

Supporting Information

A DFT Study on the Mechanism and Origins of Ligand-Controlled Regioselectivity of Palladium-Catalyzed Dearomatic Reaction of 1-(Chloromethyl)naphthalene with Phenylacetonitrile

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I. CARTESIAN COORDINATES AND ELECTRONIC ENERGIES FOR ALL OF THE CALCULATED STRUCTURES.....	S2-S22
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Cartesian coordinates and electronic energies for all of the calculated structures

4				H	-7.613900	-1.099500	0.135600
SCF done: -1541.083413				H	-4.590800	-2.911700	2.595000
Pd	0.642900	-0.395100	-1.018800	H	-6.917200	-2.057000	2.327800
C	2.825900	-1.001100	-1.187200	C	-3.433800	-1.703500	-1.735000
C	2.347200	-1.532000	-2.407700	H	-3.809800	-1.472100	-2.730900
C	3.242500	-1.929000	-0.152100	N	-0.912100	-1.777000	-1.365200
C	2.254500	-2.926500	-2.623800				
H	2.131900	-0.844600	-3.226700	TS₄₋₃			
C	3.113100	-3.325600	-0.388200	SCF done: -1541.056322			
C	2.609200	-3.797100	-1.634600	Pd	-0.406049	0.583706	-1.320132
H	1.874400	-3.292700	-3.574800	C	-2.592662	1.826031	0.143920
H	2.520600	-4.873100	-1.781600	C	-2.531851	1.211354	-1.195930
C	3.493400	-4.231300	0.626100	C	-1.753319	3.032051	0.335876
C	3.989500	-3.783600	1.828000	C	-2.308757	2.096830	-2.323652
H	3.382700	-5.299000	0.435700	H	-3.200223	0.361959	-1.350103
C	3.771300	-1.497900	1.081100	C	-1.278138	3.728095	-0.806190
C	4.135000	-2.403700	2.054100	C	-1.616381	3.261353	-2.134174
H	4.277000	-4.494500	2.600600	H	-2.565183	1.758845	-3.325125
H	3.901500	-0.432800	1.266700	H	-1.326546	3.881365	-2.980202
H	4.543700	-2.047300	2.998600	C	-0.482721	4.872538	-0.634680
C	2.605500	0.401600	-0.961900	C	-0.151674	5.326218	0.631308
H	2.932500	0.860900	-0.028000	H	-0.120294	5.395961	-1.517423
H	2.664900	1.074200	-1.822400	C	-1.411746	3.511821	1.605137
P	-0.176600	1.489900	0.121600	C	-0.618113	4.641536	1.756273
C	0.471400	1.500500	1.854500	H	0.472051	6.207817	0.748844
C	0.964800	0.290000	2.352000	H	-1.758097	2.977574	2.486212
C	0.443500	2.615300	2.703600	H	-0.357130	4.990608	2.752069
C	1.436300	0.194900	3.657400	C	-3.359358	1.299652	1.121726
H	0.975900	-0.588500	1.702900	H	-3.406715	1.725709	2.120432
C	0.916600	2.519600	4.007900	H	-3.987844	0.433673	0.926426
H	0.060400	3.570200	2.346400	P	-0.733561	-1.336654	0.020092
