

Computational insights on the mechanism of the catalytic hydrogenation with BINAP/diamine-Ru complexes: the role of base and origin of selectivity.

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1 Supporting Information

1.1 Cartesian Coordinates

1			
Num. Imaginary Frequencies: 0			
C	1.942252	-0.249500	2.802831
C	2.291322	-0.867260	1.599868
C	3.168382	-1.960426	1.619536
C	3.680213	-2.429410	2.825130
C	3.317821	-1.813540	4.024338
C	2.451707	-0.723232	4.012167
P	1.609312	-0.251557	0.006055
Ru	-0.031571	1.317981	-0.118841
N	1.340817	3.043268	0.072136
C	0.682532	4.308023	-0.319335
C	1.453196	5.518739	0.162247
C	1.303350	-1.837773	-0.895633
C	0.349495	-2.747296	-0.389811
C	0.077296	-3.912895	-1.116228
C	0.704762	-4.179478	-2.328878
C	1.652113	-3.287498	-2.819582
C	1.951238	-2.132807	-2.100313
C	-0.337247	-2.593013	0.926820
C	-1.309763	-1.608695	1.211651
C	-1.934059	-1.617085	2.463989
C	-1.601372	-2.558332	3.435380
C	-0.639264	-3.524225	3.160041
C	-0.027844	-3.541422	1.910744
P	-1.649360	-0.263815	-0.015843
C	-3.255435	0.473599	0.539647
C	-3.241927	1.315454	1.666100
C	-4.396628	1.970774	2.083908
C	-5.586177	1.813436	1.371753
C	-5.608185	0.998703	0.244022
C	-4.453170	0.332726	-0.169934
C	-2.117391	-1.229384	-1.510449
C	-1.563336	-0.874939	-2.742624
C	-1.878258	-1.597300	-3.893417
C	-2.754929	-2.676885	-3.817310
C	-3.311622	-3.039379	-2.589398
C	-2.990441	-2.322818	-1.440823
C	3.083251	0.468947	-0.838919
C	2.883147	1.017603	-2.117260
C	3.901240	1.711168	-2.763220
C	5.134800	1.883541	-2.131203
C	5.339597	1.355347	-0.860082
C	4.321312	0.649098	-0.215585
N	-1.376592	3.037047	-0.379391
C	-0.757430	4.259012	0.177522
C	-1.557059	5.501947	-0.150627
H	2.226016	2.942605	-0.434587
H	-1.571662	3.190508	-1.375884
H	-0.727977	4.115336	1.277228
H	0.648498	4.312136	-1.428457
H	-2.612515	5.367354	0.132820
H	-1.181138	6.383690	0.389055
H	-1.518699	5.721275	-1.232332
H	2.510665	5.446350	-0.135588
H	1.054823	6.453567	-0.258558
H	1.412174	5.593926	1.263139
H	2.716219	-1.455762	-2.489885
H	2.170428	-3.490127	-3.760964
H	-0.661483	-4.616163	-0.716804
H	0.459373	-5.090012	-2.882543
H	0.725325	-4.303119	1.681556
H	-0.368345	-4.270284	3.912149
H	-2.707838	-0.879305	2.692586
H	-2.104689	-2.536942	4.405983

H	-2.294379	2.887044	0.050879
H	1.604838	3.097758	1.061740
H	-3.418358	-2.619660	-0.475693
H	-3.996292	-3.890113	-2.527541
H	-3.003381	-3.244602	-4.718589
H	-1.433492	-1.317514	-4.852672
H	-0.856531	-0.036230	-2.795179
H	-4.494993	-0.298211	-1.062276
H	-6.533428	0.876220	-0.326189
H	-6.493132	2.331935	1.694765
H	-4.365973	2.612552	2.969035
H	-2.306780	1.467469	2.218691
H	3.449771	-2.453091	0.681280
H	4.363299	-3.283618	2.831264
H	3.714739	-2.187642	4.972418
H	2.166037	-0.238820	4.950198
H	1.249934	0.599816	2.789776
H	4.498107	0.243814	0.785621
H	6.301916	1.492452	-0.358825
H	5.934924	2.435032	-2.632576
H	3.732158	2.124276	-3.761604
H	1.906438	0.903518	-2.606279
H	-0.159283	1.268642	1.437055

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Num. Imaginary Frequencies: 0

C	1.903395	-0.198267	2.699114
C	2.149799	-0.980426	1.569399
C	2.875581	-2.171889	1.705269
C	3.337253	-2.575712	2.953578
C	3.079919	-1.792506	4.080278
C	2.365901	-0.604234	3.951594
P	1.605528	-0.427602	-0.100755
C	1.093721	-2.024943	-0.872346
C	0.048150	-2.768681	-0.280429
C	-0.389586	-3.936481	-0.917578
C	0.162620	-4.362655	-2.121121
C	1.199216	-3.634148	-2.694838
C	1.662500	-2.480234	-2.066659
C	-0.567404	-2.452765	1.044048
C	-1.399818	-1.342068	1.303003
C	-1.974973	-1.203818	2.570777
C	-1.727094	-2.127193	3.583681
C	-0.906410	-3.221877	3.333600
C	-0.346665	-3.380837	2.070633
P	-1.677062	-0.087298	-0.026754
C	-3.121824	0.921466	0.539376
C	-2.963523	1.794444	1.630365
C	-3.987374	2.659277	2.006761
C	-5.182779	2.685151	1.286945
C	-5.343858	1.839914	0.193757
C	-4.323285	0.963284	-0.177797
C	3.220567	0.028325	-0.883859
C	3.247672	0.415966	-2.234300
C	4.415675	0.900124	-2.815825
C	5.576282	1.030365	-2.052331
C	5.558551	0.666760	-0.709578
C	4.392080	0.166873	-0.128629
Ru	0.126673	1.298841	-0.369016
N	1.678238	2.847046	-0.158337
C	1.151611	4.186966	-0.501903
C	2.057482	5.292284	-0.003241
N	-1.036461	3.157170	-0.564680
C	-0.276010	4.278692	0.023766
C	-0.939677	5.612905	-0.242967
C	-2.427288	-1.164637	-1.323792
C	-3.407423	-2.099543	-0.959179
C	-3.983416	-2.928171	-1.915894
C	-3.581913	-2.839695	-3.250072
C	-2.607962	-1.917012	-3.620390
C	-2.036436	-1.081663	-2.659853
H	-0.018809	1.424450	1.240474
H	-1.953767	3.093095	-0.113375
H	1.977539	2.847542	0.822299
H	1.096683	4.223240	-1.609723
H	-0.243960	4.090037	1.116412
H	3.097128	5.113946	-0.318449
H	1.757666	6.274424	-0.397198
H	2.037261	5.345633	1.099425
H	-1.998253	5.582806	0.060365
H	-0.459419	6.427880	0.318350
H	-0.897815	5.865965	-1.317103
H	-2.646643	-0.366736	2.777924
H	-2.188820	-1.991704	4.565579
H	0.296844	-4.242764	1.863895
H	-0.705604	-3.957423	4.117327
H	-1.196472	-4.513203	-0.452787
H	-0.211001	-5.270707	-2.602329
H	2.497700	-1.936414	-2.515939

H	1.660372	-3.965627	-3.629270
H	2.529082	2.661883	-0.698067
H	-1.233239	3.373277	-1.547315
H	3.082486	-2.790696	0.823998
H	3.901192	-3.507867	3.050060
H	3.440056	-2.112273	5.062327
H	2.162541	0.011950	4.832072
H	1.327160	0.727957	2.594940
H	4.403699	-0.110502	0.929459
H	6.460947	0.770651	-0.100511
H	6.491973	1.419335	-2.506052
H	4.417187	1.184353	-3.871850
H	2.341662	0.345248	-2.845602
H	-3.723969	-2.181104	0.087218
H	-4.748755	-3.650954	-1.619357
H	-4.030326	-3.495493	-4.001713
H	-2.285886	-1.845396	-4.663018
H	-1.260921	-0.369660	-2.961498
H	-4.472366	0.311929	-1.043603
H	-6.273079	1.858597	-0.382581
H	-5.984589	3.369674	1.576978
H	-3.847442	3.323026	2.864700
H	-2.015066	1.811344	2.179594
H	-0.122570	0.961350	-2.122224
H	0.527020	1.513872	-2.133549

3-OMe

Num. Imaginary Frequencies: 0

C	-3.628342	1.187258	1.199654
C	-3.352587	0.361485	0.096287
C	-4.330026	0.243198	-0.898785
C	-5.551227	0.909577	-0.782595
C	-5.820036	1.701657	0.328920
C	-4.851120	1.840553	1.323307
P	-1.654359	-0.364050	-0.085808
Ru	-0.067074	1.256367	-0.088023
O	0.073050	1.784361	2.246792
C	-1.505258	-1.589328	1.295264
C	-0.442216	-2.522476	1.284474
C	-0.263512	-3.341371	2.409800
C	-1.095174	-3.260569	3.522030
C	-2.167691	-2.376452	3.506725
C	-2.366136	-1.557539	2.398383
C	0.392186	-2.851424	0.084884
C	1.336970	-2.022764	-0.566295
C	2.038052	-2.540789	-1.665757
C	1.830368	-3.835163	-2.131462
C	0.909179	-4.653342	-1.489305
C	0.212293	-4.159556	-0.393505
P	1.627530	-0.255837	-0.082260
C	2.521855	-0.389187	1.533730
C	2.682109	-1.580743	2.243509
C	3.273744	-1.581216	3.508290
C	3.729291	-0.393461	4.072725
C	3.615554	0.798912	3.355651
C	3.016858	0.797139	2.099265
C	3.030332	0.219727	-1.197851
C	2.748258	0.846424	-2.419206
C	3.775222	1.175182	-3.302893
C	5.098085	0.883553	-2.975838
C	5.389032	0.257366	-1.764859
C	4.363082	-0.074363	-0.882281
C	-1.905054	-1.492092	-1.526584
C	-2.762951	-2.593695	-1.398135
C	-3.011197	-3.426699	-2.484001
C	-2.400941	-3.171286	-3.713190
C	-1.544527	-2.081967	-3.848432
C	-1.297156	-1.245859	-2.758925
N	-1.477015	2.943116	-0.267962
C	-0.796623	4.251331	-0.201452
C	0.526030	4.125625	-0.944036
C	1.334395	5.405451	-0.965859
N	1.270197	3.012558	-0.312910
C	-1.677580	5.374292	-0.707349
H	-0.111888	1.141045	-1.665927
H	2.088896	2.784550	-0.885333
H	-1.943491	2.853424	-1.176329
H	-0.555734	4.424540	0.867342
H	0.304144	3.802917	-1.980980
H	-2.659221	5.349735	-0.209575
H	-1.233508	6.362058	-0.514431
H	-1.843843	5.281101	-1.795157
H	2.328381	5.230551	-1.406265
H	0.843428	6.187955	-1.563056
H	1.476925	5.796736	0.057465
H	2.773052	-1.919551	-2.183358
H	2.393669	-4.198084	-2.995415
H	-0.523057	-4.797503	0.107656
H	0.728388	-5.673857	-1.837682
H	0.549308	-4.075746	2.399697
H	-0.918434	-3.908881	4.384489

H	-3.225585	-0.882043	2.398079
H	-2.858177	-2.323530	4.352969
H	-2.234778	2.912182	0.419724
H	1.653671	3.367194	0.570877
H	-3.246917	-2.799766	-0.435807
H	-3.684179	-4.281623	-2.371882
H	-2.594160	-3.826844	-4.567228
H	-1.059941	-1.880698	-4.808181
H	-0.614845	-0.394984	-2.859860
H	-4.145083	-0.373666	-1.782949
H	-6.298959	0.802746	-1.573627
H	-6.779862	2.217424	0.419964
H	-5.045491	2.466783	2.198629
H	-2.867118	1.336560	1.974341
H	2.349114	-2.525908	1.806068
H	3.383062	-2.524015	4.052059
H	4.190451	-0.396098	5.064042
H	4.001911	1.732297	3.774824
H	2.974118	1.732620	1.526218
H	4.606489	-0.579232	0.058616
H	6.424788	0.021272	-1.504630
H	5.904948	1.143395	-3.666799
H	3.538808	1.661497	-4.253619
H	1.706511	1.070819	-2.678574
C	-0.284283	0.956306	3.341084
H	1.017627	1.969367	2.352589
H	-0.014738	1.431911	4.298374
H	-1.372872	0.810656	3.324987
H	0.195656	-0.037917	3.281110

3-OtBu

Num. Imaginary Frequencies: 0

C	3.778487	-0.159211	0.604227
C	3.231117	0.957505	-0.048457
C	4.106393	1.834356	-0.701128
C	5.483999	1.610623	-0.680761
C	6.013160	0.511218	-0.011317
C	5.152871	-0.377750	0.632744
P	1.380176	1.103727	-0.130556
Ru	0.331700	-0.837721	-0.680700
O	1.032202	-1.874422	1.504008
C	0.844087	1.585519	1.578087
C	-0.429643	2.169220	1.777670
C	-0.895563	2.340526	3.087417
C	-0.157385	1.920115	4.189882
C	1.095765	1.350410	3.993883
C	1.592526	1.199220	2.699100
C	-1.301945	2.680032	0.677617
C	-1.954548	1.854197	-0.263115
C	-2.797835	2.438757	-1.212857
C	-2.997024	3.817270	-1.252179
C	-2.363393	4.632362	-0.320144
C	-1.533265	4.059958	0.638637
P	-1.713439	0.025149	-0.160413
C	-2.546685	-0.281876	1.462118
C	-3.645868	0.480179	1.879196
C	-4.267886	0.211692	3.094967
C	-3.803597	-0.824080	3.907367
C	-2.720423	-1.595321	3.493254
C	-2.095820	-1.322945	2.275306
C	-2.960677	-0.676476	-1.339870
C	-2.751857	-0.528966	-2.721683
C	-3.583483	-1.161274	-3.640658
C	-4.630091	-1.971570	-3.196884
C	-4.842489	-2.132642	-1.831377
C	-4.017498	-1.486664	-0.907928
C	1.209044	2.667617	-1.086020
C	1.593634	3.889639	-0.518512
C	1.557978	5.058973	-1.271087
C	1.135760	5.020147	-2.600999
C	0.747865	3.810321	-3.171127
C	0.784739	2.637583	-2.415882
N	2.064626	-1.830021	-1.603113
C	1.787858	-3.250233	-1.903113
C	0.335199	-3.368976	-2.350416
C	-0.086138	-4.786541	-2.676089
N	-0.510895	-2.767047	-1.298504
C	2.776198	-3.820375	-2.898816
H	0.022145	-0.219671	-2.094451
H	-1.470492	-2.675239	-1.645319
H	2.248363	-1.335040	-2.481395
H	1.882372	-3.796072	-0.941603
H	0.208661	-2.728299	-3.246904
H	3.809521	-3.612837	-2.580590
H	2.674367	-4.910799	-3.000905
H	2.628654	-3.368863	-3.895846
H	-1.166013	-4.827626	-2.888588
H	0.438487	-5.176834	-3.560669
H	0.121273	-5.465647	-1.829780
H	-3.330039	1.808503	-1.930791
H	-3.659876	4.249103	-2.007122
H	-1.029709	4.695985	1.374952
H	-2.516375	5.715008	-0.334269
H	-1.878489	2.801002	3.234217
H	-0.558318	2.049078	5.198710

