

## Supporting Information

**Table S1.** Xyz coordinates and absolute energies (in a.u.) of all computed DFT species.

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Cu	-3.341675	-5.055012	2.398731
C	0.801113	4.334320	-3.387941
Cu	2.004373	3.283928	-1.060968
O	-4.399133	-3.698465	3.347460
C	-4.027248	-2.490746	3.324818
O	-3.126514	-1.992094	2.594865
C	-4.736249	-1.573239	4.269406
O	1.171780	4.641243	0.138014
C	-5.367382	-2.103692	5.400855
H	-5.352561	-3.182714	5.560502
O	1.767425	6.340919	-1.215354
C	-6.023285	0.123430	6.063218
H	-6.546581	0.785879	6.758452
C	-5.419330	0.672903	4.918499
C	-4.760039	-0.196091	4.035719
H	-4.244760	0.198185	3.157286
C	-5.487068	2.109939	4.647077
C	-5.248954	3.155511	5.531830
N	-5.508369	4.296953	4.829678
N	-5.867092	4.060869	3.548768
C	-5.856054	2.740215	3.425796
C	-6.223975	2.088411	2.145428
H	-6.792519	2.781071	1.515450
H	-6.827982	1.185184	2.311788
H	-5.335827	1.775840	1.575080
C	-4.754478	3.162341	6.928754
H	-3.878108	3.819793	7.029917

H	-4.454281	2.150795	7.227628
H	-5.516760	3.503745	7.647018
C	-5.192731	5.647943	5.211771
H	-5.967218	6.314588	4.813214
H	-5.188554	5.717175	6.306386
N	-3.911564	6.069880	4.713905
N	-2.802307	5.589111	5.318650
C	-1.800352	5.897196	4.505344
C	-2.269642	6.590178	3.349941
C	-3.648097	6.666158	3.513285
C	-4.710013	7.192358	2.623620
H	-5.214205	8.076264	3.045339
H	-5.477064	6.426956	2.432416
H	-4.281014	7.490519	1.659213
C	-0.398966	5.547606	4.852507
H	0.292335	6.371591	4.626811
H	-0.041582	4.672763	4.288980
H	-0.318699	5.305113	5.918641
C	-1.478209	7.103642	2.226091
C	-1.644559	8.418593	1.758283
H	-2.356167	9.076850	2.264744
C	-0.906565	8.896005	0.676845
H	-1.049120	9.923489	0.334134
C	0.011854	8.072442	0.033858
H	0.592767	8.427115	-0.818415
C	0.186853	6.755573	0.476878
C	-0.547747	6.283626	1.570243
H	-0.413254	5.246361	1.882351
C	1.119430	5.840943	-0.251497
C	-5.992017	-1.247660	6.303062
H	-6.477195	-1.654288	7.193380

O	-4.669163	-5.092102	0.901131
C	-4.757231	-4.077158	0.156604
O	-3.992812	-3.068268	0.172622
C	-5.884569	-4.030090	-0.824908
O	0.550895	3.606246	-2.385225
C	-6.841709	-5.050508	-0.860199
H	-6.756521	-5.885212	-0.163207
O	1.876467	4.955782	-3.611821
C	-7.982921	-3.890423	-2.650022
H	-8.826675	-3.830987	-3.341311
C	-7.028134	-2.856879	-2.639046
C	-5.976091	-2.954665	-1.714954
H	-5.196932	-2.192250	-1.683784
C	-7.123262	-1.722074	-3.560720
C	-6.786629	-0.392437	-3.313321
N	-7.039266	0.278568	-4.477152
N	-7.501257	-0.526073	-5.456440
C	-7.560436	-1.735764	-4.919209
C	-8.025433	-2.890902	-5.730602
H	-7.941959	-2.656407	-6.798455
H	-9.079019	-3.142313	-5.534163
H	-7.435970	-3.795064	-5.522898
C	-6.287596	0.269282	-2.085544
H	-5.192239	0.385903	-2.084499
H	-6.546077	-0.324402	-1.198972
H	-6.717108	1.272093	-1.946081
C	-6.890626	1.683491	-4.754738
H	-7.643843	1.925527	-5.516223
H	-7.099041	2.266142	-3.849743
N	-5.577584	2.067609	-5.211558
N	-5.174796	1.668840	-6.432479

C	-3.974784	2.206420	-6.607463
C	-3.588525	2.977292	-5.471142
C	-4.651895	2.856748	-4.584390
C	-4.828158	3.449134	-3.240099
H	-4.539228	2.757805	-2.434328
H	-5.862745	3.764581	-3.044170
H	-4.189651	4.336870	-3.138445
C	-3.223669	1.993567	-7.873747
H	-2.154866	1.828716	-7.683118
H	-3.293937	2.861665	-8.545493
H	-3.622300	1.126670	-8.414903
C	-2.408980	3.857826	-5.380619
C	-2.279175	4.918856	-6.295553
H	-3.068072	5.075225	-7.035951
C	-1.173425	5.764092	-6.268601
H	-1.093931	6.583029	-6.987351
C	-0.168429	5.562251	-5.328717
H	0.715432	6.200579	-5.299211
C	-0.282638	4.519969	-4.400507
C	-1.397503	3.674540	-4.428686
H	-1.466661	2.864595	-3.699105
C	-7.885088	-4.972486	-1.778195
H	-8.643681	-5.758068	-1.805807
Cu	3.146597	5.231197	-2.108737
C	-0.820824	-4.190908	3.326207
Cu	-2.314486	-3.143759	1.176553
O	4.348625	3.874474	-2.906293
C	3.997229	2.660914	-2.928440
O	2.996551	2.152983	-2.349769
C	4.869602	1.726555	-3.701881
O	-1.602106	-4.537251	-0.077754

C	5.689363	2.217171	-4.724255
H	5.700235	3.288229	-4.930991
O	-2.101812	-6.191587	1.370592
C	6.451252	-0.032837	-5.166309
H	7.090069	-0.718253	-5.730365
C	5.657340	-0.540610	-4.122202
C	4.855677	0.360759	-3.407493
H	4.194753	0.000800	-2.616621
C	5.668734	-1.965498	-3.783332
C	5.572390	-3.041617	-4.657955
N	5.682397	-4.157786	-3.882144
N	5.820264	-3.877869	-2.566664
C	5.817650	-2.552570	-2.490885
C	5.979101	-1.854545	-1.189162
H	6.411789	-2.518906	-0.430480
H	6.620166	-0.966749	-1.288866
H	5.013872	-1.502272	-0.792123
C	5.314783	-3.098212	-6.115958
H	4.453966	-3.747559	-6.335779
H	5.085154	-2.096171	-6.498054
H	6.177397	-3.477105	-6.686669
C	5.413010	-5.516437	-4.272275
H	6.109961	-6.184345	-3.750843
H	5.573440	-5.608489	-5.353312
N	4.064230	-5.913216	-3.973811
N	3.066306	-5.404923	-4.730890
C	1.948862	-5.701099	-4.078751
C	2.230611	-6.419405	-2.879062
C	3.616110	-6.512784	-2.832223
C	4.524666	-7.069228	-1.802384
H	5.066333	-7.961577	-2.154215

H	5.271311	-6.323125	-1.491624
H	3.952899	-7.364432	-0.913916
C	0.619154	-5.322924	-4.622726
H	-0.112852	-6.133804	-4.503408
H	0.201576	-4.442969	-4.110700
H	0.697052	-5.074746	-5.687679
C	1.286463	-6.955561	-1.893401
C	1.374263	-8.291572	-1.465143
H	2.131320	-8.942462	-1.911656
C	0.507250	-8.795980	-0.498264
H	0.591082	-9.838835	-0.183882
C	-0.457696	-7.974432	0.074154
H	-1.127837	-8.342817	0.851679
C	-0.562125	-6.639861	-0.338446
C	0.293726	-6.143581	-1.326538
H	0.210603	-5.093353	-1.613157
C	-1.512246	-5.718883	0.356385
C	6.462992	1.327899	-5.464592
H	7.097504	1.700654	-6.272007
O	4.275899	5.288667	-0.470563
C	4.334684	4.238825	0.227783
O	3.596116	3.219281	0.111965
C	5.407168	4.161482	1.265228
O	-0.723702	-3.486672	2.279746
C	6.161408	5.291901	1.600564
H	5.951106	6.240184	1.104236
O	-1.853798	-4.793288	3.728453
C	7.435618	3.952847	3.162235
H	8.250796	3.876001	3.885867
C	6.704201	2.800700	2.822772
C	5.670255	2.937459	1.884536

H	5.044999	2.081820	1.625018
C	7.002102	1.492490	3.409286
C	6.970610	0.263546	2.750611
N	7.296444	-0.668079	3.691877
N	7.526155	-0.129828	4.910729
C	7.363214	1.178412	4.751377
C	7.535167	2.104279	5.901034
H	7.449459	1.557418	6.847664
H	8.522189	2.591907	5.897010
H	6.783099	2.905680	5.889607
C	6.699284	-0.081814	1.336424
H	5.661049	-0.411352	1.178786
H	6.875802	0.786133	0.687899
H	7.331669	-0.908804	0.985143
C	7.385853	-2.099153	3.530164
H	7.895843	-2.469958	4.427849
H	7.985773	-2.355573	2.647176
N	6.115456	-2.757651	3.368102
N	5.705802	-3.120760	2.131671
C	4.488865	-3.625218	2.301956
C	4.105345	-3.589588	3.677276
C	5.191822	-3.019912	4.336639
C	5.419086	-2.683638	5.762633
H	5.953108	-3.485342	6.298707
H	6.015068	-1.766695	5.876246
H	4.461988	-2.535648	6.279016
C	3.723738	-4.158500	1.142636
H	3.179844	-5.077385	1.405357
H	2.970288	-3.444060	0.776098
H	4.395256	-4.377227	0.302907
C	2.851527	-4.057553	4.270424

C	2.813791	-4.704340	5.519897
H	3.746980	-4.884150	6.059363
C	1.611366	-5.155478	6.061391
H	1.611335	-5.660392	7.030184
C	0.416901	-4.993283	5.365031
H	-0.529840	-5.361292	5.762746
C	0.433310	-4.350881	4.121950
C	1.637877	-3.883262	3.591236
H	1.613893	-3.371548	2.628547
C	7.160659	5.181184	2.563544
H	7.749484	6.059422	2.838016

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Cu	5.462595	0.452008	3.542079
C	-5.483994	1.752846	-1.837197
Cu	-3.578068	-0.351671	-1.929125
O	6.248260	1.771073	2.292475
C	5.850205	1.776191	1.092430
O	4.832151	1.179542	0.641033
C	6.671747	2.558838	0.119647
O	-2.542470	0.452491	-3.424951
C	7.851980	3.178640	0.548351
H	8.142656	3.099350	1.596350
O	-4.427910	0.897285	-4.577366
C	8.241261	3.958470	-1.703492
H	8.852889	4.523691	-2.410907
C	7.057761	3.347396	-2.156578
C	6.282746	2.644052	-1.221248
H	5.378288	2.120269	-1.536993
C	6.672120	3.426404	-3.566921
C	5.398667	3.633332	-4.093588



N	5.553420	3.597536	-5.447448
N	6.827752	3.382650	-5.831423
C	7.520275	3.286133	-4.704422
C	8.982051	3.018713	-4.741239
H	9.259412	2.567036	-5.701257
H	9.289082	2.339906	-3.933424
H	9.578056	3.937947	-4.631483
C	4.098177	3.879826	-3.427079
H	3.544640	4.708946	-3.892928
H	4.254709	4.137484	-2.372096
H	3.440369	2.996924	-3.462598
C	4.580004	3.837296	-6.478906
H	4.343373	4.909795	-6.568830
H	5.062150	3.519251	-7.414505
N	3.341097	3.138386	-6.261988
N	3.361360	1.815294	-6.010234
C	2.086429	1.458296	-5.912615
C	1.220805	2.570523	-6.136248
C	2.076456	3.646988	-6.354973
C	1.786994	5.081952	-6.592676
H	1.968561	5.390519	-7.634640
H	2.393551	5.741619	-5.953895
H	0.734432	5.296292	-6.370341
C	1.718677	0.045864	-5.634882
H	0.843830	-0.266999	-6.221705
H	1.464315	-0.116836	-4.576554
H	2.558492	-0.617411	-5.872769
C	-0.243043	2.570475	-6.191767
C	-0.931020	3.287148	-7.188521
H	-0.359991	3.841087	-7.938423
C	-2.321645	3.267757	-7.261540

H	-2.830714	3.828460	-8.048811
C	-3.062701	2.518085	-6.353669
H	-4.151393	2.477370	-6.404037
C	-2.399298	1.795995	-5.354438
C	-1.003910	1.830255	-5.274629
H	-0.515258	1.271797	-4.474501
C	-3.183987	0.985024	-4.373763
C	8.631867	3.874158	-0.369863
H	9.552909	4.362048	-0.042794
O	4.426461	1.871427	4.423814
C	3.519862	2.474416	3.779591
O	3.080073	2.160424	2.638631
C	2.914852	3.660684	4.458487
O	-4.297701	1.472341	-1.507478
C	3.412641	4.072679	5.700943
H	4.250429	3.532095	6.142027
O	-6.263764	1.019029	-2.511610
C	1.754794	5.824025	5.768228
H	1.316633	6.685707	6.277022
C	1.237539	5.430077	4.520279
C	1.835815	4.335171	3.877286
H	1.446775	3.971999	2.923631
C	0.103813	6.152468	3.940221
C	-0.074577	6.549235	2.617066
N	-1.264194	7.224800	2.593915
N	-1.859384	7.285246	3.799827
C	-1.046091	6.644416	4.626561
C	-1.403321	6.494387	6.061945
H	-2.489034	6.579105	6.189999
H	-0.943588	7.273502	6.689298
H	-1.075811	5.524980	6.462169

C	0.804982	6.375939	1.435613
H	0.459827	5.580671	0.755873
H	1.816134	6.098243	1.759156
H	0.898828	7.296282	0.840571
C	-1.885121	7.927287	1.496033
H	-2.044699	8.975038	1.780437
H	-1.203452	7.889896	0.637084
N	-3.174642	7.412799	1.127212
N	-4.269875	7.989086	1.659938
C	-5.295252	7.291162	1.195584
C	-4.856688	6.227159	0.347083
C	-3.466452	6.338013	0.336872
C	-2.420258	5.558269	-0.365358
H	-2.012058	4.744275	0.256157
H	-1.571286	6.188517	-0.667954
H	-2.822133	5.094608	-1.275244
C	-6.675183	7.652582	1.616416
H	-7.292481	6.761449	1.796055
H	-7.199667	8.263485	0.865512
H	-6.636293	8.241485	2.540562
C	-5.681706	5.270986	-0.392693
C	-6.955049	5.644348	-0.864456
H	-7.316133	6.658200	-0.684953
C	-7.749757	4.759178	-1.585946
H	-8.733553	5.078779	-1.937094
C	-7.287217	3.482751	-1.885468
H	-7.884535	2.783284	-2.470743
C	-6.018307	3.091193	-1.441338
C	-5.237664	3.970005	-0.683630
H	-4.273252	3.614854	-0.317863
C	2.826904	5.154405	6.349663

H	3.212695	5.484063	7.316975
Cu	-5.463562	-0.452095	-3.540877
C	5.486688	-1.749048	1.834018
Cu	3.577394	0.352189	1.930166
O	-6.252478	-1.766924	-2.289185
C	-5.853466	-1.771669	-1.089442
O	-4.834049	-1.176428	-0.639344
C	-6.675685	-2.552220	-0.115520
O	2.543680	-0.454374	3.425835
C	-7.858111	-3.168834	-0.542769
H	-8.150004	-3.088498	-1.590344
O	4.429867	-0.901553	4.576086
C	-8.246243	-3.948528	1.709271
H	-8.858277	-4.512519	2.417307
C	-7.060488	-3.340754	2.160901
C	-6.285008	-2.638914	1.224809
H	-5.378740	-2.117644	1.539532
C	-6.673006	-3.421958	3.570642
C	-5.399467	-3.633449	4.095267
N	-5.552289	-3.599367	5.449400
N	-6.825379	-3.380944	5.835435
C	-7.519141	-3.280711	4.709526
C	-8.980045	-3.008892	4.748715
H	-9.254620	-2.557069	5.709467
H	-9.286186	-2.328596	3.941819
H	-9.579029	-3.926219	4.639232
C	-4.100503	-3.882747	3.426848
H	-3.548812	-4.714102	3.890905
H	-4.258996	-4.138498	2.371692
H	-3.440111	-3.001782	3.462736
C	-4.577683	-3.842236	6.478938

H	-4.341654	-4.915095	6.566085
H	-5.058379	-3.525956	7.415873
N	-3.338550	-3.143703	6.262002
N	-3.358286	-1.820077	6.013003
C	-2.083282	-1.463587	5.915062
C	-1.218045	-2.576763	6.135680
C	-2.074086	-3.653178	6.352938
C	-1.785165	-5.088697	6.587961
H	-1.966179	-5.398885	7.629540
H	-2.392437	-5.747038	5.948495
H	-0.732853	-5.303166	6.364557
C	-1.714773	-0.050861	5.639938
H	-0.840051	0.260517	6.227776
H	-1.459794	0.113647	4.582057
H	-2.554380	0.612390	5.878639
C	0.245857	-2.577484	6.189958
C	0.934370	-3.296507	7.184637
H	0.363743	-3.851837	7.933821
C	2.325066	-3.277772	7.256546
H	2.834600	-3.840349	8.042178
C	3.065647	-2.526374	6.349707
H	4.154393	-2.486145	6.399335
C	2.401696	-1.801905	5.352563
C	1.006235	-1.835581	5.273781
H	0.517045	-1.275246	4.475302
C	3.185833	-0.988918	4.373136
C	-8.638558	-3.862630	0.376259
H	-9.561303	-4.348016	0.050273
O	-4.431398	-1.875669	-4.420206
C	-3.524539	-2.477825	-3.775583
O	-3.082906	-2.161285	-2.636050

C	-2.921847	-3.666539	-4.452308
O	4.299324	-1.470232	1.506623
C	-3.424185	-4.082880	-5.691492
H	-4.263475	-3.543717	-6.131450
O	6.265778	-1.015242	2.509206
C	-1.766900	-5.834680	-5.758577
H	-1.330763	-6.698303	-6.265809
C	-1.244847	-5.436185	-4.514073
C	-1.840738	-4.339053	-3.872643
H	-1.448237	-3.972677	-2.921623
C	-0.108717	-6.156629	-3.936215
C	0.074854	-6.550040	-2.612788
N	1.264534	-7.225650	-2.592595
N	1.854951	-7.289176	-3.800684
C	1.038488	-6.650339	-4.625815
C	1.390187	-6.503835	-6.062941
H	2.475496	-6.587848	-6.194848
H	0.928903	-7.285094	-6.686479
H	1.060268	-5.535825	-6.464541
C	-0.799952	-6.373523	-1.428307
H	-0.451469	-5.577141	-0.751589
H	-1.812123	-6.095661	-1.748498
H	-0.892266	-7.292535	-0.830951
C	1.889644	-7.925511	-1.495400
H	2.049664	-8.973440	-1.778866
H	1.210439	-7.887770	-0.634556
N	3.179482	-7.408784	-1.130731
N	4.273782	-7.981638	-1.669099
C	5.299539	-7.282179	-1.207923
C	4.862178	-6.220618	-0.355785
C	3.472254	-6.334641	-0.339809

C	2.427730	-5.558262	0.368636
H	2.017341	-4.741851	-0.248236
H	1.579950	-6.190006	0.671375
H	2.832236	-5.097978	1.279099
C	6.678511	-7.639739	-1.635106
H	7.292901	-6.746855	-1.816049
H	7.207638	-8.250449	-0.887312
H	6.637108	-8.227413	-2.559922
C	5.688000	-5.263809	0.382253
C	6.964304	-5.634686	0.847926
H	7.327419	-6.647160	0.664752
C	7.759589	-4.748825	1.567960
H	8.745708	-5.066464	1.914339
C	7.294837	-3.474281	1.872099
H	7.892631	-2.774406	2.456418
C	6.023157	-3.085194	1.433797
C	5.241803	-3.964565	0.677486
H	4.275061	-3.611143	0.316252
C	-2.841114	-5.167090	-6.338434
H	-3.230623	-5.500254	-7.303051

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Cu	-6.092323	-0.975328	-2.349618
C	5.313914	2.531957	0.672956
Cu	3.806182	0.241025	1.387202
O	-6.763265	0.604492	-1.365593
C	-6.146462	1.002914	-0.337042
O	-5.041687	0.565477	0.092316
C	-6.774018	2.130054	0.415965
O	2.978299	1.191746	2.946000
C	-8.088437	2.518030	0.132621

H	-8.657069	1.967077	-0.617335
O	4.998394	1.798217	3.751182
C	-7.879150	4.317950	1.731093
H	-8.310902	5.197263	2.213493
C	-6.552065	3.952088	2.024647
C	-6.026641	2.827011	1.369399
H	-5.020948	2.470642	1.597496
C	-5.743981	4.735847	2.959015
C	-4.381359	5.014122	2.864728
N	-4.092400	5.816419	3.930051
N	-5.163361	6.064102	4.710256
C	-6.171622	5.425327	4.134501
C	-7.525261	5.469010	4.747770
H	-7.446087	5.733185	5.808962
H	-8.038898	4.501115	4.665542
H	-8.175829	6.220701	4.274590
C	-3.364463	4.631883	1.857208
H	-2.663976	5.455441	1.649733
H	-3.842120	4.359345	0.907363
H	-2.759215	3.766798	2.174814
C	-2.824475	6.384775	4.294977
H	-2.314528	6.772174	3.403221
H	-3.052022	7.222089	4.966609
N	-1.926351	5.469893	4.957921
N	-2.263171	5.028086	6.185296
C	-1.212339	4.343643	6.614201
C	-0.168800	4.338022	5.642227
C	-0.670091	5.081153	4.577089
C	-0.030111	5.460599	3.294164
H	-0.192284	6.516952	3.033131
H	-0.384306	4.854275	2.445036



H	1.054923	5.307983	3.360339
C	-1.231000	3.688199	7.948295
H	-0.774262	4.318963	8.726324
H	-0.679519	2.738198	7.940247
H	-2.263968	3.492772	8.259689
C	1.171834	3.761374	5.772649
C	1.899509	3.949503	6.962083
H	1.443649	4.513564	7.779451
C	3.197057	3.466141	7.097406
H	3.745623	3.635467	8.026678
C	3.806334	2.790951	6.044497
H	4.830347	2.423853	6.122756
C	3.088323	2.560835	4.865543
C	1.778555	3.033521	4.736887
H	1.228990	2.817082	3.817692
C	3.734082	1.788332	3.759961
C	-8.638390	3.602334	0.809101
H	-9.664309	3.912181	0.597555
O	-5.323591	0.214845	-3.733145
C	-4.397161	1.015410	-3.419278
O	-3.759806	1.028615	-2.328392
C	-4.021747	2.036039	-4.443869
O	4.158462	2.034301	0.571668
C	-4.688403	2.065971	-5.674506
H	-5.486558	1.347282	-5.863098
O	6.292950	2.031448	1.298610
C	-3.296215	3.913984	-6.364961
H	-3.033141	4.663483	-7.114783
C	-2.615019	3.906428	-5.133551
C	-2.991672	2.945580	-4.183007
H	-2.466770	2.875865	-3.228238