C	1.415300	1.311000	4.486400	C	-0.606583	-0.925436	1.844068
H	1.821700	-0.757000	4.019700	C	-0.078383	0.323802	2.181840
H	0.895100	3.396200	4.653400	C	-0.935614	-1.831420	2.859982
H	1.786100	1.241200	5.507700	C	0.106066	0.670370	3.517833
C	0.497200	2.998600	-0.717100	H	0.179747	1.029726	1.392141
C	0.149100	3.193000	-2.061600	C	-0.752098	-1.478900	4.195188
C	1.419500	3.870600	-0.133200	H	-1.335742	-2.812712	2.616032
C	0.669700	4.260000	-2.782300	C	-0.233148	-0.228714	4.525404
H	-0.515300	2.485600	-2.557500	H	0.516293	1.646437	3.765203
C	1.948900	4.933200	-0.861500	H	-1.009979	-2.186460	4.978773
H	1.749400	3.714800	0.892200	H	-0.090847	0.041571	5.568324
C	1.568100	5.138600	-2.182000	C	-2.408052	-2.147563	-0.216759
H	0.382300	4.397500	-3.823400	C	-2.725322	-2.629391	-1.494264
H	2.668000	5.601100	-0.389900	C	-3.380520	-2.181791	0.786112
H	1.981400	5.971100	-2.748600	C	-3.980689	-3.171245	-1.749044
C	-2.055200	1.759600	0.311500	H	-1.998416	-2.554140	-2.300762
C	-2.559800	0.612100	1.183800	C	-4.641851	-2.715746	0.522035
H	-3.659100	0.641500	1.232300	H	-3.162350	-1.775164	1.769765
H	-2.287200	-0.369000	0.773700	C	-4.941413	-3.218469	-0.739685
H	-2.172600	0.679800	2.209600	H	-4.213976	-3.546628	-2.741952
C	-2.385500	3.098600	0.961100	H	-5.392137	-2.733377	1.308049
H	-1.939300	3.945100	0.419400	H	-5.924146	-3.634777	-0.942653
H	-3.477600	3.235600	0.952500	C	0.602109	-2.715334	-0.240210
H	-2.062900	3.139300	2.009100	C	1.883677	-2.210835	0.440122
C	-2.699500	1.693000	-1.072800	H	2.713226	-2.881637	0.172236
H	-2.371500	0.815900	-1.646000	H	2.151778	-1.205214	0.094270
H	-3.789700	1.600000	-0.952000	H	1.776868	-2.197380	1.531695
H	-2.502700	2.604000	-1.654100	C	0.170633	-4.056448	0.360424
C	-2.092400	-1.734500	-1.553700	H	-0.768015	-4.414726	-0.082970
C	-4.371900	-1.847200	-0.644000	H	0.958806	-4.796270	0.152436
C	-5.696800	-1.392900	-0.780900	H	0.055378	-3.989068	1.449710
C	-4.006400	-2.408900	0.595400	C	0.844942	-2.871985	-1.748919
C	-6.597200	-1.468000	0.273200	H	1.082185	-1.906654	-2.213277
H	-6.008000	-0.962100	-1.734200	H	1.702352	-3.546433	-1.891783
C	-4.907500	-2.474900	1.647700	H	-0.024565	-3.315486	-2.252770
H	-2.994200	-2.798400	0.717900	C	2.647970	0.205817	-1.927432
C	-6.210600	-2.000800	1.501400	C	4.829692	-0.341604	-0.926238