H	2.596379	0.781931	2.567287
H	1.701798	1.033875	4.847731
H	2.934339	-1.747533	-1.067745
H	-0.571913	-3.411223	-0.502032
H	1.931220	3.925598	0.524491
H	1.861436	6.007478	-0.818718
H	1.107531	5.939343	-3.193144
H	0.412487	3.776719	-4.211646
H	0.473790	1.684505	-2.858565
H	3.721142	2.703543	-1.241043
H	6.148353	2.308233	-1.198726
H	7.093332	0.341821	0.002833
H	5.552080	-1.252313	1.156396
H	3.109857	-0.877526	1.086892
H	-4.021303	1.294545	1.249027
H	-5.123453	0.814748	3.412482
H	-4.292072	-1.031536	4.863674
H	-2.358545	-2.416355	4.121095
H	-1.236520	-1.915366	1.947988
H	-4.202779	-1.629020	0.161231
H	-5.658429	-2.767131	-1.473654
H	-5.277411	-2.477711	-3.918471
H	-3.409497	-1.026163	-4.711990
H	-1.916440	0.082304	-3.081379
C	1.411937	-3.025718	2.302401
H	0.970172	-1.097724	2.081578
C	1.178237	-2.692052	3.764692
C	0.547122	-4.195690	1.870591
C	2.879374	-3.335689	2.055000
H	1.449612	-3.545706	4.404848
H	1.799354	-1.832732	4.072000
H	0.121115	-2.442122	3.954226
H	0.793167	-5.090786	2.462792
H	-0.525203	-3.981512	2.012108
H	0.727057	-4.451267	0.812452
H	3.170265	-4.265345	2.569518
H	3.075713	-3.468994	0.977063
H	3.527787	-2.527252	2.431947

3

Num. Imaginary Frequencies: 0

C	2.771285	0.984595	-2.341238
C	3.032498	0.331382	-1.128983
C	4.361007	0.042728	-0.790778
C	5.402446	0.401735	-1.644194
C	5.131986	1.051311	-2.847406
C	3.813898	1.340716	-3.195293
P	1.610508	-0.184412	-0.055896
C	1.339905	-1.935459	-0.590645
C	1.999481	-2.416874	-1.729550
C	1.772065	-3.699826	-2.218932
C	0.883809	-4.539782	-1.557639
C	0.234683	-4.082648	-0.416716
C	0.427967	-2.784895	0.077092
C	-0.331665	-2.452474	1.321201
C	-0.060115	-3.235313	2.451560
C	-0.762040	-3.079849	3.642868
C	-1.792002	-2.149685	3.709173
C	-2.100934	-1.382146	2.586864
C	-1.379962	-1.504295	1.391225
P	-1.673649	-0.362516	-0.042013
C	-1.944793	-1.555428	-1.418565
C	-2.777769	-2.667399	-1.231442
C	-3.012163	-3.554883	-2.276110
C	-2.411015	-3.344087	-3.518474
C	-1.577309	-2.245480	-3.709433
C	-1.345609	-1.352459	-2.662605
Ru	-0.120418	1.287150	-0.086385
N	-1.550428	2.947755	-0.315687
C	-0.901323	4.260317	-0.130556
C	-1.766476	5.396811	-0.633313
N	1.189621	3.061782	-0.163114
C	0.471915	4.195657	-0.785221
C	1.257835	5.485514	-0.683679
C	2.486355	-0.373649	1.566821
C	2.833150	-1.604593	2.129034
C	3.482708	-1.665347	3.362799
C	3.807210	-0.496384	4.045590
C	3.494583	0.740878	3.481709
C	2.840181	0.797648	2.254108
C	-3.386364	0.304776	0.220182
C	-4.427331	0.080720	-0.688715
C	-5.669320	0.694403	-0.518692
C	-5.896263	1.540551	0.561862
C	-4.865171	1.786428	1.468596
C	-3.622086	1.185001	1.291619
H	-0.094155	1.193089	-1.669887
O	-0.255977	1.599359	2.276115
H	2.060459	2.886267	-0.673482
H	-1.923563	2.890527	-1.268413
H	-0.737719	4.375144	0.961058
H	0.327957	3.926093	-1.850937
H	-2.778465	5.331069	-0.204683
H	-1.354553	6.378852	-0.357607
H	-1.858608	5.360701	-1.733165
H	2.281088	5.347306	-1.066165
H	0.794765	6.293776	-1.268646
H	1.327221	5.820932	0.366400
H	2.711760	-1.776603	-2.257159
H	2.297029	-4.039739	-3.115867
H	-0.470891	-4.738112	0.104900
H	0.693907	-5.551747	-1.925869
H	0.732088	-3.989079	2.387740
H	-0.512504	-3.698014	4.509312

H	-2.947772	-0.693301	2.645758
H	-2.373648	-2.026882	4.626872
H	-2.369413	2.878992	0.295295
H	1.480038	3.358753	0.775800
H	-3.250427	-2.839644	-0.256812
H	-3.665922	-4.418094	-2.121612
H	-2.593084	-4.043369	-4.339667
H	-1.099345	-2.081317	-4.679538
H	-0.679090	-0.493548	-2.801211
H	-4.276333	-0.578842	-1.547825
H	-6.466206	0.503977	-1.243189
H	-6.871836	2.015873	0.695465
H	-5.025911	2.457481	2.317139
H	-2.818608	1.423491	1.997855
H	2.609679	-2.531788	1.592749
H	3.743124	-2.638848	3.788319
H	4.315904	-0.546522	5.012139
H	3.768575	1.665845	3.996912
H	2.640233	1.776640	1.801278
H	4.591026	-0.476163	0.145728
H	6.434465	0.169488	-1.366214
H	5.951044	1.332341	-3.515396
H	3.593620	1.847087	-4.139442
H	1.733146	1.207704	-2.615395
H	-0.613823	0.782540	2.660262
H	0.622178	1.656021	2.684716

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Num. Imaginary Frequencies: 0

C	-3.286212	1.589798	1.223906
C	-3.313879	0.499994	0.336322
C	-4.549750	0.078759	-0.168501
C	-5.730299	0.716356	0.215575
C	-5.694965	1.782498	1.110536
C	-4.468423	2.218471	1.611470
P	-1.674242	-0.263671	-0.110960
Ru	-0.015333	1.268821	-0.217600
O	-0.192290	2.092317	1.843450
C	-1.439120	-1.527309	1.228212
C	-0.458558	-2.536058	1.088678
C	-0.227418	-3.404160	2.163949
C	-0.920738	-3.283233	3.364545
C	-1.894065	-2.298273	3.494151
C	-2.150190	-1.437542	2.429542
C	0.273250	-2.815474	-0.183473
C	1.219949	-1.955413	-0.783518
C	1.828989	-2.353463	-1.980775
C	1.528190	-3.571579	-2.584528
C	0.617995	-4.432350	-1.980047
C	0.008846	-4.052223	-0.788923
P	1.595098	-0.291548	-0.058090
C	2.381855	-0.745157	1.557725
C	2.831930	-2.028153	1.884926
C	3.478965	-2.263878	3.097810
C	3.695236	-1.215476	3.990676
C	3.258180	0.069136	3.668512
C	2.600473	0.299457	2.462550
C	3.149108	0.179389	-0.989681
C	3.042330	0.962742	-2.147781
C	4.172620	1.311274	-2.885249
C	5.434955	0.884564	-2.476453
C	5.556229	0.107476	-1.326521
C	4.424787	-0.241274	-0.589844
C	-2.163218	-1.360649	-1.525103
C	-2.928899	-2.517540	-1.323405
C	-3.316880	-3.309893	-2.400046
C	-2.937051	-2.960416	-3.696789
C	-2.171409	-1.816268	-3.907357
C	-1.789400	-1.020087	-2.826790
N	-1.282671	3.002043	-0.767949
C	-0.613855	4.274553	-0.444266
C	0.860534	4.143234	-0.810639
C	1.668978	5.381279	-0.475183
N	1.371267	2.948729	-0.125296
C	-1.297309	5.457402	-1.099734
H	0.146747	0.994231	-1.815533
H	2.352942	2.787424	-0.359427
H	-1.450074	2.952119	-1.776009
H	-0.665368	4.369224	0.657459
H	0.923918	3.944883	-1.901611
H	-2.377079	5.449859	-0.882394
H	-0.896358	6.417127	-0.740124
H	-1.171258	5.425421	-2.196989
H	2.741394	5.202885	-0.652819
H	1.373766	6.247213	-1.087196
H	1.541066	5.651769	0.587914
H	2.563602	-1.697764	-2.457780
H	2.016227	-3.848523	-3.523481
H	-0.720358	-4.718279	-0.314593
H	0.376382	-5.397340	-2.434856
H	0.525821	-4.191352	2.048286
H	-0.707033	-3.967183	4.190849

H	-2.921779	-0.669853	2.543770
H	-2.461097	-2.197225	4.424156
H	-2.204412	2.975675	-0.325112
H	1.280382	3.063233	0.898111
H	-3.221693	-2.806653	-0.306649
H	-3.914799	-4.209791	-2.226704
H	-3.236193	-3.585679	-4.543344
H	-1.864786	-1.540807	-4.921009
H	-1.169295	-0.128853	-2.978828
H	-4.604834	-0.753278	-0.876171
H	-6.685975	0.373618	-0.192503
H	-6.622039	2.279015	1.412113
H	-4.429465	3.061423	2.308379
H	-2.311802	1.948967	1.588911
H	2.687302	-2.855354	1.180646
H	3.822439	-3.273485	3.343520
H	4.204493	-1.400649	4.941150
H	3.419992	0.895611	4.367390
H	2.220953	1.299692	2.222372
H	4.546751	-0.852370	0.309876
H	6.542176	-0.232080	-0.995144
H	6.323709	1.158991	-3.052335
H	4.064847	1.921200	-3.787384
H	2.046081	1.292771	-2.464795
C	-0.357822	1.392809	3.002700
H	0.067695	0.359216	2.995302
H	0.114695	1.895859	3.884465
H	-1.431378	1.245356	3.300295

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Num. Imaginary Frequencies: 0			
C	3.159615	1.138125	-1.945867
C	3.209604	0.408291	-0.745808
C	4.432912	0.332966	-0.069370
C	5.574299	0.952005	-0.583267
C	5.514624	1.653168	-1.783560
C	4.300049	1.744141	-2.465255
P	1.618688	-0.266820	-0.052261
C	1.268619	-1.750847	-1.111663
C	1.867474	-1.908356	-2.366843
C	1.536525	-2.969670	-3.206252
C	0.599891	-3.910659	-2.790953
C	0.012339	-3.778456	-1.537561
C	0.318666	-2.706828	-0.687416
C	-0.347414	-2.709275	0.649805
C	-0.065707	-3.796263	1.487757
C	-0.668533	-3.935912	2.733511
C	-1.593505	-2.985204	3.151784
C	-1.903429	-1.909597	2.322160
C	-1.290372	-1.746035	1.074842
P	-1.609864	-0.268620	-0.003854
C	-2.255583	-1.138175	-1.510505
C	-3.154711	-2.206570	-1.387856
C	-3.656727	-2.842174	-2.519251
C	-3.263350	-2.418562	-3.790677
C	-2.371325	-1.357175	-3.921161
C	-1.870413	-0.720002	-2.784460
Ru	0.008574	1.297492	-0.038052
N	-1.347208	3.034900	-0.293664
C	-0.668225	4.302975	0.038371
C	-1.420851	5.502911	-0.499448
N	1.360540	2.994285	0.104477
C	0.776920	4.223148	-0.445508
C	1.587774	5.452786	-0.083730
C	2.216098	-1.092469	1.489750
C	3.034800	-2.229582	1.451856
C	3.476312	-2.820411	2.631738
C	3.097658	-2.280607	3.863062
C	2.283759	-1.151117	3.905216
C	1.839487	-0.550308	2.723810
C	-3.172526	0.473690	0.664685
C	-4.336300	0.614218	-0.100511
C	-5.422656	1.345989	0.383870
C	-5.365923	1.941246	1.640644
C	-4.207964	1.813911	2.410529
C	-3.117927	1.098123	1.922821
H	0.109514	1.192905	-1.670841
O	0.016110	1.808401	2.120281
H	2.323735	2.872271	-0.214283
H	-1.631822	3.050730	-1.276645
H	-0.632253	4.356203	1.144348
H	0.757738	4.107088	-1.549728
H	-2.479650	5.462350	-0.198618
H	-1.008170	6.451825	-0.125398
H	-1.381157	5.525280	-1.603207
H	2.644988	5.311349	-0.358771
H	1.230092	6.354147	-0.604605
H	1.543103	5.642148	1.003403
H	2.619510	-1.188302	-2.701973
H	2.019931	-3.060881	-4.183390
H	-0.724943	-4.515604	-1.200863
H	0.328256	-4.750072	-3.437537
H	0.662118	-4.541179	1.147632
H	-0.417407	-4.787937	3.371760

H	-2.653411	-1.188733	2.658016
H	-2.087842	-3.081085	4.122939
H	-2.215659	2.955583	0.244425
H	1.340485	3.006277	1.138723
H	-3.466663	-2.544937	-0.392220
H	-4.358668	-3.674633	-2.411163
H	-3.655140	-2.920344	-4.680601
H	-2.057683	-1.023929	-4.915198
H	-1.154180	0.106329	-2.867807
H	-4.401964	0.156129	-1.092367
H	-6.321453	1.448878	-0.231631
H	-6.219446	2.510889	2.019654
H	-4.150190	2.285237	3.396417
H	-2.184694	1.045757	2.496527
H	3.329393	-2.658829	0.485992
H	4.115458	-3.708030	2.593828
H	3.439682	-2.746936	4.792292
H	1.983862	-0.732365	4.871181
H	1.173246	0.328740	2.743898
H	4.504361	-0.208167	0.878524
H	6.517948	0.883726	-0.033717
H	6.410051	2.136078	-2.185638
H	4.238663	2.299672	-3.405967
H	2.197858	1.245077	-2.461260
H	-0.743334	2.367125	2.316204

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Num. Imaginary Frequencies: 0

Ru	0.149226	1.353462	-0.261896
N	1.693696	2.786776	0.045704
N	-0.973738	3.236818	-0.383814
C	-0.122430	4.342560	0.108980
C	1.277298	4.081200	-0.433297
H	1.161020	4.128253	-1.558936
H	2.546366	2.537797	-0.462640
H	-1.220113	3.428729	-1.359794
H	-1.863700	3.221232	0.121725
H	-0.068076	4.217651	1.208901
C	2.261286	5.173653	-0.041841
H	2.030854	6.147842	-0.507142
H	2.273039	5.301924	1.055207
H	3.280330	4.890417	-0.352937
C	-0.711288	5.694537	-0.234933
H	-0.164422	6.513535	0.257151
H	-1.764046	5.761525	0.085626
H	-0.676138	5.873107	-1.325232
H	-0.028383	1.199799	-2.063791
H	0.634631	1.728826	-1.976564
P	1.610636	-0.372972	-0.067961
P	-1.692486	-0.034498	-0.047999
C	-3.180174	0.901693	0.557375
C	-4.418018	0.878303	-0.096137
C	-3.024107	1.770968	1.651680
C	-4.079183	2.565140	2.092790
C	-5.309534	2.524863	1.435609
C	-5.471537	1.684614	0.338508
H	-4.571766	0.228285	-0.962324
H	-6.428395	1.651617	-0.190896
H	-6.137001	3.153877	1.776016
H	-3.936375	3.226557	2.952422
H	-2.050246	1.833077	2.152811
C	-2.441361	-1.047765	-1.408542
C	-2.106248	-0.791818	-2.738398
C	-2.668486	-1.540641	-3.773338
C	-3.575148	-2.556671	-3.483495
C	-3.922340	-2.818647	-2.156789
C	-3.358963	-2.070085	-1.128193
H	-3.635217	-2.283596	-0.088676
H	-4.636271	-3.614206	-1.923638
H	-4.014357	-3.148131	-4.292189
H	-2.391079	-1.330320	-4.810381
H	-1.381930	-0.001983	-2.969196
C	-1.459275	-1.360674	1.229061
C	-0.605685	-2.451348	0.951735
C	-0.397576	-3.415902	1.947181
C	-0.983867	-3.310328	3.203869
C	-1.818510	-2.231662	3.476650
C	-2.057375	-1.276389	2.491365
H	-2.737203	-0.450168	2.716587
H	-2.297823	-2.133674	4.454984
H	-0.789857	-4.071740	3.964688
H	0.260182	-4.262655	1.722139
C	1.095996	-1.943769	-0.914519
C	0.041196	-2.712155	-0.370279
C	-0.384254	-3.857357	-1.056293
C	0.182253	-4.239564	-2.268053
C	1.217255	-3.480835	-2.803882
C	1.671428	-2.352727	-2.123509
H	2.507728	-1.788045	-2.544605
H	1.686950	-3.770216	-3.748457
H	-0.181949	-5.131116	-2.786419

