -1.506846 0.205261
 C -3.470633 0.750933 0.968755
 C -4.218635 -1.679699 -0.201582
 C -4.782759 0.531184 0.543411
 C -5.177540 -0.675696 -0.037569
 H -4.506636 -2.623568 -0.662445
 H -5.515475 1.326652 0.670292
 C 2.364363 -0.249230 0.914918
 C 3.177730 0.891374 0.915362
 C 2.884102 -1.523934 0.614812
 C 4.508691 0.745737 0.503492
 C 4.216902 -1.618413 0.230313
 C 5.041184 -0.489273 0.144463
 H 5.147349 1.627690 0.483989
 H 4.624833 -2.598123 -0.014720
 C 2.021329 -2.742279 0.714120
 H 1.613654 -2.872872 1.723867

H 1.167676 -2.677842 0.032242
 H 2.586764 -3.643103 0.464955
 C 2.697615 2.222041 1.406395
 H 1.616791 2.251988 1.546805
 H 3.174213 2.463571 2.363461
 H 2.958634 3.024443 0.710349
 C 6.462067 -0.617586 -0.312067
 H 7.016144 0.314323 -0.175288
 H 6.989299 -1.409078 0.229512
 H 6.514386 -0.879487 -1.374486
 C -3.059184 2.054473 1.577641
 H -2.705850 1.927863 2.607547
 H -2.232148 2.509790 1.020793
 H -3.893680 2.758948 1.598457
 C -1.869972 -2.569968 -0.039579
 H -1.150455 -2.254109 -0.807667
 H -1.281858 -2.799138 0.856264
 H -2.337001 -3.496888 -0.379576
 C -6.599166 -0.901647 -0.452450
 H -6.664061 -1.509835 -1.358864
 H -7.156621 -1.434889 0.326156
 H -7.122054 0.040812 -0.633679
 H -1.603804 0.877998 -3.084739

TS(C2-C3)

C 1.266348 -1.775157 -0.396068
 H 1.602991 -2.429538 0.425291
 Ru -0.347703 -0.946645 -0.339625
 Cl -0.094132 -0.301684 -2.600936
 C 0.326948 0.817285 0.323753
 C 1.444119 2.731561 1.066104
 C -0.038941 3.061902 0.913202
 H 1.758390 2.700203 2.119858
 H 2.101119 3.433469 0.543294
 H -0.472115 3.518121 1.809165
 H -0.233913 3.730159 0.061137
 N -0.609726 1.738980 0.666553
 N 1.540455 1.389327 0.473661
 Cl -1.122198 -2.322378 1.829836
 O -2.032446 -1.997747 -0.707749
 H -1.903279 -2.545792 0.734740
 C -2.648569 -2.258166 -1.939544
 H -1.923557 -2.570602 -2.702157
 H -3.394062 -3.055625 -1.813737
 H -3.167006 -1.364723 -2.321254
 C 2.798813 0.741110 0.307827
 C 3.292711 -0.083389 1.329894
 C 3.504353 0.950261 -0.883758

C 4.521975 -0.709480 1.129579
 C 4.735056 0.309646 -1.033742
 C 5.258078 -0.523240 -0.043532
 H 4.911688 -1.364317 1.908014
 H 5.291914 0.452939 -1.958698
 C -1.994436 1.419037 0.506861
 C -2.610939 1.583520 -0.747029
 C -2.666163 0.829103 1.590826
 C -3.888815 1.050972 -0.914345
 C -3.939377 0.308932 1.367558
 C -4.549559 0.378230 0.114099
 H -4.364843 1.135485 -1.890592
 H -4.454573 -0.190361 2.186723
 C 2.916332 1.781605 -1.978870
 H 2.014382 1.300897 -2.381216
 H 2.611637 2.774818 -1.627842
 H 3.627998 1.918801 -2.796258
 C 6.586774 -1.192369 -0.223453
 H 6.575240 -2.219654 0.152468
 H 6.884778 -1.221560 -1.274585
 H 7.377183 -0.665073 0.323242
 C 2.492505 -0.317162 2.573498
 H 2.229420 0.619197 3.079536
 H 1.544854 -0.821167 2.342579
 H 3.039810 -0.938407 3.286206
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 C -1.946977 2.328006 -1.863409
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 H -0.857273 2.308382 -1.788390
 C -5.870147 -0.279886 -0.140497
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 H -5.752755 -1.117280 -0.838373
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 H 1.907740 -1.767728 -1.289389

C3

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 C 0.556899 0.579794 2.653604
 N 0.978230 0.426601 1.253793
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 C 3.264787 1.105682 0.627241
 C 2.336495 0.101164 0.933995

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 C -4.277943 -1.629642 0.130273
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 C -2.551244 -0.098301 0.793237
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 C 6.376654 -1.006015 -0.028028
 C -1.953854 -2.528735 0.462448
 C -3.033471 2.356634 1.119615
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 Ru 0.205738 0.296689 -1.507851
 C -1.495134 0.331475 -2.128501
 Cl 0.986567 -1.960772 -1.922821
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 H -3.893366 3.012464 1.273076
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 H 6.416944 -1.443191 -1.032125
 H 7.050971 -0.145964 -0.021060
 H 6.776823 -1.759535 0.656747
 H 4.341477 -2.630984 0.756083
 H -2.439273 0.121419 -1.616604
 C 0.058650 3.159985 -0.813625
 O 0.722444 2.178050 -1.549587
 H 0.635603 4.095725 -0.851026
 H -0.069651 2.891009 0.249036
 H -0.945102 3.362761 -1.227243

H -1.594783 0.610497 -3.194031

TS(C3-C4)

C 0.172549 0.361946 0.334273
N 1.287279 1.062975 0.655542
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C -0.507171 2.286892 1.508685
N -0.892931 1.016685 0.872133
C -4.979087 0.755931 -0.163079
C -4.520099 0.256449 1.054704
C -3.169665 0.306721 1.414500
C -2.267654 0.863078 0.499883
C -2.695785 1.395613 -0.729317
C -4.051008 1.329405 -1.037885
C 5.327100 0.275334 -0.278904
C 4.549470 1.127588 -1.073401
C 3.213695 1.382252 -0.779457
C 2.645594 0.756760 0.346435
C 3.395056 -0.088393 1.172745
C 4.733055 -0.320042 0.831494
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