C	-1.549701	4.875892	-4.871489
C	-1.307188	5.578564	-3.692998
N	-0.229409	6.378824	-3.957539
N	0.234869	6.238667	-5.213203
C	-0.551335	5.335529	-5.781162
C	-0.311019	4.910886	-7.185398
H	0.729649	5.112136	-7.465836
H	-0.948309	5.454698	-7.899502
H	-0.512790	3.839962	-7.325658
C	-2.034563	5.568994	-2.400199
H	-1.524918	4.971389	-1.626975
H	-3.031255	5.129117	-2.532932
H	-2.181111	6.579004	-1.989846
C	0.374830	7.387032	-3.118676
H	0.328817	8.359477	-3.625268
H	-0.200950	7.442816	-2.186029
N	1.762322	7.153656	-2.831475
N	2.687897	7.776027	-3.587314
C	3.856697	7.345989	-3.136297
C	3.688225	6.411398	-2.067371
C	2.307102	6.309358	-1.906626
C	1.479178	5.530494	-0.955872
H	1.126646	4.578229	-1.385543
H	0.586153	6.089067	-0.636655
H	2.051563	5.283021	-0.052616
C	5.110587	7.824431	-3.776888
H	5.854307	7.020442	-3.865384
H	5.585382	8.643571	-3.215107
H	4.889972	8.207324	-4.780375
C	4.732853	5.747159	-1.285711
C	5.954552	6.399516	-1.030949

H	6.107750	7.412890	-1.405926
C	6.958550	5.791843	-0.283637
H	7.895761	6.323293	-0.103530
C	6.765590	4.524025	0.254128
H	7.532762	4.039714	0.858685
C	5.553372	3.860529	0.030136
C	4.558555	4.460624	-0.748723
H	3.644741	3.895983	-0.940157
C	-4.315946	3.004839	-6.631224
H	-4.832031	3.036145	-7.593444
Cu	5.978025	0.557617	2.565028
C	-5.634263	-2.642659	-0.171632
Cu	-3.967193	-0.558467	-1.133985
O	6.717995	-0.733398	1.278327
C	6.072811	-0.996732	0.222603
O	4.886184	-0.651820	-0.033693
C	6.806992	-1.790868	-0.810647
O	-3.129804	-1.664701	-2.556751
C	8.161487	-2.087433	-0.612719
H	8.650498	-1.748075	0.300696
O	-5.125686	-2.502559	-3.186269
C	8.208793	-3.225301	-2.739714
H	8.758501	-3.805818	-3.484304
C	6.847529	-2.945179	-2.959107
C	6.159921	-2.214225	-1.976626
H	5.113386	-1.938961	-2.123633
C	6.194311	-3.399716	-4.188267
C	4.923258	-3.952845	-4.327496
N	4.783466	-4.217912	-5.657242
N	5.863549	-3.871267	-6.385192
C	6.731653	-3.383072	-5.509651

C	8.049815	-2.870190	-5.967497
H	8.003091	-2.606045	-7.030795
H	8.357136	-1.981228	-5.399426
H	8.851588	-3.616291	-5.854833
C	3.875853	-4.260953	-3.325836
H	3.425009	-5.251248	-3.490335
H	4.300913	-4.254320	-2.314242
H	3.053295	-3.528257	-3.346961
C	3.693067	-4.861540	-6.336609
H	3.648358	-5.936948	-6.100778
H	3.915403	-4.758540	-7.408328
N	2.411813	-4.292471	-6.008614
N	2.242048	-2.959345	-6.092012
C	0.968446	-2.748778	-5.783894
C	0.291223	-3.977966	-5.523592
C	1.267001	-4.959468	-5.675809
C	1.199544	-6.429268	-5.490366
H	1.228216	-6.984578	-6.441467
H	2.026630	-6.810825	-4.872696
H	0.265843	-6.702994	-4.983831
C	0.414779	-1.369988	-5.775899
H	-0.597744	-1.337763	-6.201758
H	0.344235	-0.955908	-4.758747
H	1.061910	-0.700458	-6.354526
C	-1.129486	-4.166768	-5.222937
C	-1.872919	-5.202406	-5.818758
H	-1.379956	-5.876857	-6.524074
C	-3.233388	-5.353970	-5.560521
H	-3.789189	-6.162139	-6.041475
C	-3.893458	-4.464381	-4.718271
H	-4.962774	-4.553506	-4.522442

C	-3.171831	-3.429693	-4.111498
C	-1.802855	-3.292732	-4.357087
H	-1.263141	-2.487763	-3.856026
C	-3.863563	-2.457700	-3.211671
C	8.856444	-2.800136	-1.583769
H	9.912775	-3.035597	-1.435436
O	5.420053	-0.913604	3.743599
C	4.447358	-1.649205	3.407676
O	3.692749	-1.481129	2.410194
C	4.178080	-2.813960	4.306624
O	-4.441286	-2.225360	-0.152385
C	5.044657	-3.064364	5.378147
H	5.913304	-2.420707	5.517917
O	-6.583827	-2.154761	-0.849214
C	3.657934	-4.918591	6.049772
H	3.467379	-5.755576	6.725472
C	2.771834	-4.687953	4.981385
C	3.052531	-3.622309	4.111482
H	2.375770	-3.385733	3.287301
C	1.595936	-5.547362	4.824514
C	1.097535	-6.124634	3.659672
N	0.027997	-6.882568	4.053880
N	-0.195782	-6.827034	5.380405
C	0.742883	-6.026397	5.862938
C	0.789130	-5.716238	7.316360
H	-0.203802	-5.851421	7.761525
H	1.478950	-6.378287	7.862001
H	1.120491	-4.685079	7.500499
C	1.589734	-6.041454	2.263394
H	0.977705	-5.379603	1.630678
H	2.609542	-5.636249	2.251188

H	1.626686	-7.023450	1.768677
C	-0.789626	-7.775186	3.267725
H	-0.777128	-8.769334	3.731594
H	-0.354651	-7.843972	2.263276
N	-2.171669	-7.389672	3.178358
N	-3.031290	-7.880493	4.092763
C	-4.204092	-7.339317	3.799805
C	-4.105306	-6.467722	2.671302
C	-2.761185	-6.524344	2.301293
C	-2.018771	-5.875317	1.194929
H	-1.573546	-4.911918	1.492989
H	-1.199887	-6.506140	0.820491
H	-2.683416	-5.668357	0.346244
C	-5.386864	-7.656411	4.643645
H	-6.016924	-6.771794	4.810739
H	-6.028740	-8.430935	4.196148
H	-5.054357	-8.036411	5.616934
C	-5.177955	-5.726909	2.006621
C	-6.494101	-6.227571	1.985676
H	-6.712900	-7.179976	2.471216
C	-7.516363	-5.551733	1.325825
H	-8.526909	-5.966554	1.327783
C	-7.252492	-4.372236	0.637880
H	-8.033457	-3.846802	0.087588
C	-5.950935	-3.856850	0.638609
C	-4.935699	-4.514913	1.339179
H	-3.945193	-4.059156	1.352861
C	4.779367	-4.118937	6.244409
H	5.454436	-4.323131	7.078531

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Cu	6.176291	2.097942	-1.160157
C	-4.858974	-3.610507	-0.777355
Cu	-3.903881	-1.291148	0.528715
O	6.864271	0.557133	-0.158621
C	6.119039	-0.038517	0.672293
O	4.888466	0.169309	0.859284
C	6.779087	-1.112404	1.475147
O	-3.223651	-2.368379	2.079664
C	8.175790	-1.204569	1.490064
H	8.763921	-0.469333	0.940266
O	-5.223128	-3.369758	2.388272
C	8.012193	-3.187220	2.856861
H	8.504955	-4.019451	3.363426
C	6.606305	-3.120702	2.850200
C	6.006164	-2.047944	2.169496
H	4.922043	-1.921568	2.174860
C	5.813168	-4.159060	3.508510
C	4.603978	-4.701805	3.077117
N	4.296646	-5.682151	3.976201
N	5.208081	-5.799106	4.962253
C	6.134205	-4.890935	4.692532
C	7.300007	-4.728609	5.600998
H	7.057556	-5.124895	6.594212
H	7.588358	-3.673636	5.706033
H	8.188323	-5.272427	5.244146
C	3.758886	-4.407254	1.896376
H	3.318160	-5.320355	1.467786
H	4.349792	-3.926019	1.106427
H	2.924179	-3.727545	2.134865
C	3.152537	-6.550921	3.989899
H	2.916803	-6.876204	2.968526

H	3.442493	-7.426169	4.584530
N	1.962189	-5.965833	4.558029
N	1.954578	-5.700676	5.878658
C	0.718702	-5.308207	6.152455
C	-0.095253	-5.315481	4.981515
C	0.748849	-5.748986	3.962904
C	0.463425	-6.003157	2.529739
H	0.900260	-6.947008	2.170827
H	0.830397	-5.200265	1.870198
H	-0.620936	-6.069969	2.372530
C	0.342009	-4.911821	7.534787
H	-0.108535	-5.743999	8.097134
H	-0.387888	-4.090842	7.535897
H	1.231033	-4.593232	8.091850
C	-1.526092	-5.018318	4.886421
C	-2.413967	-5.535156	5.847859
H	-2.018160	-6.147973	6.661236
C	-3.784251	-5.311481	5.757178
H	-4.454389	-5.732584	6.509982
C	-4.305001	-4.573461	4.698923
H	-5.377419	-4.402491	4.599054
C	-3.436690	-4.022743	3.749449
C	-2.058855	-4.236826	3.849753
H	-1.399800	-3.771485	3.113038
C	-3.999327	-3.185266	2.646604
C	8.784245	-2.234599	2.199047
H	9.873569	-2.313264	2.218651
O	5.924860	0.946653	-2.758934
C	5.076753	0.010314	-2.723722
O	4.215175	-0.182553	-1.819716
C	5.099510	-0.951720	-3.866742



O	-3.808769	-2.934746	-0.588947
C	6.014355	-0.765585	-4.909996
H	6.706903	0.075376	-4.863952
O	-6.000203	-3.373640	-0.287374
C	5.125616	-2.717964	-6.016310
H	5.156662	-3.421168	-6.851726
C	4.201150	-2.929450	-4.976468
C	4.199417	-2.021774	-3.906460
H	3.475014	-2.122036	-3.095585
C	3.278436	-4.065351	-5.032006
C	2.918180	-4.926091	-3.997544
N	2.069244	-5.840785	-4.559150
N	1.858322	-5.626467	-5.871279
C	2.581839	-4.558565	-6.175166
C	2.571078	-4.015262	-7.558937
H	1.655505	-4.324535	-8.076905
H	3.419079	-4.382869	-8.156845
H	2.625526	-2.917925	-7.564461
C	3.351059	-4.958151	-2.579049
H	2.595195	-4.546101	-1.890763
H	4.258243	-4.354071	-2.449747
H	3.589838	-5.974683	-2.232806
C	1.492461	-7.023917	-3.964535
H	1.809131	-7.907211	-4.533799
H	1.869837	-7.107694	-2.937639
N	0.056332	-7.042400	-3.966012
N	-0.575065	-7.675959	-4.973465
C	-1.867573	-7.498124	-4.745494
C	-2.084110	-6.721242	-3.564928
C	-0.802655	-6.438941	-3.092149
C	-0.332035	-5.699881	-1.896655

H	-0.089006	-4.647750	-2.119251
H	0.572031	-6.153715	-1.463167
H	-1.101633	-5.692633	-1.113985
C	-2.862889	-8.056925	-5.698645
H	-3.702459	-7.366941	-5.861192
H	-3.290389	-9.010259	-5.351718
H	-2.380514	-8.252174	-6.663754
C	-3.364004	-6.347809	-2.960122
C	-4.480742	-7.199337	-3.066229
H	-4.380077	-8.151200	-3.590403
C	-5.702402	-6.868129	-2.488042
H	-6.550480	-7.549162	-2.589077
C	-5.841656	-5.690160	-1.761957
H	-6.784008	-5.424833	-1.281975
C	-4.742337	-4.834079	-1.628093
C	-3.526068	-5.152278	-2.240961
H	-2.705400	-4.438858	-2.154535
C	6.017174	-1.649687	-5.983749
H	6.728182	-1.512082	-6.801511
Cu	-6.161353	-2.100371	1.210700
C	4.983538	3.465203	0.959002
Cu	3.925239	1.277540	-0.497074
O	-6.894461	-0.729560	0.014904
C	-6.127897	-0.134984	-0.796241
O	-4.878591	-0.281622	-0.895257
C	-6.787100	0.862448	-1.692030
O	3.248936	2.444692	-1.983595
C	-8.180571	0.860416	-1.825528
H	-8.764961	0.103420	-1.301463
O	5.221989	3.529130	-2.123019
C	-8.027790	2.811009	-3.240534

H	-8.528523	3.595695	-3.811280
C	-6.626956	2.839625	-3.112931
C	-6.020031	1.826332	-2.351489
H	-4.933841	1.772125	-2.261483
C	-5.842558	3.905792	-3.735775
C	-4.712200	4.537723	-3.220212
N	-4.385787	5.506808	-4.124223
N	-5.211910	5.537126	-5.188929
C	-6.103186	4.582035	-4.966699
C	-7.168928	4.318858	-5.969684
H	-6.858069	4.698527	-6.950222
H	-7.382450	3.245042	-6.061548
H	-8.118037	4.816422	-5.717042
C	-3.966911	4.350210	-1.952850
H	-3.693206	5.313790	-1.495729
H	-4.574853	3.805018	-1.220579
H	-3.034161	3.778610	-2.090801
C	-3.287489	6.432828	-4.081638
H	-3.140064	6.794443	-3.054974
H	-3.578952	7.277955	-4.718443
N	-2.033188	5.892526	-4.546116
N	-1.920607	5.566357	-5.849908
C	-0.641576	5.267618	-6.029426
C	0.095126	5.411361	-4.816508
C	-0.842358	5.818138	-3.875459
C	-0.672293	6.187359	-2.449209
H	-0.922876	7.242401	-2.254611
H	-1.289918	5.575379	-1.774019
H	0.373578	6.045015	-2.150375
C	-0.157643	4.789246	-7.350419
H	0.756934	5.302777	-7.675037

H	0.079365	3.714950	-7.325936
H	-0.931003	4.943238	-8.111579
C	1.540820	5.243780	-4.620393
C	2.439518	5.970340	-5.421656
H	2.043675	6.650121	-6.180756
C	3.814996	5.861546	-5.238974
H	4.495196	6.444526	-5.864047
C	4.325228	5.028302	-4.249203
H	5.398939	4.937621	-4.081589
C	3.449120	4.279111	-3.454853
C	2.066860	4.386286	-3.644668
H	1.401455	3.778158	-3.026671
C	4.010477	3.341244	-2.438127
C	-8.790330	1.826910	-2.618251
H	-9.876885	1.833404	-2.730053
O	-6.029701	-0.758804	2.659473
C	-5.158658	0.156345	2.605254
O	-4.223083	0.249097	1.763181
C	-5.258754	1.219691	3.651873
O	3.903046	2.867964	0.686544
C	-6.305180	1.170308	4.580786
H	-7.035945	0.364110	4.512706
O	6.124502	3.197393	0.485719
C	-5.443085	3.160067	5.636538
H	-5.532847	3.931994	6.404210
C	-4.382905	3.233152	4.713722
C	-4.306282	2.242749	3.721915
H	-3.482440	2.238602	3.004836
C	-3.403816	4.318023	4.819797
C	-2.869085	5.101795	3.799780
N	-2.052256	6.007614	4.421908

N	-2.021683	5.856121	5.759039
C	-2.832488	4.841093	6.018148
C	-3.024918	4.375825	7.417118
H	-2.160551	4.659488	8.029232
H	-3.913043	4.825239	7.887213
H	-3.150361	3.285627	7.468748
C	-3.119547	5.076250	2.337774
H	-2.297561	4.614027	1.766975
H	-4.022350	4.489404	2.124705
H	-3.282472	6.081436	1.920220
C	-1.336118	7.125096	3.853405
H	-1.635145	8.041611	4.377229
H	-1.616369	7.210198	2.796486
N	0.093606	7.038684	3.975403
N	0.674873	7.587084	5.060228
C	1.968216	7.330807	4.934715
C	2.236950	6.590943	3.741494
C	0.985797	6.415728	3.149338
C	0.580904	5.759157	1.883574
H	0.310931	4.699399	2.023662
H	-0.286603	6.254190	1.423031
H	1.399150	5.784561	1.151873
C	2.909224	7.783275	5.993501
H	3.679327	7.028075	6.203563
H	3.433402	8.712750	5.722802
H	2.355178	7.982884	6.918351
C	3.535220	6.156169	3.223592
C	4.700967	6.905162	3.476103
H	4.631455	7.825284	4.058481
C	5.936941	6.515786	2.968075
H	6.822447	7.118637	3.181869

C	6.045534	5.384164	2.166666
H	6.999665	5.080165	1.734946
C	4.899720	4.628882	1.891959
C	3.666936	5.000012	2.437510
H	2.806166	4.361267	2.237652
C	-6.389936	2.142850	5.570983
H	-7.206182	2.113560	6.296262

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Cu	5.462595	0.452008	3.542079
C	-5.483994	1.752846	-1.837197
Cu	-3.578068	-0.351671	-1.929125
O	6.248260	1.771073	2.292475
C	5.850205	1.776191	1.092430
O	4.832151	1.179542	0.641033
C	6.671747	2.558838	0.119647
O	-2.542470	0.452491	-3.424951
C	7.851980	3.178640	0.548351
H	8.142656	3.099350	1.596350
O	-4.427910	0.897285	-4.577366
C	8.241261	3.958470	-1.703492
H	8.852889	4.523691	-2.410907
C	7.057761	3.347396	-2.156578
C	6.282746	2.644052	-1.221248
H	5.378288	2.120269	-1.536993
C	6.672120	3.426404	-3.566921
C	5.398667	3.633332	-4.093588
N	5.553420	3.597536	-5.447448
N	6.827752	3.382650	-5.831423
C	7.520275	3.286133	-4.704422
C	8.982051	3.018713	-4.741239

H	9.259412	2.567036	-5.701257
H	9.289082	2.339906	-3.933424
H	9.578056	3.937947	-4.631483
C	4.098177	3.879826	-3.427079
H	3.544640	4.708946	-3.892928
H	4.254709	4.137484	-2.372096
H	3.440369	2.996924	-3.462598
C	4.580004	3.837296	-6.478906
H	4.343373	4.909795	-6.568830
H	5.062150	3.519251	-7.414505
N	3.341097	3.138386	-6.261988
N	3.361360	1.815294	-6.010234
C	2.086429	1.458296	-5.912615
C	1.220805	2.570523	-6.136248
C	2.076456	3.646988	-6.354973
C	1.786994	5.081952	-6.592676
H	1.968561	5.390519	-7.634640
H	2.393551	5.741619	-5.953895
H	0.734432	5.296292	-6.370341
C	1.718677	0.045864	-5.634882
H	0.843830	-0.266999	-6.221705
H	1.464315	-0.116836	-4.576554
H	2.558492	-0.617411	-5.872769
C	-0.243043	2.570475	-6.191767
C	-0.931020	3.287148	-7.188521
H	-0.359991	3.841087	-7.938423
C	-2.321645	3.267757	-7.261540
H	-2.830714	3.828460	-8.048811
C	-3.062701	2.518085	-6.353669
H	-4.151393	2.477370	-6.404037
C	-2.399298	1.795995	-5.354438

C	-1.003910	1.830255	-5.274629
H	-0.515258	1.271797	-4.474501
C	-3.183987	0.985024	-4.373763
C	8.631867	3.874158	-0.369863
H	9.552909	4.362048	-0.042794
O	4.426461	1.871427	4.423814
C	3.519862	2.474416	3.779591
O	3.080073	2.160424	2.638631
C	2.914852	3.660684	4.458487
O	-4.297701	1.472341	-1.507478
C	3.412641	4.072679	5.700943
H	4.250429	3.532095	6.142027
O	-6.263764	1.019029	-2.511610
C	1.754794	5.824025	5.768228
H	1.316633	6.685707	6.277022
C	1.237539	5.430077	4.520279
C	1.835815	4.335171	3.877286
H	1.446775	3.971999	2.923631
C	0.103813	6.152468	3.940221
C	-0.074577	6.549235	2.617066
N	-1.264194	7.224800	2.593915
N	-1.859384	7.285246	3.799827
C	-1.046091	6.644416	4.626561
C	-1.403321	6.494387	6.061945
H	-2.489034	6.579105	6.189999
H	-0.943588	7.273502	6.689298
H	-1.075811	5.524980	6.462169
C	0.804982	6.375939	1.435613
H	0.459827	5.580671	0.755873
H	1.816134	6.098243	1.759156
H	0.898828	7.296282	0.840571



C	-1.885121	7.927287	1.496033
H	-2.044699	8.975038	1.780437
H	-1.203452	7.889896	0.637084
N	-3.174642	7.412799	1.127212
N	-4.269875	7.989086	1.659938
C	-5.295252	7.291162	1.195584
C	-4.856688	6.227159	0.347083
C	-3.466452	6.338013	0.336872
C	-2.420258	5.558269	-0.365358
H	-2.012058	4.744275	0.256157
H	-1.571286	6.188517	-0.667954
H	-2.822133	5.094608	-1.275244
C	-6.675183	7.652582	1.616416
H	-7.292481	6.761449	1.796055
H	-7.199667	8.263485	0.865512
H	-6.636293	8.241485	2.540562
C	-5.681706	5.270986	-0.392693
C	-6.955049	5.644348	-0.864456
H	-7.316133	6.658200	-0.684953
C	-7.749757	4.759178	-1.585946
H	-8.733553	5.078779	-1.937094
C	-7.287217	3.482751	-1.885468
H	-7.884535	2.783284	-2.470743
C	-6.018307	3.091193	-1.441338
C	-5.237664	3.970005	-0.683630
H	-4.273252	3.614854	-0.317863
C	2.826904	5.154405	6.349663
H	3.212695	5.484063	7.316975
Cu	-5.463562	-0.452095	-3.540877
C	5.486688	-1.749048	1.834018
Cu	3.577394	0.352189	1.930166

O	-6.252478	-1.766924	-2.289185
C	-5.853466	-1.771669	-1.089442
O	-4.834049	-1.176428	-0.639344
C	-6.675685	-2.552220	-0.115520
O	2.543680	-0.454374	3.425835
C	-7.858111	-3.168834	-0.542769
H	-8.150004	-3.088498	-1.590344
O	4.429867	-0.901553	4.576086
C	-8.246243	-3.948528	1.709271
H	-8.858277	-4.512519	2.417307
C	-7.060488	-3.340754	2.160901
C	-6.285008	-2.638914	1.224809
H	-5.378740	-2.117644	1.539532
C	-6.673006	-3.421958	3.570642
C	-5.399467	-3.633449	4.095267
N	-5.552289	-3.599367	5.449400
N	-6.825379	-3.380944	5.835435
C	-7.519141	-3.280711	4.709526
C	-8.980045	-3.008892	4.748715
H	-9.254620	-2.557069	5.709467
H	-9.286186	-2.328596	3.941819
H	-9.579029	-3.926219	4.639232
C	-4.100503	-3.882747	3.426848
H	-3.548812	-4.714102	3.890905
H	-4.258996	-4.138498	2.371692
H	-3.440111	-3.001782	3.462736
C	-4.577683	-3.842236	6.478938
H	-4.341654	-4.915095	6.566085
H	-5.058379	-3.525956	7.415873
N	-3.338550	-3.143703	6.262002
N	-3.358286	-1.820077	6.013003