H	-1.194770	-4.453010	-0.622135
C	3.258780	0.037741	-0.819766
C	4.443977	0.044093	-0.075678
C	5.670743	0.946654	-1.954618
C	5.638498	0.497460	-0.638485
C	4.495267	0.952202	-2.706710
C	3.302135	0.516099	-2.139404
H	2.383236	0.557689	-2.734203
H	4.505226	1.310665	-3.740229
H	6.607695	1.300419	-2.394336
H	6.550825	0.500398	-0.034762
H	4.444004	-0.296973	0.963600
H	-0.009331	1.386882	1.351246
C	2.136668	-1.042280	1.573810
C	2.811965	-2.267829	1.656439
C	1.909256	-0.312773	2.742138
C	2.334340	-0.806718	3.976604
C	2.994662	-2.030488	4.051363
C	3.237614	-2.760020	2.886147
H	3.006387	-2.846377	0.745206
H	3.760891	-3.719544	2.937792
H	3.324556	-2.418666	5.019625
H	2.145348	-0.229213	4.886362
H	1.379755	0.644110	2.676108

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Num. Imaginary Frequencies: 0

C	3.395275	0.569484	-1.973385
C	3.280835	0.070447	-0.664038
C	4.422383	0.078555	0.146258
C	5.642449	0.552275	-0.340816
C	5.745524	1.021829	-1.646524
C	4.614411	1.028500	-2.463796
P	1.592732	-0.372351	-0.025467
C	1.158419	-1.938622	-0.917647
C	1.805884	-2.308787	-2.102582
C	1.393859	-3.411643	-2.845916
C	0.324675	-4.182776	-2.400626
C	-0.310345	-3.842073	-1.211640
C	0.076760	-2.722705	-0.460290
C	-0.639236	-2.513079	0.834255
C	-0.497965	-3.540797	1.778211
C	-1.158668	-3.514819	3.000982
C	-2.006462	-2.450694	3.288169
C	-2.172959	-1.429653	2.355960
C	-1.494466	-1.426040	1.130088
P	-1.645169	0.000451	-0.063985
C	-2.279423	-0.917307	-1.545445
C	-3.220344	-1.946359	-1.402959
C	-3.701909	-2.625778	-2.517647
C	-3.246068	-2.286412	-3.793004
C	-2.317298	-1.260075	-3.945157
C	-1.838908	-0.577163	-2.825812
Ru	0.156238	1.368915	-0.219642
N	-0.760287	3.019460	0.368346
C	-0.096761	4.309898	0.356058
C	-1.025965	5.429798	-0.078236
N	1.740603	2.889096	-0.306667
C	1.124931	4.208828	-0.552205
C	2.120794	5.338471	-0.391242
C	2.007478	-1.042122	1.651967
C	2.733275	-2.229009	1.815477
C	3.045479	-2.695699	3.088945
C	2.631428	-1.981448	4.215205
C	1.910361	-0.799610	4.061494
C	1.601873	-0.332281	2.783125
C	-3.190922	0.863894	0.498969
C	-4.339963	0.957883	-0.295384
C	-5.436609	1.714477	0.119538
C	-5.406381	2.389373	1.336566
C	-4.263847	2.316076	2.133270
C	-3.164841	1.571879	1.712188
H	0.468364	0.818307	-1.700822
H	2.474270	2.698535	-0.994278
H	0.289479	4.569217	1.375742
H	0.752582	4.176865	-1.595268
H	-1.902073	5.485003	0.588775
H	-0.536539	6.417635	-0.059478
H	-1.394522	5.240671	-1.101809
H	2.986061	5.204146	-1.060265
H	1.669340	6.314545	-0.627693
H	2.496596	5.384032	0.646280
H	2.662353	-1.729221	-2.457449
H	1.919090	-3.670760	-3.769846
H	-1.147459	-4.448300	-0.848364
H	-0.011476	-5.052944	-2.971690
H	0.166174	-4.378203	1.537355
H	-1.016376	-4.326809	3.719767
H	-2.868138	-0.621563	2.594112
H	-2.552492	-2.413760	4.235336

H	-1.749741	3.118624	0.599449
H	2.218317	2.903969	0.601768
H	-3.580483	-2.221035	-0.404140
H	-4.435248	-3.428165	-2.392385
H	-3.619633	-2.824207	-4.669552
H	-1.959084	-0.987814	-4.942495
H	-1.099589	0.224250	-2.934453
H	-4.386925	0.438933	-1.257380
H	-6.323052	1.773710	-0.519052
H	-6.268186	2.979126	1.662150
H	-4.223180	2.850748	3.086954
H	-2.260023	1.552072	2.330136
H	3.058018	-2.795074	0.933661
H	3.612884	-3.623863	3.206617
H	2.872697	-2.350754	5.216444
H	1.581714	-0.238880	4.941658
H	1.020301	0.589860	2.648549
H	4.367802	-0.283352	1.177240
H	6.519667	0.552212	0.313025
H	6.702676	1.389821	-2.027008
H	4.679508	1.402710	-3.489764
H	2.505704	0.615779	-2.611800

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Num. Imaginary Frequencies: 0

C	-2.111753	-0.897622	-2.719230
C	-2.376093	-1.164082	-1.375444
C	-3.204874	-2.248351	-1.053723
C	-3.746341	-3.049379	-2.054243
C	-3.464560	-2.780095	-3.394535
C	-2.648895	-1.701492	-3.725495
P	-1.669703	-0.081677	-0.047365
C	-1.355127	-1.358732	1.263794
C	-0.479362	-2.438774	1.011453
C	-0.232818	-3.360618	2.038450
C	-0.801906	-3.224330	3.300200
C	-1.654700	-2.154131	3.549126
C	-1.930875	-1.240807	2.534027
C	0.160296	-2.733656	-0.307397
C	1.196240	-1.961631	-0.881555
C	1.773831	-2.393387	-2.081370
C	1.336491	-3.548969	-2.725480
C	0.318384	-4.310773	-2.161240
C	-0.246366	-3.906889	-0.955515
P	1.642702	-0.346673	-0.090702
C	3.266315	0.135375	-0.857471
C	3.288043	0.547099	-2.201138
C	4.445555	1.062451	-2.777055
C	5.604703	1.205666	-2.013337
C	5.593022	0.823191	-0.675647
C	4.436818	0.289592	-0.103197
C	-3.193481	0.794693	0.555202
C	-3.048493	1.758754	1.566811
C	-4.142483	2.488530	2.021480
C	-5.402181	2.289339	1.454833
C	-5.554710	1.355361	0.435157
C	-4.459880	0.612058	-0.010751
Ru	0.090350	1.336481	-0.347961
N	-1.104000	3.047455	-0.666345
C	-0.501959	4.194264	-0.031568
C	-1.250960	5.477056	-0.359179
N	1.560572	2.947915	-0.108340
C	0.955416	4.249365	-0.475939
C	1.759473	5.408462	0.073702
C	2.220168	-0.933748	1.566795
C	2.980571	-2.103042	1.700017
C	3.443082	-2.505959	2.948932
C	3.152585	-1.741728	4.081166
C	2.402792	-0.574906	3.956638
C	1.938377	-0.173323	2.702993
H	-0.112125	1.496148	1.258522
H	2.448685	2.814164	-0.599781
H	-0.460644	4.110477	1.094254
H	0.948827	4.282840	-1.584236
H	-2.317983	5.361573	-0.104290
H	-0.872219	6.352826	0.195681
H	-1.188983	5.690482	-1.441211
H	2.824198	5.318602	-0.197785
H	1.399854	6.373129	-0.316398
H	1.691856	5.444450	1.176191
H	2.596197	-1.824027	-2.523736
H	1.805029	-3.857148	-3.664683
H	-1.041257	-4.506255	-0.498205
H	-0.032392	-5.222980	-2.652243
H	0.442438	-4.198637	1.833164
H	-0.578826	-3.954030	4.083774
H	-2.623241	-0.419734	2.740370
H	-2.118859	-2.030179	4.531802

H	-2.043249	2.951207	-0.276140
H	1.798840	2.966988	0.887757
H	-3.428772	-2.470548	-0.003583
H	-4.390292	-3.892612	-1.787321
H	-3.884666	-3.413289	-4.181460
H	-2.426719	-1.480934	-4.773556
H	-1.472622	-0.049806	-2.988824
H	-4.605911	-0.111906	-0.817463
H	-6.534806	1.199492	-0.025270
H	-6.261246	2.869787	1.803653
H	-4.008154	3.227735	2.816847
H	-2.053687	1.943326	1.988238
H	3.214517	-2.704741	0.813296
H	4.034639	-3.421654	3.042580
H	3.514310	-2.059756	5.063545
H	2.171800	0.025831	4.841413
H	1.328509	0.731887	2.594797
H	4.454710	-0.002335	0.951160
H	6.492641	0.938868	-0.063809
H	6.511927	1.621098	-2.461242
H	4.438870	1.364787	-3.828378
H	2.379275	0.474585	-2.808384
H	-0.102212	1.010740	-2.125067
H	0.509313	1.593068	-2.111488

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Num. Imaginary Frequencies: 0

Ru	-0.160867	1.249138	-0.594428
H	-0.231094	0.535537	-2.032111
P	-1.545695	-0.466077	-0.062005
C	-2.086856	-1.885149	-1.133657
C	-3.184676	0.269939	0.399444
P	1.688106	0.036376	-0.166843
C	3.189281	0.645458	-1.075049
C	2.322053	-0.093670	1.566993
N	-1.724063	2.706770	-1.132596
H	-2.688282	2.385678	-1.007871
N	0.683826	2.983726	-0.132534
C	-0.001899	4.232974	-0.405630
H	0.222556	4.608570	-1.438142
C	-1.499169	3.949465	-0.366220
H	-1.752005	3.706726	0.685647
C	0.393322	5.324075	0.574129
H	1.485098	5.476257	0.559410
H	-0.074844	6.294467	0.340079
H	0.108683	5.035614	1.601552
C	-2.380796	5.080062	-0.852640
H	-3.443703	4.787410	-0.817731
H	-2.266918	5.982460	-0.232161
H	-2.135952	5.352578	-1.894570
C	-1.017980	-1.424156	1.440411
C	-1.639319	-1.258947	2.683888
C	0.082273	-2.305841	1.344239
C	-1.180787	-1.918326	3.822300
H	-2.513351	-0.608262	2.772761
C	0.514335	-2.978673	2.494361
C	-0.094625	-2.782101	3.729363
H	-1.685303	-1.761789	4.780235
H	1.365214	-3.663603	2.408779
H	0.275692	-3.309104	4.613382
C	0.780907	-2.644351	0.068229
C	0.662164	-3.966516	-0.381175
C	1.597361	-1.749081	-0.658382
C	1.302881	-4.408073	-1.534456
H	0.032534	-4.656428	0.191525
C	2.246801	-2.209858	-1.809628
C	2.098800	-3.522101	-2.253556
H	1.180312	-5.442779	-1.867116
H	2.890665	-1.530285	-2.376036
H	2.616306	-3.850695	-3.159545
H	1.676357	3.149957	0.045038
H	-1.622767	2.910216	-2.131973
C	3.239484	-1.076421	1.960705
C	3.685070	-1.140576	3.278083
C	3.213016	-0.224867	4.219904
C	2.302054	0.757078	3.836635
C	1.860265	0.823869	2.514826
H	3.604409	-1.807017	1.228164
H	4.400348	-1.913595	3.575076
H	3.557297	-0.279773	5.257004
H	1.930280	1.476911	4.572024
H	1.142219	1.592221	2.200025
C	4.458129	0.773941	-0.499746
C	5.528336	1.276275	-1.242131
C	5.348015	1.649828	-2.570744
C	4.085975	1.531178	-3.154393
C	3.015756	1.045847	-2.408687
H	4.623202	0.488510	0.543221
H	6.511528	1.376025	-0.772507
H	6.188411	2.041280	-3.151514

H	3.932133	1.829320	-4.195763
H	2.017450	0.977099	-2.856777
C	-2.787476	-2.972603	-0.593820
C	-3.188595	-4.029764	-1.405044
C	-2.892070	-4.014633	-2.769579
C	-2.201458	-2.935902	-3.316006
C	-1.802150	-1.876068	-2.499901
H	-3.021356	-2.992098	0.477594
H	-3.734589	-4.873348	-0.971899
H	-3.202540	-4.848061	-3.406822
H	-1.966574	-2.919252	-4.384532
H	-1.246041	-1.029843	-2.920049
C	-4.356962	0.010457	-0.320749
C	-5.517447	0.751686	-0.086801
C	-5.528800	1.756823	0.876209
C	-4.368673	2.023076	1.605871
C	-3.208328	1.294278	1.361342
H	-4.367901	-0.771253	-1.087047
H	-6.419667	0.538935	-0.667948
H	-6.438755	2.335850	1.058050
H	-4.364348	2.812445	2.363709
H	-2.290322	1.541288	1.908704

6b-OMe

Num. Imaginary Frequencies: 0

C	1.923556	-0.355500	2.859423
C	2.262263	-0.946951	1.641114
C	3.106944	-2.065199	1.644720
C	3.591772	-2.587065	2.840852
C	3.236641	-1.995451	4.054645
C	2.405061	-0.878185	4.060882
P	1.623469	-0.210439	0.056792
C	1.363562	-1.781121	-0.918097
C	0.452028	-2.756120	-0.449646
C	0.219125	-3.898073	-1.227517
C	0.830429	-4.081592	-2.464048
C	1.710245	-3.112284	-2.934969
C	1.975356	-1.983845	-2.161343
C	-0.245004	-2.699617	0.870698
C	-1.260613	-1.770112	1.193365
C	-1.885854	-1.875407	2.442198
C	-1.519000	-2.849414	3.368725
C	-0.520531	-3.764511	3.050204
C	0.092677	-3.690052	1.803495
P	-1.621620	-0.360919	0.025355
C	-3.262856	0.285311	0.642133
C	-3.273500	1.058800	1.817082
C	-4.434913	1.688058	2.257600
C	-5.615526	1.577241	1.521091
C	-5.617444	0.831432	0.345957
C	-4.454638	0.190234	-0.087346
C	3.202949	0.451050	-0.665697
C	3.079216	1.112743	-1.897880
C	4.188462	1.704841	-2.496410
C	5.432414	1.671648	-1.863212
C	5.557290	1.040522	-0.628422
C	4.450015	0.431398	-0.033157
Ru	-0.059909	1.273527	-0.008154
O	0.029841	1.601024	-2.276657
C	0.289653	2.798931	-2.841319
N	-1.453777	2.937405	-0.052153
C	-0.881978	4.061839	0.710012
C	0.556104	4.228900	0.224521
C	1.291084	5.313813	1.006879
N	1.231715	2.952692	0.297873
C	-1.741382	5.306046	0.597030
C	-2.191303	-1.334097	-1.452986
C	-2.963052	-2.499079	-1.350909
C	-3.366042	-3.184171	-2.493935
C	-2.996183	-2.709897	-3.754691
C	-2.231223	-1.550350	-3.862661
C	-1.826259	-0.857786	-2.717664
H	-0.193462	1.206667	1.606999
H	-2.400558	2.726422	0.272066
H	0.453923	4.610820	-0.827665
H	-0.846026	3.726336	1.766731
H	2.345745	5.350202	0.686985
H	0.864784	6.324132	0.865095
H	1.284656	5.077579	2.087240
H	-2.785007	5.093190	0.886505
H	-1.378311	6.118145	1.246648
H	-1.748451	5.681949	-0.442866
H	-2.688487	-1.179940	2.704286
H	-2.024622	-2.894548	4.338296
H	0.877871	-4.407466	1.539169
H	-0.221162	-4.537138	3.764664
H	-0.482129	-4.650659	-0.849429
H	0.616526	-4.977123	-3.055097