C	6.043294	-1.050155	-1.051519
C	4.616928	0.385832	0.265791
C	6.990067	-1.035860	-0.037747
H	6.228177	-1.615624	-1.963336
C	5.568763	0.394004	1.274470
H	3.694319	0.954058	0.381155
C	6.762412	-0.316123	1.135346
H	7.916689	-1.592135	-0.161240
H	5.382617	0.965482	2.181147
H	7.505541	-0.305087	1.927904
C	3.853686	-0.396490	-1.987547
H	4.095958	-0.967380	-2.882603
N	1.585832	0.746018	-1.860730

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SCF done: -1541.067654

Pd	-0.592855	0.598699	-1.361410
C	-2.976927	1.568833	0.062506
C	-2.833187	0.884093	-1.225430
C	-2.148846	2.776951	0.260544
C	-2.314226	1.558423	-2.353786
H	-3.447360	-0.005816	-1.373291
C	-1.361954	3.257600	-0.816178
C	-1.414174	2.602296	-2.114434
H	-2.452280	1.158469	-3.356697
H	-0.862059	3.054152	-2.937129
C	-0.497597	4.341696	-0.617420
C	-0.417353	4.967213	0.615299
H	0.121717	4.674631	-1.450018
C	-2.059920	3.432620	1.490831
C	-1.208582	4.513814	1.671529
H	0.262666	5.804697	0.758702
H	-2.644308	3.073138	2.336464
H	-1.150579	4.998429	2.644879
C	-3.809350	1.061192	0.993966
H	-3.945863	1.510974	1.974324
H	-4.389566	0.164650	0.782757
P	-0.481296	-1.330531	0.020518
C	-0.277768	-0.803943	1.779861
C	0.040492	0.535498	2.023872
C	-0.380335	-1.683375	2.865867
C	0.237661	0.989935	3.324924
H	0.134988	1.233417	1.188337
C	-0.177457	-1.229421	4.163612
H	-0.628279	-2.731333	2.699101
C	0.129824	0.109286	4.394876
H	0.476644	2.038666	3.494171
H	-0.259237	-1.924693	4.997449
H	0.286831	0.463810	5.412326
C	-2.105531	-2.216360	-0.053963
C	-2.508331	-2.731515	-1.295060
C	-2.996172	-2.287945	1.019355
C	-3.754208	-3.324024	-1.449499
H	-1.849388	-2.637254	-2.159197
C	-4.251224	-2.874019	0.860119
H	-2.722747	-1.869310	1.985976
C	-4.632748	-3.395321	-0.369302
H	-4.047302	-3.720854	-2.420117
H	-4.933833	-2.915724	1.707674
H	-5.613879	-3.850966	-0.491603
C	0.866598	-2.649870	-0.291570
C	2.142089	-2.136251	0.372419
H	3.001019	-2.734922	0.033196
H	2.359224	-1.095773	0.101199
H	2.089643	-2.200742	1.466723
C	0.493712	-4.020913	0.259998
H	-0.429011	-4.414548	-0.186802
H	1.306434	-4.728076	0.033366
H	0.371304	-4.011917	1.350999
C	1.081630	-2.742752	-1.802772
H	1.348170	-1.770590	-2.237593

H	1.912332	-3.436804	-2.001249
H	0.198090	-3.133704	-2.326288
C	2.464327	0.636005	-1.872496
C	4.653505	0.003643	-0.937338
C	5.879918	-0.660148	-1.130348
C	4.420859	0.573504	0.331080
C	6.819210	-0.751578	-0.113559
H	6.084887	-1.107548	-2.104254
C	5.361235	0.474499	1.344944
H	3.483884	1.105825	0.508130
C	6.570700	-0.187090	1.135836
H	7.759583	-1.270861	-0.298979
H	5.150492	0.927427	2.313913
H	7.308588	-0.259591	1.933021
C	3.689455	0.074318	-2.010396
H	3.965721	-0.306370	-2.992882
N	1.413185	1.190795	-1.739545