C	-2.083282	-1.463587	5.915062
C	-1.218045	-2.576763	6.135680
C	-2.074086	-3.653178	6.352938
C	-1.785165	-5.088697	6.587961
H	-1.966179	-5.398885	7.629540
H	-2.392437	-5.747038	5.948495
H	-0.732853	-5.303166	6.364557
C	-1.714773	-0.050861	5.639938
H	-0.840051	0.260517	6.227776
H	-1.459794	0.113647	4.582057
H	-2.554380	0.612390	5.878639
C	0.245857	-2.577484	6.189958
C	0.934370	-3.296507	7.184637
H	0.363743	-3.851837	7.933821
C	2.325066	-3.277772	7.256546
H	2.834600	-3.840349	8.042178
C	3.065647	-2.526374	6.349707
H	4.154393	-2.486145	6.399335
C	2.401696	-1.801905	5.352563
C	1.006235	-1.835581	5.273781
H	0.517045	-1.275246	4.475302
C	3.185833	-0.988918	4.373136
C	-8.638558	-3.862630	0.376259
H	-9.561303	-4.348016	0.050273
O	-4.431398	-1.875669	-4.420206
C	-3.524539	-2.477825	-3.775583
O	-3.082906	-2.161285	-2.636050
C	-2.921847	-3.666539	-4.452308
O	4.299324	-1.470232	1.506623
C	-3.424185	-4.082880	-5.691492
H	-4.263475	-3.543717	-6.131450

O	6.265778	-1.015242	2.509206
C	-1.766900	-5.834680	-5.758577
H	-1.330763	-6.698303	-6.265809
C	-1.244847	-5.436185	-4.514073
C	-1.840738	-4.339053	-3.872643
H	-1.448237	-3.972677	-2.921623
C	-0.108717	-6.156629	-3.936215
C	0.074854	-6.550040	-2.612788
N	1.264534	-7.225650	-2.592595
N	1.854951	-7.289176	-3.800684
C	1.038488	-6.650339	-4.625815
C	1.390187	-6.503835	-6.062941
H	2.475496	-6.587848	-6.194848
H	0.928903	-7.285094	-6.686479
H	1.060268	-5.535825	-6.464541
C	-0.799952	-6.373523	-1.428307
H	-0.451469	-5.577141	-0.751589
H	-1.812123	-6.095661	-1.748498
H	-0.892266	-7.292535	-0.830951
C	1.889644	-7.925511	-1.495400
H	2.049664	-8.973440	-1.778866
H	1.210439	-7.887770	-0.634556
N	3.179482	-7.408784	-1.130731
N	4.273782	-7.981638	-1.669099
C	5.299539	-7.282179	-1.207923
C	4.862178	-6.220618	-0.355785
C	3.472254	-6.334641	-0.339809
C	2.427730	-5.558262	0.368636
H	2.017341	-4.741851	-0.248236
H	1.579950	-6.190006	0.671375
H	2.832236	-5.097978	1.279099

C	6.678511	-7.639739	-1.635106
H	7.292901	-6.746855	-1.816049
H	7.207638	-8.250449	-0.887312
H	6.637108	-8.227413	-2.559922
C	5.688000	-5.263809	0.382253
C	6.964304	-5.634686	0.847926
H	7.327419	-6.647160	0.664752
C	7.759589	-4.748825	1.567960
H	8.745708	-5.066464	1.914339
C	7.294837	-3.474281	1.872099
H	7.892631	-2.774406	2.456418
C	6.023157	-3.085194	1.433797
C	5.241803	-3.964565	0.677486
H	4.275061	-3.611143	0.316252
C	-2.841114	-5.167090	-6.338434
H	-3.230623	-5.500254	-7.303051

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Cu	-2.179469	-5.524163	2.448896
C	-0.058400	4.066519	-3.379925
Cu	1.515011	3.534418	-1.109616
O	-3.557724	-4.356349	3.216715
C	-3.460305	-3.100861	3.099247
O	-2.626125	-2.472968	2.391730
C	-4.447628	-2.293948	3.879066
O	0.477148	4.841252	0.006386
C	-5.096418	-2.868064	4.978753
H	-4.877629	-3.902877	5.244955
O	0.683595	6.445000	-1.565274
C	-6.288069	-0.798585	5.333938
H	-7.034128	-0.224152	5.889908

C	-5.661092	-0.208705	4.221512
C	-4.724810	-0.974977	3.510380
H	-4.189863	-0.543478	2.662118
C	-5.988623	1.158786	3.812999
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N	-6.522990	3.287726	3.813148
N	-6.590797	2.922209	2.513367
C	-6.267549	1.635279	2.496676
C	-6.254805	0.864099	1.227668
H	-6.825703	1.377708	0.443527
H	-6.670415	-0.143928	1.370189
H	-5.232579	0.731349	0.839394
C	-5.906805	2.454917	6.087631
H	-5.237242	3.309459	6.266666
H	-5.431631	1.561884	6.511099
H	-6.836898	2.630155	6.651435
C	-6.583642	4.689199	4.132497
H	-7.410122	5.142905	3.571792
H	-6.775284	4.803336	5.206291
N	-5.362487	5.372178	3.804374
N	-4.284910	5.167831	4.595278
C	-3.254775	5.647936	3.910777
C	-3.674949	6.172379	2.653071
C	-5.046254	5.956521	2.611781
C	-6.042851	6.205440	1.543804
H	-6.776512	6.978312	1.822569
H	-6.597650	5.286697	1.300634
H	-5.539943	6.547619	0.630855
C	-1.880693	5.625645	4.474998
H	-1.353487	6.573100	4.295812
H	-1.265149	4.832477	4.024669

H	-1.913361	5.441750	5.555233
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C	-3.206997	8.038826	1.056851
H	-4.084982	8.562719	1.445352
C	-2.448214	8.612463	0.038593
H	-2.736138	9.582431	-0.373355
C	-1.330589	7.951553	-0.459422
H	-0.737726	8.373257	-1.271742
C	-0.966084	6.709218	0.075870
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C	0.163741	5.940396	-0.528770
C	-6.002385	-2.108165	5.711649
H	-6.508972	-2.547128	6.574269
O	-3.397622	-5.968694	0.909324
C	-3.685825	-5.028561	0.120653
O	-3.142482	-3.885770	0.085035
C	-4.780518	-5.252518	-0.871893
O	-0.057690	3.442297	-2.279242
C	-5.339769	-6.521022	-1.060957
H	-4.975824	-7.359614	-0.465261
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H	-7.616745	-5.743324	-3.473776
C	-6.274197	-4.312712	-2.560773
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H	-6.256833	-4.764884	-5.594765
C	-6.756024	-1.326090	-1.405219
H	-5.783992	-0.826859	-1.270832
H	-6.819071	-2.135452	-0.666296
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C	-7.684339	0.313210	-3.800462
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H	-8.377057	0.539252	-2.978870
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C	-5.211391	2.449340	-2.553090
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C	-5.675544	1.053909	-5.954491
H	-6.311147	1.688699	-6.593474
H	-6.077696	0.032533	-6.016002
H	-4.672223	1.054397	-6.399378
C	-4.661477	3.223733	-1.407407
H	-4.288398	4.207961	-1.726244
H	-3.815341	2.711663	-0.923217
H	-5.430241	3.373559	-0.638486
C	-3.554781	3.050240	-4.464582
C	-3.573333	3.580043	-5.768384
H	-4.484988	3.501672	-6.366028
C	-2.463926	4.237609	-6.296002
H	-2.508611	4.644301	-7.308972
C	-1.311393	4.402924	-5.533357



H	-0.441723	4.934720	-5.922040
C	-1.269622	3.880203	-4.236047
C	-2.378232	3.204612	-3.716899
H	-2.306602	2.790707	-2.710631
C	-6.341846	-6.686302	-2.014349
H	-6.778526	-7.674589	-2.175773
Cu	2.178991	5.524357	-2.448645
C	0.057722	-4.066740	3.380312
Cu	-1.515521	-3.534409	1.109584
O	3.557003	4.356500	-3.216816
C	3.459434	3.101000	-3.099622
O	2.625241	2.473050	-2.392172
C	4.446591	2.294154	-3.879728
O	-0.476807	-4.840684	-0.006357
C	5.094991	2.868329	-4.979613
H	4.876002	3.903111	-5.245772
O	-0.683404	-6.443966	1.565751
C	6.286837	0.799010	-5.335055
H	7.032860	0.224682	-5.891180
C	5.660259	0.209076	-4.222431
C	4.724039	0.975229	-3.511086
H	4.189373	0.543698	-2.662660
C	5.988243	-1.158311	-3.813913
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C	6.255089	-0.863383	-1.228674
H	6.825452	-1.377349	-0.444373
H	6.671341	0.144396	-1.371096
H	5.232836	-0.730016	-0.840688

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H	5.236515	-3.309248	-6.267086
H	5.430810	-1.561727	-6.511881
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C	6.584138	-4.688570	-4.133204
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C	3.255445	-5.647012	-3.908734
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C	6.045371	-6.204265	-1.543848
H	6.778718	-6.977283	-1.823038
H	6.600451	-5.285510	-1.301356
H	5.543211	-6.546179	-0.630393
C	1.880809	-5.624337	-4.471606
H	1.351077	-6.569055	-4.285672
H	1.268183	-4.826398	-4.025707
H	1.912620	-5.447339	-5.553030
C	2.857398	-6.794170	-1.607529
C	3.210091	-8.036343	-1.052996
H	4.088554	-8.559942	-1.440806
C	2.451559	-8.609591	-0.034345
H	2.740242	-9.578875	0.378680
C	1.333158	-7.949210	0.462639
H	0.740422	-8.370632	1.275194
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H	1.428020	-5.167198	-1.497523
C	-0.163125	-5.939437	0.529414

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O	3.397338	5.968541	-0.909059
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O	3.142246	3.885385	-0.085353
C	4.780264	5.251911	0.871951
O	0.056834	-3.442450	2.279658
C	5.339302	6.520432	1.061529
H	4.975273	7.359187	0.466113
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C	6.807357	5.598507	2.753340
H	7.616107	5.742232	3.474347
C	6.273899	4.311732	2.560669
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C	6.758812	3.140508	3.293656
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H	6.255768	4.762818	5.594802
C	6.756576	1.325688	1.404115
H	5.784658	0.826368	1.269247
H	6.819736	2.135354	0.665531
H	7.517165	0.571771	1.158130
C	7.684235	-0.314478	3.799078
H	8.185752	-0.517324	4.753674
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N	6.320386	-1.734637	2.407407
C	5.210325	-2.449507	2.551756
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H	6.312493	-1.691512	6.592091
H	6.078911	-0.034993	6.015613
H	4.673544	-1.056890	6.399223
C	4.659578	-3.222855	1.405763
H	4.286056	-4.207134	1.723950
H	3.813513	-2.709960	0.922329
H	5.427949	-3.372486	0.636404
C	3.554717	-3.051388	4.463826
C	3.573771	-3.581750	5.767395
H	4.485718	-3.503843	6.364654
C	2.464484	-4.239314	6.295264
H	2.509567	-4.646419	7.308051
C	1.311554	-4.404089	5.533101
H	0.441961	-4.935867	5.921983
C	1.269302	-3.880861	4.236013
C	2.377796	-3.205267	3.716620
H	2.305752	-2.790945	2.710562
C	6.341246	6.685525	2.015093
H	6.777746	7.673824	2.176928

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Cu	1.801887	-5.767419	-1.749694
C	0.299668	4.226067	2.962799
Cu	-1.231621	3.517136	0.695889
O	3.291341	-4.777563	-2.588691

C	3.281359	-3.513143	-2.626676
O	2.476096	-2.748736	-2.036141
C	4.350814	-2.886548	-3.467886
O	-0.099975	4.704289	-0.511069
C	4.988095	-3.643504	-4.458548
H	4.707433	-4.689496	-4.589072
O	-0.205704	6.423849	0.939127
C	6.335708	-1.729943	-5.046237
H	7.134557	-1.286937	-5.647341
C	5.727794	-0.957056	-4.041111
C	4.718393	-1.553486	-3.269404
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C	6.154080	0.422808	-3.798447
C	6.400246	1.409195	-4.746731
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H	6.982315	0.980930	-0.466170
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C	6.188238	1.433538	-6.212977
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H	7.132080	1.489421	-6.778202
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C	3.709293	4.939144	-4.389706

C	4.160231	5.576674	-3.195805
C	5.525667	5.328240	-3.147897
C	6.544246	5.656778	-2.123076
H	7.299908	6.367998	-2.492463
H	7.070208	4.750859	-1.785852
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C	2.328110	4.899893	-4.935429
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C	3.370804	6.323235	-2.213018
C	3.782840	7.589826	-1.764991
H	4.684670	8.037117	-2.192466
C	3.050272	8.284045	-0.804617
H	3.383726	9.271192	-0.475868
C	1.897956	7.723776	-0.263741
H	1.318636	8.246519	0.498390
C	1.470845	6.460946	-0.694440
C	2.198366	5.777148	-1.671322
H	1.857868	4.785307	-1.975890
C	0.286089	5.809730	-0.052338
C	5.964153	-3.055304	-5.256307
H	6.458413	-3.640870	-6.035070
O	2.867247	-6.005733	-0.049602
C	3.214966	-4.999139	0.620082
O	2.767379	-3.821849	0.498428
C	4.278904	-5.194680	1.654634
O	0.306647	3.498759	1.929593
C	4.708887	-6.478553	2.007520
H	4.253869	-7.343333	1.522241
O	-0.594727	5.048533	3.293458

C	6.291686	-5.505574	3.559680
H	7.097263	-5.638336	4.286145
C	5.889120	-4.206496	3.203129
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H	4.478808	-3.090914	1.992914
C	6.517613	-3.011318	3.769359
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C	6.947390	-2.770080	5.106397
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H	5.944504	-4.267977	6.274286
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C	5.861405	1.457616	5.874646
H	6.508737	2.149486	6.438001
H	6.241460	0.442121	6.055421
H	4.857625	1.530796	6.312582
C	4.901573	3.128365	1.109477

H	4.559057	4.153874	1.310764
H	4.037361	2.592718	0.685294
H	5.672164	3.163636	0.328561
C	3.787220	3.314945	4.169070
C	3.800870	3.968099	5.415559
H	4.708094	3.945108	6.024348
C	2.688093	4.672620	5.870773
H	2.725713	5.171299	6.842238
C	1.539057	4.760827	5.089599
H	0.662416	5.317143	5.426526
C	1.504075	4.120609	3.845669
C	2.616991	3.402561	3.401573
H	2.550482	2.900078	2.436351
C	5.702273	-6.624041	2.972732
H	6.037169	-7.623433	3.260282
O	2.312559	-7.529660	-3.055048
O	-0.908017	1.418972	-0.046353
Cu	-1.843706	5.736805	1.808000
C	-0.308190	-4.307036	-2.959689
Cu	1.189705	-3.543101	-0.653996
O	-3.338452	4.754449	2.606976
C	-3.314391	3.492769	2.664901
O	-2.493227	2.725813	2.096228
C	-4.390745	2.867840	3.496935
O	0.048454	-4.714205	0.551397
C	-5.033343	3.626802	4.482339
H	-4.743768	4.669299	4.620471
O	0.183605	-6.450518	-0.879328
C	-6.399445	1.717003	5.045676
H	-7.209306	1.277326	5.634457
C	-5.782273	0.943061	4.046938



C	-4.760085	1.536779	3.290767
H	-4.230802	0.955155	2.533124
C	-6.209853	-0.433648	3.790511
C	-6.483796	-1.423008	4.728067
N	-6.923698	-2.497841	4.011758
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C	-6.486434	-1.037468	2.527567
C	-6.368335	-0.421906	1.181285
H	-6.958113	-0.971787	0.436572
H	-6.695396	0.627944	1.194079
H	-5.326593	-0.422089	0.821311
C	-6.307104	-1.454925	6.198835
H	-5.700810	-2.322602	6.499391
H	-5.788057	-0.549825	6.536512
H	-7.264367	-1.506211	6.741502
C	-7.081242	-3.849101	4.481797
H	-7.925797	-4.311293	3.955995
H	-7.295724	-3.830713	5.557169
N	-5.898835	-4.633249	4.254698
N	-4.816822	-4.385996	5.028289
C	-3.801275	-4.965556	4.401733
C	-4.233497	-5.596293	3.197513
C	-5.596455	-5.340964	3.126228
C	-6.597611	-5.660989	2.081772
H	-7.364723	-6.367950	2.435418
H	-7.111354	-4.751191	1.736218
H	-6.105565	-6.120702	1.215877
C	-2.429663	-4.935353	4.971678
H	-1.928219	-5.908071	4.871731
H	-1.790332	-4.198294	4.462921
H	-2.461734	-4.664133	6.033450

C	-3.430930	-6.342314	2.224507
C	-3.838576	-7.607530	1.768667
H	-4.746038	-8.054622	2.184505
C	-3.096664	-8.299264	0.813657
H	-3.428292	-9.284220	0.476629
C	-1.938176	-7.738965	0.285935
H	-1.353123	-8.255096	-0.476029
C	-1.515380	-6.478256	0.726886
C	-2.252182	-5.795591	1.697715
H	-1.914794	-4.804601	2.008556
C	-0.323463	-5.827548	0.096898
C	-6.022214	3.039452	5.265307
H	-6.522240	3.624854	6.040504
O	-2.898125	6.021905	0.106376
C	-3.258062	5.013910	-0.554279
O	-2.826348	3.831707	-0.417705
C	-4.312080	5.210045	-1.598376
O	-0.319193	-3.585375	-1.922339
C	-4.743907	6.493555	-1.950393
H	-4.300169	7.358087	-1.454373
O	0.585090	-5.132298	-3.285784
C	-6.299877	5.520623	-3.529666
H	-7.095593	5.653115	-4.266992
C	-5.895053	4.221756	-3.174883
C	-4.876942	4.093741	-2.219028
H	-4.497810	3.106877	-1.950033
C	-6.506505	3.025687	-3.757616
C	-6.797142	1.840841	-3.084158
N	-7.327615	1.002615	-4.018980
N	-7.390595	1.557659	-5.250385
C	-6.909900	2.787739	-5.103303

C	-6.823178	3.707493	-6.267299
H	-6.855495	3.140827	-7.205628
H	-7.658521	4.424150	-6.292455
H	-5.896676	4.298241	-6.245823
C	-6.648727	1.461773	-1.661116
H	-5.725904	0.890151	-1.474637
H	-6.620691	2.356154	-1.024855
H	-7.471398	0.818597	-1.319870
C	-7.767724	-0.358708	-3.834042
H	-8.299511	-0.631289	-4.754302
H	-8.460965	-0.433006	-2.985679
N	-6.702684	-1.290845	-3.565507
N	-6.484444	-1.700880	-2.295754
C	-5.405407	-2.473451	-2.357514
C	-4.920267	-2.570866	-3.698276
C	-5.790496	-1.785397	-4.450773
C	-5.827370	-1.458243	-5.896382
H	-6.484072	-2.141888	-6.458988
H	-6.194273	-0.437840	-6.077186
H	-4.824907	-1.544766	-6.334872
C	-4.884213	-3.134893	-1.129888
H	-4.552879	-4.164168	-1.330797
H	-4.013526	-2.609596	-0.706303
H	-5.654733	-3.161938	-0.348546
C	-3.771089	-3.335451	-4.186853
C	-3.792931	-3.994543	-5.429977
H	-4.698104	-3.959539	-6.041318
C	-2.692648	-4.723820	-5.876409
H	-2.737985	-5.231156	-6.843025
C	-1.549238	-4.831157	-5.089606
H	-0.688318	-5.417246	-5.415038

C	-1.504550	-4.182315	-3.850911
C	-2.604478	-3.438789	-3.416162
H	-2.531643	-2.931526	-2.454085
C	-5.725281	6.638963	-2.927841
H	-6.062354	7.638068	-3.213847
O	-1.925588	7.658503	2.980630
O	0.762891	-1.469613	0.094089
C	2.496932	-7.268815	-4.216592
H	2.730885	-8.070847	-4.957131
H	2.442541	-6.225966	-4.605868
C	1.667148	-0.693838	0.283686
H	1.465438	0.365589	0.563297
H	2.735467	-1.003882	0.185736
C	-1.860201	0.686625	-0.159450
H	-2.905351	1.060803	-0.040682
H	-1.727173	-0.396057	-0.386247
C	-0.872853	8.044399	3.422532
H	-0.815169	8.972124	4.041080
H	0.083567	7.502496	3.239167

4

CH2OSVP SCF Done: -114.400758933 A.U.

O	-0.674156	0.000002	-0.000007
C	0.522066	-0.000011	0.000028
H	1.130418	0.942811	-0.000055
H	1.130435	-0.942760	-0.000055

3

trosSVP+CuCl2metal SCF Done: -2560.41522075 A.U.

Cu	0.000000	0.000000	0.000000
Cl	0.000000	0.000000	2.095716
Cl	0.000000	0.000000	-2.095716

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troSVP+CuCl2 SCF Done: -3669.46230368 A.U.

C	-5.407863	-3.516167	-0.832395
C	-6.574300	-2.804652	-1.110512
H	-7.478483	-3.331550	-1.422947
C	-5.425650	-0.741667	-0.592065
H	-5.444156	0.344944	-0.479322
C	-4.242794	-1.444027	-0.305378
C	-4.253796	-2.843087	-0.439094
H	-3.334201	-3.406731	-0.258778
C	-3.032603	-0.732763	0.118089
C	-2.146285	-1.108105	1.125356
N	-1.187375	-0.141147	1.160461
N	-1.399357	0.818438	0.232150
C	-2.517747	0.485689	-0.409321
C	-3.054993	1.303517	-1.521429
H	-2.254106	1.850376	-2.031914
H	-3.743539	2.075243	-1.148715
H	-3.593399	0.673453	-2.242021
C	-2.166585	-2.251287	2.067621
H	-1.447397	-3.040136	1.795258
H	-3.161283	-2.712860	2.076781
H	-1.942450	-1.942649	3.098986
C	0.000003	-0.033149	1.964268
H	-0.000037	0.946913	2.470232
H	-0.000003	-0.821520	2.724107
N	1.187434	-0.141087	1.160531
N	1.399428	0.818518	0.232238
C	2.517812	0.485760	-0.409242
C	3.032651	-0.732709	0.118145
C	2.146326	-1.108061	1.125401
C	2.166610	-2.251280	2.067621

H	1.447537	-3.040189	1.795125
H	1.942310	-1.942713	3.098970
H	3.161351	-2.712760	2.076890
C	3.055077	1.303570	-1.521355
H	3.593501	0.673487	-2.241916
H	3.743614	2.075307	-1.148648
H	2.254202	1.850416	-2.031871
C	4.242835	-1.443981	-0.305328
C	5.425699	-0.741633	-0.592013
H	5.444219	0.344978	-0.479262
C	6.576823	-1.414982	-0.991637
H	7.486521	-0.849137	-1.204965
C	6.574325	-2.804627	-1.110476
H	7.478501	-3.331533	-1.422918
C	5.407881	-3.516131	-0.832358
C	4.253823	-2.843040	-0.439049
H	3.334224	-3.406677	-0.258732
C	-6.576783	-1.415007	-0.991681
H	-7.486475	-0.849153	-1.205010
Cu	-0.000026	2.402521	0.077889
Cl	1.677701	3.870972	0.042526
Cl	-1.677901	3.870834	0.043039
H	5.392167	-4.603722	-0.934669
H	-5.392161	-4.603759	-0.934701

3

trosSVP+PdCl<sub>2</sub>metal SCF Done: -1048.10818946 A.U.

Pd	-0.000000	-0.000000	0.622407
Cl	-0.000000	-1.675354	-0.842080
Cl	0.000000	1.675354	-0.842080

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trosSVP+PdCl<sub>2</sub> SCF Done: -2157.20273611 A.U.