H	2.689334	-1.245430	-2.537052
H	2.204260	-3.234476	-3.903755
H	1.975229	2.957698	-0.405934
H	-1.531035	3.198651	-1.040799
H	3.386065	-2.537926	0.694840
H	4.247926	-3.463193	2.828653
H	3.611975	-2.407745	4.996499
H	2.124924	-0.409299	5.009437
H	1.248319	0.508795	2.845100
H	4.569200	-0.055110	0.939954
H	6.524791	1.022630	-0.116494
H	6.301552	2.147548	-2.328192
H	4.077322	2.212062	-3.460815
H	2.076560	1.168911	-2.350246
H	-3.252055	-2.874518	-0.360823
H	-3.968626	-4.093973	-2.404687
H	-3.307085	-3.249983	-4.654837
H	-1.939112	-1.181783	-4.851591
H	-1.204331	0.052811	-2.782327
H	-4.482212	-0.385547	-1.017534
H	-6.533134	0.745618	-0.247528
H	-6.527359	2.078349	1.859508
H	-4.415758	2.278492	3.179056
H	-2.337117	1.188553	2.373181
H	0.302562	2.765492	-3.963913
H	-0.451528	3.622011	-2.613265
H	1.280751	3.257528	-2.560588

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Num. Imaginary Frequencies: 0

C	-3.156987	1.186944	1.832438
C	-3.226848	0.467614	0.627356
C	-4.455549	0.393103	-0.036725
C	-5.593402	1.001344	0.499000
C	-5.520121	1.686493	1.708174
C	-4.296072	1.776707	2.374027
P	-1.621459	-0.192052	-0.046051
Ru	0.021919	1.333662	-0.045739
N	1.374238	3.016462	0.109464
C	0.769903	4.237695	-0.441947
C	1.573378	5.474768	-0.088119
C	-1.319492	-1.684272	1.033334
C	-0.375329	-2.661227	0.637803
C	-0.105694	-3.735352	1.496318
C	-0.710258	-3.847198	2.744352
C	-1.626504	-2.878864	3.141044
C	-1.930746	-1.821351	2.286087
C	0.315020	-2.679226	-0.686635
C	1.295148	-1.742304	-1.086649
C	1.895966	-1.901050	-2.341952
C	1.544489	-2.943357	-3.197153
C	0.589902	-3.873383	-2.796829
C	-0.002077	-3.740910	-1.545000
P	1.630141	-0.248551	-0.024026
C	2.222353	-1.090372	1.523896
C	2.990349	-2.262343	1.518557
C	3.407821	-2.842745	2.713248
C	3.054719	-2.256575	3.930762
C	2.289160	-1.092353	3.943028
C	1.870797	-0.504265	2.745903
C	3.258427	0.367866	-0.710063
C	3.217437	1.159948	-1.870639
C	4.376756	1.714873	-2.406399
C	5.607241	1.508992	-1.780791
C	5.661660	0.745155	-0.618559
C	4.499542	0.178735	-0.089967
C	-2.246276	-1.050717	-1.575294
C	-3.026605	-2.212365	-1.505459
C	-3.501702	-2.821093	-2.663890
C	-3.200662	-2.274803	-3.913107
C	-2.436098	-1.112968	-3.992220
C	-1.966746	-0.501690	-2.828143
N	-1.295496	3.000979	-0.301152
C	-0.677420	4.258680	0.043303
C	-1.450292	5.445340	-0.520790
H	0.148298	1.243429	-1.676567
H	2.342267	2.902896	-0.196885
H	-0.592117	4.437272	1.154904
H	0.748623	4.114272	-1.544811
H	-2.509037	5.377132	-0.219644
H	-1.069273	6.423390	-0.174327
H	-1.421156	5.426217	-1.625327
H	2.629960	5.357771	-0.383061
H	1.188632	6.374527	-0.594487
H	1.546284	5.660015	1.001044
H	2.662774	-1.190598	-2.665933
H	2.027871	-3.030663	-4.175127
H	-0.756884	-4.465843	-1.219703
H	0.306136	-4.701006	-3.453821
H	0.619601	-4.490334	1.172292
H	-0.464912	-4.687575	3.400614
H	-2.672964	-1.085674	2.608009
H	-2.118853	-2.946949	4.116005

H	-2.143254	2.909012	0.265518
H	1.345262	3.028593	1.142167
H	-3.263877	-2.649161	-0.527369
H	-4.107549	-3.730194	-2.594175
H	-3.567131	-2.756124	-4.825190
H	-2.201838	-0.676967	-4.968458
H	-1.351387	0.406399	-2.868152
H	-4.536036	-0.139015	-0.989693
H	-6.544675	0.937293	-0.038768
H	-6.413099	2.159184	2.128830
H	-4.226517	2.324453	3.319428
H	-2.176044	1.291041	2.318443
H	3.263349	-2.728996	0.563259
H	4.007353	-3.758781	2.697976
H	3.376832	-2.713625	4.871968
H	2.006432	-0.637373	4.898030
H	1.233572	0.396157	2.741363
H	4.569916	-0.414228	0.826725
H	6.618388	0.585663	-0.111278
H	6.518568	1.950874	-2.195002
H	4.317833	2.321349	-3.315673
H	2.243536	1.352210	-2.338017
O	-0.030991	1.830113	2.141747
H	-0.673944	2.548058	2.132594

8-OMe

Num. Imaginary Frequencies: 0

C	-1.587040	-0.973411	-2.701173
C	-1.988458	-1.482122	-1.463043
C	-2.701915	-2.687007	-1.410626
C	-3.025558	-3.367731	-2.581273
C	-2.631051	-2.851088	-3.818089
C	-1.913236	-1.658474	-3.874883
P	-1.528303	-0.514789	0.052233
Ru	-0.226934	1.288199	-0.070051
N	0.709022	3.273813	-0.192513
C	-0.175704	4.373484	0.247137
C	0.490218	5.158090	1.357026
C	-0.975400	-1.930992	1.130718
C	0.118634	-2.737305	0.737873
C	0.531740	-3.773798	1.588022
C	-0.083753	-4.014081	2.812086
C	-1.154877	-3.215991	3.200372
C	-1.593956	-2.196296	2.358830
C	0.837452	-2.632810	-0.569353
C	1.648859	-1.540160	-0.959090
C	2.322010	-1.611532	-2.185058
C	2.211619	-2.720691	-3.020646
C	1.424785	-3.801078	-2.633015
C	0.756202	-3.749336	-1.413516
P	1.665842	0.017670	0.062391
C	3.212905	0.877818	-0.527983
C	3.098563	1.608274	-1.724395
C	4.183254	2.332924	-2.215015
C	5.389434	2.366297	-1.513393
C	5.501421	1.670614	-0.312626
C	4.422849	0.930296	0.175517
C	2.297881	-0.709427	1.661631
C	1.812856	-0.229880	2.879727
C	2.283975	-0.744773	4.089072
C	3.254608	-1.743768	4.092807
C	3.751608	-2.228094	2.881078
C	3.273482	-1.716038	1.678055
C	-3.207999	-0.091877	0.741196
C	-3.261869	0.625982	1.948409
C	-4.467606	1.108200	2.446492
C	-5.650794	0.911418	1.730825
C	-5.610222	0.224868	0.521697
C	-4.399877	-0.275011	0.032996
N	-1.824462	2.657644	-0.164248
C	-1.536849	3.797634	0.665395
C	-2.628482	4.857264	0.572836
O	0.120720	1.687922	-2.338967
H	-0.383776	1.292453	1.542447
H	-2.710860	2.272316	0.168327
H	1.666881	3.403953	0.133665
H	-0.350506	5.047076	-0.618624
H	-1.436068	3.534829	1.757313
H	1.411486	5.658258	1.013624
H	-0.181777	5.931626	1.761799
H	0.758734	4.481225	2.188058
H	-3.593437	4.439990	0.911022
H	-2.419740	5.749508	1.191324
H	-2.755755	5.179964	-0.476826
H	-2.454800	-1.597460	2.668820
H	-1.661501	-3.390215	4.154557
H	1.378182	-4.395398	1.274955
H	0.273075	-4.823174	3.456392
H	0.130797	-4.593312	-1.100662
H	1.328568	-4.681625	-3.275142

H	2.956228	-0.776732	-2.498233
H	2.750277	-2.739245	-3.973077
H	0.734699	3.162945	-1.217321
H	3.664554	-2.107045	0.730440
H	4.513652	-3.013978	2.875538
H	3.624578	-2.149532	5.039558
H	1.886478	-0.363500	5.035029
H	1.032738	0.540862	2.860096
H	4.535885	0.393699	1.122267
H	6.437090	1.701065	0.254935
H	6.236779	2.943013	-1.897362
H	4.081681	2.889994	-3.152312
H	2.123080	1.622343	-2.242219
H	-3.010071	-3.096850	-0.440382
H	-3.586531	-4.306580	-2.532338
H	-2.883559	-3.385839	-4.739384
H	-1.593952	-1.258861	-4.843027
H	-0.982056	-0.052984	-2.717704
H	-4.393249	-0.802630	-0.925471
H	-6.527602	0.076681	-0.056538
H	-6.598671	1.302798	2.112565
H	-4.482892	1.658820	3.392380
H	-2.327240	0.837583	2.480599
C	-0.767524	2.390669	-3.093751
H	-0.374270	2.628300	-4.116900
H	-1.744090	1.860499	-3.275007
H	-1.081823	3.371240	-2.652407

8-OtBu

Num. Imaginary Frequencies: 0

C	1.326625	-1.004681	2.648540
C	1.653226	-1.763863	1.522488
C	2.177480	-3.052873	1.687681
C	2.395887	-3.568559	2.962404
C	2.080701	-2.801023	4.086646
C	1.543648	-1.525464	3.926941
P	1.320696	-1.025533	-0.148538
Ru	0.423503	0.993729	-0.435867
N	-0.167498	3.057229	-0.882821
C	0.749133	3.742981	-1.815558
C	0.015242	4.085848	-3.094043
C	0.389492	-2.465327	-0.881206
C	-0.812015	-2.907284	-0.277350
C	-1.528627	-3.948888	-0.885153
C	-1.107888	-4.539498	-2.071986
C	0.075392	-4.107320	-2.661734
C	0.813095	-3.089953	-2.060732
C	-1.358749	-2.403812	1.021476
C	-1.870100	-1.100482	1.228601
C	-2.409732	-0.781247	2.480424
C	-2.460059	-1.712519	3.515045
C	-1.977167	-3.000817	3.306998
C	-1.441285	-3.333951	2.066614
P	-1.680788	0.181449	-0.103563
C	-2.931040	1.478609	0.389634
C	-2.512759	2.400026	1.366398
C	-3.352208	3.440024	1.760774
C	-4.609543	3.597576	1.175350
C	-5.019682	2.706468	0.186923
C	-4.188476	1.653589	-0.202509
C	-2.647209	-0.676632	-1.451974
C	-2.266269	-0.526170	-2.787252
C	-2.990563	-1.141760	-3.810225
C	-4.110477	-1.912935	-3.509052
C	-4.507434	-2.062487	-2.179078
C	-3.780520	-1.449364	-1.162657
C	3.003337	-1.109321	-0.936382
C	3.124602	-0.766347	-2.293884
C	4.372364	-0.628023	-2.893326
C	5.535386	-0.792171	-2.137982
C	5.431862	-1.097223	-0.784214
C	4.177743	-1.258396	-0.189929
N	2.202934	2.049637	-0.898470
C	1.983142	2.856335	-2.066864
C	3.199237	3.704615	-2.420781
O	0.432956	1.964270	1.692347
H	0.370369	0.534550	-1.982724
H	3.011119	1.451628	-1.088087
H	-1.144573	3.255808	-1.101432
H	1.099165	4.683711	-1.337735
H	1.741827	2.249895	-2.986123
H	-0.800320	4.808922	-2.923151
H	0.698299	4.519710	-3.841906
H	-0.422531	3.170940	-3.533618
H	4.062294	3.056073	-2.653026
H	3.029169	4.354655	-3.298927
H	3.486068	4.342330	-1.564724
H	1.753900	-2.782374	-2.525220
H	0.435266	-4.565814	-3.587935
H	-2.457388	-4.285738	-0.411074
H	-1.700618	-5.338226	-2.527881
H	-1.052344	-4.344425	1.896280
H	-2.013254	-3.746800	4.106647

H	-2.810185	0.222958	2.650936
H	-2.887935	-1.429240	4.481704
H	-0.010452	3.325770	0.095780
H	-4.098176	-1.576162	-0.120344
H	-5.388058	-2.664659	-1.933543
H	-4.676731	-2.398866	-4.309709
H	-2.672903	-1.020164	-4.850645
H	-1.370070	0.065361	-3.010986
H	-4.533533	0.968801	-0.983277
H	-5.997301	2.828176	-0.290674
H	-5.263907	4.420096	1.481127
H	-3.013426	4.145865	2.527753
H	-1.487573	2.303536	1.773443
H	2.420183	-3.659894	0.806196
H	2.812523	-4.573798	3.083028
H	2.250943	-3.205223	5.089751
H	1.285003	-0.928007	4.808252
H	0.897178	-0.000652	2.492525
H	4.121657	-1.489407	0.878618
H	6.335181	-1.209886	-0.176514
H	6.518102	-0.668820	-2.603109
H	4.438842	-0.368678	-3.954731
H	2.218078	-0.564859	-2.875656
C	1.311678	2.716594	2.440203
C	0.860346	2.672535	3.909855
C	2.764032	2.222765	2.351222
C	1.303297	4.192989	1.997753
H	1.518059	3.254245	4.583486
H	-0.166258	3.074605	3.998301
H	0.837387	1.627228	4.266561
H	1.932010	4.838157	2.640294
H	1.684137	4.272023	0.964494
H	0.269638	4.588890	2.029082
H	3.453513	2.851996	2.945916
H	2.845501	1.186001	2.723293
H	3.066814	2.239333	1.290612

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Num. Imaginary Frequencies: 0

C	-1.894065	-0.530810	-2.850990
C	-2.285550	-0.975688	-1.586675
C	-3.150659	-2.074748	-1.498858
C	-3.611622	-2.713055	-2.647295
C	-3.209300	-2.261986	-3.906123
C	-2.350684	-1.169333	-4.005452
P	-1.656975	-0.068334	-0.080791
C	-1.488959	-1.516139	1.078635
C	-0.607333	-2.577130	0.763764
C	-0.427784	-3.608979	1.695019
C	-1.062536	-3.598919	2.933664
C	-1.911880	-2.543154	3.251454
C	-2.122701	-1.522112	2.327193
C	0.103735	-2.721257	-0.542644
C	1.131865	-1.860839	-0.993936
C	1.746793	-2.140499	-2.220154
C	1.369255	-3.231242	-3.000332
C	0.368948	-4.087075	-2.550112
C	-0.242926	-3.830583	-1.327128
P	1.581155	-0.339369	-0.014312
C	3.246407	0.121758	-0.734280
C	3.265664	0.832001	-1.946701
C	4.462280	1.269886	-2.506105
C	5.672193	1.032060	-1.851616
C	5.667521	0.353434	-0.637108
C	4.466206	-0.098852	-0.085340
C	-3.244200	0.722702	0.502468
C	-3.129522	1.602015	1.595014
C	-4.251376	2.274745	2.077423
C	-5.496992	2.103830	1.471217
C	-5.612786	1.254207	0.374216
C	-4.495744	0.566789	-0.105391
Ru	0.122804	1.343469	-0.061231
N	1.628370	2.810384	0.170948
C	1.238391	4.050702	-0.454663
C	2.208438	5.179310	-0.130608
O	-0.163892	1.805769	2.076213
N	-1.023854	3.209016	-0.325320
C	-0.178766	4.372197	0.007564
C	-0.759095	5.660458	-0.541443
C	2.111621	-1.155204	1.567429
C	2.822113	-2.362806	1.604146
C	3.202995	-2.923069	2.820295
C	2.870823	-2.280545	4.015217
C	2.159127	-1.083141	3.984355
C	1.774633	-0.516165	2.766036
H	0.345196	1.299773	-1.705254
H	2.515671	2.533600	-0.255247
H	-1.330786	3.277576	-1.298158
H	-0.146201	4.414126	1.113468
H	1.178737	3.976993	-1.579994
H	-1.816875	5.773062	-0.250588
H	-0.218902	6.546384	-0.171660
H	-0.709257	5.673536	-1.646059
H	3.238252	4.873668	-0.382081
H	1.995075	6.111322	-0.683835
H	2.184189	5.399430	0.952305
H	2.551263	-1.491979	-2.579176
H	1.868355	-3.414726	-3.956838
H	-1.035926	-4.495079	-0.965582
H	0.063614	-4.952285	-3.146231
H	0.250419	-4.430492	1.437196
H	-0.890035	-4.411213	3.646045