TS₃₋₅

SCF done: -1541.037312

Pd	0.288941	-1.466312	-0.591220
C	-0.392884	-0.464863	2.169830
C	-0.149440	-1.780460	1.569480
C	-1.767801	0.063242	2.085505
C	-1.224108	-2.618825	1.278667
H	0.813122	-2.240852	1.810410
C	-2.831264	-0.811461	1.763955
C	-2.560820	-2.155144	1.274448
H	-1.025733	-3.663076	1.042371
H	-3.347132	-2.897308	1.405186
C	-4.149093	-0.346014	1.864459
C	-4.425590	0.969288	2.195661
H	-4.964117	-1.037953	1.646101
C	-2.064268	1.398147	2.383816
C	-3.372710	1.855272	2.422396
H	-5.456980	1.313656	2.247799
H	-1.248657	2.094417	2.577608
H	-3.575260	2.902126	2.644322
C	0.596487	0.157400	2.841548
H	0.453821	1.105650	3.354964
H	1.593837	-0.279547	2.901279
P	2.026174	0.119778	-0.631134
C	1.564944	1.905114	-0.390326
C	0.225000	2.154243	-0.079043
C	2.436222	2.999375	-0.487432
C	-0.241537	3.451460	0.115404
H	-0.459097	1.312958	0.041458
C	1.970846	4.297520	-0.301538
H	3.494629	2.845805	-0.691957
C	0.630378	4.527981	-0.004605
H	-1.291251	3.605459	0.371590
H	2.663931	5.133625	-0.381770
H	0.270750	5.545125	0.143311
C	3.363740	-0.195802	0.616853
C	3.715954	-1.537209	0.823513
C	3.928655	0.776238	1.446931
C	4.631956	-1.891843	1.806282
H	3.232080	-2.313316	0.228134
C	4.836563	0.419280	2.441047
H	3.641372	1.820888	1.341094
C	5.193920	-0.912247	2.621322
H	4.894206	-2.939155	1.948184
H	5.253713	1.188704	3.089139
H	5.895020	-1.189954	3.406609
C	2.874034	0.027194	-2.344135
C	1.808978	0.441712	-3.359374
H	2.228461	0.381756	-4.375604
H	0.929882	-0.218450	-3.317090
H	1.472029	1.475593	-3.197329
C	4.110972	0.900993	-2.504101
H	4.868786	0.685585	-1.737264

H	4.567090	0.705698	-3.487512
H	3.869617	1.969954	-2.476106
C	3.259846	-1.431659	-2.583036
H	2.392020	-2.102695	-2.498582
H	3.672439	-1.533646	-3.598594
H	4.033684	-1.772426	-1.881171
C	-2.152610	-2.506635	-1.480179
C	-3.716338	-0.653689	-1.158110
C	-5.076978	-0.319042	-1.191736
C	-2.775938	0.371429	-1.342660
C	-5.485922	0.991705	-1.399082
H	-5.820340	-1.106552	-1.055565
C	-3.184857	1.681994	-1.543490
H	-1.709915	0.122926	-1.331933
C	-4.541804	2.000935	-1.568605
H	-6.548868	1.227429	-1.431071
H	-2.428915	2.459154	-1.666189
H	-4.861911	3.029257	-1.728482
C	-3.309447	-2.028989	-0.868169
H	-4.128348	-2.743638	-0.761150
N	-1.058341	-2.807626	-1.801721

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SCF done: -1541.061882

Pd	0.259250	-0.093085	0.919991
C	-0.946340	2.542776	1.490050
C	-0.779734	1.304536	2.251153
C	-1.752082	2.443653	0.253302
C	-1.605173	0.213817	2.036364
H	-0.157127	1.356363	3.145825
C	-2.647410	1.370082	0.059962
C	-2.813617	0.314083	1.137137
H	-1.641948	-0.575958	2.791426
H	-3.661058	0.629839	1.775665
C	-3.398731	1.326733	-1.115489
C	-3.259492	2.293797	-2.102995
H	-4.110465	0.519552	-1.273082
C	-1.611692	3.399776	-0.758389
C	-2.354118	3.333452	-1.927213
H	-3.852001	2.224823	-3.013554
H	-0.880125	4.197223	-0.631476
H	-2.219475	4.087042	-2.701422
C	-0.384329	3.684243	1.924171
H	-0.515503	4.637468	1.417216
H	0.224421	3.692647	2.826705
P	2.285689	-0.426669	-0.293410
C	3.305294	1.114178	-0.092223
C	2.646777	2.330704	-0.321034
C	4.623941	1.149732	0.366298
C	3.301109	3.542087	-0.141030
H	1.594326	2.325715	-0.608332
C	5.275171	2.365969	0.561385
H	5.148808	0.226127	0.602018
C	4.621991	3.564254	0.299336
H	2.766952	4.473726	-0.325208
H	6.301156	2.371105	0.926904
H	5.132341	4.513481	0.455059
C	3.366591	-1.841418	0.219643
C	4.666560	-2.087865	-0.242227
C	2.784377	-2.762163	1.096585
C	5.362250	-3.219174	0.169547
H	5.147251	-1.391958	-0.928174
C	3.477969	-3.897188	1.505123
H	1.772525	-2.571353	1.461141
C	4.769342	-4.126427	1.043428
H	6.372582	-3.393890	-0.197417
H	3.007796	-4.602284	2.188760
H	5.316177	-5.012261	1.362906
C	2.085522	-0.646815	-2.184856
C	0.982286	0.307214	-2.644402
H	0.764602	0.116585	-3.706939