C	-5.406691	-3.670077	-0.871038
C	-6.585319	-2.963964	-1.108564
H	-7.488796	-3.491782	-1.421453
C	-5.450825	-0.904164	-0.548718
H	-5.478743	0.178512	-0.403894
C	-4.255893	-1.601389	-0.302714
C	-4.253408	-2.995826	-0.477349
H	-3.324627	-3.553698	-0.329184
C	-3.046888	-0.888274	0.121383
C	-2.142787	-1.278563	1.106047
N	-1.193387	-0.301942	1.158509
N	-1.436555	0.678637	0.255279
C	-2.557518	0.348431	-0.386035
C	-3.110394	1.177218	-1.481042
H	-2.312608	1.717040	-2.004945
H	-3.789209	1.950553	-1.094767
H	-3.665686	0.552877	-2.193536
C	-2.140602	-2.446033	2.017991
H	-1.412624	-3.217661	1.721029
H	-3.128908	-2.921124	2.019606
H	-1.915645	-2.161855	3.056192
C	0.000044	-0.204268	1.958376
H	0.000055	0.768628	2.476026
H	0.000067	-1.010411	2.699482
N	1.193466	-0.301889	1.158456
N	1.436684	0.678778	0.255331
C	2.557689	0.348655	-0.385920
C	3.047045	-0.888102	0.121379
C	2.142890	-1.278497	1.105959
C	2.140763	-2.446158	2.017656
H	1.413754	-3.218352	1.719793

H	1.914596	-2.162458	3.055716
H	3.129470	-2.920423	2.020077
C	3.110549	1.177609	-1.480836
H	3.665436	0.553302	-2.193680
H	3.789800	1.950575	-1.094581
H	2.312789	1.717870	-2.004317
C	4.256069	-1.601186	-0.302692
C	5.450918	-0.903913	-0.548977
H	5.478765	0.178796	-0.404410
C	6.601264	-1.578248	-0.949060
H	7.520480	-1.016828	-1.130852
C	6.585538	-2.963738	-1.108484
H	7.489025	-3.491554	-1.421347
C	5.406993	-3.669897	-0.870689
C	4.253695	-2.995663	-0.477028
H	3.324985	-3.553595	-0.328653
C	-6.601150	-1.578510	-0.948837
H	-7.520437	-1.017138	-1.130419
Pd	-0.000119	2.208929	0.084437
Cl	1.663695	3.812463	-0.014235
Cl	-1.664294	3.812121	-0.014170
H	5.381320	-4.753768	-1.005189
H	-5.380943	-4.753918	-1.005766

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trosSVP SCF Done: -1108.98179886 A.U.

C	5.491307	1.986157	1.117591
C	6.511927	1.826440	0.180859
H	7.439885	2.394871	0.274645
C	5.152664	0.211943	-0.998751
H	5.035838	-0.498973	-1.820187
C	4.114019	0.356710	-0.062144



C	4.306069	1.265329	0.994302
H	3.497985	1.427881	1.712988
C	2.868790	-0.403403	-0.194635
C	2.131419	-1.005956	0.821697
N	1.046970	-1.567748	0.208500
N	1.030644	-1.368572	-1.122576
C	2.130153	-0.673347	-1.385458
C	2.439429	-0.257133	-2.778299
H	1.525310	-0.255724	-3.383945
H	3.149875	-0.941212	-3.267190
H	2.887716	0.745537	-2.811195
C	2.405970	-1.134155	2.273576
H	1.748785	-0.504448	2.895826
H	3.437713	-0.830474	2.489007
H	2.291934	-2.168675	2.628830
C	-0.044120	-2.281974	0.822957
H	-0.078114	-3.328046	0.489033
H	0.124211	-2.269758	1.911363
N	-1.326080	-1.727098	0.484371
N	-2.270689	-2.542277	-0.024099
C	-3.326407	-1.764968	-0.229211
C	-3.051038	-0.412711	0.133484
C	-1.737051	-0.432355	0.595663
C	-0.873026	0.637010	1.148946
H	-0.138642	1.006445	0.414561
H	-0.301838	0.289197	2.023037
H	-1.480010	1.492273	1.471677
C	-4.571848	-2.332203	-0.809481
H	-5.039270	-1.636367	-1.520138
H	-5.326429	-2.558546	-0.040332
H	-4.351037	-3.270702	-1.332107

C	-3.936334	0.748247	0.023225
C	-5.305862	0.646881	0.326309
H	-5.706977	-0.308315	0.673300
C	-6.150370	1.748461	0.218046
H	-7.209803	1.643104	0.464370
C	-5.648665	2.983501	-0.192221
H	-6.311288	3.847878	-0.275914
C	-4.293657	3.102584	-0.499858
C	-3.450151	1.999158	-0.398879
H	-2.398482	2.096007	-0.680984
C	6.334486	0.938187	-0.879692
H	7.128225	0.803051	-1.618372
H	-3.891035	4.061567	-0.835275
H	5.613298	2.688881	1.945477

Truncated structures:

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troscis SCF Done: -1108.98192213 A.U.

C	5.578554	1.914106	1.095555
C	6.553529	1.770205	0.108903
H	7.495960	2.317876	0.181770
C	5.111247	0.227433	-1.066104
H	4.944292	-0.451362	-1.905850
C	4.116886	0.358141	-0.080557
C	4.374055	1.221473	0.999497
H	3.602068	1.372222	1.759407
C	2.853434	-0.375051	-0.192480
C	2.145346	-1.010592	0.824802
N	1.034158	-1.537148	0.228204
N	0.972339	-1.283625	-1.091736
C	2.068774	-0.588567	-1.366121

C	2.329793	-0.117069	-2.751021
H	1.395984	-0.100792	-3.325742
H	3.029047	-0.775454	-3.288933
H	2.768679	0.890401	-2.761370
C	2.465520	-1.195528	2.260957
H	1.842665	-0.573991	2.925330
H	3.510226	-0.920524	2.451615
H	2.341048	-2.239183	2.584707
C	-0.040176	-2.275765	0.847876
H	-0.057961	-3.321220	0.509964
H	0.133550	-2.263457	1.935249
N	-1.329075	-1.739210	0.516238
N	-2.233622	-2.534149	-0.088128
C	-3.287009	-1.757810	-0.306596
C	-3.048518	-0.423613	0.142022
C	-1.761030	-0.455533	0.671298
C	-0.934349	0.588732	1.319909
H	-0.181739	1.013408	0.635300
H	-0.388735	0.195245	2.191058
H	-1.564723	1.414880	1.672853
C	-4.490726	-2.307702	-0.982577
H	-4.914221	-1.591604	-1.700720
H	-5.292911	-2.559635	-0.271852
H	-4.231346	-3.228364	-1.519296
C	-3.938590	0.734567	0.043685
C	-5.324561	0.605536	0.245055
H	-5.738156	-0.372250	0.503520
C	-6.171421	1.705962	0.146810
H	-7.244210	1.578295	0.311845
C	-5.656743	2.967476	-0.150495
H	-6.321933	3.830778	-0.225052

C	-4.285472	3.114335	-0.357323
C	-3.439225	2.012488	-0.267661
H	-2.372320	2.133685	-0.472973
C	6.311964	0.925172	-0.973642
H	7.070329	0.801327	-1.750611
H	-3.871422	4.095010	-0.605154
H	5.751534	2.583263	1.942147

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trosisomer000TScistrans SCF Done: -1108.97904770 A.U.

C	5.268329	-2.583557	-0.597228
C	6.561004	-2.082560	-0.446185
H	7.424687	-2.740143	-0.568983
C	5.639248	0.101320	0.024490
H	5.792716	1.160193	0.246869
C	4.328750	-0.385175	-0.126410
C	4.166561	-1.747558	-0.435694
H	3.156966	-2.158418	-0.522233
C	3.175472	0.501047	0.044460
C	2.012644	0.534838	-0.717139
N	1.245377	1.524837	-0.175532
N	1.814947	2.111807	0.899546
C	2.990804	1.515212	1.033481
C	3.911278	1.914403	2.129614
H	3.352981	2.423482	2.924547
H	4.692767	2.609503	1.785722
H	4.425490	1.044967	2.562415
C	1.577107	-0.257313	-1.888422
H	0.885740	-1.062728	-1.595608
H	2.438846	-0.715521	-2.390047
H	1.050614	0.361544	-2.630380
C	-0.059944	1.923985	-0.571180

H	-0.255152	2.889873	-0.083737
H	-0.100169	2.080275	-1.663060
N	-1.091845	0.961920	-0.200269
N	-0.788834	-0.187894	0.423934
C	-1.955767	-0.796844	0.616226
C	-3.033358	-0.028066	0.089514
C	-2.424895	1.112875	-0.433195
C	-2.984229	2.325847	-1.075591
H	-2.827316	2.341667	-2.166824
H	-2.535341	3.247490	-0.675757
H	-4.065884	2.386564	-0.903905
C	-2.003394	-2.125313	1.280802
H	-2.760125	-2.779244	0.825039
H	-2.250325	-2.046646	2.350838
H	-1.026003	-2.618529	1.213640
C	-4.459683	-0.358852	0.077349
C	-5.070885	-0.973470	1.184584
H	-4.473599	-1.186007	2.074511
C	-6.427190	-1.287292	1.174718
H	-6.878853	-1.759535	2.050709
C	-7.211037	-0.992316	0.059465
H	-8.275743	-1.236340	0.053572
C	-6.621542	-0.386988	-1.049756
C	-5.263554	-0.079587	-1.043063
H	-4.806090	0.361798	-1.932891
C	6.740116	-0.735673	-0.132127
H	7.748306	-0.330356	-0.014974
H	-7.222454	-0.162140	-1.934484
H	5.115423	-3.640211	-0.831022

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trosisomer000 SCF Done: -1108.97904344 A.U.

C	-5.246199	-2.596666	0.604086
C	-6.542107	-2.103484	0.455018
H	-7.401596	-2.766322	0.578961
C	-5.634211	0.086016	-0.016470
H	-5.794427	1.143961	-0.238364
C	-4.320503	-0.392567	0.132271
C	-4.149711	-1.754056	0.440992
H	-3.137572	-2.158970	0.525690
C	-3.173000	0.500667	-0.040544
C	-2.006590	0.537909	0.715421
N	-1.247502	1.534229	0.174059
N	-1.825263	2.122050	-0.896012
C	-2.998496	1.519598	-1.026628
C	-3.926039	1.917967	-2.117071
H	-3.373807	2.432060	-2.913015
H	-4.709024	2.608415	-1.767271
H	-4.438276	1.047507	-2.550156
C	-1.559931	-0.256707	1.880896
H	-0.868720	-1.059627	1.580673
H	-2.416406	-0.718948	2.387830
H	-1.029409	0.361357	2.620639
C	0.058748	1.936381	0.563600
H	0.249232	2.902360	0.074158
H	0.104382	2.093525	1.655095
N	1.089706	0.974656	0.189426
N	0.787309	-0.162848	-0.457294
C	1.953061	-0.774321	-0.648306
C	3.029232	-0.019938	-0.098126
C	2.421143	1.115114	0.437781
C	2.979733	2.314234	1.106412
H	2.812624	2.311749	2.196264

H	2.538834	3.244827	0.718647
H	4.063232	2.372967	0.946079
C	2.000141	-2.092167	-1.333766
H	2.749579	-2.757202	-0.882039
H	2.256834	-1.997574	-2.400215
H	1.019668	-2.581215	-1.283135
C	4.453494	-0.358884	-0.077232
C	5.071634	-0.961176	-1.187439
H	4.481819	-1.157001	-2.086123
C	6.425841	-1.283670	-1.169195
H	6.882809	-1.746265	-2.047585
C	7.200785	-1.009678	-0.042505
H	8.263856	-1.260471	-0.030037
C	6.604411	-0.416617	1.069656
C	5.248384	-0.100786	1.054602
H	4.785242	0.330147	1.946578
C	-6.729765	-0.757646	0.141481
H	-7.740545	-0.358386	0.025838
H	7.198167	-0.208226	1.963211
H	-5.086565	-3.652420	0.837417

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troisomer020 SCF Done: -1108.97988240 A.U.

C	4.760592	-2.905929	-0.342887
C	6.111404	-2.564247	-0.401527
H	6.873666	-3.341705	-0.490406
C	5.508405	-0.229486	-0.230816
H	5.809149	0.820629	-0.210751
C	4.141490	-0.554537	-0.172438
C	3.789028	-1.915219	-0.224819
H	2.736257	-2.197745	-0.141160
C	3.122589	0.489906	-0.049663

C	1.874451	0.527788	-0.662443
N	1.288047	1.681469	-0.233612
N	2.052589	2.380144	0.630348
C	3.173934	1.680006	0.738410
C	4.265316	2.154092	1.628580
H	3.869465	2.868971	2.360074
H	5.066061	2.666694	1.073471
H	4.734901	1.321361	2.170608
C	1.197530	-0.396632	-1.600542
H	0.513103	-1.083295	-1.076421
H	1.929145	-1.005071	-2.147622
H	0.592555	0.145718	-2.343151
C	-0.023214	2.140031	-0.546532
H	-0.112560	3.141860	-0.099652
H	-0.162596	2.239774	-1.635925
N	-1.055902	1.244242	-0.047070
N	-0.791890	0.370244	0.938782
C	-1.926037	-0.297483	1.125099
C	-2.938754	0.140009	0.222761
C	-2.327746	1.145062	-0.526291
C	-2.845865	2.032050	-1.595428
H	-2.464267	1.763098	-2.594798
H	-2.580094	3.085659	-1.423038
H	-3.940156	1.973855	-1.642951
C	-1.998867	-1.371744	2.149471
H	-2.595698	-2.226122	1.800472
H	-2.458970	-1.021827	3.086518
H	-0.990595	-1.723898	2.399413
C	-4.308145	-0.360636	0.083865
C	-5.078228	-0.693560	1.212011
H	-4.652476	-0.558364	2.209189



C	-6.381853	-1.163763	1.078951
H	-6.961161	-1.409822	1.972245
C	-6.953136	-1.310967	-0.184858
H	-7.977099	-1.677459	-0.287805
C	-6.202427	-0.992221	-1.315680
C	-4.895973	-0.529181	-1.183110
H	-4.304823	-0.318385	-2.078429
C	6.479649	-1.220563	-0.342257
H	7.534818	-0.940163	-0.390329
H	-6.633810	-1.116853	-2.312068
H	4.460422	-3.956246	-0.375760

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trosisomer040 SCF Done: -1108.98141032 A.U.

C	-4.342480	-3.101119	-0.144959
C	-5.711527	-2.928417	0.056129
H	-6.384442	-3.788798	0.041859
C	-5.357571	-0.547450	0.290092
H	-5.762517	0.448876	0.483199
C	-3.973422	-0.702682	0.094811
C	-3.486823	-2.003278	-0.131534
H	-2.421807	-2.147700	-0.330617
C	-3.066690	0.446456	0.117575
C	-1.777530	0.488125	0.640977
N	-1.324007	1.751500	0.405441
N	-2.215522	2.525046	-0.244141
C	-3.282651	1.754575	-0.412230
C	-4.480850	2.283725	-1.113926
H	-4.210392	3.168107	-1.703476
H	-5.274818	2.588528	-0.414675
H	-4.919620	1.534422	-1.787761
C	-0.958379	-0.525274	1.345933

H	-0.235849	-1.015561	0.673129
H	-1.596032	-1.307827	1.776773
H	-0.375957	-0.081063	2.167661
C	-0.031299	2.277429	0.722230
H	-0.032653	3.313880	0.354335
H	0.142163	2.297706	1.809980
N	1.034953	1.499272	0.128486
N	0.894683	1.023049	-1.121761
C	2.000539	0.327106	-1.356240
C	2.866820	0.334061	-0.222754
C	2.198740	1.105992	0.724787
C	2.591375	1.524347	2.091985
H	2.002824	1.023444	2.878725
H	2.479158	2.607855	2.244876
H	3.644781	1.277469	2.272755
C	2.190815	-0.364650	-2.657571
H	2.702738	-1.328758	-2.530586
H	2.796977	0.229630	-3.358468
H	1.221098	-0.538668	-3.139550
C	4.157121	-0.344455	-0.077097
C	5.090485	-0.350019	-1.128352
H	4.857521	0.185689	-2.051921
C	6.313630	-1.002384	-1.000055
H	7.023572	-0.987484	-1.830670
C	6.637735	-1.665058	0.183433
H	7.597710	-2.176776	0.283813
C	5.723329	-1.673287	1.235773
C	4.496804	-1.026292	1.105272
H	3.772046	-1.072329	1.923022
C	-6.214036	-1.644924	0.268707
H	-7.285105	-1.496815	0.427922

H	5.960564	-2.201295	2.162760
H	-3.937534	-4.099759	-0.327167

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trosisomer060 SCF Done: -1108.98167784 A.U.

C	-4.290850	-3.084785	-0.624991
C	-5.642347	-2.985396	-0.296644
H	-6.302908	-3.848112	-0.409631
C	-5.303213	-0.672416	0.319665
H	-5.704002	0.265976	0.710786
C	-3.936895	-0.754457	-0.003087
C	-3.450905	-1.983061	-0.486126
H	-2.402669	-2.061804	-0.786310
C	-3.056204	0.406094	0.143843
C	-1.735997	0.415123	0.588770
N	-1.331873	1.715452	0.519457
N	-2.288604	2.542762	0.053430
C	-3.343611	1.768665	-0.165414
C	-4.598499	2.350389	-0.709143
H	-4.390492	3.315666	-1.186609
H	-5.350509	2.530534	0.074574
H	-5.063519	1.685509	-1.450515
C	-0.866922	-0.674603	1.091655
H	-0.120859	-0.996305	0.346469
H	-1.470000	-1.550938	1.360404
H	-0.309332	-0.371138	1.990460
C	-0.046992	2.276198	0.849127
H	-0.082174	3.317639	0.503543
H	0.121313	2.274244	1.937495
N	1.044132	1.562473	0.240527
N	1.094200	1.480653	-1.102780
C	2.194134	0.789493	-1.370661

C	2.871838	0.410727	-0.172282
C	2.096011	0.940949	0.854868
C	2.316211	0.954659	2.321143
H	1.644098	0.273983	2.869320
H	2.181154	1.957193	2.752840
H	3.343047	0.641078	2.546783
C	2.564825	0.484174	-2.776921
H	2.996056	-0.522062	-2.872239
H	3.311511	1.190063	-3.171894
H	1.682254	0.552981	-3.424002
C	4.107451	-0.366378	-0.050088
C	5.179006	-0.154189	-0.935523
H	5.092079	0.619306	-1.702283
C	6.353823	-0.893179	-0.833571
H	7.172831	-0.705461	-1.532269
C	6.491571	-1.862920	0.159233
H	7.413569	-2.443288	0.239487
C	5.438970	-2.088997	1.045420
C	4.260339	-1.354849	0.938724
H	3.427755	-1.567943	1.615373
C	-6.144298	-1.771805	0.173060
H	-7.201560	-1.682214	0.435005
H	5.531276	-2.854588	1.819782
H	-3.888600	-4.026302	-1.007345

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troisomer080TSciscis SCF Done: -1108.97793847 A.U.

C	5.118615	2.698655	-0.640474
C	6.373036	2.138291	-0.879003
H	7.224245	2.776428	-1.126850
C	5.444012	-0.057999	-0.484481
H	5.587035	-1.137683	-0.401806

C	4.171080	0.488075	-0.238267
C	4.031769	1.885143	-0.330087
H	3.046944	2.336642	-0.184952
C	3.038615	-0.376927	0.098099
C	2.016579	-0.120022	1.009018
N	1.214415	-1.228947	0.990726
N	1.645100	-2.171758	0.129837
C	2.747686	-1.677619	-0.413290
C	3.488866	-2.460648	-1.436565
H	2.825807	-3.208859	-1.887037
H	4.346033	-3.003040	-1.008515
H	3.884261	-1.814860	-2.233181
C	1.800911	1.038943	1.907542
H	1.130562	1.799641	1.476835
H	2.756497	1.539567	2.112609
H	1.373786	0.744932	2.877227
C	0.000000	-1.486034	1.723131
H	-0.000010	-2.548379	1.993061
H	-0.000010	-0.881826	2.637813
N	-1.214394	-1.228935	0.990697
N	-1.645095	-2.171770	0.129841
C	-2.747692	-1.677652	-0.413278
C	-3.038621	-0.376947	0.098083
C	-2.016565	-0.120011	1.008977
C	-1.800962	1.038942	1.907534
H	-1.130887	1.799834	1.476745
H	-1.373557	0.744963	2.877104
H	-2.756618	1.539336	2.112840
C	-3.488851	-2.460716	-1.436543
H	-3.884085	-1.814978	-2.233279
H	-4.346121	-3.002976	-1.008534

H	-2.825813	-3.209044	-1.886854
C	-4.171084	0.488059	-0.238270
C	-5.443998	-0.058003	-0.484614
H	-5.587030	-1.137691	-0.402038
C	-6.528034	0.754526	-0.802860
H	-7.506493	0.302570	-0.983530
C	-6.373021	2.138317	-0.878987
H	-7.224220	2.776467	-1.126832
C	-5.118622	2.698669	-0.640319
C	-4.031789	1.885138	-0.329940
H	-3.046980	2.336636	-0.184701
C	6.528061	0.754509	-0.802737
H	7.506535	0.302546	-0.983304
H	-4.981396	3.780767	-0.708140
H	4.981383	3.780746	-0.708410

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trosisomer080 SCF Done: -1108.97771131 A.U.

C	5.006018	2.721261	-0.317404
C	6.222323	2.206827	-0.765015
H	7.059679	2.875762	-0.976232
C	5.290699	-0.022739	-0.676362
H	5.417396	-1.100939	-0.799076
C	4.057007	0.476734	-0.221891
C	3.936947	1.868814	-0.054719
H	2.977389	2.288974	0.258563
C	2.934559	-0.421556	0.055200
C	2.009738	-0.323462	1.092076
N	1.157123	-1.382981	0.930493
N	1.465648	-2.146388	-0.134255
C	2.540229	-1.586234	-0.670372
C	3.159178	-2.171827	-1.887939

H	2.430283	-2.798213	-2.415935
H	4.023204	-2.811218	-1.649366
H	3.518171	-1.392366	-2.574456
C	1.947636	0.622750	2.232516
H	1.219242	1.435953	2.088985
H	2.926975	1.097528	2.375575
H	1.690598	0.122528	3.177876
C	-0.010583	-1.715153	1.709897
H	0.006279	-2.794143	1.907716
H	0.038977	-1.175372	2.662442
N	-1.263757	-1.426816	1.061648
N	-1.725985	-2.299126	0.142992
C	-2.781610	-1.712868	-0.401213
C	-2.990622	-0.410682	0.146219
C	-1.975037	-0.257574	1.085138
C	-1.678764	0.867672	2.002724
H	-0.935528	1.568935	1.589898
H	-1.297740	0.527561	2.976712
H	-2.589555	1.450360	2.194103
C	-3.560183	-2.406132	-1.460102
H	-3.884310	-1.708980	-2.245516
H	-4.468183	-2.886293	-1.063519
H	-2.950923	-3.194241	-1.918542
C	-4.024456	0.564276	-0.208121
C	-5.347705	0.165063	-0.467062
H	-5.614828	-0.890685	-0.376895
C	-6.324235	1.095312	-0.812118
H	-7.346599	0.759516	-1.002821
C	-6.006083	2.449989	-0.906445
H	-6.773416	3.178937	-1.177038
C	-4.698473	2.864206	-0.656662

C	-3.720929	1.933590	-0.315985
H	-2.691149	2.265887	-0.160058
C	6.357126	0.830372	-0.945773
H	7.306232	0.415359	-1.293964
H	-4.433918	3.921332	-0.739474
H	4.883839	3.799158	-0.184651

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troisomer100 SCF Done: -1108.98054737 A.U.