H	-2.804552	-0.707000	2.587300
H	-2.420992	-2.513078	4.219745
H	-1.869093	3.206138	0.250657
H	-3.465444	-2.439204	-0.512916
H	-4.285883	-3.571304	-2.562162
H	-3.566059	-2.766304	-4.809610
H	-2.028744	-0.813613	-4.989394
H	-1.194856	0.313673	-2.907348
H	-4.612321	-0.094086	-0.969608
H	-6.581760	1.121594	-0.117810
H	-6.373932	2.639287	1.848490
H	-4.149545	2.950185	2.933491
H	-2.126668	1.766112	2.032121
H	3.080373	-2.872218	0.666858
H	3.758544	-3.866359	2.839577
H	3.166688	-2.720936	4.972987
H	1.889727	-0.586732	4.922561
H	1.160690	0.402968	2.715340
H	4.490807	-0.624173	0.873693
H	6.606963	0.172846	-0.105217
H	6.613391	1.385073	-2.284145
H	4.450052	1.814287	-3.455698
H	2.309409	1.058813	-2.433635
H	0.596738	2.404716	2.075087

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Num. Imaginary Frequencies: 0

Ru	0.000009	1.357279	-0.000487
H	-0.129056	1.473792	1.716280
H	0.129129	1.473686	-1.717317
P	-1.612126	-0.202569	0.020770
C	-2.231263	-1.071761	-1.503860
C	-3.217366	0.482934	0.677781
P	1.612106	-0.202655	-0.020987
C	3.217369	0.482486	-0.678317
C	2.231198	-1.071009	1.504151
N	-1.375659	3.085228	-0.105398
H	-2.216494	2.943913	0.460680
N	1.375823	3.085145	0.104317
H	1.699144	3.187574	1.069641
C	0.695221	4.322209	-0.312794
H	0.561337	4.246163	-1.411614
C	-0.695076	4.322095	0.312283
H	-0.561228	4.245559	1.411073
C	1.508319	5.557859	0.017533
H	2.537910	5.454120	-0.359606
H	1.082203	6.466750	-0.433418
H	1.560254	5.711482	1.110459
C	-1.508158	5.557892	-0.017541
H	-2.537765	5.453982	0.359510
H	-1.082076	6.466591	0.433828
H	-1.560055	5.711993	-1.110401
C	-1.288094	-1.691733	1.084092
C	-1.907891	-1.854164	2.328517
C	-0.341723	-2.654346	0.665088
C	-1.605944	-2.929704	3.160691
H	-2.656134	-1.128422	2.659437
C	-0.066645	-3.741015	1.507409
C	-0.678927	-3.881511	2.748141
H	-2.106570	-3.024924	4.128763
H	0.664980	-4.485456	1.174414
H	-0.432888	-4.734295	3.387422
C	0.341621	-2.654729	-0.663992
C	0.066482	-3.741820	-1.505743
C	1.288079	-1.692414	-1.083479
C	0.678790	-3.883019	-2.746383
H	-0.665214	-4.486025	-1.172377
C	1.907886	-1.855535	-2.327806
C	1.605889	-2.931498	-3.159414
H	0.432704	-4.736120	-3.385222
H	2.656165	-1.129991	-2.659093
H	2.106527	-3.027266	-4.127426
H	2.216441	2.943890	-0.462099
H	-1.698616	3.187962	-1.070813
C	3.057854	-2.199442	1.412629
C	3.532324	-2.825267	2.561541
C	3.184323	-2.330863	3.820401
C	2.368087	-1.206827	3.920231
C	1.894893	-0.579950	2.765863
H	3.334833	-2.594477	0.427446
H	4.175958	-3.706293	2.476881
H	3.552685	-2.825638	4.724242
H	2.091175	-0.816700	4.904572
H	1.229881	0.291990	2.822179
C	4.413260	0.464109	0.050263
C	5.556473	1.104125	-0.432735
C	5.528351	1.769387	-1.654557
C	4.342009	1.803300	-2.388746
C	3.198310	1.177010	-1.900282
H	4.462530	-0.049527	1.014809

H	6.477295	1.080028	0.157846
H	6.425708	2.267951	-2.032504
H	4.304192	2.329844	-3.347246
H	2.254286	1.243669	-2.454177
C	-3.058039	-2.200058	-1.411757
C	-3.532479	-2.826475	-2.560358
C	-3.184324	-2.332813	-3.819470
C	-2.367967	-1.208916	-3.919871
C	-1.894799	-0.581444	-2.765816
H	-3.335122	-2.594513	-0.426371
H	-4.176206	-3.707391	-2.475260
H	-3.552664	-2.828062	-4.723060
H	-2.090941	-0.819370	-4.904408
H	-1.229752	0.290443	-2.822563
C	-4.413207	0.464387	-0.050875
C	-5.556416	1.104638	0.431821
C	-5.528340	1.770322	1.653415
C	-4.342041	1.804435	2.387662
C	-3.198346	1.177905	1.899495
H	-4.462439	-0.049579	-1.015247
H	-6.477198	1.080383	-0.158814
H	-6.425697	2.269059	2.031132
H	-4.304257	2.331315	3.345979
H	-2.254361	1.244710	2.453441

acroleine

Num. Imaginary Frequencies: 0

C	0.000000	0.720499	0.000000
C	-0.157136	-0.739093	0.000000
C	1.216888	1.273001	0.000000
H	-0.920098	1.316192	0.000000
H	1.369828	2.355302	0.000000
H	2.115134	0.643677	0.000000
O	-1.217529	-1.317577	0.000000
H	0.816852	-1.300999	0.000000

CH3OH2

Num. Imaginary Frequencies: 0

C	0.770333	0.000000	0.018276
O	-0.700497	0.000000	-0.088725
H	1.105623	0.900767	-0.502575
H	1.055792	0.000007	1.075227
H	1.105621	-0.900775	-0.502562
H	-1.142530	-0.799621	0.265028
H	-1.142528	0.799622	0.265027

H2			
Num.	Imaginary	Frequencies:	0
H	0.000000	0.000000	-0.009028
H	0.000000	0.000000	0.749028
H	0.000000	0.000000	0.379028
H	0.000000	0.000000	-0.379028

H30

Num. Imaginary Frequencies: 0

O	-0.000124	0.000092	-0.085441
H	0.642448	0.673003	0.227808
H	0.263026	-0.892286	0.227622
H	-0.904483	0.218551	0.228097

HOH

Num. Imaginary Frequencies: 0

O	0.000000	0.000000	0.120409
H	0.000000	0.752856	-0.481637
H	0.000000	-0.752856	-0.481637

MeOH

Num. Imaginary Frequencies: 0

C	-0.649294	-0.019594	0.000000
H	-1.095941	0.986679	-0.000001
H	-1.035906	-0.547700	0.893277
O	0.741175	0.122905	0.000000
H	-1.035906	-0.547702	-0.893276
H	1.134120	-0.756952	0.000001

MeO

Num. Imaginary Frequencies: 0

C	0.518237	0.000009	-0.000097
H	1.058847	-0.042661	1.023236
H	1.059228	0.907375	-0.474384
O	-0.785838	0.000000	-0.000004
H	1.059208	-0.864770	-0.548234

complex 6-acrolein-b

Num. Imaginary Frequencies: 0

Ru	-0.145923	1.041999	-0.603118
H	-0.419496	1.799557	1.220224
H	0.038108	0.500099	-2.095271
P	-1.594163	-0.647909	-0.151485
C	-1.912261	-2.086061	-1.266267
C	-3.324797	-0.010989	0.069105
P	1.654035	-0.257488	-0.138535
C	3.144177	0.223965	-1.146320
C	2.393387	-0.277751	1.553687
N	-1.619660	2.486706	-1.379210
H	-2.516198	2.479854	-0.882418
N	1.039795	2.821993	-0.860994
H	1.028934	3.244642	0.120489
C	0.404931	3.778424	-1.781070
H	0.466987	3.358267	-2.808146
C	-1.068967	3.861311	-1.399784
H	-1.103249	4.229814	-0.356685
C	1.095788	5.128100	-1.742219
H	2.174499	5.013746	-1.934021
H	0.698049	5.822431	-2.498243
H	0.975303	5.586861	-0.745267
C	-1.881164	4.773877	-2.294439
H	-2.950167	4.724778	-2.033504
H	-1.567783	5.824403	-2.200972
H	-1.774215	4.479350	-3.353924
C	-1.173301	-1.506627	1.437679
C	-1.815100	-1.177781	2.636935
C	-0.099620	-2.425921	1.470756
C	-1.408689	-1.719267	3.854100
H	-2.657486	-0.481776	2.631996
C	0.266768	-2.991967	2.698863
C	-0.362609	-2.634806	3.886966
H	-1.922902	-1.427880	4.774719
H	1.089457	-3.715096	2.715461
H	-0.037572	-3.076167	4.833275
C	0.649537	-2.890039	0.265307
C	0.552942	-4.250585	-0.055491
C	1.498831	-2.067399	-0.508682
C	1.241894	-4.800057	-1.131749
H	-0.100146	-4.884113	0.554748
C	2.189887	-2.634601	-1.586065
C	2.060515	-3.984193	-1.905768
H	1.136217	-5.863637	-1.363760
H	2.857626	-2.013217	-2.189962
H	2.612079	-4.396570	-2.755460
H	2.013554	2.675518	-1.135693
H	-1.838197	2.200316	-2.337880
C	-0.484572	2.831235	1.826249
O	0.566111	3.610366	1.661886
H	-1.474587	3.239614	1.456047
C	-0.713871	2.341221	3.235355
C	-1.828234	2.546656	3.940077
H	0.133642	1.810607	3.694712
H	-1.942277	2.193641	4.970915
H	-2.678193	3.093183	3.508327
C	3.079944	-1.384670	2.067676
C	3.662993	-1.331624	3.331246
C	3.572763	-0.166479	4.093072
C	2.908760	0.944876	3.578353
C	2.320176	0.894498	2.313888
H	3.164323	-2.301562	1.472774
H	4.191508	-2.205625	3.723935
H	4.026912	-0.124662	5.087575

H	2.840491	1.867307	4.164163
H	1.810651	1.793654	1.933839
C	4.442245	0.234055	-0.621179
C	5.528916	0.602621	-1.414768
C	5.337517	0.964253	-2.745501
C	4.049591	0.960482	-3.280628
C	2.963918	0.599571	-2.486480
H	4.617388	-0.044621	0.422276
H	6.534353	0.607731	-0.983693
H	6.190789	1.253678	-3.365692
H	3.887584	1.244441	-4.324678
H	1.950467	0.606382	-2.904533
C	-2.624504	-3.201398	-0.805679
C	-2.923340	-4.252882	-1.666034
C	-2.514968	-4.200427	-3.000381
C	-1.808504	-3.094687	-3.466619
C	-1.506810	-2.041778	-2.600955
H	-2.952447	-3.244540	0.240134
H	-3.479617	-5.119326	-1.296166
H	-2.749748	-5.027041	-3.677491
H	-1.484334	-3.051115	-4.510596
H	-0.939474	-1.173135	-2.955374
C	-4.394537	-0.419024	-0.737595
C	-5.638533	0.207717	-0.643285
C	-5.838166	1.249349	0.257961
C	-4.779289	1.671226	1.062696
C	-3.535712	1.054185	0.960097
H	-4.264638	-1.232355	-1.457840
H	-6.458732	-0.125905	-1.285849
H	-6.814460	1.737003	0.330164
H	-4.917706	2.493008	1.772437
H	-2.710215	1.418014	1.580084

complex 6-acrolein

Num. Imaginary Frequencies: 0

Ru	0.254682	-0.987469	-0.618517
H	0.695174	-1.845662	1.142783
H	0.033381	-0.438175	-2.098902
P	1.519684	0.839127	-0.146935
C	1.575880	2.369715	-1.180235
C	3.334566	0.449351	-0.050132
P	-1.681555	0.092418	-0.099598
C	-3.094497	-0.436944	-1.193262
C	-2.476018	-0.116349	1.558660
N	1.865860	-2.256125	-1.419417
H	2.761788	-2.156849	-0.932049
N	-0.743989	-2.867737	-0.927300
H	-0.693778	-3.310883	0.048688
C	-0.006679	-3.735789	-1.857991
H	-0.088212	-3.298445	-2.876744
C	1.457830	-3.678266	-1.441449
H	1.489753	-4.034563	-0.392832
C	-0.562540	-5.146770	-1.866719
H	-1.644779	-5.131958	-2.071980
H	-0.089477	-5.774806	-2.637332
H	-0.410591	-5.624007	-0.883069
C	2.379564	-4.511969	-2.305458
H	3.431182	-4.355071	-2.017493
H	2.169154	-5.587638	-2.208988
H	2.273369	-4.237806	-3.370560
C	1.080483	1.520060	1.521109
C	1.816211	1.177754	2.661791
C	-0.100991	2.281488	1.676198
C	1.401673	1.554410	3.937144
H	2.742705	0.605757	2.562005
C	-0.482719	2.678907	2.964496
C	0.244155	2.309339	4.091454
H	1.994809	1.261263	4.808261
H	-1.390026	3.282089	3.077623
H	-0.091804	2.617845	5.085297
C	-0.945965	2.767299	0.544074
C	-1.018852	4.155816	0.369612
C	-1.721283	1.935787	-0.295527
C	-1.804515	4.730149	-0.624113
H	-0.422074	4.795201	1.029391
C	-2.510205	2.527699	-1.289531
C	-2.550122	3.909114	-1.463346
H	-1.830994	5.817276	-0.740933
H	-3.122324	1.898741	-1.942633
H	-3.174923	4.339966	-2.250884
H	-1.726570	-2.818037	-1.205146
H	2.045092	-1.946823	-2.379285
C	0.512834	-2.699207	1.960647
O	-0.251560	-3.693402	1.545111
H	0.093353	-2.058276	2.789904
C	1.907043	-3.106061	2.368295
C	2.487011	-2.795565	3.529428
H	2.444982	-3.739815	1.643609
H	3.493661	-3.138998	3.792221
H	1.963372	-2.179141	4.272271
C	-3.203451	0.902922	2.185930
C	-3.838745	0.674330	3.404659
C	-3.762062	-0.580458	4.007879
C	-3.054028	-1.603840	3.381380
C	-2.413668	-1.377618	2.163019
H	-3.285276	1.889144	1.715604
H	-4.400741	1.481727	3.883970
H	-4.258470	-0.760282	4.966180

H	-2.990985	-2.593743	3.843962
H	-1.861145	-2.209332	1.702038
C	-4.411474	-0.539270	-0.727111
C	-5.444454	-0.909415	-1.587945
C	-5.179945	-1.181600	-2.928177
C	-3.873023	-1.086655	-3.403951
C	-2.840403	-0.722397	-2.542740
H	-4.643100	-0.328830	0.321623
H	-6.465869	-0.986065	-1.203710
H	-5.991701	-1.472080	-3.601408
H	-3.653746	-1.300344	-4.454309
H	-1.811438	-0.655359	-2.914285
C	2.149440	3.547846	-0.683632
C	2.265357	4.673476	-1.493057
C	1.806640	4.635471	-2.811315
C	1.232565	3.469768	-3.312083
C	1.118843	2.340913	-2.498824
H	2.515967	3.581861	0.349728
H	2.716438	5.587342	-1.095114
H	1.896626	5.520494	-3.448085
H	0.868104	3.436676	-4.343060
H	0.659604	1.422311	-2.882461
C	4.312556	1.100461	-0.812043
C	5.640799	0.670671	-0.782806
C	6.017811	-0.412197	0.006580
C	5.051907	-1.076268	0.763188
C	3.726161	-0.654485	0.723660
H	4.045823	1.952116	-1.444676
H	6.387555	1.193013	-1.388192
H	7.060167	-0.742754	0.027762
H	5.325582	-1.933742	1.386805
H	2.979706	-1.203336	1.306721