H	0.051127	0.161439	-2.077019
H	1.284307	1.359845	-2.555984
C	3.363700	-0.361926	-2.961731
H	4.185940	-1.026686	-2.667457
H	3.182672	-0.531584	-4.034924
H	3.696486	0.677858	-2.837135
C	1.629554	-2.086208	-2.418955
H	0.735406	-2.334222	-1.829938
H	1.361083	-2.208962	-3.479390
H	2.420212	-2.811882	-2.185127
C	-2.313605	-1.557132	-0.435591
C	-4.676272	-1.304348	0.273377
C	-5.652481	-0.946585	1.206814
C	-5.083186	-1.887728	-0.926976
C	-7.001392	-1.144503	0.938308
H	-5.358955	-0.518596	2.165737
C	-6.434200	-2.085542	-1.196834
H	-4.337172	-2.182404	-1.664589
C	-7.398571	-1.711950	-0.268443
H	-7.745186	-0.856674	1.679395
H	-6.730238	-2.537298	-2.142140
H	-8.454909	-1.867137	-0.480563
C	-3.206341	-1.104936	0.633489
H	-3.005549	-1.775563	1.487525
N	-1.667042	-1.952178	-1.318194

TS4-6

SCF done: -1541.071225

Pd	-0.270861	-0.969051	0.076925
C	0.803083	-1.718241	-1.710654
C	1.160438	-2.950528	-1.064119
C	1.882242	-0.765480	-1.974700
C	2.414651	-3.180602	-0.555988
H	0.394368	-3.725019	-1.005596
C	3.164262	-1.008029	-1.421388
C	3.370406	-2.138290	-0.542275
H	2.636250	-4.121981	-0.055517
H	4.410732	-2.382908	-0.320727
C	4.220697	-0.128588	-1.717001
C	4.026709	0.975322	-2.523934
H	5.202763	-0.324354	-1.285301
C	1.706300	0.367513	-2.788970
C	2.756999	1.226059	-3.054957
H	4.855679	1.648507	-2.735097
H	0.732744	0.558506	-3.238755
H	2.594859	2.091482	-3.696455
C	-0.562852	-1.452218	-1.985075
H	-0.859422	-0.600100	-2.596688
H	-1.260354	-2.292077	-2.022301
P	-2.247680	0.257771	0.576476
C	-2.173557	1.926425	-0.234753
C	-0.953226	2.276052	-0.824692
C	-3.216383	2.862628	-0.261312
C	-0.781084	3.514440	-1.435435
H	-0.127323	1.560640	-0.801841
C	-3.045033	4.100723	-0.871750
H	-4.177558	2.628741	0.192934
C	-1.827814	4.429072	-1.461995
H	0.178098	3.761280	-1.889175
H	-3.868698	4.812860	-0.884738
H	-1.696774	5.399334	-1.938686
C	-3.731701	-0.604476	-0.131667
C	-3.841055	-1.975092	0.142499
C	-4.693601	-0.011525	-0.953118
C	-4.904587	-2.719320	-0.352848
H	-3.063640	-2.467348	0.728839
C	-5.750583	-0.761710	-1.462816
H	-4.614177	1.039394	-1.223372
C	-5.865965	-2.112482	-1.156713
H	-4.973136	-3.781622	-0.123471
H	-6.485983	-0.283016	-2.107849