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troisomer080 SCF Done: -1108.97771131 A.U.

C	5.165770	2.315239	0.714020
C	6.182306	2.108737	-0.217830
H	7.048646	2.773589	-0.244729
C	4.976127	0.200723	-1.083659
H	4.920461	-0.640388	-1.778700
C	3.940631	0.392784	-0.151878
C	4.057177	1.473225	0.741906
H	3.246186	1.673910	1.447802
C	2.768900	-0.485248	-0.131814
C	2.067173	-0.937692	0.983267
N	1.037614	-1.692960	0.491931
N	1.021770	-1.750538	-0.851784
C	2.067744	-1.037153	-1.246824
C	2.352910	-0.875399	-2.696098
H	1.457695	-1.117308	-3.281485
H	3.156520	-1.543946	-3.041015
H	2.664756	0.150543	-2.937283
C	2.339607	-0.773597	2.432259
H	1.656705	-0.062124	2.924776
H	3.358231	-0.394494	2.581975



H	2.266709	-1.725249	2.978794
C	-0.055270	-2.288867	1.226330
H	-0.088408	-3.373028	1.055982
H	0.115230	-2.102473	2.295487
N	-1.335024	-1.781957	0.818113
N	-2.089474	-2.512243	-0.029559
C	-3.075029	-1.708329	-0.400466
C	-2.931444	-0.409494	0.177574
C	-1.778729	-0.496148	0.950106
C	-1.084324	0.498423	1.800056
H	-0.182994	0.908927	1.312400
H	-0.764473	0.064411	2.760122
H	-1.747916	1.341921	2.028182
C	-4.125244	-2.191390	-1.334090
H	-4.412458	-1.413455	-2.055303
H	-5.043567	-2.496364	-0.808742
H	-3.762838	-3.065978	-1.887773
C	-3.781581	0.766212	-0.023061
C	-5.181866	0.652617	-0.076184
H	-5.643957	-0.328022	0.062066
C	-5.986196	1.771023	-0.277113
H	-7.072507	1.656577	-0.309473
C	-5.413143	3.033765	-0.428026
H	-6.045386	3.910618	-0.585561
C	-4.025879	3.165137	-0.382176
C	-3.221053	2.046055	-0.187419
H	-2.133345	2.155748	-0.193148
C	6.079336	1.048880	-1.118289
H	6.870749	0.876118	-1.851800
H	-3.564255	4.147033	-0.513326
H	5.228479	3.150316	1.416302

trosisomer120 SCF Done: -1108.98191671 A.U.

C	-5.550289	1.949809	-1.063742
C	-6.529087	1.796374	-0.082277
H	-7.465893	2.354654	-0.146572
C	-5.104687	0.217447	1.066339
H	-4.946351	-0.478706	1.893471
C	-4.106415	0.358053	0.086215
C	-4.352711	1.244060	-0.977900
H	-3.577107	1.401694	-1.732747
C	-2.848149	-0.385347	0.188330
C	-2.141577	-1.007682	-0.838022
N	-1.033333	-1.548376	-0.248412
N	-0.971749	-1.315387	1.075255
C	-2.065845	-0.620433	1.359255
C	-2.327641	-0.169986	2.751000
H	-1.394178	-0.161105	3.326414
H	-3.026327	-0.837331	3.278546
H	-2.767844	0.836640	2.776123
C	-2.461319	-1.169427	-2.277082
H	-1.836746	-0.539277	-2.931679
H	-3.505323	-0.889270	-2.464255
H	-2.339014	-2.208277	-2.616696
C	0.041763	-2.276241	-0.879784
H	0.061366	-3.326073	-0.556055
H	-0.132784	-2.249073	-1.966545
N	1.330082	-1.742242	-0.542334
N	2.225427	-2.533005	0.080950
C	3.274481	-1.754505	0.312026
C	3.041066	-0.422141	-0.144886
C	1.761613	-0.457899	-0.693042

C	0.940103	0.583620	-1.352497
H	0.182527	1.011201	-0.675016
H	0.400717	0.186462	-2.225862
H	1.572585	1.408650	-1.704415
C	4.468996	-2.300604	1.007086
H	4.881793	-1.581409	1.728362
H	5.281255	-2.554574	0.308643
H	4.202814	-3.219438	1.543591
C	3.928111	0.737611	-0.037977
C	5.316872	0.609988	-0.220163
H	5.735375	-0.368077	-0.469446
C	6.160677	1.712088	-0.114725
H	7.235770	1.585513	-0.264852
C	5.640114	2.973945	0.170791
H	6.302947	3.838561	0.250918
C	4.265968	3.119388	0.358783
C	3.422665	2.015909	0.261788
H	2.352910	2.136242	0.452084
C	-6.298675	0.928001	0.984076
H	-7.060273	0.796561	1.756622
H	3.847077	4.100347	0.597161
H	-5.714493	2.636977	-1.897561

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trosisomer140 SCF Done: -1108.98147178 A.U.

C	-5.480049	1.957127	-1.252587
C	-6.542729	1.785092	-0.366204
H	-7.474397	2.337144	-0.509834
C	-5.217564	0.201629	0.889699
H	-5.128275	-0.502061	1.720948
C	-4.137241	0.358214	0.003693
C	-4.290695	1.256825	-1.066727

H	-3.450935	1.425142	-1.747034
C	-2.890666	-0.386049	0.203275
C	-2.117284	-1.019119	-0.765288
N	-1.056294	-1.561723	-0.095592
N	-1.090082	-1.321496	1.229565
C	-2.197524	-0.618291	1.429047
C	-2.559025	-0.159195	2.795264
H	-1.671492	-0.154942	3.439374
H	-3.300597	-0.818646	3.271489
H	-2.991586	0.850916	2.782968
C	-2.336639	-1.183203	-2.222490
H	-1.642406	-0.583343	-2.833984
H	-3.353270	-0.866661	-2.486125
H	-2.228897	-2.228893	-2.545851
C	0.043946	-2.308800	-0.641044
H	0.079148	-3.327757	-0.231589
H	-0.112077	-2.380785	-1.729386
N	1.324685	-1.723867	-0.334556
N	2.332662	-2.559818	-0.016923
C	3.400447	-1.784497	0.121138
C	3.074091	-0.414418	-0.103531
C	1.714396	-0.418930	-0.410274
C	0.803072	0.681931	-0.804071
H	0.105615	0.960233	0.002157
H	0.189081	0.413995	-1.677000
H	1.381660	1.574880	-1.071317
C	4.707918	-2.375259	0.508866
H	5.241491	-1.740066	1.229864
H	5.378275	-2.510943	-0.353839
H	4.555736	-3.363544	0.959432
C	3.959917	0.748299	-0.015043

C	5.280288	0.688151	-0.494520
H	5.638866	-0.235353	-0.955590
C	6.125366	1.791631	-0.417111
H	7.145696	1.718904	-0.801896
C	5.672263	2.988363	0.137672
H	6.334607	3.855239	0.194629
C	4.367966	3.065146	0.624380
C	3.525082	1.958881	0.554986
H	2.517835	2.020234	0.975435
C	-6.404061	0.905950	0.707219
H	-7.231066	0.761832	1.406782
H	4.005608	3.992799	1.074666
H	-5.573075	2.653133	-2.089859

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trosisomer160TStranscis SCF Done: -1108.98022875 A.U.

C	-4.986122	2.259453	-1.419338
C	-6.214857	2.093590	-0.781256
H	-7.057726	2.741429	-1.032538
C	-5.283906	0.270272	0.504530
H	-5.412274	-0.521719	1.246655
C	-4.040482	0.418502	-0.133258
C	-3.911094	1.435962	-1.095215
H	-2.941235	1.597652	-1.574842
C	-2.908813	-0.450503	0.201495
C	-2.004398	-1.034587	-0.677911
N	-1.118212	-1.723932	0.102534
N	-1.386640	-1.622203	1.421464
C	-2.474001	-0.865497	1.496994
C	-3.071250	-0.537921	2.817248
H	-2.331871	-0.683481	3.613867
H	-3.931694	-1.182636	3.052857

H	-3.430746	0.499856	2.853656
C	-1.927184	-1.021679	-2.157467
H	-1.051701	-0.465872	-2.532486
H	-2.822084	-0.551734	-2.582205
H	-1.861151	-2.037062	-2.576127
C	0.021110	-2.466974	-0.326482
H	0.098118	-3.389020	0.264230
H	-0.124011	-2.754098	-1.378669
N	1.292808	-1.771798	-0.194078
N	2.371955	-2.557809	-0.366816
C	3.418187	-1.744061	-0.302000
C	3.006411	-0.402901	-0.066518
C	1.612325	-0.455153	-0.008489
C	0.642353	0.652918	0.172834
H	0.040372	0.540721	1.087017
H	-0.065113	0.741508	-0.664643
H	1.183232	1.604451	0.238599
C	4.798532	-2.279862	-0.431121
H	5.493612	-1.778895	0.257089
H	5.204578	-2.146933	-1.445805
H	4.808659	-3.355733	-0.218220
C	3.877626	0.768504	0.074616
C	4.940178	0.961216	-0.825586
H	5.079076	0.248700	-1.642648
C	5.798113	2.050203	-0.707726
H	6.613660	2.177555	-1.423967
C	5.613007	2.981868	0.313330
H	6.284885	3.838164	0.407578
C	4.565152	2.807537	1.216793
C	3.710458	1.712977	1.102835
H	2.914820	1.567250	1.838752

C	-6.356972	1.097931	0.184974
H	-7.316090	0.958722	0.689801
H	4.418529	3.524938	2.028222
H	-4.859458	3.045663	-2.167602

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trosisomer160 SCF Done: -1108.98047094 A.U.

C	-5.093381	2.187003	-1.379897
C	-6.283758	2.029915	-0.671241
H	-7.145910	2.661959	-0.895818
C	-5.264899	0.255645	0.617132
H	-5.345000	-0.514058	1.388929
C	-4.059964	0.394456	-0.092376
C	-3.993766	1.383510	-1.089960
H	-3.052970	1.539167	-1.626162
C	-2.901340	-0.452316	0.204354
C	-2.040932	-1.053987	-0.706958
N	-1.101116	-1.705246	0.042869
N	-1.294163	-1.562525	1.370521
C	-2.386441	-0.817930	1.485098
C	-2.910136	-0.452334	2.826344
H	-2.126262	-0.571887	3.583725
H	-3.753750	-1.091330	3.128909
H	-3.271501	0.585226	2.851643
C	-2.061031	-1.094537	-2.188235
H	-1.225493	-0.537034	-2.643151
H	-2.991520	-0.655600	-2.567374
H	-2.005559	-2.123252	-2.574259
C	0.034228	-2.437272	-0.422314
H	0.105808	-3.400055	0.100506
H	-0.108696	-2.645833	-1.493928
N	1.303707	-1.766177	-0.210766

N	2.384793	-2.569271	-0.239133
C	3.431199	-1.756786	-0.166034
C	3.017386	-0.397433	-0.079142
C	1.623445	-0.440087	-0.124734
C	0.646379	0.676226	-0.127709
H	-0.006937	0.668957	0.758317
H	-0.011773	0.660246	-1.008969
H	1.182482	1.632707	-0.144999
C	4.811931	-2.306539	-0.141410
H	5.471053	-1.712011	0.506177
H	5.273047	-2.318426	-1.141242
H	4.803079	-3.341839	0.220713
C	3.883374	0.779248	0.040958
C	5.039364	0.886837	-0.751993
H	5.260679	0.100617	-1.478281
C	5.888677	1.984081	-0.644275
H	6.778362	2.043814	-1.276119
C	5.602366	3.007758	0.258251
H	6.267621	3.870123	0.343605
C	4.461402	2.918116	1.054845
C	3.614870	1.816334	0.952111
H	2.743815	1.739310	1.608653
C	-6.362546	1.063523	0.331234
H	-7.291068	0.931629	0.892158
H	4.234403	3.708206	1.775157
H	-5.015025	2.951327	-2.156922

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trosisomer180 SCF Done: -1108.98069383 A.U.

C	-4.911233	-2.246664	1.556473
C	-6.166200	-2.097959	0.966672
H	-6.994931	-2.743812	1.265523



C	-5.297230	-0.298366	-0.392460
H	-5.459429	0.478784	-1.143433
C	-4.026402	-0.432064	0.192929
C	-3.853151	-1.427163	1.171265
H	-2.863613	-1.576236	1.613442
C	-2.915404	0.428933	-0.221241
C	-1.965726	1.039275	0.590289
N	-1.131192	1.713617	-0.256168
N	-1.473490	1.577234	-1.555360
C	-2.558446	0.813510	-1.549349
C	-3.229595	0.449105	-2.823814
H	-2.528213	0.536063	-3.662365
H	-4.080885	1.110822	-3.045650
H	-3.622061	-0.576825	-2.794559
C	-1.785338	1.049099	2.060080
H	-0.905712	0.465425	2.378210
H	-2.664339	0.621434	2.557131
H	-1.646539	2.067390	2.452755
C	0.009037	2.495940	0.089445
H	0.124513	3.273509	-0.677527
H	-0.159059	2.997431	1.053275
N	1.262742	1.758353	0.189151
N	2.319142	2.527018	0.517051
C	3.372191	1.721360	0.474295
C	2.993127	0.407302	0.081847
C	1.609537	0.467936	-0.103558
C	0.668693	-0.618029	-0.474313
H	0.172423	-0.437191	-1.439290
H	-0.130191	-0.761877	0.267664
H	1.215190	-1.565696	-0.546226
C	4.729938	2.241703	0.781464

H	5.493948	1.772884	0.146008
H	5.023567	2.052357	1.825619
H	4.763231	3.327553	0.629934
C	3.883570	-0.746781	-0.078349
C	4.891946	-0.990548	0.871111
H	4.970457	-0.335645	1.742436
C	5.772613	-2.058766	0.732053
H	6.545476	-2.224918	1.486627
C	5.664908	-2.919970	-0.359196
H	6.354930	-3.759623	-0.470332
C	4.671026	-2.695560	-1.311520
C	3.795578	-1.620122	-1.177375
H	3.048322	-1.432291	-1.953177
C	-6.353147	-1.121444	-0.011506
H	-7.333457	-0.994385	-0.477257
H	4.585501	-3.356277	-2.177980
H	-4.751307	-3.016796	2.315014

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troisomer200 SCF Done: -1108.98320549 A.U.

C	-4.490990	-2.476286	1.545271
C	-5.810231	-2.387639	1.102517
H	-6.554549	-3.112182	1.440482
C	-5.222138	-0.443125	-0.208364
H	-5.522048	0.365498	-0.879359
C	-3.888571	-0.514667	0.230396
C	-3.541839	-1.555014	1.110988
H	-2.502748	-1.655544	1.436886
C	-2.885625	0.451445	-0.224198
C	-1.864571	1.022334	0.530050
N	-1.167085	1.818227	-0.331807
N	-1.660014	1.799405	-1.587784

C	-2.709341	0.987621	-1.535591
C	-3.508858	0.718833	-2.758814
H	-2.926155	0.967451	-3.653987
H	-4.429304	1.321360	-2.793991
H	-3.814884	-0.334983	-2.818804
C	-1.488623	0.883662	1.955978
H	-0.674738	0.154870	2.104261
H	-2.345902	0.545850	2.551777
H	-1.134048	1.833873	2.380783
C	0.001120	2.587084	-0.033667
H	0.180782	3.226178	-0.910650
H	-0.150577	3.240562	0.837339
N	1.167967	1.776139	0.267970
N	2.146490	2.408741	0.949018
C	3.191366	1.593702	0.908579
C	2.901531	0.427103	0.143861
C	1.581703	0.588987	-0.276645
C	0.727714	-0.317877	-1.083065
H	0.391748	0.142857	-2.023977
H	-0.182793	-0.628954	-0.548057
H	1.286509	-1.228117	-1.329650
C	4.462006	1.962252	1.585129
H	5.337094	1.663015	0.991516
H	4.565476	1.481617	2.570281
H	4.502734	3.045998	1.748729
C	3.806963	-0.690652	-0.143988
C	4.601992	-1.250582	0.871292
H	4.515451	-0.863359	1.889859
C	5.476014	-2.300915	0.604695
H	6.079561	-2.720934	1.413242
C	5.576134	-2.822732	-0.684642

H	6.260375	-3.648244	-0.893598
C	4.799940	-2.276156	-1.705906
C	3.931540	-1.220366	-1.440637
H	3.357020	-0.775062	-2.257296
C	-6.169774	-1.368099	0.221689
H	-7.201518	-1.287496	-0.129353
H	4.880702	-2.666946	-2.723351
H	-4.194481	-3.278379	2.225594

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trosisomer220 SCF Done: -1108.98629967 A.U.

C	-4.080089	-2.848351	1.160405
C	-5.442231	-2.775375	0.871360
H	-6.105496	-3.604052	1.129494
C	-5.105048	-0.579284	-0.082509
H	-5.519678	0.317249	-0.549874
C	-3.729538	-0.634818	0.202299
C	-3.234730	-1.793736	0.826773
H	-2.162764	-1.877232	1.025826
C	-2.833773	0.467366	-0.155568
C	-1.755777	0.951101	0.582351
N	-1.203745	1.940000	-0.177199
N	-1.836913	2.125708	-1.352960
C	-2.837443	1.251962	-1.348122
C	-3.758476	1.163687	-2.510741
H	-3.292879	1.612191	-3.396710
H	-4.703720	1.699873	-2.334884
H	-4.021138	0.121431	-2.740092
C	-1.212560	0.575404	1.909246
H	-0.360924	-0.121027	1.829684
H	-1.984106	0.087532	2.518499
H	-0.840488	1.449144	2.463232

C	-0.027048	2.702367	0.133400
H	0.122467	3.387413	-0.714635
H	-0.146486	3.302487	1.047030
N	1.124168	1.860360	0.365089
N	1.961577	2.202199	1.365810
C	2.968742	1.340902	1.287985
C	2.796355	0.444679	0.192983
C	1.588715	0.820908	-0.392042
C	0.835643	0.241065	-1.530778
H	0.554524	0.996393	-2.279466
H	-0.104702	-0.232029	-1.204089
H	1.432941	-0.531424	-2.027959
C	4.095935	1.408179	2.254084
H	5.055686	1.177327	1.771135
H	3.976411	0.693675	3.082981
H	4.157440	2.409476	2.697539
C	3.709244	-0.620383	-0.236720
C	4.286498	-1.498458	0.697008
H	4.024902	-1.401005	1.753937
C	5.164114	-2.501507	0.293641
H	5.595127	-3.174698	1.038891
C	5.484934	-2.655693	-1.054451
H	6.171134	-3.444537	-1.371045
C	4.926839	-1.789473	-1.994335
C	4.056027	-0.781452	-1.589823
H	3.655454	-0.083386	-2.329816
C	-5.949218	-1.636509	0.246612
H	-7.015869	-1.566903	0.019367
H	5.182438	-1.890997	-3.052000
H	-3.668585	-3.740260	1.639415

trosisomer240 SCF Done: -1108.98629983 A.U.

C	-4.079633	-2.848586	1.160167
C	-5.441828	-2.775638	0.871365
H	-6.105002	-3.604394	1.129481
C	-5.104943	-0.579372	-0.082200
H	-5.519690	0.317219	-0.549351
C	-3.729380	-0.634890	0.202342
C	-3.234390	-1.793870	0.826557
H	-2.162385	-1.877309	1.025428
C	-2.833738	0.467405	-0.155511
C	-1.755733	0.951184	0.582355
N	-1.203800	1.940118	-0.177220
N	-1.837082	2.125857	-1.352914
C	-2.837561	1.252053	-1.348025
C	-3.758734	1.163770	-2.510528
H	-3.293149	1.611962	-3.396662
H	-4.703812	1.700247	-2.334658
H	-4.021696	0.121532	-2.739611
C	-1.212426	0.575471	1.909206
H	-0.360576	-0.120690	1.829564
H	-1.983840	0.087291	2.518382
H	-0.840627	1.449252	2.463313
C	-0.027054	2.702459	0.133276
H	0.122462	3.387425	-0.714823
H	-0.146429	3.302669	1.046855
N	1.124112	1.860418	0.365016
N	1.961556	2.202314	1.365682
C	2.968711	1.341011	1.287864
C	2.796290	0.444740	0.192897
C	1.588643	0.820954	-0.392111
C	0.835512	0.241050	-1.530776

H	0.554279	0.996335	-2.279463
H	-0.104779	-0.232090	-1.203989
H	1.432820	-0.531414	-2.027985
C	4.095934	1.408391	2.253921
H	5.055767	1.178165	1.770832
H	3.976784	0.693509	3.082544
H	4.157006	2.409548	2.697749
C	3.709153	-0.620366	-0.236757
C	4.286414	-1.498366	0.697038
H	4.024856	-1.400800	1.753964
C	5.163985	-2.501484	0.293746
H	5.595000	-3.174612	1.039052
C	5.484742	-2.655829	-1.054342
H	6.170896	-3.444735	-1.370880
C	4.926636	-1.789693	-1.994293
C	4.055870	-0.781600	-1.589858
H	3.655287	-0.083610	-2.329915
C	-5.948997	-1.636699	0.246895
H	-7.015694	-1.567118	0.019858
H	5.182184	-1.891338	-3.051959
H	-3.668002	-3.740547	1.638972

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trosisomer260 SCF Done: -1108.98772935 A.U.

C	-5.099373	2.366201	1.181328
C	-6.317546	1.727191	1.410086
H	-7.171318	2.289571	1.795100
C	-5.346723	-0.352944	0.652857
H	-5.459895	-1.415501	0.424937
C	-4.111236	0.274645	0.413417
C	-4.009892	1.649225	0.694457
H	-3.051186	2.155124	0.552746

C	-2.969547	-0.481146	-0.106582
C	-2.026749	-0.052609	-1.039736
N	-1.166092	-1.098318	-1.203552
N	-1.475332	-2.163616	-0.432580
C	-2.571273	-1.809600	0.228011
C	-3.201497	-2.750516	1.190240
H	-2.476442	-3.507994	1.511887
H	-4.055386	-3.287130	0.748651
H	-3.579869	-2.226104	2.078742
C	-1.900775	1.215924	-1.793865
H	-1.178948	1.907878	-1.333858
H	-2.870989	1.726214	-1.848385
H	-1.542531	1.052104	-2.819685
C	-0.000088	-1.150054	-2.048030
H	0.239837	-2.212899	-2.177818
H	-0.219050	-0.709827	-3.028685
N	1.139972	-0.440386	-1.529567
N	1.414921	0.793882	-2.005007
C	2.494627	1.188555	-1.340035
C	2.940650	0.181408	-0.433549
C	2.030947	-0.862128	-0.585726
C	1.923771	-2.186024	0.072389
H	2.415469	-2.981116	-0.512034
H	0.875196	-2.486521	0.210836
H	2.409656	-2.165969	1.056328
C	3.101273	2.516718	-1.617094
H	4.199247	2.469807	-1.613364
H	2.812402	3.270825	-0.868648
H	2.769793	2.887729	-2.594610
C	4.118165	0.206675	0.437427
C	4.493013	1.372252	1.128732



H	3.877626	2.270480	1.036461
C	5.617255	1.389945	1.950319
H	5.883103	2.307124	2.481868
C	6.395237	0.243337	2.105992
H	7.276373	0.258366	2.751491
C	6.039870	-0.921353	1.426715
C	4.918741	-0.938027	0.601541
H	4.670633	-1.847320	0.048018
C	-6.433725	0.362895	1.146250
H	-7.384228	-0.148561	1.317866
H	6.648022	-1.823301	1.531335
H	-4.992561	3.432668	1.394896

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trosisomer280 SCF Done: -1108.98835069 A.U.