OH

Num. Imaginary Frequencies: 0

O	0.000000	0.000000	-0.009113
H	0.000000	0.000000	0.959113
O	0.000000	0.000000	0.107581
H	0.000000	0.000000	-0.860645

ts12

Num. Imaginary Frequencies: 1

C	-4.310732	1.083641	-0.184009
C	-3.113686	1.004270	0.536726
C	-2.952046	1.838490	1.657259
C	-3.968602	2.701149	2.058151
C	-5.160629	2.762819	1.335151
C	-5.324399	1.957218	0.212926
P	-1.679989	-0.016662	-0.038289
C	-1.475176	-1.321249	1.259440
C	-0.683306	-2.457681	0.984861
C	-0.519071	-3.422298	1.988302
C	-1.096355	-3.277374	3.244835
C	-1.876535	-2.157504	3.511459
C	-2.067408	-1.196940	2.521117
C	-0.052853	-2.764674	-0.334385
C	1.031115	-2.047522	-0.888263
C	1.613771	-2.502986	-2.076026
C	1.125585	-3.628127	-2.736456
C	0.048715	-4.327676	-2.202451
C	-0.516248	-3.903968	-1.004251
P	1.579556	-0.484268	-0.075106
C	2.060080	-1.084475	1.597401
C	1.810693	-0.321132	2.738968
C	2.229739	-0.770836	3.991837
C	2.903241	-1.983629	4.109090
C	3.163490	-2.748276	2.970385
C	2.744978	-2.301405	1.721713
C	-2.427795	-1.030032	-1.387747
C	-1.988053	-0.908818	-2.706237
C	-2.548778	-1.692372	-3.715473
C	-3.560134	-2.599480	-3.412770
C	-4.009343	-2.725913	-2.096898
C	-3.443887	-1.950192	-1.090647
Ru	0.161233	1.314827	-0.338434
N	1.803181	2.782939	-0.253815
C	1.322764	4.146574	-0.562315
C	2.330650	5.203582	-0.163449
N	-0.915224	3.235157	-0.397175
C	-0.038947	4.317370	0.099498
C	-0.655347	5.682854	-0.116696
C	3.231665	-0.072044	-0.806991
C	3.322345	0.315469	-2.154868
C	4.522428	0.773476	-2.690433
C	5.655416	0.875186	-1.882804
C	5.576682	0.509630	-0.542789
C	4.377078	0.037217	-0.008144
H	0.074458	1.461984	1.273413
H	-1.771331	3.203345	0.164764
H	2.175965	2.769331	0.701403
H	1.164580	4.180740	-1.660251
H	0.092339	4.133589	1.185333
H	3.324517	4.966810	-0.573751
H	2.048382	6.198928	-0.536773
H	2.419427	5.263046	0.935577
H	-1.679654	5.712031	0.286411
H	-0.081252	6.474726	0.386386
H	-0.703068	5.926461	-1.192657
H	-2.709510	-0.340663	2.741781
H	-2.351549	-2.030677	4.488176
H	0.093205	-4.303399	1.768131
H	-0.940790	-4.042814	4.010012
H	-1.353180	-4.460213	-0.568746
H	-0.345607	-5.212522	-2.709617
H	2.480118	-1.984094	-2.494142

H	1.598621	-3.960008	-3.664754
H	2.599795	2.551019	-0.855044
H	-1.227737	3.474581	-1.343190
H	2.953862	-2.906294	0.831338
H	3.695660	-3.699791	3.057588
H	3.229033	-2.337367	5.091463
H	2.024249	-0.168959	4.881635
H	1.268808	0.626102	2.642429
H	4.342034	-0.240866	1.049231
H	6.456840	0.590789	0.101174
H	6.596816	1.243216	-2.299755
H	4.570465	1.058612	-3.745023
H	2.442112	0.267460	-2.805755
H	-3.797176	-2.061912	-0.058789
H	-4.803784	-3.437281	-1.853932
H	-4.000675	-3.213947	-4.203063
H	-2.189641	-1.592320	-4.743662
H	-1.185108	-0.206795	-2.949844
H	-4.462928	0.462957	-1.071456
H	-6.250918	2.004443	-0.366214
H	-5.957375	3.444345	1.645471
H	-3.826021	3.333894	2.938778
H	-2.007664	1.822790	2.214598
H	0.636277	1.067856	-2.074140
H	-0.132676	1.421748	-2.125684

ts26

Num. Imaginary Frequencies: 1

C	-4.380675	0.138636	-0.040491
C	-3.174976	0.258596	0.660732
C	-3.137736	1.103491	1.782532
C	-4.273988	1.789713	2.199904
C	-5.469069	1.663672	1.489792
C	-5.516726	0.839629	0.369442
P	-1.585341	-0.448280	0.020168
C	-1.074741	-1.707592	1.280506
C	-0.043145	-2.621529	0.969124
C	0.351839	-3.548489	1.942826
C	-0.222045	-3.569644	3.209882
C	-1.233181	-2.664717	3.515246
C	-1.658350	-1.753210	2.551245
C	0.614948	-2.734268	-0.368489
C	1.486614	-1.765604	-0.916661
C	2.093473	-2.021293	-2.151276
C	1.848419	-3.200428	-2.851701
C	0.996072	-4.158443	-2.312377
C	0.399363	-3.923410	-1.077641
P	1.686340	-0.125373	-0.077315
C	2.307436	-0.652271	1.580906
C	1.928673	0.042800	2.731021
C	2.424870	-0.333092	3.980077
C	3.308024	-1.404292	4.088235
C	3.696890	-2.101347	2.943072
C	3.198517	-1.728023	1.698936
C	-2.200788	-1.581149	-1.309772
C	-1.979920	-1.274047	-2.653299
C	-2.442638	-2.122286	-3.660500
C	-3.135882	-3.283661	-3.330147
C	-3.375912	-3.591310	-1.989632
C	-2.910936	-2.745844	-0.987140
Ru	-0.115648	1.241417	-0.340878
N	0.949703	3.152782	-0.468028
C	0.263587	4.218805	0.281677
C	0.890016	4.435417	1.641328
N	-1.592244	2.835004	-0.544925
C	-1.244522	3.903763	0.399398
C	-2.095640	5.141681	0.192058
C	3.225345	0.594900	-0.829786
C	3.127253	1.187061	-2.099647
C	4.227649	1.799341	-2.692272
C	5.446597	1.854333	-2.016807
C	5.552428	1.292286	-0.748046
C	4.452745	0.666253	-0.159245
O	-0.290212	3.442207	-2.754161
H	-0.207710	1.413884	1.266447
H	-2.578639	2.587171	-0.442570
H	1.951561	3.165475	-0.271555
H	0.359139	5.156343	-0.306110
H	-1.427592	3.505630	1.416616
H	1.937542	4.768153	1.556290
H	0.341418	5.202983	2.211330
H	0.868397	3.497587	2.223422
H	-3.163552	4.920905	0.357211
H	-1.807827	5.950075	0.884781
H	-1.973118	5.514831	-0.839788
H	-2.475996	-1.070542	2.798197
H	-1.705795	-2.671842	4.501626
H	1.146510	-4.259927	1.692541
H	0.118794	-4.295891	3.953225
H	-0.271151	-4.673836	-0.644633
H	0.796261	-5.090743	-2.848071

H	2.781967	-1.286515	-2.579365
H	2.334679	-3.369882	-3.816657
H	0.772686	3.364325	-1.492205
H	-1.392338	3.179406	-1.527751
H	3.505994	-2.282514	0.804007
H	4.390889	-2.943420	3.021837
H	3.695505	-1.699995	5.067657
H	2.115528	0.215052	4.874891
H	1.221533	0.874688	2.638428
H	4.562137	0.236461	0.840371
H	6.500089	1.339610	-0.203462
H	6.310038	2.343247	-2.477048
H	4.127473	2.246269	-3.685527
H	2.169707	1.180902	-2.630640
H	-3.100774	-2.995880	0.063534
H	-3.927221	-4.498552	-1.725125
H	-3.495505	-3.951602	-4.118377
H	-2.256930	-1.872262	-4.709086
H	-1.433436	-0.362415	-2.916118
H	-4.440789	-0.497731	-0.928691
H	-6.445962	0.738856	-0.198973
H	-6.359767	2.212611	1.808591
H	-4.223007	2.438319	3.079635
H	-2.192138	1.245924	2.317451
H	-0.108167	1.623890	-2.232297
H	0.049706	0.801057	-2.120494
H	-0.296448	3.963648	-3.561795

ts45-OMe

Num. Imaginary Frequencies: 1

C	-4.545606	0.106918	-0.316057
C	-3.335117	0.480004	0.279757
C	-3.330428	1.589273	1.144818
C	-4.507303	2.280364	1.423869
C	-5.708849	1.891688	0.830413
C	-5.721503	0.808745	-0.043640
P	-1.697228	-0.326022	-0.089237
Ru	-0.054918	1.215809	-0.375200
N	1.233536	2.906147	-0.170964
C	0.770237	4.070060	-0.913024
C	1.510080	5.332224	-0.502058
C	-1.392639	-1.369080	1.417707
C	-0.397970	-2.374743	1.389597
C	-0.124215	-3.084531	2.566231
C	-0.775361	-2.800467	3.763125
C	-1.750377	-1.809585	3.789064
C	-2.057642	-1.113168	2.622131
C	0.301736	-2.816966	0.145260
C	1.219677	-2.038046	-0.596553
C	1.782399	-2.588153	-1.756386
C	1.479145	-3.880074	-2.178288
C	0.609045	-4.661882	-1.426236
C	0.035158	-4.127470	-0.277580
P	1.608205	-0.283493	-0.130553
C	2.514814	-0.479139	1.478305
C	2.922607	0.699134	2.116807
C	3.645005	0.652903	3.305523
C	3.963119	-0.576952	3.882393
C	3.568726	-1.755362	3.253078
C	2.856695	-1.705892	2.054073
C	3.094777	0.063828	-1.204934
C	4.345789	-0.507813	-0.932492
C	5.435306	-0.270030	-1.766408
C	5.294851	0.550341	-2.885812
C	4.058927	1.129201	-3.163512
C	2.967455	0.887627	-2.328681
C	-2.214014	-1.618250	-1.309414
C	-1.858574	-1.465459	-2.650943
C	-2.270280	-2.398905	-3.603299
C	-3.042616	-3.492795	-3.220290
C	-3.402802	-3.654042	-1.881037
C	-2.989032	-2.723381	-0.932735
N	-1.342878	2.883890	-1.027719
C	-0.735774	4.190599	-0.695962
C	-1.387257	5.319442	-1.468131
O	-0.191529	2.308868	1.704164
H	0.094970	0.818584	-1.919543
H	2.235579	2.789427	-0.328817
H	-1.416445	2.800421	-2.044975
H	-0.897876	4.335584	0.389129
H	0.918432	3.922547	-2.013263
H	-2.482467	5.297309	-1.347302
H	-1.038759	6.305775	-1.125539
H	-1.162979	5.237309	-2.547101
H	2.598548	5.181134	-0.587611
H	1.249103	6.202407	-1.126453
H	1.288744	5.579360	0.551645
H	2.482938	-1.994137	-2.350675
H	1.933382	-4.274415	-3.091802
H	-0.668817	-4.728993	0.308018
H	0.367214	-5.682925	-1.734920
H	0.628813	-3.879716	2.535832
H	-0.527013	-3.362270	4.667984

H	-2.841150	-0.350647	2.656466
H	-2.284338	-1.579893	4.715790
H	-2.302481	2.844113	-0.672954
H	-3.273959	-2.855154	0.118438
H	-4.008677	-4.512392	-1.575302
H	-3.364725	-4.225702	-3.966051
H	-1.982099	-2.271397	-4.651079
H	-1.237687	-0.608746	-2.939335
H	-4.582498	-0.739149	-1.008566
H	-6.655775	0.501563	-0.523257
H	-6.631890	2.438404	1.044300
H	-4.483696	3.135677	2.106036
H	-2.380478	1.922580	1.583802
H	2.577060	-2.639952	1.555637
H	3.823035	-2.724558	3.693091
H	4.523292	-0.615645	4.821254
H	3.955927	1.583799	3.789604
H	2.663883	1.670499	1.677904
H	4.473363	-1.156916	-0.059388
H	6.402588	-0.728264	-1.539380
H	6.151463	0.739398	-3.539639
H	3.940405	1.776256	-4.037939
H	1.991305	1.338266	-2.539198
H	0.653392	2.745203	1.105595
C	0.022103	1.821382	2.988406
H	0.739656	2.443831	3.560646
H	-0.926720	1.818563	3.562194
H	0.405049	0.779484	3.007342

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Num. Imaginary Frequencies: 1

C	4.409686	-0.255387	-0.702041
C	3.158423	0.305085	-0.991186
C	3.067663	1.247052	-2.022947
C	4.198289	1.615707	-2.751745
C	5.436502	1.048788	-2.457651
C	5.539257	0.111747	-1.429955
P	1.613753	-0.194795	-0.077073
C	1.278922	-1.870915	-0.803045
C	0.380185	-2.780420	-0.198875
C	0.149553	-4.015356	-0.821211
C	0.741295	-4.347067	-2.035277
C	1.592575	-3.434391	-2.649795
C	1.860788	-2.216776	-2.029830
C	-0.304840	-2.541395	1.105170
C	-1.259709	-1.520826	1.318696
C	-1.834064	-1.390228	2.588359
C	-1.492333	-2.245122	3.634370
C	-0.584816	-3.275660	3.414421
C	-0.012286	-3.421699	2.154962
P	-1.649675	-0.315368	-0.039217
C	-2.194577	-1.474111	-1.376977
C	-1.898669	-1.166341	-2.706332
C	-2.332122	-1.998395	-3.739976
C	-3.067287	-3.145364	-3.450986
C	-3.370074	-3.460266	-2.124834
C	-2.935019	-2.630314	-1.095973
C	2.383841	-0.612045	1.561274
C	2.584678	0.447281	2.455826
C	3.179455	0.232894	3.697747
C	3.583647	-1.049815	4.064706
C	3.408513	-2.108016	3.175084
C	2.818005	-1.889241	1.931052
Ru	-0.064790	1.294511	-0.235650
N	-1.433757	2.944210	-0.754655
C	-0.876562	4.255683	-0.362155
C	-1.595730	5.396361	-1.052417
O	-0.160277	2.204262	1.903697
N	1.152637	3.034304	0.044761
C	0.627947	4.217333	-0.619702
C	1.321987	5.485670	-0.153165
C	-3.284919	0.405498	0.484975
C	-3.258350	1.424253	1.454666
C	-4.434297	2.057643	1.851080
C	-5.654731	1.702552	1.275522
C	-5.688881	0.709784	0.300595
C	-4.514475	0.064922	-0.091558
H	0.088570	0.999912	-1.812407
H	2.163086	2.974941	-0.087002
H	-1.532966	2.916674	-1.772803
H	-1.019038	4.335381	0.732942
H	0.758349	4.133361	-1.727814
H	-2.685286	5.317347	-0.907860
H	-1.282107	6.376103	-0.660841
H	-1.395370	5.385617	-2.139034
H	2.413693	5.388597	-0.269224
H	1.008905	6.375533	-0.723122
H	1.113630	5.665256	0.916597
H	2.549037	-1.519008	-2.516917
H	2.060618	-3.670309	-3.609847
H	-0.537867	-4.719848	-0.340058
H	0.528917	-5.313086	-2.502232
H	0.707910	-4.228022	1.976986
H	-0.320641	-3.966646	4.219953

H	-2.578325	-0.608827	2.767890
H	-1.953449	-2.111907	4.617309
H	-2.378915	2.838906	-0.375814
H	-3.174793	-2.884322	-0.056112
H	-3.947748	-4.360144	-1.892828
H	-3.405779	-3.799199	-4.260300
H	-2.089650	-1.749452	-4.777482
H	-1.305972	-0.269067	-2.921010
H	-4.568267	-0.707724	-0.863860
H	-6.638592	0.430718	-0.165767
H	-6.576522	2.205550	1.582333
H	-4.395286	2.842635	2.612608
H	-2.293506	1.731757	1.882408
H	2.702641	-2.727313	1.235037
H	3.737100	-3.115225	3.449406
H	4.043918	-1.223212	5.041755
H	3.328446	1.073493	4.381838
H	2.287988	1.461928	2.167848
H	4.508624	-0.994425	0.100094
H	6.507988	-0.337424	-1.191400
H	6.324228	1.338529	-3.027694
H	4.109666	2.352888	-3.555513
H	2.088590	1.687151	-2.244611
H	0.635560	2.779327	1.228542
H	0.287454	1.629197	2.535437

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Num. Imaginary Frequencies: 1

C	-3.150432	1.461675	1.694158
C	-3.235753	0.516916	0.658914
C	-4.501958	0.191516	0.159279
C	-5.651122	0.780268	0.689700
C	-5.553929	1.701077	1.728886
C	-4.297223	2.040388	2.230774
P	-1.641675	-0.175374	-0.009191
Ru	0.004258	1.365973	-0.070201
N	1.362691	3.078262	0.209682
C	0.725883	4.339308	-0.227575
C	1.442445	5.549027	0.334807
C	-1.296263	-1.603532	1.122240
C	-0.362294	-2.597747	0.754219
C	-0.086733	-3.630824	1.660617
C	-0.679559	-3.679340	2.918081
C	-1.584332	-2.687765	3.284812
C	-1.892043	-1.668455	2.386930
C	0.314372	-2.669273	-0.575918
C	1.275789	-1.737797	-1.030352
C	1.879829	-1.942935	-2.275954
C	1.547281	-3.034829	-3.074971
C	0.611685	-3.960379	-2.623956
C	0.015652	-3.776674	-1.380183
P	1.632453	-0.226249	-0.015085
C	2.258582	-1.027909	1.535167
C	3.038517	-2.191597	1.487785
C	3.519776	-2.769773	2.658452
C	3.226321	-2.191310	3.894797
C	2.458282	-1.030976	3.951211
C	1.978778	-0.451166	2.775392
C	3.221784	0.429071	-0.729285
C	3.158593	1.139220	-1.940243
C	4.293330	1.735761	-2.482716
C	5.515182	1.654296	-1.813343
C	5.588800	0.970134	-0.603934
C	4.453488	0.359881	-0.067101
C	-2.239133	-1.081573	-1.512713
C	-2.993703	-2.258846	-1.415386
C	-3.443430	-2.909755	-2.560497
C	-3.139122	-2.394670	-3.821655
C	-2.388768	-1.226342	-3.928764
C	-1.943008	-0.572931	-2.778951
N	-1.284880	3.061316	-0.477558
C	-0.756711	4.256734	0.131244
C	-1.520612	5.497827	-0.300938
H	-0.118144	1.332577	1.571654
H	2.278850	2.974170	-0.235165
H	-0.795016	4.196528	1.253382
H	0.788953	4.349395	-1.334920
H	-2.599044	5.358637	-0.120506
H	-1.209095	6.402656	0.246727
H	-1.382474	5.675678	-1.382218
H	2.525126	5.491806	0.137614
H	1.075228	6.486400	-0.109966
H	1.298633	5.614131	1.428472
H	2.637857	-1.239839	-2.633477
H	2.033147	-3.165093	-4.046338
H	-0.722938	-4.500143	-1.017548
H	0.345487	-4.826751	-3.236214
H	0.631280	-4.404336	1.366427
H	-0.432556	-4.490851	3.608627
H	-2.620053	-0.905866	2.680656
H	-2.062730	-2.709009	4.268305

H	-2.269662	2.924016	-0.252822
H	1.545141	3.130096	1.215394
H	-3.228440	-2.676173	-0.428593
H	-4.031160	-3.828295	-2.469947
H	-3.486981	-2.909239	-4.722323
H	-2.144186	-0.819735	-4.914606
H	-1.337155	0.337484	-2.857835
H	-4.606067	-0.523624	-0.661378
H	-6.630636	0.514705	0.280900
H	-6.455747	2.161106	2.143483
H	-4.208431	2.768836	3.042424
H	-2.158133	1.742621	2.067068
H	3.271126	-2.653142	0.520362
H	4.125794	-3.679449	2.608328
H	3.599458	-2.648718	4.816002
H	2.225166	-0.574137	4.917727
H	1.354411	0.449941	2.808243
H	4.537380	-0.169645	0.886452
H	6.539240	0.908162	-0.065536
H	6.406027	2.130691	-2.232767
H	4.221196	2.275543	-3.431596
H	2.194777	1.235998	-2.454875
H	0.018358	1.696551	-1.900667
H	-0.597116	2.350619	-1.509040

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Num. Imaginary Frequencies: 1

C	-1.819475	-1.187121	-2.649007
C	-2.206157	-1.411567	-1.326510
C	-3.014224	-2.518406	-1.034212
C	-3.427224	-3.381023	-2.044968
C	-3.034244	-3.148665	-3.364587
C	-2.230632	-2.051657	-3.665034
P	-1.695717	-0.207876	-0.011452
Ru	-0.018829	1.340016	-0.191925
N	-1.289207	3.094734	-0.569590
C	-0.586206	4.324052	-0.145025
C	-1.258240	5.570120	-0.682706
C	-1.415641	-1.373477	1.411983
C	-0.429479	-2.383521	1.308825
C	-0.164763	-3.184410	2.428032
C	-0.815774	-2.990356	3.642293
C	-1.781724	-1.995344	3.743358
C	-2.080142	-1.207908	2.633549
C	0.276531	-2.744472	0.041388
C	1.220022	-1.934235	-0.631788
C	1.806235	-2.422058	-1.807952
C	1.495846	-3.680992	-2.315621
C	0.593659	-4.492309	-1.636045
C	0.000441	-4.020963	-0.469894
P	1.610473	-0.213790	-0.057775
C	3.122820	0.177458	-1.068903
C	2.998039	1.000407	-2.194712
C	4.102108	1.274266	-3.001383
C	5.348250	0.734790	-2.688969
C	5.485661	-0.079393	-1.565299
C	4.381558	-0.354838	-0.761469
C	2.413317	-0.494904	1.586862
C	2.656046	0.642634	2.368116
C	3.294007	0.527111	3.601196
C	3.688210	-0.725533	4.071753
C	3.457234	-1.860363	3.296377
C	2.829200	-1.744562	2.056624
C	-3.344930	0.572568	0.371746
C	-3.397896	1.554732	1.376666
C	-4.573092	2.252200	1.643786
C	-5.722222	2.000037	0.893948
C	-5.680214	1.047290	-0.119320
C	-4.505100	0.338937	-0.377032
N	1.329708	2.895289	0.005606
C	0.872473	4.149662	-0.550357
C	1.735111	5.318158	-0.100195
H	0.013747	1.097851	-1.753292
H	-2.234236	3.064176	-0.175896
H	0.869127	4.150934	-1.677896
H	-0.614885	4.330496	0.964355
H	2.794168	5.116539	-0.330862
H	1.465817	6.267534	-0.593748
H	1.653860	5.453936	0.993104
H	-2.331857	5.581037	-0.432827
H	-0.812599	6.485637	-0.263934
H	-1.165053	5.622005	-1.782460
H	-2.863652	-0.450373	2.725772
H	-2.317425	-1.834130	4.683385
H	0.584411	-3.978581	2.336758
H	-0.573758	-3.622732	4.501056
H	-0.724260	-4.647531	0.061549
H	0.343926	-5.487959	-2.013668
H	2.532148	-1.805169	-2.345935
H	1.969667	-4.026870	-3.238768

H	2.288017	2.739687	-0.315169
H	-1.418287	3.130306	-1.585286
H	2.670623	-2.639932	1.444992
H	3.772294	-2.844613	3.656348
H	4.181038	-0.816920	5.044273
H	3.482610	1.422074	4.201900
H	2.343407	1.625793	1.989241
H	4.505147	-0.999518	0.115338
H	6.461552	-0.503578	-1.310797
H	6.215727	0.952228	-3.319147
H	3.987396	1.918040	-3.878617
H	2.017555	1.431394	-2.426156
H	-3.327433	-2.704606	0.000536
H	-4.059017	-4.241376	-1.804192
H	-3.356143	-3.827761	-4.159742
H	-1.917509	-1.867252	-4.697073
H	-1.176499	-0.328299	-2.875305
H	-4.500789	-0.402323	-1.181421
H	-6.571632	0.847740	-0.721571
H	-6.644935	2.551303	1.096265
H	-4.588659	3.002932	2.439462
H	-2.497624	1.785104	1.957227
H	-0.193727	2.036219	2.188569
H	-0.174970	1.272602	2.261549

ts65b

Num. Imaginary Frequencies: 1

C	-3.329904	1.567763	1.159462
C	-3.309582	0.558007	0.182516
C	-4.438171	0.402382	-0.630670
C	-5.557475	1.220021	-0.461514
C	-5.571289	2.202148	0.524054
C	-4.450520	2.373994	1.337714
P	-1.715709	-0.349680	-0.107832
C	-1.514569	-1.430184	1.385955
C	-2.252078	-1.215770	2.554893
C	-2.018765	-1.954194	3.713173
C	-1.038726	-2.939437	3.714177
C	-0.328869	-3.195322	2.545073
C	-0.544906	-2.460192	1.371825
C	0.155550	-2.941638	0.141400
C	-0.162983	-4.249369	-0.255318
C	0.421757	-4.846784	-1.366475
C	1.363542	-4.136642	-2.102561
C	1.710447	-2.845919	-1.712159
C	1.122722	-2.227114	-0.600641
P	1.570760	-0.481227	-0.167854
C	2.384380	-0.670913	1.478354
C	2.802088	-1.906942	1.985200
C	3.498761	-1.979285	3.189804
C	3.798472	-0.813509	3.893376
C	3.392724	0.420796	3.389718
C	2.683168	0.496046	2.191993
Ru	-0.010002	1.110862	-0.479256
N	1.428167	2.674457	-0.802458
C	0.887388	3.748492	-1.649301
C	1.810058	4.951744	-1.679965
N	-1.277308	2.822771	-1.055912
C	-0.496577	4.079579	-1.103442
C	-1.221981	5.159766	-1.877036
C	-2.258149	-1.608447	-1.352398
C	-3.154417	-2.623335	-0.989527
C	-3.597644	-3.546281	-1.931428
C	-3.147825	-3.467995	-3.250798
C	-2.258254	-2.462700	-3.620652
C	-1.816331	-1.536506	-2.674586
C	3.074590	-0.204828	-1.232162
C	4.374998	-0.478143	-0.790488
C	5.469294	-0.274355	-1.631319
C	5.282314	0.203037	-2.926116
C	3.992397	0.479729	-3.377832
C	2.900136	0.281438	-2.536445
O	1.262020	3.530152	1.686455
C	0.230539	2.795088	2.058157
H	-0.787052	3.278588	1.931246
H	0.070631	1.800506	1.416083
H	-0.005939	0.662018	-2.008422
H	-2.103865	2.949612	-0.463566
H	1.552466	3.078679	0.183958
H	0.763079	3.350165	-2.679699
H	-0.342610	4.395855	-0.053699
H	2.825973	4.650279	-1.981485
H	1.468933	5.719216	-2.391902
H	1.874412	5.407237	-0.676630
H	-2.250428	5.283435	-1.502250
H	-0.720211	6.134904	-1.787129
H	-1.278607	4.903539	-2.950509
H	-3.040174	-0.457073	2.566617
H	-2.608900	-1.754854	4.612429
H	0.418169	-3.996310	2.529301

H	-0.837022	-3.524244	4.615852
H	-0.911886	-4.799768	0.324406
H	0.139720	-5.863840	-1.653075
H	2.468772	-2.312056	-2.291504
H	1.840057	-4.585752	-2.978578
H	2.339789	2.378902	-1.157620
H	-1.644761	2.620682	-1.990584
C	0.308325	2.273842	3.482320
H	2.594095	-2.826869	1.427648
H	3.816084	-2.952329	3.576868
H	4.349879	-0.868318	4.836743
H	3.623971	1.340286	3.936764
H	2.368053	1.483851	1.824602
H	4.545656	-0.854662	0.223045
H	6.477741	-0.491017	-1.266817
H	6.142043	0.363066	-3.583198
H	3.834588	0.855493	-4.393127
H	1.886135	0.503755	-2.889502
H	-3.511576	-2.691007	0.045252
H	-4.297542	-4.333535	-1.635901
H	-3.493363	-4.195436	-3.991279
H	-1.900371	-2.398923	-4.652521
H	-1.106089	-0.750725	-2.955763
H	-4.451662	-0.361058	-1.414317
H	-6.426811	1.083297	-1.111430
H	-6.450315	2.839390	0.655680
H	-4.443805	3.146907	2.111803
H	-2.442713	1.740681	1.779824
C	-0.561339	1.472897	4.097261
H	1.192717	2.645246	4.021054
H	-0.428444	1.159415	5.138030
H	-1.446442	1.080844	3.581288

ts65

Num. Imaginary Frequencies: 1

Ru	0.252946	-0.974921	-0.646690
H	0.744058	-1.853842	1.149025
H	0.018893	-0.380869	-2.100384
P	1.512712	0.853330	-0.140956
C	1.578323	2.415398	-1.128539
C	3.325590	0.453410	-0.039235
P	-1.691812	0.074707	-0.102163
C	-3.110809	-0.444775	-1.191745
C	-2.480006	-0.149366	1.557594
N	1.869391	-2.194473	-1.506038
H	2.785643	-2.067884	-1.064772
N	-0.686475	-2.864454	-0.893393
H	-0.550586	-3.331843	0.188005
C	0.020064	-3.725827	-1.847130
H	-0.115240	-3.325352	-2.878238
C	1.504392	-3.628624	-1.515078
H	1.613921	-3.988793	-0.473535
C	-0.496594	-5.151932	-1.795660
H	-1.585494	-5.170422	-1.963275
H	-0.034123	-5.795207	-2.560733
H	-0.300930	-5.587001	-0.800552
C	2.401204	-4.427654	-2.436437
H	3.462883	-4.242786	-2.207327
H	2.226847	-5.509799	-2.339252
H	2.226818	-4.148617	-3.491239
C	1.061208	1.499637	1.538073
C	1.785459	1.140510	2.680796
C	-0.121274	2.259753	1.691903
C	1.360479	1.504842	3.956541
H	2.711400	0.566928	2.582361
C	-0.510938	2.648684	2.979914
C	0.206107	2.265253	4.108876
H	1.944339	1.199733	4.829881
H	-1.416231	3.255340	3.091417
H	-0.135336	2.566597	5.103086
C	-0.953710	2.748928	0.551893
C	-1.000609	4.135654	0.359396
C	-1.727263	1.918696	-0.290969
C	-1.749087	4.708203	-0.663446
H	-0.405855	4.773505	1.022534
C	-2.485793	2.509974	-1.308601
C	-2.491543	3.888587	-1.506413
H	-1.749528	5.793476	-0.799618
H	-3.094661	1.882091	-1.966003
H	-3.088240	4.319021	-2.315771
H	-1.683811	-2.861454	-1.118402
H	1.988154	-1.877100	-2.472610
C	0.545626	-2.719324	1.916496
O	-0.218421	-3.700635	1.417231
H	0.086194	-2.136892	2.760142
C	1.913775	-3.163978	2.356095
C	2.476998	-2.863063	3.527698
H	2.456634	-3.798715	1.636727
H	3.475348	-3.218451	3.804345
H	1.948732	-2.242940	4.263864
C	-3.195920	0.865572	2.204138
C	-3.822192	0.625087	3.425324
C	-3.748204	-0.637630	4.011856
C	-3.052836	-1.657871	3.365912
C	-2.422070	-1.418689	2.145245
H	-3.275546	1.857784	1.746281
H	-4.374911	1.429680	3.919920
H	-4.237327	-0.826629	4.972097