C	5.386562	2.256410	-0.779121
C	6.494940	1.529161	-1.212141
H	7.402070	2.046335	-1.533323
C	5.277116	-0.522108	-0.823657
H	5.248830	-1.614481	-0.822559
C	4.151546	0.193975	-0.379935
C	4.228158	1.598094	-0.373886
H	3.352935	2.179604	-0.071706
C	2.938053	-0.507310	0.048398
C	2.129444	-0.218696	1.145050
N	1.138345	-1.156145	1.128678
N	1.230180	-2.007941	0.084914
C	2.324681	-1.639670	-0.568497
C	2.752813	-2.369692	-1.789888
H	1.902872	-2.905014	-2.230455
H	3.531150	-3.118358	-1.576363
H	3.166632	-1.686082	-2.544095

C	2.238529	0.806850	2.208454
H	1.411639	1.531387	2.162985
H	3.187614	1.348572	2.121905
H	2.209755	0.356083	3.212398
C	-0.016913	-1.225429	1.981622
H	-0.306969	-2.278725	2.071904
H	0.246572	-0.840117	2.974602
N	-1.141300	-0.466925	1.501954
N	-1.165120	0.867427	1.707749
C	-2.233735	1.301256	1.050489
C	-2.917020	0.225727	0.407680
C	-2.161766	-0.905067	0.709369
C	-2.283754	-2.318268	0.279132
H	-2.673808	-2.972845	1.075520
H	-1.309319	-2.719911	-0.036888
H	-2.973162	-2.397679	-0.570322
C	-2.602094	2.740563	1.082802
H	-3.688944	2.878345	1.170507
H	-2.286770	3.270901	0.171039
H	-2.116379	3.238097	1.931066
C	-4.160407	0.279699	-0.363989
C	-4.424216	1.338025	-1.251137
H	-3.674179	2.121082	-1.386625
C	-5.609823	1.386489	-1.979399
H	-5.787240	2.216554	-2.667803
C	-6.562970	0.377495	-1.842743
H	-7.491883	0.415125	-2.416434
C	-6.320416	-0.677768	-0.964327
C	-5.137746	-0.723291	-0.231440
H	-4.974354	-1.537218	0.480126
C	6.432225	0.136426	-1.236202

H	7.295027	-0.444923	-1.570795
H	-7.065336	-1.467538	-0.838807
H	5.419285	3.348667	-0.768756

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trosisomer300 SCF Done: -1108.98563539 A.U.

C	5.508006	-2.267864	0.008754
C	6.586883	-1.679798	0.668479
H	7.512610	-2.240020	0.819322
C	5.292538	0.342408	0.943768
H	5.222936	1.375463	1.293308
C	4.195639	-0.232271	0.277949
C	4.326058	-1.556296	-0.178813
H	3.473771	-2.039604	-0.664022
C	2.956818	0.525047	0.081355
C	2.155343	0.563862	-1.056637
N	1.129342	1.411309	-0.753866
N	1.191016	1.894247	0.506191
C	2.302194	1.382200	1.017978
C	2.708223	1.704397	2.410706
H	1.839843	2.038777	2.991272
H	3.455853	2.511584	2.451264
H	3.152803	0.833653	2.912688
C	2.289798	-0.083167	-2.382074
H	1.504563	-0.838230	-2.539590
H	3.268727	-0.567859	-2.475835
H	2.206673	0.645569	-3.202788
C	-0.040019	1.696282	-1.530544
H	-0.362816	2.721120	-1.318669
H	0.221326	1.623407	-2.595680
N	-1.135019	0.798302	-1.259273
N	-0.955065	-0.520677	-1.477329

C	-2.028572	-1.109418	-0.965161
C	-2.917816	-0.152324	-0.392125
C	-2.284863	1.073634	-0.576911
C	-2.630229	2.433623	-0.099546
H	-2.907645	3.120524	-0.914886
H	-1.789637	2.887822	0.446886
H	-3.482161	2.385507	0.589137
C	-2.201869	-2.582195	-1.059902
H	-3.250358	-2.852976	-1.247803
H	-1.900953	-3.095200	-0.133566
H	-1.584254	-2.988943	-1.869805
C	-4.221562	-0.389139	0.232149
C	-4.430004	-1.473510	1.101715
H	-3.595571	-2.139922	1.333981
C	-5.671856	-1.691189	1.693064
H	-5.805533	-2.536867	2.372178
C	-6.737926	-0.830709	1.431833
H	-7.711107	-1.001418	1.897807
C	-6.551010	0.247148	0.567590
C	-5.311190	0.461648	-0.028134
H	-5.184428	1.289810	-0.730933
C	6.470856	-0.372243	1.138966
H	7.310117	0.099879	1.655764
H	-7.381947	0.921549	0.345779
H	5.582645	-3.296660	-0.352627

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troisomer320 SCF Done: -1108.98217620 A.U.

C	5.452533	-2.354895	-0.404745
C	6.645649	-1.847567	0.109038
H	7.550238	-2.460064	0.110023
C	5.519141	0.229527	0.623960

H	5.558797	1.251328	1.009770
C	4.309330	-0.262840	0.104269
C	4.298997	-1.575141	-0.401619
H	3.360024	-1.995925	-0.771243
C	3.092831	0.553709	0.096329
C	2.150133	0.644255	-0.921617
N	1.194837	1.505649	-0.464248
N	1.437005	1.951383	0.788905
C	2.593144	1.400765	1.132082
C	3.193140	1.676847	2.463098
H	2.427266	2.048728	3.154378
H	3.984840	2.440319	2.413459
H	3.648278	0.774189	2.894471
C	2.095976	0.032600	-2.268600
H	1.328779	-0.754697	-2.319623
H	3.065446	-0.408710	-2.529997
H	1.853796	0.773873	-3.045267
C	-0.056940	1.817694	-1.071665
H	-0.374675	2.809439	-0.730369
H	0.081573	1.855122	-2.164294
N	-1.097782	0.861281	-0.744534
N	-0.797318	-0.448398	-0.696984
C	-1.928165	-1.055935	-0.355496
C	-2.987028	-0.116773	-0.189599
C	-2.400404	1.123318	-0.440150
C	-2.948963	2.497227	-0.350534
H	-3.074997	2.976419	-1.334612
H	-2.304974	3.155127	0.252342
H	-3.934425	2.478767	0.130285
C	-1.973961	-2.535082	-0.220993
H	-2.913607	-2.948445	-0.613717

H	-1.895361	-2.859697	0.827912
H	-1.137127	-2.992110	-0.763019
C	-4.385405	-0.389116	0.151350
C	-4.721748	-1.354139	1.117040
H	-3.923866	-1.883010	1.643840
C	-6.051126	-1.625290	1.429958
H	-6.284493	-2.377546	2.187471
C	-7.080692	-0.935740	0.789929
H	-8.123498	-1.148425	1.036216
C	-6.766411	0.024805	-0.170712
C	-5.437105	0.290576	-0.489386
H	-5.204774	1.018590	-1.271521
C	6.671013	-0.553501	0.627657
H	7.600545	-0.144744	1.031853
H	-7.564593	0.563330	-0.687635
H	5.415986	-3.373085	-0.800261

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troisomer340 SCF Done: -1108.97987042 A.U.

C	5.415060	-2.386741	-0.701136
C	6.647684	-1.909188	-0.256696
H	7.541896	-2.531500	-0.337622
C	5.586399	0.160134	0.402324
H	5.666150	1.168360	0.816039
C	4.335459	-0.303295	-0.042199
C	4.273365	-1.597363	-0.590189
H	3.305866	-1.998750	-0.903180
C	3.136856	0.529308	0.078743
C	2.098475	0.658616	-0.837278
N	1.218402	1.539010	-0.276501
N	1.595147	1.955765	0.953117
C	2.763233	1.370534	1.171559

C	3.494680	1.610762	2.442473
H	2.802109	1.966397	3.214909
H	4.280276	2.374513	2.333890
H	3.986495	0.696808	2.803681
C	1.877104	0.051209	-2.168512
H	1.150765	-0.774805	-2.117289
H	2.815811	-0.345284	-2.574791
H	1.486626	0.780519	-2.893558
C	-0.070525	1.902232	-0.753609
H	-0.339631	2.862830	-0.296319
H	-0.030272	2.042433	-1.847114
N	-1.094256	0.917841	-0.425884
N	-0.753310	-0.343303	-0.113297
C	-1.902327	-0.964561	0.134812
C	-3.011060	-0.087004	-0.037643
C	-2.438736	1.133788	-0.396317
C	-3.040904	2.463274	-0.654715
H	-3.040849	2.733912	-1.723262
H	-2.508923	3.265554	-0.121728
H	-4.083487	2.482231	-0.315163
C	-1.908678	-2.401651	0.513481
H	-2.749940	-2.938655	0.053208
H	-1.995393	-2.543421	1.601764
H	-0.972918	-2.881184	0.201489
C	-4.436594	-0.391369	0.105231
C	-4.904213	-1.222580	1.138441
H	-4.192749	-1.625818	1.863010
C	-6.259404	-1.513862	1.268762
H	-6.596768	-2.158497	2.084202
C	-7.185434	-0.979158	0.373099
H	-8.248828	-1.206289	0.477841

C	-6.739984	-0.155790	-0.660057
C	-5.383991	0.128750	-0.795711
H	-5.044241	0.743854	-1.633423
C	6.726053	-0.632606	0.299090
H	7.686571	-0.246249	0.649114
H	-7.453965	0.258416	-1.376336
H	5.338410	-3.391203	-1.125114

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trosSVP SCF Done: -1108.98192241 A.U.

C	-5.577252	1.915373	-1.095021
C	-6.552617	1.771015	-0.108807
H	-7.494877	2.318986	-0.181632
C	-5.111148	0.227060	1.065630
H	-4.944656	-0.452359	1.904961
C	-4.116408	0.358236	0.080541
C	-4.372967	1.222375	-0.999015
H	-3.600653	1.373404	-1.758538
C	-2.853161	-0.375310	0.192432
C	-2.145032	-1.010679	-0.824937
N	-1.034115	-1.537758	-0.228296
N	-0.972518	-1.284753	1.091737
C	-2.068833	-0.589537	1.366163
C	-2.330105	-0.118567	2.751196
H	-1.396408	-0.102481	3.326111
H	-3.029407	-0.777217	3.288726
H	-2.769008	0.888888	2.761886
C	-2.465062	-1.195078	-2.261192
H	-1.841929	-0.573563	-2.925333
H	-3.509656	-0.919676	-2.451900
H	-2.340880	-2.238674	-2.585240
C	0.040249	-2.276250	-0.848008



H	0.058244	-3.321661	-0.509984
H	-0.133561	-2.264025	-1.935360
N	1.329136	-1.739479	-0.516509
N	2.233884	-2.534310	0.087734
C	3.287169	-1.757808	0.306171
C	3.048359	-0.423582	-0.142236
C	1.760814	-0.455736	-0.671405
C	0.933963	0.588485	-1.319897
H	0.181752	1.013518	-0.635065
H	0.387888	0.194869	-2.190695
H	1.564335	1.414425	-1.673364
C	4.490981	-2.307635	0.982032
H	4.913317	-1.592328	1.701659
H	5.293916	-2.557626	0.271479
H	4.232072	-3.229393	1.517088
C	3.938111	0.734821	-0.043627
C	5.324151	0.606213	-0.244831
H	5.738030	-0.371391	-0.503490
C	6.170701	1.706845	-0.146282
H	7.243544	1.579505	-0.311211
C	5.655651	2.968168	0.151186
H	6.320610	3.831624	0.226020
C	4.284307	3.114622	0.357829
C	3.438366	2.012569	0.267838
H	2.371402	2.133487	0.472987
C	-6.311672	0.925152	0.973216
H	-7.070358	0.800949	1.749814
H	3.869964	4.095148	0.605760
H	-5.749779	2.585171	-1.941196

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trostrANS SCF Done: -1108.98846668 A.U.

C	5.317195	-2.266931	0.915405
C	6.443271	-1.543903	1.308166
H	7.335685	-2.064062	1.663914
C	5.280949	0.511450	0.791917
H	5.281663	1.602217	0.725664
C	4.137493	-0.200594	0.389231
C	4.177352	-1.604112	0.467395
H	3.287481	-2.179574	0.198159
C	2.940288	0.504099	-0.077726
C	2.119185	0.172673	-1.152765
N	1.146262	1.129185	-1.182392
N	1.263216	2.035916	-0.188658
C	2.354270	1.681686	0.478144
C	2.806799	2.468132	1.654903
H	1.969525	3.034463	2.080723
H	3.589689	3.196287	1.392453
H	3.225607	1.818069	2.435623
C	2.202476	-0.908316	-2.162288
H	1.355316	-1.606767	-2.088026
H	3.135609	-1.471165	-2.044286
H	2.190641	-0.507006	-3.187453
C	-0.013064	1.169601	-2.033033
H	-0.295452	2.221430	-2.160912
H	0.240731	0.744511	-3.011761
N	-1.138291	0.432799	-1.522260
N	-1.217698	-0.892610	-1.769037
C	-2.284667	-1.307768	-1.097034
C	-2.913923	-0.227937	-0.408549
C	-2.127936	0.884763	-0.698611
C	-2.200614	2.292915	-0.241279
H	-2.626849	2.963797	-1.005072

H	-1.202676	2.675501	0.019793
H	-2.838604	2.370708	0.647882
C	-2.704838	-2.731700	-1.161291
H	-3.797544	-2.828492	-1.229199
H	-2.389746	-3.298954	-0.271947
H	-2.255003	-3.221126	-2.033762
C	-4.141372	-0.259844	0.389422
C	-4.424228	-1.332385	1.253211
H	-3.699276	-2.144008	1.352367
C	-5.596270	-1.360319	2.004270
H	-5.789060	-2.202519	2.673523
C	-6.516383	-0.316275	1.913846
H	-7.434841	-0.338095	2.504883
C	-6.254108	0.754388	1.059984
C	-5.085040	0.779807	0.304593
H	-4.906739	1.607403	-0.387348
C	6.417618	-0.151139	1.247113
H	7.294837	0.426410	1.549165
H	-6.973324	1.572511	0.971354
H	5.321193	-3.358330	0.970550

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troTSscis SCF Done: -1108.97793840 A.U.

C	5.118913	2.698490	-0.640045
C	6.373193	2.137977	-0.878957
H	7.224467	2.776034	-1.126784
C	5.443864	-0.058261	-0.484872
H	5.586714	-1.137992	-0.402521
C	4.171069	0.487964	-0.238282
C	4.031984	1.885080	-0.329682
H	3.047261	2.336703	-0.184232
C	3.038518	-0.376939	0.098034

C	2.016672	-0.120114	1.009194
N	1.214307	-1.228895	0.990701
N	1.644682	-2.171521	0.129459
C	2.747269	-1.677424	-0.413697
C	3.488157	-2.460297	-1.437302
H	2.824924	-3.208336	-1.887806
H	4.345351	-3.002875	-1.009544
H	3.883462	-1.814375	-2.233854
C	1.801461	1.038593	1.908166
H	1.131349	1.799699	1.477814
H	2.757242	1.538808	2.113330
H	1.374322	0.744369	2.877779
C	-0.000021	-1.486030	1.723240
H	0.000016	-2.548370	1.993194
H	0.000065	-0.881802	2.637907
N	-1.214505	-1.229001	0.990942
N	-1.645339	-2.171917	0.130241
C	-2.747874	-1.677733	-0.412944
C	-3.038616	-0.376903	0.098204
C	-2.016505	-0.119952	1.009026
C	-1.800641	1.039135	1.907341
H	-1.130356	1.799751	1.476388
H	-1.373331	0.745253	2.876983
H	-2.756168	1.539822	2.112531
C	-3.489188	-2.460858	-1.436050
H	-3.884565	-1.815154	-2.232743
H	-4.346383	-3.003102	-1.007868
H	-2.826224	-3.209201	-1.886442
C	-4.170976	0.488183	-0.238296
C	-5.443952	-0.057797	-0.484502
H	-5.587081	-1.137458	-0.401726

C	-6.527918	0.754778	-0.802868
H	-7.506425	0.302884	-0.983430
C	-6.372770	2.138539	-0.879253
H	-7.223915	2.776728	-1.127183
C	-5.118306	2.698810	-0.640733
C	-4.031540	1.885230	-0.330242
H	-3.046682	2.336660	-0.185119
C	6.527994	0.754148	-0.803097
H	7.506360	0.302067	-0.983960
H	-4.980975	3.780883	-0.708761
H	4.981855	3.780623	-0.707658

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Cu	1.668414	-5.772602	-1.915187
C	0.406564	4.201669	2.994302
Cu	-1.066037	3.603136	0.665112
O	3.233135	-4.829771	-2.665125
C	3.277565	-3.565515	-2.678450
O	2.479552	-2.778263	-2.108352
C	4.409530	-2.970188	-3.457842
O	0.166925	4.751857	-0.481352
C	5.059841	-3.734827	-4.434012
H	4.740956	-4.764672	-4.600330
O	0.074843	6.458410	0.985047
C	6.516006	-1.871647	-4.915348
H	7.361402	-1.452703	-5.468099
C	5.894718	-1.092820	-3.923086
C	4.824486	-1.658989	-3.213253
H	4.292477	-1.071989	-2.461617
C	6.369019	0.260897	-3.628174
C	6.701327	1.256613	-4.539593

N	7.168568	2.298462	-3.792620
N	7.127211	2.057430	-2.462945
C	6.644546	0.827094	-2.347698
C	6.476883	0.188952	-1.017649
H	7.059175	0.710764	-0.247411
H	6.780097	-0.867790	-1.041875
H	5.426404	0.206656	-0.686111
C	6.557437	1.324532	-6.012706
H	5.984593	2.216692	-6.307233
H	6.018983	0.443079	-6.381058
H	7.527502	1.358406	-6.533475
C	7.383908	3.652426	-4.230336
H	8.231982	4.073565	-3.676551
H	7.621604	3.648970	-5.300945
N	6.224409	4.472973	-4.013148
N	5.155040	4.284309	-4.819919
C	4.145932	4.890202	-4.208146
C	4.570015	5.478960	-2.979994
C	5.919826	5.169071	-2.878355
C	6.904248	5.428391	-1.801497
H	7.700674	6.121430	-2.115762
H	7.381658	4.493730	-1.470609
H	6.405428	5.877307	-0.933712
C	2.790207	4.925078	-4.814610
H	2.324560	5.914860	-4.709261
H	2.108840	4.204457	-4.337933
H	2.840672	4.672789	-5.880293
C	3.772371	6.242315	-2.016854
C	4.220917	7.481879	-1.530006
H	5.159554	7.893957	-1.911160
C	3.479481	8.193949	-0.589832

H	3.841955	9.159975	-0.230539
C	2.281460	7.677934	-0.107584
H	1.693883	8.214728	0.638246
C	1.817883	6.441840	-0.576632
C	2.555076	5.740982	-1.534055
H	2.184240	4.770160	-1.869409
C	0.580429	5.834473	0.006492
C	6.097522	-3.174671	-5.171992
H	6.602619	-3.765994	-5.939358
O	2.650628	-6.100664	-0.179863
C	3.019211	-5.123247	0.521316
O	2.633623	-3.923637	0.403533
C	4.028823	-5.385889	1.594577
O	0.418940	3.487581	1.951685
C	4.387934	-6.694228	1.936849
H	3.918922	-7.528392	1.412805
O	-0.458608	5.063272	3.301148
C	5.938077	-5.822826	3.579640
H	6.702701	-6.005031	4.338943
C	5.606940	-4.500401	3.235552
C	4.626129	-4.308063	2.251707
H	4.302178	-3.300152	1.988842
C	6.256482	-3.345598	3.858962
C	6.624174	-2.164038	3.218318
N	7.165888	-1.370131	4.185212
N	7.163920	-1.950634	5.406632
C	6.628987	-3.152549	5.220660
C	6.461621	-4.088367	6.362811
H	6.489720	-3.541375	7.312847
H	7.261454	-4.843958	6.399827
H	5.509805	-4.634163	6.300088

C	6.536640	-1.752432	1.799288
H	5.642774	-1.142062	1.594947
H	6.493724	-2.633190	1.145057
H	7.394337	-1.136183	1.496844
C	7.677760	-0.029221	4.041432
H	8.190381	0.200544	4.983994
H	8.402311	0.026506	3.218151
N	6.668227	0.958316	3.755803
N	6.511324	1.398418	2.487084
C	5.462843	2.213242	2.526175
C	4.935759	2.308185	3.851066
C	5.746319	1.474420	4.618321
C	5.717606	1.119277	6.057489
H	6.375140	1.769389	6.657540
H	6.042672	0.083624	6.231332
H	4.702796	1.231356	6.460382
C	5.008927	2.912910	1.292990
H	4.696487	3.946338	1.502561
H	4.142659	2.418514	0.824940
H	5.809668	2.934460	0.542309
C	3.797498	3.104126	4.314100
C	3.794434	3.734797	5.572111
H	4.675244	3.657860	6.214352
C	2.699572	4.484310	5.998260
H	2.723264	4.963611	6.979834
C	1.586796	4.641204	5.176311
H	0.725089	5.232975	5.490665
C	1.569223	4.024293	3.920382
C	2.662908	3.260787	3.505317
H	2.610083	2.777528	2.529628
C	5.329928	-6.902408	2.941307



H	5.609218	-7.921053	3.220503
O	2.162677	-7.526356	-3.239028
O	-0.821841	1.497775	-0.097290
Cu	-1.621198	5.835222	1.781843
C	-0.330304	-4.202303	-3.167040
Cu	1.113770	-3.546070	-0.793965
O	-3.192735	4.925151	2.510774
C	-3.233666	3.662876	2.549758
O	-2.421463	2.865392	2.010723
C	-4.386277	3.082150	3.308823
O	-0.119653	-4.692783	0.344142
C	-5.097173	3.881788	4.212024
H	-4.797505	4.921661	4.347600
O	-0.018819	-6.394402	-1.130292
C	-6.552766	2.017496	4.700465
H	-7.422847	1.612768	5.224552
C	-5.862067	1.200843	3.788129
C	-4.764218	1.752410	3.109850
H	-4.181153	1.138304	2.420258
C	-6.286505	-0.176933	3.530160
C	-6.653986	-1.144143	4.460381
N	-7.024107	-2.234617	3.724664
N	-6.897838	-2.044532	2.391919
C	-6.448677	-0.803755	2.259373
C	-6.206510	-0.215251	0.917533
H	-6.798805	-0.720084	0.143165
H	-6.445715	0.857544	0.906772
H	-5.150381	-0.307584	0.616033
C	-6.664697	-1.115763	5.941551
H	-6.103066	-1.948027	6.395243
H	-6.195709	-0.191766	6.299825

H	-7.687761	-1.139981	6.349994
C	-7.252755	-3.577333	4.186890
H	-8.125536	-3.997604	3.670373
H	-7.451819	-3.552811	5.265390
N	-6.118047	-4.428585	3.941831
N	-5.027305	-4.276131	4.726048
C	-4.035036	-4.888838	4.093207
C	-4.491782	-5.444895	2.864055
C	-5.838728	-5.110303	2.791690
C	-6.843213	-5.343038	1.728043
H	-7.645479	-6.025330	2.050201
H	-7.306565	-4.396369	1.413343
H	-6.364447	-5.793319	0.849967
C	-2.680358	-4.956118	4.698722
H	-2.252457	-5.965280	4.620961
H	-1.975325	-4.276143	4.198629
H	-2.722033	-4.666279	5.756103
C	-3.716087	-6.194723	1.871988
C	-4.183497	-7.414751	1.355427
H	-5.123826	-7.826988	1.732447
C	-3.458066	-8.107676	0.388571
H	-3.835779	-9.057594	0.003136
C	-2.256542	-7.593779	-0.088113
H	-1.681516	-8.112126	-0.856219
C	-1.774868	-6.378011	0.413991
C	-2.497342	-5.693783	1.393992
H	-2.112805	-4.736491	1.751802
C	-0.529490	-5.772815	-0.155504
C	-6.167387	3.338448	4.915641
H	-6.723085	3.956999	5.624289
O	-2.603432	6.180184	0.045659