H	-2.993920	-2.654202	3.814838
H	-1.879464	-2.242884	1.662233
C	-4.435354	-0.477660	-0.736853
C	-5.474425	-0.833079	-1.595899
C	-5.207983	-1.160500	-2.923690
C	-3.893888	-1.135119	-3.387704
C	-2.855173	-0.784746	-2.527590
H	-4.667694	-0.222552	0.301898
H	-6.501962	-0.854705	-1.220965
H	-6.024476	-1.439766	-3.595992
H	-3.673583	-1.393101	-4.427866
H	-1.820680	-0.771038	-2.888955
C	2.179887	3.569868	-0.609269
C	2.278903	4.723572	-1.380384
C	1.774382	4.738430	-2.682334
C	1.172089	3.597073	-3.205077
C	1.075291	2.440053	-2.429979
H	2.580031	3.563486	0.412141
H	2.752459	5.618261	-0.965200
H	1.851060	5.645637	-3.289002
H	0.771597	3.605231	-4.223180
H	0.592539	1.541036	-2.830919
C	4.307790	1.105475	-0.795058
C	5.632468	0.664307	-0.775683
C	6.002630	-0.431959	-0.001761
C	5.032919	-1.097625	0.748544
C	3.710620	-0.664354	0.718249
H	4.046116	1.967291	-1.415894
H	6.381688	1.188067	-1.376815
H	7.042082	-0.771915	0.011908
H	5.300666	-1.966010	1.359492
H	2.962149	-1.218046	1.293564

3-OtBu

Num. Imaginary Frequencies: 0

C	3.778487	-0.159211	0.604227
C	3.231117	0.957505	-0.048457
C	4.106393	1.834356	-0.701128
C	5.483999	1.610623	-0.680761
C	6.013160	0.511218	-0.011317
C	5.152871	-0.377750	0.632744
P	1.380176	1.103727	-0.130556
Ru	0.331700	-0.837721	-0.680700
O	1.032202	-1.874422	1.504008
C	0.844087	1.585519	1.578087
C	-0.429643	2.169220	1.777670
C	-0.895563	2.340526	3.087417
C	-0.157385	1.920115	4.189882
C	1.095765	1.350410	3.993883
C	1.592526	1.199220	2.699100
C	-1.301945	2.680032	0.677617
C	-1.954548	1.854197	-0.263115
C	-2.797835	2.438757	-1.212857
C	-2.997024	3.817270	-1.252179
C	-2.363393	4.632362	-0.320144
C	-1.533265	4.059958	0.638637
P	-1.713439	0.025149	-0.160413
C	-2.546685	-0.281876	1.462118
C	-3.645868	0.480179	1.879196
C	-4.267886	0.211692	3.094967
C	-3.803597	-0.824080	3.907367
C	-2.720423	-1.595321	3.493254
C	-2.095820	-1.322945	2.275306
C	-2.960677	-0.676476	-1.339870
C	-2.751857	-0.528966	-2.721683
C	-3.583483	-1.161274	-3.640658
C	-4.630091	-1.971570	-3.196884
C	-4.842489	-2.132642	-1.831377
C	-4.017498	-1.486664	-0.907928
C	1.209044	2.667617	-1.086020
C	1.593634	3.889639	-0.518512
C	1.557978	5.058973	-1.271087
C	1.135760	5.020147	-2.600999
C	0.747865	3.810321	-3.171127
C	0.784739	2.637583	-2.415882
N	2.064626	-1.830021	-1.603113
C	1.787858	-3.250233	-1.903113
C	0.335199	-3.368976	-2.350416
C	-0.086138	-4.786541	-2.676089
N	-0.510895	-2.767047	-1.298504
C	2.776198	-3.820375	-2.898816
H	0.022145	-0.219671	-2.094451
H	-1.470492	-2.675239	-1.645319
H	2.248363	-1.335040	-2.481395
H	1.882372	-3.796072	-0.941603
H	0.208661	-2.728299	-3.246904
H	3.809521	-3.612837	-2.580590
H	2.674367	-4.910799	-3.000905
H	2.628654	-3.368863	-3.895846
H	-1.166013	-4.827626	-2.888588
H	0.438487	-5.176834	-3.560669
H	0.121273	-5.465647	-1.829780
H	-3.330039	1.808503	-1.930791
H	-3.659876	4.249103	-2.007122
H	-1.029709	4.695985	1.374952
H	-2.516375	5.715008	-0.334269
H	-1.878489	2.801002	3.234217
H	-0.558318	2.049078	5.198710

H	2.596379	0.781931	2.567287
H	1.701798	1.033875	4.847731
H	2.934339	-1.747533	-1.067745
H	-0.571913	-3.411223	-0.502032
H	1.931220	3.925598	0.524491
H	1.861436	6.007478	-0.818718
H	1.107531	5.939343	-3.193144
H	0.412487	3.776719	-4.211646
H	0.473790	1.684505	-2.858565
H	3.721142	2.703543	-1.241043
H	6.148353	2.308233	-1.198726
H	7.093332	0.341821	0.002833
H	5.552080	-1.252313	1.156396
H	3.109857	-0.877526	1.086892
H	-4.021303	1.294545	1.249027
H	-5.123453	0.814748	3.412482
H	-4.292072	-1.031536	4.863674
H	-2.358545	-2.416355	4.121095
H	-1.236520	-1.915366	1.947988
H	-4.202779	-1.629020	0.161231
H	-5.658429	-2.767131	-1.473654
H	-5.277411	-2.477711	-3.918471
H	-3.409497	-1.026163	-4.711990
H	-1.916440	0.082304	-3.081379
C	1.411937	-3.025718	2.302401
H	0.970172	-1.097724	2.081578
C	1.178237	-2.692052	3.764692
C	0.547122	-4.195690	1.870591
C	2.879374	-3.335689	2.055000
H	1.449612	-3.545706	4.404848
H	1.799354	-1.832732	4.072000
H	0.121115	-2.442122	3.954226
H	0.793167	-5.090786	2.462792
H	-0.525203	-3.981512	2.012108
H	0.727057	-4.451267	0.812452
H	3.170265	-4.265345	2.569518
H	3.075713	-3.468994	0.977063
H	3.527787	-2.527252	2.431947

4-OtBu

Num. Imaginary Frequencies: 0

C	1.513065	2.117519	-2.550215
C	1.957394	2.080383	-1.226811
C	2.696395	3.163691	-0.731858
C	2.985879	4.256696	-1.543441
C	2.536180	4.284027	-2.864384
C	1.799856	3.213521	-3.365564
P	1.639404	0.584752	-0.177915
C	1.468547	1.366441	1.495648
C	0.410969	2.271677	1.742239
C	0.237870	2.761028	3.044349
C	1.070836	2.376320	4.090931
C	2.128606	1.510870	3.837309
C	2.320317	1.016720	2.549215
C	-0.411695	2.895606	0.659366
C	-1.330665	2.241789	-0.195090
C	-1.971569	2.997162	-1.188143
C	-1.743175	4.361360	-1.342679
C	-0.868486	5.011835	-0.480078
C	-0.221377	4.278474	0.506841
P	-1.651238	0.411521	-0.100337
C	-3.127346	0.251662	-1.242640
C	-2.962852	-0.228820	-2.547050
C	-4.046562	-0.317450	-3.421513
C	-5.315427	0.078500	-3.006402
C	-5.493086	0.565602	-1.711792
C	-4.410697	0.649204	-0.839232
C	3.343302	-0.152919	-0.103519
C	3.454629	-1.396737	0.541283
C	4.691834	-2.029021	0.645806
C	5.831831	-1.442209	0.094563
C	5.723987	-0.221624	-0.566723
C	4.488762	0.422296	-0.664713
Ru	0.052596	-0.964543	-0.659369
N	-1.226878	-2.672858	-1.128790
C	-0.640949	-3.534263	-2.168217
C	-1.364758	-4.862318	-2.271941
O	0.575836	-2.494818	0.955061
C	0.326278	-2.889301	2.253621
N	1.426058	-2.342374	-1.704561
C	0.840123	-3.687703	-1.843353
C	1.595944	-4.533693	-2.847280
C	-2.586005	0.256813	1.498112
C	-2.769893	1.282868	2.426491
C	-3.443869	1.044043	3.626138
C	-3.965440	-0.217592	3.899760
C	-3.820319	-1.241194	2.961765
C	-3.132128	-1.002089	1.777734
H	-0.170411	-0.244494	-2.081394
H	-2.218345	-2.513345	-1.318192
H	1.645203	-1.962350	-2.629033
H	0.902295	-4.133568	-0.832318
H	-0.727342	-2.987222	-3.130671
H	2.673982	-4.530088	-2.621321
H	1.262126	-5.582403	-2.837616
H	1.462598	-4.144189	-3.872887
H	-2.448357	-4.707502	-2.396194
H	-1.017047	-5.457375	-3.130182
H	-1.209259	-5.459288	-1.355264
H	-2.674961	2.509812	-1.868608
H	-2.257376	4.911864	-2.135692
H	0.489622	4.779779	1.172390
H	-0.679838	6.084677	-0.578051
H	-0.570211	3.476473	3.233558

H	0.901814	2.770580	5.096914
H	3.155377	0.334026	2.365638
H	2.809027	1.214196	4.640727
H	2.314395	-2.411243	-1.201622
H	-1.126492	-3.136686	-0.215169
H	3.051482	3.151947	0.305863
H	3.563760	5.094941	-1.142640
H	2.759958	5.144217	-3.502392
H	1.441280	3.230605	-4.399187
H	0.921711	1.277730	-2.933071
H	4.429884	1.380865	-1.188777
H	6.609728	0.240229	-1.013469
H	6.802499	-1.941078	0.172382
H	4.762819	-2.995461	1.156458
H	2.535336	-1.873414	0.927412
H	-2.393219	2.287470	2.214239
H	-3.568045	1.857367	4.347696
H	-4.493427	-0.403090	4.839625
H	-4.235474	-2.234333	3.159898
H	-3.010530	-1.813904	1.050154
H	-4.570097	1.042224	0.170526
H	-6.484590	0.884490	-1.376641
H	-6.166590	0.009473	-3.690152
H	-3.894532	-0.697147	-4.436428
H	-1.960407	-0.525201	-2.875066
C	0.059548	-1.712968	3.197904
C	-0.872191	-3.851765	2.304506
C	1.548829	-3.653590	2.788710
H	-0.161909	-2.047484	4.228423
H	0.943155	-1.054088	3.235119
H	-0.790411	-1.107641	2.843851
H	1.376863	-4.080971	3.793531
H	1.802204	-4.479097	2.098858
H	2.424526	-2.983552	2.854073
H	-1.082342	-4.229678	3.322070
H	-1.785676	-3.348859	1.943483
H	-0.677384	-4.722353	1.650199

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C	1.326625	-1.004681	2.648540
C	1.653226	-1.763863	1.522488
C	2.177480	-3.052873	1.687681
C	2.395887	-3.568559	2.962404
C	2.080701	-2.801023	4.086646
C	1.543648	-1.525464	3.926941
P	1.320696	-1.025533	-0.148538
Ru	0.423503	0.993729	-0.435867
N	-0.167498	3.057229	-0.882821
C	0.749133	3.742981	-1.815558
C	0.015242	4.085848	-3.094043
C	0.389492	-2.465327	-0.881206
C	-0.812015	-2.907284	-0.277350
C	-1.528627	-3.948888	-0.885153
C	-1.107888	-4.539498	-2.071986
C	0.075392	-4.107320	-2.661734
C	0.813095	-3.089953	-2.060732
C	-1.358749	-2.403812	1.021476
C	-1.870100	-1.100482	1.228601
C	-2.409732	-0.781247	2.480424
C	-2.460059	-1.712519	3.515045
C	-1.977167	-3.000817	3.306998
C	-1.441285	-3.333951	2.066614
P	-1.680788	0.181449	-0.103563
C	-2.931040	1.478609	0.389634
C	-2.512759	2.400026	1.366398
C	-3.352208	3.440024	1.760774
C	-4.609543	3.597576	1.175350
C	-5.019682	2.706468	0.186923
C	-4.188476	1.653589	-0.202509
C	-2.647209	-0.676632	-1.451974
C	-2.266269	-0.526170	-2.787252
C	-2.990563	-1.141760	-3.810225
C	-4.110477	-1.912935	-3.509052
C	-4.507434	-2.062487	-2.179078
C	-3.780520	-1.449364	-1.162657
C	3.003337	-1.109321	-0.936382
C	3.124602	-0.766347	-2.293884
C	4.372364	-0.628023	-2.893326
C	5.535386	-0.792171	-2.137982
C	5.431862	-1.097223	-0.784214
C	4.177743	-1.258396	-0.189929
N	2.202934	2.049637	-0.898470
C	1.983142	2.856335	-2.066864
C	3.199237	3.704615	-2.420781
O	0.432956	1.964270	1.692347
H	0.370369	0.534550	-1.982724
H	3.011119	1.451628	-1.088087
H	-1.144573	3.255808	-1.101432
H	1.099165	4.683711	-1.337735
H	1.741827	2.249895	-2.986123
H	-0.800320	4.808922	-2.923151
H	0.698299	4.519710	-3.841906
H	-0.422531	3.170940	-3.533618
H	4.062294	3.056073	-2.653026
H	3.029169	4.354655	-3.298927
H	3.486068	4.342330	-1.564724
H	1.753900	-2.782374	-2.525220
H	0.435266	-4.565814	-3.587935
H	-2.457388	-4.285738	-0.411074
H	-1.700618	-5.338226	-2.527881
H	-1.052344	-4.344425	1.896280
H	-2.013254	-3.746800	4.106647

H	-2.810185	0.222958	2.650936
H	-2.887935	-1.429240	4.481704
H	-0.010452	3.325770	0.095780
H	-4.098176	-1.576162	-0.120344
H	-5.388058	-2.664659	-1.933543
H	-4.676731	-2.398866	-4.309709
H	-2.672903	-1.020164	-4.850645
H	-1.370070	0.065361	-3.010986
H	-4.533533	0.968801	-0.983277
H	-5.997301	2.828176	-0.290674
H	-5.263907	4.420096	1.481127
H	-3.013426	4.145865	2.527753
H	-1.487573	2.303536	1.773443
H	2.420183	-3.659894	0.806196
H	2.812523	-4.573798	3.083028
H	2.250943	-3.205223	5.089751
H	1.285003	-0.928007	4.808252
H	0.897178	-0.000652	2.492525
H	4.121657	-1.489407	0.878618
H	6.335181	-1.209886	-0.176514
H	6.518102	-0.668820	-2.603109
H	4.438842	-0.368678	-3.954731
H	2.218078	-0.564859	-2.875656
C	1.311678	2.716594	2.440203
C	0.860346	2.672535	3.909855
C	2.764032	2.222765	2.351222
C	1.303297	4.192989	1.997753
H	1.518059	3.254245	4.583486
H	-0.166258	3.074605	3.998301
H	0.837387	1.627228	4.266561
H	1.932010	4.838157	2.640294
H	1.684137	4.272023	0.964494
H	0.269638	4.588890	2.029082
H	3.453513	2.851996	2.945916
H	2.845501	1.186001	2.723293
H	3.066814	2.239333	1.290612

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C	0.007197	0.000000	0.019394
O	-0.066335	-0.000006	1.441369
C	1.487347	-0.000017	-0.310631
C	-0.665232	1.251167	-0.526596
C	-0.665264	-1.251145	-0.526607
H	1.648163	-0.000015	-1.400388
H	1.973861	0.892428	0.115179
H	1.973837	-0.892480	0.115172
H	-0.594315	-1.300941	-1.625715
H	-0.193831	-2.153745	-0.105133
H	-1.736343	-1.265900	-0.258777
H	-0.594277	1.300975	-1.625703
H	-1.736311	1.265947	-0.258771
H	-0.193778	2.153750	-0.105108
H	-1.000619	-0.000002	1.684933