C	-2.983917	5.194743	-0.636755
O	-2.599996	3.995440	-0.505143
C	-4.006821	5.441401	-1.701023
O	-0.348025	-3.503949	-2.113858
C	-4.391462	6.743815	-2.037811
H	-3.930434	7.585003	-1.517986
O	0.542906	-5.051551	-3.485321
C	-5.948776	5.848190	-3.660395
H	-6.727349	6.018560	-4.408137
C	-5.590960	4.530982	-3.322708
C	-4.594326	4.354193	-2.351998
H	-4.250796	3.351439	-2.093977
C	-6.231154	3.367209	-3.939338
C	-6.572160	2.177839	-3.298040
N	-7.116988	1.379962	-4.259819
N	-7.142606	1.965148	-5.478609
C	-6.622022	3.173820	-5.295933
C	-6.485795	4.115943	-6.437121
H	-6.516747	3.571347	-7.388484
H	-7.299170	4.857465	-6.461648
H	-5.543035	4.678314	-6.384820
C	-6.456869	1.758411	-1.883370
H	-5.565990	1.135839	-1.704430
H	-6.390047	2.634516	-1.225060
H	-7.314320	1.149839	-1.564133
C	-7.612661	0.033345	-4.111944
H	-8.138517	-0.198113	-5.046860
H	-8.323024	-0.032153	-3.277089
N	-6.589729	-0.945807	-3.846188
N	-6.418618	-1.402418	-2.584991
C	-5.369075	-2.214796	-2.646065

C	-4.855352	-2.289972	-3.977460
C	-5.676415	-1.449477	-4.725233
C	-5.666691	-1.081144	-6.161263
H	-6.332533	-1.725893	-6.757999
H	-5.994295	-0.044202	-6.322033
H	-4.657389	-1.190631	-6.578490
C	-4.904528	-2.938351	-1.430485
H	-4.610024	-3.972414	-1.662436
H	-4.023754	-2.465171	-0.968222
H	-5.693643	-2.962105	-0.667653
C	-3.722014	-3.081419	-4.459898
C	-3.733971	-3.708616	-5.719384
H	-4.620677	-3.626407	-6.352952
C	-2.647933	-4.465400	-6.155379
H	-2.685060	-4.947213	-7.135304
C	-1.530201	-4.632322	-5.342292
H	-0.681949	-5.241008	-5.659579
C	-1.495566	-4.014521	-4.087582
C	-2.579976	-3.242939	-3.663240
H	-2.514709	-2.759253	-2.688514
C	-5.350120	6.937220	-3.029283
H	-5.650802	7.951250	-3.302997
O	-1.647976	7.734974	2.992406
O	0.719336	-1.474992	-0.014657
C	2.410961	-7.244833	-4.383801
H	2.654947	-8.036783	-5.131907
H	2.408182	-6.192029	-4.749329
C	1.635387	-0.732531	0.240690
H	1.452031	0.328776	0.525181
H	2.697268	-1.076091	0.202069
C	-1.816237	0.831473	-0.249379

H	-2.837024	1.272352	-0.151303
H	-1.747600	-0.253989	-0.493281
C	-0.594597	8.054965	3.482824
H	-0.513826	8.962525	4.128092
H	0.339371	7.469261	3.319686
H	-4.789520	-3.706852	6.514093
O	-4.645272	-3.428891	7.441493
H	-5.081998	-4.124921	7.942343

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Cu	2.372023	5.307747	2.654869
C	0.146011	-3.892347	-3.519194
Cu	-1.506804	-3.406669	-1.292782
O	3.680721	4.075980	3.438474
C	3.543578	2.830154	3.267790
O	2.728044	2.262039	2.491333
C	4.449090	1.958861	4.077727
O	-0.577815	-4.807204	-0.192625
C	5.057507	2.477245	5.227390
H	4.870278	3.514883	5.505997
O	-0.758256	-6.331158	-1.844768
C	6.127383	0.346179	5.601828
H	6.810817	-0.275554	6.186651
C	5.539968	-0.189563	4.441342
C	4.686114	0.636382	3.693752
H	4.182578	0.249158	2.805688
C	5.823721	-1.564702	4.025972
C	5.870698	-2.694258	4.836250
N	6.250007	-3.718148	4.018733
N	6.420081	-3.335264	2.733115
C	6.163251	-2.033115	2.721170

C	6.275041	-1.238249	1.471482
H	6.868342	-1.765845	0.713859
H	6.735380	-0.258464	1.664315
H	5.289465	-1.039301	1.021790
C	5.533165	-2.890521	6.265789
H	4.815297	-3.715480	6.386925
H	5.072505	-1.982692	6.673624
H	6.416274	-3.116322	6.884553
C	6.222609	-5.125377	4.318393
H	7.058756	-5.612931	3.802424
H	6.342987	-5.260987	5.400132
N	4.991654	-5.744577	3.907622
N	3.876170	-5.476181	4.623761
C	2.868180	-5.885870	3.865108
C	3.340743	-6.427828	2.633078
C	4.722727	-6.301438	2.690252
C	5.775285	-6.614480	1.695706
H	6.444928	-7.421845	2.031499
H	6.394679	-5.730015	1.484614
H	5.318817	-6.940928	0.753281
C	1.462543	-5.779711	4.334064
H	0.884805	-6.682231	4.090712
H	0.937428	-4.933175	3.866626
H	1.431151	-5.625160	5.418961
C	2.555858	-6.978557	1.524448
C	2.869911	-8.225203	0.956500
H	3.687573	-8.812243	1.384198
C	2.147692	-8.723851	-0.125889
H	2.405641	-9.697492	-0.548865
C	1.103815	-7.985073	-0.672524
H	0.541364	-8.349058	-1.532943

C	0.774828	-6.740446	-0.120124
C	1.488314	-6.252633	0.977865
H	1.230016	-5.269191	1.375509
C	-0.278797	-5.894595	-0.758557
C	5.882554	1.659926	5.993058
H	6.357104	2.055729	6.893928
O	3.676631	5.779489	1.194493
C	3.980423	4.863185	0.383997
O	3.402795	3.742813	0.267379
C	5.142158	5.085389	-0.529240
O	0.122766	-3.324385	-2.388760
C	5.766428	6.333971	-0.622798
H	5.400593	7.162015	-0.013642
O	-0.763861	-4.615663	-4.009738
C	7.306478	5.419120	-2.254164
H	8.169317	5.556614	-2.910796
C	6.705161	4.151607	-2.157973
C	5.605249	4.016358	-1.299874
H	5.078665	3.064013	-1.231195
C	7.184070	2.989223	-2.908558
C	7.249616	1.678843	-2.437510
N	7.705066	0.932245	-3.482493
N	7.930700	1.664640	-4.597032
C	7.629253	2.913930	-4.259731
C	7.752451	4.015280	-5.249756
H	7.759305	3.614028	-6.270265
H	8.684599	4.586403	-5.119284
H	6.923974	4.731902	-5.160411
C	6.954160	1.098568	-1.108081
H	5.947500	0.655094	-1.060221
H	7.014099	1.869565	-0.328995

H	7.650482	0.288677	-0.849837
C	7.956564	-0.488185	-3.508149
H	8.488889	-0.681567	-4.448003
H	8.598254	-0.784586	-2.667535
N	6.774015	-1.305886	-3.414910
N	6.467241	-1.894510	-2.236951
C	5.325390	-2.537155	-2.453504
C	4.890537	-2.371265	-3.804223
C	5.859574	-1.561737	-4.394050
C	5.990042	-1.010568	-5.764337
H	6.609473	-1.651917	-6.412549
H	6.453694	-0.013818	-5.763035
H	5.004924	-0.929191	-6.241415
C	4.694176	-3.333169	-1.366510
H	4.278341	-4.277656	-1.745657
H	3.862966	-2.797241	-0.882118
H	5.428108	-3.562489	-0.583804
C	3.711589	-2.958247	-4.444863
C	3.749443	-3.418574	-5.774324
H	4.681627	-3.347041	-6.340220
C	2.631910	-4.001246	-6.368312
H	2.691604	-4.355613	-7.399973
C	1.451799	-4.160836	-5.648047
H	0.575247	-4.637495	-6.088900
C	1.390224	-3.705441	-4.326109
C	2.506616	-3.101346	-3.740589
H	2.419799	-2.737175	-2.716347
C	6.837463	6.493525	-1.499229
H	7.326753	7.466507	-1.585164
Cu	-2.172489	-5.312207	-2.748830
C	0.043577	3.852271	3.386971



Cu	1.717179	3.403943	1.190676
O	-3.474172	-4.066805	-3.524868
C	-3.331673	-2.820263	-3.360699
O	-2.515263	-2.251958	-2.585959
C	-4.234472	-1.948593	-4.173313
O	0.783734	4.812964	0.101883
C	-4.839606	-2.466681	-5.324829
H	-4.652818	-3.504722	-5.602232
O	0.954018	6.331063	1.760307
C	-5.905655	-0.334409	-5.703447
H	-6.586190	0.288272	-6.290659
C	-5.322862	0.200434	-4.540189
C	-4.471677	-0.625908	-3.789989
H	-3.971976	-0.238719	-2.899700
C	-5.612908	1.573827	-4.122694
C	-5.666225	2.704892	-4.930766
N	-6.055729	3.723515	-4.111975
N	-6.225117	3.337402	-2.827726
C	-5.961240	2.036823	-2.818510
C	-6.073923	1.240815	-1.570402
H	-6.680232	1.763198	-0.819305
H	-6.520700	0.255641	-1.767803
H	-5.089474	1.054415	-1.112712
C	-5.325367	2.908085	-6.358556
H	-4.610198	3.736337	-6.474073
H	-4.860978	2.003624	-6.769529
H	-6.207562	3.134559	-6.978395
C	-6.038380	5.132331	-4.405144
H	-6.880544	5.610504	-3.890176
H	-6.154150	5.273758	-5.486551
N	-4.813696	5.756137	-3.985022

N	-3.696282	5.511928	-4.707109
C	-2.691466	5.912563	-3.939607
C	-3.168267	6.423396	-2.695589
C	-4.548956	6.287683	-2.755209
C	-5.602964	6.563839	-1.751056
H	-6.270062	7.386281	-2.054201
H	-6.223936	5.672116	-1.578082
H	-5.148065	6.848715	-0.794316
C	-1.285585	5.830415	-4.412447
H	-0.721669	6.741076	-4.166469
H	-0.745028	4.990840	-3.950269
H	-1.255429	5.681830	-5.498179
C	-2.388390	6.964042	-1.579511
C	-2.725213	8.192599	-0.985654
H	-3.557386	8.770562	-1.397472
C	-2.006555	8.686262	0.101063
H	-2.282090	9.646146	0.543941
C	-0.943787	7.959473	0.626605
H	-0.383256	8.318733	1.490225
C	-0.593747	6.731520	0.050089
C	-1.304087	6.248797	-1.051958
H	-1.028377	5.277864	-1.468206
C	0.475386	5.894727	0.674373
C	-5.660448	-1.648311	-6.094006
H	-6.132145	-2.043708	-6.996540
O	-3.477940	-5.765644	-1.289219
C	-3.783701	-4.845538	-0.483635
O	-3.195943	-3.731641	-0.358085
C	-4.977552	-5.054879	0.391252
O	0.074688	3.285505	2.256422
C	-5.658501	-6.276971	0.401431

H	-5.294991	-7.096486	-0.220246
O	0.951510	4.572131	3.886997
C	-7.260136	-5.348573	1.961848
H	-8.174842	-5.468262	2.546988
C	-6.597734	-4.107591	1.954911
C	-5.434429	-3.996058	1.179885
H	-4.857391	-3.071284	1.182895
C	-7.102565	-2.949890	2.695102
C	-7.034220	-1.615879	2.283280
N	-7.622052	-0.889431	3.269687
N	-8.066784	-1.656800	4.287556
C	-7.766543	-2.909323	3.953353
C	-8.103546	-4.031666	4.866217
H	-8.263219	-3.664676	5.887960
H	-9.024658	-4.551060	4.560560
H	-7.304353	-4.785679	4.889657
C	-6.524073	-0.989805	1.042363
H	-5.490096	-0.624364	1.149521
H	-6.533758	-1.709217	0.213450
H	-7.125577	-0.117030	0.754690
C	-7.820553	0.544387	3.335388
H	-8.312481	0.727126	4.302736
H	-8.475069	0.887652	2.521863
N	-6.607264	1.307303	3.221248
N	-6.380030	2.038459	2.104435
C	-5.230692	2.665237	2.328014
C	-4.715248	2.350734	3.623409
C	-5.636396	1.459031	4.168488
C	-5.652895	0.707515	5.446136
H	-6.506359	0.970519	6.090861
H	-5.721297	-0.376763	5.268979

H	-4.729216	0.886317	6.009059
C	-4.658538	3.579754	1.302603
H	-4.223682	4.480510	1.759961
H	-3.852198	3.105135	0.722049
H	-5.431228	3.887493	0.586748
C	-3.526793	2.907872	4.276696
C	-3.561039	3.313735	5.623978
H	-4.492864	3.217049	6.187361
C	-2.441816	3.871515	6.238042
H	-2.498902	4.184657	7.283039
C	-1.263019	4.057006	5.521586
H	-0.383490	4.512935	5.978462
C	-1.205353	3.654602	4.182873
C	-2.325876	3.080183	3.573863
H	-2.244936	2.761206	2.533686
C	-6.787592	-6.418773	1.204211
H	-7.322981	-7.370750	1.224254
O	-8.653594	-0.082137	6.653369
H	-8.509898	-0.783630	5.984495
H	-9.611987	-0.025576	6.708492

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Cu	5.580479	0.302703	3.416205
C	-5.598892	1.472005	-1.307765
Cu	-3.484191	-0.325122	-1.894850
O	6.302246	1.661862	2.164305
C	5.810159	1.730616	1.002909
O	4.743243	1.180167	0.606092
C	6.579420	2.513228	-0.010144
O	-2.657841	0.862796	-3.281641
C	7.900705	2.889714	0.255698

H	8.342701	2.639909	1.220900
O	-4.693705	1.254353	-4.165302
C	8.045801	3.849433	-1.957669
H	8.647927	4.335942	-2.726742
C	6.710224	3.502710	-2.239774
C	5.990514	2.834561	-1.236166
H	4.944952	2.565250	-1.388064
C	6.105406	3.814421	-3.535455
C	6.394092	4.913837	-4.402859
N	5.658323	4.864314	-5.503135
N	4.906871	3.752650	-5.380139
C	5.125049	3.085513	-4.209793
C	4.423091	1.823834	-3.875295
H	3.451514	1.997635	-3.384382
H	5.022378	1.208762	-3.192220
H	4.225523	1.216979	-4.771030
C	7.335981	6.047098	-4.203802
H	8.375067	5.779702	-4.449982
H	7.332295	6.402274	-3.163779
H	7.053811	6.880973	-4.857536
C	3.939103	3.463093	-6.401206
H	4.294743	3.965983	-7.309337
H	3.893467	2.382287	-6.585008
N	2.604659	3.922879	-6.089870
N	2.405874	5.248820	-5.967841
C	1.100156	5.394561	-5.793935
C	0.434828	4.132875	-5.798262
C	1.448873	3.197169	-5.992776
C	1.379141	1.722499	-6.133477
H	1.683137	1.189393	-5.218690
H	2.006276	1.345468	-6.954344

H	0.348148	1.415124	-6.349481
C	0.516964	6.749008	-5.603777
H	-0.331787	6.731414	-4.906278
H	0.148241	7.179676	-6.547408
H	1.278480	7.435852	-5.215340
C	-1.005258	3.887095	-5.687936
C	-1.912329	4.716022	-6.374300
H	-1.526321	5.529413	-6.992946
C	-3.284746	4.496532	-6.307228
H	-3.966345	5.150929	-6.855328
C	-3.789542	3.437124	-5.560799
H	-4.860774	3.241517	-5.504443
C	-2.908332	2.606439	-4.857874
C	-1.529493	2.837668	-4.916685
H	-0.866569	2.192501	-4.335787
C	-3.456565	1.484029	-4.036335
C	8.625868	3.556856	-0.726540
H	9.664005	3.839993	-0.538295
O	4.596554	1.680240	4.403201
C	3.628841	2.290075	3.861222
O	3.094974	2.007457	2.753460
C	3.074203	3.443139	4.633971
O	-4.360355	1.296412	-1.129192
C	3.718706	3.853040	5.807798
H	4.625606	3.336495	6.122642
O	-6.354431	0.761275	-2.031893
C	2.024714	5.539175	6.131707
H	1.628361	6.375262	6.712243
C	1.356567	5.143951	4.957911
C	1.904085	4.085766	4.215079
H	1.404121	3.724960	3.313552

C	0.122470	5.822864	4.556897
C	-0.259022	6.231946	3.281265
N	-1.469610	6.850100	3.440699
N	-1.890486	6.861194	4.719845
C	-0.940386	6.246915	5.408986
C	-1.084295	6.056694	6.876556
H	-2.143434	6.093832	7.157916
H	-0.570577	6.842434	7.451532
H	-0.666573	5.094467	7.203504
C	0.454891	6.123184	1.986016
H	0.064780	5.317188	1.344942
H	1.515658	5.902560	2.160238
H	0.411887	7.053562	1.400790
C	-2.276645	7.532160	2.457413
H	-2.507293	8.538128	2.828834
H	-1.694233	7.617167	1.532294
N	-3.540235	6.901841	2.183204
N	-4.606786	7.268523	2.920904
C	-5.609210	6.518484	2.489051
C	-5.184581	5.635021	1.448722
C	-3.826971	5.912912	1.285161
C	-2.820321	5.360783	0.347967
H	-2.276782	4.500143	0.770959
H	-2.066749	6.107658	0.060304
H	-3.298245	5.010238	-0.575984
C	-6.948524	6.655270	3.120995
H	-7.438302	5.680468	3.252877
H	-7.632288	7.283321	2.529272
H	-6.845065	7.129229	4.104319
C	-5.998135	4.691462	0.680778
C	-7.358477	4.955292	0.428552

H	-7.804241	5.877222	0.805292
C	-8.139536	4.082887	-0.323473
H	-9.191761	4.316642	-0.500983
C	-7.581907	2.934208	-0.874182
H	-8.170635	2.253760	-1.489965
C	-6.229221	2.653996	-0.646941
C	-5.457324	3.511859	0.142814
H	-4.418994	3.237874	0.332565
C	3.189500	4.903092	6.549640
H	3.690926	5.233566	7.462072
Cu	-5.472713	-0.385260	-3.376658
C	5.535606	-1.807707	1.586034
Cu	3.596465	0.252285	1.919633
O	-5.989223	-1.990043	-2.354165
C	-5.524848	-2.131398	-1.185530
O	-4.553540	-1.496111	-0.688312
C	-6.211208	-3.137851	-0.319057
O	2.682026	-0.669393	3.418242
C	-7.281701	-3.878470	-0.836300
H	-7.574772	-3.731018	-1.876210
O	4.632815	-1.104198	4.461159
C	-7.570906	-4.934522	1.314304
H	-8.099716	-5.650063	1.948719
C	-6.499935	-4.201351	1.857112
C	-5.823967	-3.303884	1.015178
H	-5.011071	-2.687199	1.404468
C	-6.142756	-4.355990	3.269182
C	-4.870011	-4.445277	3.829314
N	-5.070345	-4.548337	5.174262
N	-6.372883	-4.532409	5.520271
C	-7.037015	-4.425478	4.377308



C	-8.521547	-4.348997	4.374855
H	-8.884668	-4.027220	5.358276
H	-8.888894	-3.642046	3.617985
H	-8.990186	-5.321577	4.159025
C	-3.531649	-4.467214	3.193037
H	-2.896060	-5.273161	3.589608
H	-3.630226	-4.625468	2.111840
H	-2.983840	-3.523969	3.345554
C	-4.112487	-4.764377	6.227388
H	-3.785390	-5.815950	6.264007
H	-4.650838	-4.547517	7.161098
N	-2.935466	-3.949619	6.099228
N	-3.064083	-2.615991	5.958366
C	-1.822574	-2.149545	5.899525
C	-0.869484	-3.202785	6.034516
C	-1.633391	-4.359538	6.157249
C	-1.225933	-5.780592	6.274566
H	-1.393934	-6.194180	7.281701
H	-1.765729	-6.429569	5.568303
H	-0.155993	-5.884886	6.056186
C	-1.568415	-0.694209	5.742944
H	-0.719281	-0.364461	6.357472
H	-1.330507	-0.423797	4.703059
H	-2.456832	-0.120730	6.032064
C	0.590305	-3.092331	6.085884
C	1.340385	-3.811864	7.034272
H	0.819632	-4.448519	7.754728
C	2.727140	-3.696644	7.094644
H	3.285810	-4.260938	7.844781
C	3.400807	-2.851447	6.218522
H	4.485143	-2.740494	6.255765

C	2.673962	-2.125831	5.267109
C	1.282938	-2.249791	5.204528
H	0.744471	-1.686160	4.440908
C	3.385280	-1.227781	4.307064
C	-7.953966	-4.776775	-0.014577
H	-8.786395	-5.361435	-0.412769
O	-4.359667	-1.483176	-4.578930
C	-3.358872	-2.082628	-4.092090
O	-2.875496	-1.913528	-2.937278
C	-2.688756	-3.078956	-4.981605
O	4.333399	-1.525917	1.323546
C	-3.156806	-3.270133	-6.287265
H	-4.016619	-2.694713	-6.631780
O	6.331294	-1.112895	2.282701
C	-1.422433	-4.909386	-6.652913
H	-0.944801	-5.643475	-7.306019
C	-0.939026	-4.739883	-5.342407
C	-1.586081	-3.804602	-4.520302
H	-1.222788	-3.610481	-3.509049
C	0.204310	-5.520068	-4.866068
C	0.358917	-6.125837	-3.620939
N	1.572378	-6.754991	-3.667320
N	2.204644	-6.595188	-4.845075
C	1.390848	-5.853959	-5.583427
C	1.781183	-5.460211	-6.962864
H	2.871977	-5.495018	-7.069778
H	1.362106	-6.137269	-7.723050
H	1.434684	-4.447075	-7.209571
C	-0.563845	-6.188404	-2.461384
H	-0.287079	-5.494863	-1.651549
H	-1.579516	-5.916899	-2.775587

H	-0.621202	-7.195613	-2.023441
C	2.190981	-7.597480	-2.671511
H	2.403777	-8.581464	-3.107890
H	1.483691	-7.719129	-1.841380
N	3.445956	-7.098202	-2.182490
N	4.581428	-7.563902	-2.738227
C	5.562063	-6.912460	-2.131546
C	5.051775	-5.991379	-1.163716
C	3.667192	-6.138679	-1.236369
C	2.565605	-5.491641	-0.486353
H	2.134681	-4.634285	-1.029288
H	1.740790	-6.190405	-0.283075
H	2.919641	-5.114878	0.481422
C	6.970521	-7.172561	-2.532547
H	7.567561	-6.250184	-2.543290
H	7.478644	-7.878094	-1.857191
H	6.993219	-7.614562	-3.535780
C	5.817597	-5.131639	-0.259478
C	7.069914	-5.556962	0.224453
H	7.448054	-6.539383	-0.062550
C	7.820986	-4.766682	1.088072
H	8.789121	-5.124548	1.445662
C	7.335204	-3.535970	1.514490
H	7.901462	-2.908426	2.202914
C	6.083270	-3.097897	1.065298
C	5.343016	-3.881926	0.174295
H	4.390481	-3.490458	-0.186983
C	-2.514037	-4.181868	-7.118414
H	-2.873594	-4.336837	-8.138201

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Cu	5.938003	-0.217656	-2.796133
C	-5.373034	2.478321	1.242202
Cu	-3.745043	0.197877	1.622879
O	4.903781	-0.720648	-4.394888
C	3.741846	-1.200102	-4.255508
O	3.079536	-1.252744	-3.181787
C	3.100525	-1.741170	-5.492320
O	-4.694365	-0.907654	0.249721
C	3.790000	-1.684636	-6.709783
H	4.795774	-1.264131	-6.730463
O	-6.717174	-0.339083	1.066365
C	1.893339	-2.689304	-7.813245
H	1.432978	-3.079523	-8.723934
C	1.183127	-2.763042	-6.600875
C	1.807789	-2.273738	-5.443247
H	1.281050	-2.277227	-4.486586
C	-0.167938	-3.327526	-6.575004
C	-1.207042	-3.121926	-7.530297
N	-2.292763	-3.812259	-7.213373
N	-1.982603	-4.465194	-6.077638
C	-0.710550	-4.209498	-5.643203
C	-0.100297	-4.843282	-4.449315
H	-0.451745	-4.405850	-3.501649
H	0.988999	-4.715186	-4.472402
H	-0.295331	-5.924816	-4.401011
C	-1.195452	-2.255524	-8.738514
H	-0.752637	-2.761699	-9.610067
H	-0.615542	-1.336936	-8.573222
H	-2.220571	-1.980823	-9.014264
C	-2.952165	-5.388633	-5.536787
H	-3.252253	-6.093897	-6.321931

H	-2.476020	-5.944958	-4.720206
N	-4.161505	-4.768430	-5.069534
N	-5.195673	-4.661928	-5.926491
C	-6.145422	-4.028308	-5.255325
C	-5.716486	-3.705929	-3.930125
C	-4.414288	-4.200153	-3.853184
C	-3.432358	-4.214177	-2.743468
H	-2.739474	-3.357544	-2.781264
H	-2.817766	-5.125965	-2.747305
H	-3.940447	-4.170708	-1.771749
C	-7.434875	-3.720728	-5.929628
H	-7.813053	-2.726940	-5.652369
H	-8.224344	-4.447182	-5.682572
H	-7.298425	-3.751239	-7.017190
C	-6.488761	-3.052179	-2.872522
C	-7.884437	-3.226312	-2.797657
H	-8.383061	-3.870084	-3.523964
C	-8.638406	-2.622841	-1.796110
H	-9.719419	-2.777093	-1.766173
C	-8.021005	-1.846628	-0.821537
H	-8.591832	-1.381281	-0.017617
C	-6.632359	-1.672761	-0.861893
C	-5.881438	-2.253627	-1.888778
H	-4.807803	-2.061445	-1.911132
C	-5.957357	-0.905614	0.228570
C	3.178174	-2.156840	-7.866062
H	3.710449	-2.117806	-8.819153
O	5.565242	1.688890	-3.162805
C	4.377701	2.118006	-3.091665
O	3.382289	1.486356	-2.639549
C	4.151399	3.511371	-3.583516

O	-4.395583	1.856890	0.737637
C	5.244442	4.280545	-4.001093
H	6.241931	3.841027	-3.976836
O	-6.073004	2.100602	2.225384
C	3.755393	6.124220	-4.454443
H	3.603039	7.142865	-4.818703
C	2.639733	5.367991	-4.049814
C	2.862602	4.055588	-3.604614
H	2.032132	3.444031	-3.245409
C	1.300293	5.958205	-4.099718
C	0.123009	5.371599	-4.558771
N	-0.836161	6.341808	-4.452741
N	-0.360840	7.500124	-3.956955
C	0.929035	7.287706	-3.740668
C	1.780097	8.365390	-3.170489
H	1.160264	9.080768	-2.616815
H	2.308806	8.934951	-3.950217
H	2.545508	7.963140	-2.492572
C	-0.119620	4.020261	-5.119384
H	-0.599296	3.335942	-4.402120
H	0.833041	3.558152	-5.407511
H	-0.751153	4.043347	-6.019537
C	-2.214394	6.303214	-4.881759
H	-2.398916	7.144888	-5.560716
H	-2.378899	5.364158	-5.423786
N	-3.169930	6.429102	-3.815213
N	-3.614197	7.661635	-3.500513
C	-4.435559	7.489208	-2.476064
C	-4.522371	6.110497	-2.107778
C	-3.676321	5.454816	-3.002574
C	-3.347591	4.019542	-3.170507

H	-2.449707	3.722480	-2.604078
H	-3.165653	3.756808	-4.222430
H	-4.171101	3.386593	-2.815816
C	-5.089468	8.673511	-1.858293
H	-5.125443	8.594404	-0.762828
H	-6.124691	8.813247	-2.205902
H	-4.534894	9.581153	-2.124646
C	-5.345587	5.512898	-1.055598
C	-6.579671	6.089083	-0.696171
H	-6.931909	6.975045	-1.226665
C	-7.376671	5.534450	0.300482
H	-8.328234	6.006105	0.556127
C	-6.980246	4.373223	0.955318
H	-7.598536	3.914520	1.727457
C	-5.768935	3.768083	0.600589
C	-4.955958	4.344638	-0.380059
H	-4.000149	3.866998	-0.598702
C	5.039235	5.588212	-4.428000
H	5.887248	6.194745	-4.753887
Cu	-5.936570	0.216654	2.791622
C	5.372140	-2.483521	-1.254486
Cu	3.747362	-0.198834	-1.625526
O	-4.901072	0.728322	4.385854
C	-3.740601	1.211608	4.246567
O	-3.075589	1.259637	3.174373
C	-3.106113	1.763892	5.482027
O	4.694081	0.898664	-0.245979
C	-3.805311	1.722397	6.694576
H	-4.812035	1.304148	6.712095
O	6.715337	0.328925	-1.065634
C	-1.915638	2.736206	7.801188

H	-1.461757	3.136166	8.710801
C	-1.194905	2.794054	6.593934
C	-1.811860	2.293209	5.436909
H	-1.278468	2.284642	4.484034
C	0.156686	3.356755	6.574187
C	0.714580	4.214215	5.628253
N	1.978130	4.485068	6.078467
N	2.268902	3.863131	7.236810
C	1.178939	3.179426	7.553050
C	1.148637	2.347014	8.784607
H	2.169478	2.080132	9.083045
H	0.693379	2.877780	9.634910
H	0.570711	1.424203	8.636719
C	0.123089	4.807948	4.404737
H	0.449719	4.305547	3.480707
H	-0.970587	4.725335	4.439035
H	0.361399	5.876076	4.295864
C	2.959834	5.391354	5.531235
H	2.493931	5.946988	4.708589
H	3.264755	6.098398	6.312567
N	5.191206	4.636229	5.936553
N	4.164177	4.754058	5.072340
C	4.420837	4.185706	3.856722
C	5.717905	3.679262	3.942280
C	6.139746	3.994593	5.271350
C	7.420969	3.673825	5.955110
H	8.220569	4.389999	5.710653
H	7.277772	3.709797	7.041624
H	7.789221	2.674669	5.683775
C	3.447766	4.207560	2.739295
H	3.964278	4.185371	1.771109



H	2.764928	3.342325	2.757035
H	2.821711	5.111223	2.752887
C	6.491288	3.020017	2.888814
C	7.889611	3.176766	2.825746
H	8.390661	3.810788	3.558851
C	8.643845	2.568362	1.827331
H	9.726874	2.709377	1.806437
C	8.024582	1.804318	0.844367
H	8.595864	1.335762	0.042618
C	6.633721	1.647134	0.873543
C	5.882014	2.233139	1.896935
H	4.805967	2.054458	1.909489
C	5.957093	0.891743	-0.224017
C	-3.201845	2.207130	7.850028
H	-3.741742	2.180542	8.799258
O	-5.561088	-1.687625	3.166114
C	-4.372738	-2.114943	3.096971
O	-3.378196	-1.483063	2.643340
C	-4.144612	-3.506381	3.593465
O	4.396266	-1.861868	-0.747021
C	-5.236223	-4.273691	4.018226
H	-6.233687	-3.834022	3.996058
O	6.071727	-2.104122	-2.237233
C	-3.746044	-6.116098	4.472589
H	-3.592490	-7.133455	4.839951
C	-2.631811	-5.361859	4.060411
C	-2.855878	-4.050911	3.611579
H	-2.026508	-3.440903	3.247183
C	-1.292660	-5.953193	4.106462
C	-0.113062	-5.367346	4.560347
N	0.844513	-6.338984	4.452587

N	0.365947	-7.497535	3.960526
C	-0.924389	-7.283793	3.748347
C	-1.778820	-8.361352	3.182969
H	-1.161844	-9.078241	2.628055
H	-2.305220	-8.929196	3.965500
H	-2.546280	-7.959316	2.507262
C	0.133368	-4.015384	5.117749
H	0.615277	-3.334246	4.398964
H	-0.818014	-3.549861	5.404542
H	0.764583	-4.038152	6.018163
C	2.224125	-6.301603	4.877194
H	2.409620	-7.142515	5.556834
H	2.391650	-5.361986	5.417308
N	3.176165	-6.430238	3.807797
N	3.616439	-7.663960	3.492225
C	4.434603	-7.494028	2.464810
C	4.523290	-6.115740	2.095359
C	3.681975	-5.457569	2.992882
C	3.357327	-4.021431	3.161537
H	2.459120	-3.721971	2.596886
H	3.178078	-3.758334	4.213820
H	4.181755	-3.390516	2.805369
C	5.083576	-8.680295	1.845610
H	5.114477	-8.602825	0.749864
H	6.120195	-8.821340	2.188496
H	4.528664	-9.586566	2.115894
C	5.344066	-5.520490	1.039950
C	6.574732	-6.100432	0.674861
H	6.926322	-6.987988	1.203093
C	7.369391	-5.547575	-0.324667
H	8.318258	-6.022240	-0.584720

C	6.974304	-4.384302	-0.976696
H	7.591066	-3.926749	-1.750750
C	5.766368	-3.775626	-0.616555
C	4.955406	-4.350616	0.366667
H	4.001914	-3.870258	0.589224
C	-5.029776	-5.579702	4.449504
H	-5.876668	-6.184611	4.781266

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CO SCF Done: -113.209487992 A.U.

O	0.000000	0.000000	0.485740
C	0.000000	0.000000	-0.647654

3

CO2 SCF Done: -188.435335300 A.U.

O	0.000000	0.000000	1.162407
C	0.000000	0.000000	0.000000
O	0.000000	0.000000	-1.162407

2

N2 SCF Done: -109.427342079 A.U.

N	0.000000	0.000000	0.552185
N	0.000000	0.000000	-0.552185

2

H2 SCF Done: -1.16720776949 A.U.

H	0.000000	0.000000	0.377264
H	0.000000	0.000000	-0.377264

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trosTRANS+CO2 SCF Done: -1297.43342243 A.U.

C	-5.805124	-1.923627	-1.797606
C	-6.691798	-0.847600	-1.806105
H	-7.625920	-0.907453	-2.369429
C	-5.188105	0.377849	-0.365012
H	-4.968479	1.271242	0.225743

C	-4.278166	-0.694186	-0.351226
C	-4.613002	-1.847700	-1.081950
H	-3.915495	-2.688747	-1.103926
C	-3.033175	-0.613595	0.416796
C	-2.190085	0.487564	0.544779
N	-1.205962	0.102021	1.406850
N	-1.346918	-1.170968	1.834907
C	-2.444523	-1.620432	1.238979
C	-2.931170	-2.999713	1.499653
H	-2.517583	-3.377576	2.442704
H	-4.027865	-3.036422	1.556863
H	-2.628972	-3.702562	0.708035
C	-2.205425	1.822858	-0.098109
H	-1.207372	2.084686	-0.479865
H	-2.906921	1.831665	-0.941287
H	-2.514322	2.622080	0.595132
C	-0.053052	0.859317	1.819535
H	0.200498	0.542094	2.838323
H	-0.302677	1.926253	1.831095
N	1.099619	0.693298	0.970459
N	1.250768	1.498114	-0.106705
C	2.320518	1.031913	-0.744791
C	2.878136	-0.087126	-0.060490
C	2.048235	-0.283448	1.040726
C	2.055772	-1.311206	2.108627
H	2.480515	-0.931178	3.052213
H	1.038545	-1.670970	2.321526
H	2.666012	-2.170353	1.803718
C	2.809292	1.679278	-1.989645
H	3.906620	1.662437	-2.044973
H	2.437547	1.165090	-2.889455

H	2.469625	2.719482	-2.048396
C	4.083788	-0.844398	-0.405018
C	4.981588	-1.265989	0.592120
H	4.786692	-0.999276	1.634219
C	6.128979	-1.985873	0.270491
H	6.811809	-2.297979	1.064629
C	6.415797	-2.294741	-1.058822
H	7.317952	-2.856241	-1.312242
C	5.541435	-1.877532	-2.061687
C	4.389864	-1.163962	-1.739652
H	3.699849	-0.866085	-2.532792
C	-6.376702	0.304357	-1.086187
H	-7.069015	1.149887	-1.075782
O	1.314000	4.601090	-0.802073
C	0.755350	4.352364	0.185070
O	0.183795	4.160603	1.180914
H	5.753269	-2.117304	-3.106610
H	-6.039779	-2.829791	-2.361615

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trosTRANS+CO SCF Done: -1222.20347959 A.U.

C	-5.751230	-1.896755	-1.747703
C	-6.647588	-0.829295	-1.782837
H	-7.583940	-0.913977	-2.339255
C	-5.148103	0.450484	-0.385347
H	-4.933573	1.362653	0.177944
C	-4.229316	-0.613241	-0.343598
C	-4.556718	-1.789922	-1.039996
H	-3.852144	-2.625262	-1.040508
C	-2.984154	-0.501562	0.420083
C	-2.151821	0.610894	0.521488
N	-1.165139	0.255077	1.393656

N	-1.293395	-1.008821	1.852011
C	-2.386251	-1.482722	1.266530
C	-2.859610	-2.860070	1.559866
H	-2.444668	-3.210709	2.512787
H	-3.956044	-2.906518	1.615169
H	-2.548139	-3.578803	0.786293
C	-2.180175	1.930604	-0.152606
H	-1.180671	2.206808	-0.520432
H	-2.865622	1.905611	-1.008548
H	-2.520423	2.739567	0.514676
C	-0.017789	1.029360	1.788395
H	0.242906	0.729613	2.810807
H	-0.280656	2.094160	1.786202
N	1.131982	0.866596	0.936508
N	1.266611	1.665761	-0.144363
C	2.355699	1.231746	-0.768853
C	2.941339	0.132927	-0.073512
C	2.108741	-0.081248	1.022952
C	2.135013	-1.100444	2.098735
H	2.554433	-0.707250	3.039393
H	1.124045	-1.475380	2.315638
H	2.759029	-1.951865	1.799718
C	2.832166	1.906936	-2.003548
H	3.929446	1.950193	-2.041018
H	2.501598	1.383773	-2.914123
H	2.438713	2.929772	-2.055186
C	4.167904	-0.594546	-0.407501
C	5.067045	-0.998277	0.595918
H	4.859109	-0.737064	1.636858
C	6.231594	-1.693453	0.281899
H	6.914941	-1.992057	1.080802

C	6.534655	-1.994843	-1.045546
H	7.449981	-2.537581	-1.292603
C	5.659664	-1.593968	-2.054572
C	4.491295	-0.905070	-1.740253
H	3.801177	-0.620741	-2.538322
C	-6.339260	0.345782	-1.098390
H	-7.038615	1.185440	-1.109434
C	0.834800	4.649052	-0.158459
O	0.062136	4.606702	0.672777
H	5.884402	-1.827711	-3.098164
H	-5.980178	-2.820796	-2.284452

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trosTRANS+H2O SCF Done: -1185.35452718 A.U.

C	-5.565164	-1.512956	-2.072056
C	-6.534766	-0.526932	-1.891639
H	-7.448272	-0.535546	-2.490618
C	-5.163765	0.479986	-0.173639
H	-5.029545	1.248132	0.592162
C	-4.169652	-0.498941	-0.350371
C	-4.398151	-1.497947	-1.313475
H	-3.633219	-2.259100	-1.485198
C	-2.934355	-0.486313	0.436747
C	-2.184225	0.624394	0.818178
N	-1.145641	0.129169	1.556006
N	-1.170247	-1.217614	1.667496
C	-2.243531	-1.604746	0.990733
C	-2.609746	-3.043210	0.920879
H	-2.163622	-3.592058	1.759220
H	-3.699240	-3.182991	0.947639
H	-2.249691	-3.518177	-0.004760
C	-2.380545	2.067983	0.548085

H	-1.445725	2.613226	0.357516
H	-3.014024	2.200784	-0.337814
H	-2.890158	2.578563	1.381755
C	-0.016662	0.833769	2.099148
H	0.247255	0.361525	3.053775
H	-0.295845	1.878685	2.281792
N	1.144003	0.838062	1.242696
N	1.256576	1.800509	0.303611
C	2.328854	1.486598	-0.413690
C	2.930618	0.290961	0.076434
C	2.125562	-0.104926	1.144267
C	2.184941	-1.287436	2.035056
H	2.626024	-1.049445	3.016711
H	1.181124	-1.702476	2.205140
H	2.806297	-2.070850	1.583980
C	2.760104	2.370368	-1.527659
H	3.851579	2.497581	-1.544517
H	2.470579	1.963878	-2.508377
H	2.283243	3.354865	-1.435664
C	4.141297	-0.368640	-0.418507
C	5.071546	-0.947565	0.463444
H	4.904547	-0.875349	1.541324
C	6.216611	-1.580013	-0.013141
H	6.925649	-2.018111	0.693633
C	6.468126	-1.641262	-1.383145
H	7.368429	-2.134180	-1.757096
C	5.561672	-1.063221	-2.271601
C	4.413351	-0.437006	-1.796128
H	3.698554	-0.012079	-2.504526
C	-6.328059	0.468689	-0.937421
H	-7.085490	1.240444	-0.779437



H	0.492019	3.501199	-0.010346
O	0.130631	4.375149	-0.260244
H	0.384816	4.933335	0.481271
H	5.746071	-1.107513	-3.347745
H	-5.713596	-2.296215	-2.819528

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trostrANS+H2 SCF Done: -1110.15829259 A.U.

C	-5.632085	1.419683	1.980228
C	-6.546998	0.371116	1.889681
H	-7.466799	0.389599	2.478744
C	-5.107172	-0.721384	0.285212
H	-4.923475	-1.549347	-0.404909
C	-4.168651	0.322693	0.370695
C	-4.458371	1.395540	1.231799
H	-3.737203	2.210557	1.330930
C	-2.937604	0.297364	-0.422317
C	-2.135624	-0.807050	-0.699207
N	-1.143801	-0.347263	-1.516518
N	-1.240901	0.975036	-1.774361
C	-2.318059	1.380933	-1.113869
C	-2.757109	2.798381	-1.191429
H	-2.312363	3.286403	-2.067234
H	-3.850880	2.879664	-1.261574
H	-2.450585	3.377255	-0.306660
C	-2.194734	-2.213620	-0.235603
H	-1.200094	-2.572685	0.067734
H	-2.867979	-2.301958	0.625999
H	-2.570334	-2.899168	-1.013017
C	-0.005716	-1.072225	-2.015745
H	0.263631	-0.634284	-2.984674
H	-0.281160	-2.123608	-2.163404

N	1.141545	-1.042317	-1.145507
N	1.250039	-1.973293	-0.173195
C	2.329293	-1.632346	0.519918
C	2.936327	-0.457911	-0.018147
C	2.126244	-0.099382	-1.094154
C	2.180423	1.047945	-2.030685
H	2.608785	0.771578	-3.008082
H	1.177132	1.461592	-2.209348
H	2.810156	1.845589	-1.617411
C	2.779176	-2.464661	1.665696
H	3.875103	-2.529844	1.711771
H	2.442181	-2.057017	2.631228
H	2.370683	-3.479503	1.584112
C	4.158557	0.208950	0.435542
C	5.086491	0.732405	-0.482829
H	4.904131	0.612704	-1.554033
C	6.247776	1.367044	-0.050557
H	6.954237	1.760902	-0.785439
C	6.518343	1.487002	1.311979
H	7.431298	1.981442	1.651725
C	5.613785	0.966179	2.237021
C	4.449023	0.337887	1.805282
H	3.736128	-0.042216	2.540855
C	-6.277952	-0.699836	1.038256
H	-6.993241	-1.521394	0.949720
H	0.506296	-4.317496	-1.026299
H	0.231396	-4.941682	-1.359348
H	5.812887	1.057245	3.307719
H	-5.830290	2.262306	2.647360

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C	-5.753520	-1.843028	-1.803036
C	-6.646553	-0.772247	-1.799448
H	-7.582270	-0.832847	-2.360045
C	-5.145091	0.449795	-0.353224
H	-4.928472	1.339572	0.244028
C	-4.228987	-0.617166	-0.351052
C	-4.559535	-1.766328	-1.090582
H	-3.857284	-2.603067	-1.122302
C	-2.983140	-0.535322	0.415109
C	-2.152390	0.573493	0.558032
N	-1.164201	0.186483	1.414825
N	-1.289602	-1.094179	1.824346
C	-2.382185	-1.547423	1.222037
C	-2.852445	-2.936030	1.462544
H	-2.429680	-3.324623	2.397111
H	-3.948416	-2.985740	1.524701
H	-2.546965	-3.622407	0.657849
C	-2.181604	1.917959	-0.065291
H	-1.181122	2.208483	-0.419787
H	-2.865505	1.925605	-0.922969
H	-2.524656	2.699384	0.632816
C	-0.016322	0.947405	1.833445
H	0.246165	0.615113	2.845265
H	-0.278322	2.012026	1.864929
N	1.131129	0.812645	0.974150
N	1.260480	1.645230	-0.080939
C	2.349996	1.234385	-0.718967
C	2.942836	0.117713	-0.057619
C	2.112202	-0.132861	1.032741
C	2.144479	-1.183837	2.077446
H	2.558107	-0.816171	3.030923

H	1.136154	-1.573698	2.279760
H	2.776223	-2.020563	1.754213
C	2.821379	1.950768	-1.932637
H	3.917804	2.017508	-1.962423
H	2.506856	1.447247	-2.859806
H	2.407232	2.966619	-1.960822
C	4.173825	-0.590541	-0.415054
C	5.078491	-1.017149	0.573721
H	4.870491	-0.789870	1.622581
C	6.248805	-1.691474	0.236512
H	6.936429	-2.008411	1.024589
C	6.552060	-1.949227	-1.099988
H	7.471744	-2.475861	-1.365126
C	5.671420	-1.525406	-2.094658
C	4.497491	-0.857188	-1.757307
H	3.803436	-0.553595	-2.544857
C	-6.335553	0.375538	-1.071085
H	-7.032669	1.216965	-1.051300
N	0.588317	5.010127	-0.132211
N	0.116649	4.585084	0.771287
H	5.896175	-1.724650	-3.145435
H	-5.984819	-2.745729	-2.373934