H	-6.694256	-2.695915	-1.555302
C	-2.696183	0.600316	2.402390
C	-1.616390	1.534697	2.945371
H	-1.795098	1.707218	4.018007
H	-0.615529	1.094704	2.837624
H	-1.629549	2.511868	2.443374
C	-4.079052	1.206937	2.600906
H	-4.865993	0.611283	2.116940
H	-4.305261	1.243850	3.678082
H	-4.137175	2.237383	2.227585
C	-2.617478	-0.739279	3.134524
H	-1.638764	-1.217897	2.995331
H	-2.760339	-0.566310	4.212447
H	-3.407265	-1.430474	2.808727
C	1.915520	-1.077882	1.802069
C	4.159685	-0.155161	1.456128
C	5.536783	-0.343681	1.641201
C	3.701152	1.132620	1.140548
C	6.424397	0.717781	1.520023
H	5.907119	-1.341264	1.884933
C	4.589515	2.193572	1.030001
H	2.634762	1.289481	0.961000
C	5.955496	1.993624	1.214594
H	7.490003	0.549487	1.671290
H	4.211900	3.185028	0.783388
H	6.650941	2.826145	1.122912
C	3.255333	-1.304437	1.489785
H	3.659222	-2.222772	1.920931
N	0.781276	-0.865559	2.069653

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SCF done: -1541.101805

Pd	0.351515	-0.677407	-0.370335
C	0.948199	-0.760889	-2.157170
C	1.488406	-2.116852	-2.187909
C	1.937343	0.326220	-1.991539
C	2.739550	-2.417249	-1.807823
H	0.821433	-2.900514	-2.551646
C	3.253415	0.018605	-1.588900
C	3.634380	-1.386589	-1.202742
H	3.101280	-3.445293	-1.844520
H	4.683210	-1.565758	-1.493468
C	4.211363	1.034037	-1.525619
C	3.886594	2.352806	-1.809754
H	5.233596	0.779523	-1.240599
C	1.625043	1.665850	-2.269946
C	2.578400	2.666472	-2.172111
H	4.647466	3.128896	-1.749738
H	0.614789	1.925272	-2.583311
H	2.304405	3.695927	-2.399996
C	0.395453	-0.543405	-2.513719
H	0.761394	0.437713	-2.816909
H	0.974014	-1.382490	-2.905135
P	2.390315	-0.099655	0.691402
C	2.808001	1.661078	0.259884
C	1.753606	2.516104	-0.075976
C	4.113103	2.164089	0.257013
C	1.994547	3.850070	-0.390652
H	0.736715	2.115461	-0.098282
C	4.354968	3.495566	-0.065516
H	4.949924	1.505596	0.492338
C	3.296464	4.341128	-0.386814
H	1.162186	4.503518	-0.649262
H	5.376254	3.873894	-0.068865
H	3.489014	5.382510	-0.640932
C	3.880149	-0.983663	0.013935
C	4.692065	-1.884522	0.706616
C	4.126396	-0.785640	-1.352688
C	5.724813	-2.558723	0.057079
H	4.529558	-2.079096	1.763979
C	5.159720	-1.450180	-1.998046

H	3.493153	-0.096470	-1.913617
C	5.964445	-2.343328	-1.293534
H	6.344862	-3.255657	0.619192
H	5.335418	-1.273811	-3.058329
H	6.772531	-2.869793	-1.798899
C	2.477881	-0.099460	2.598989
C	1.392347	0.877273	3.058554
H	1.326650	0.847901	4.157175
H	0.406014	0.607704	2.655813
H	1.618753	1.911016	2.764735
C	3.816966	0.348179	3.172029
H	4.654464	-0.292267	2.868470
H	3.767806	0.328583	4.272345
H	4.054426	1.378104	2.873130
C	2.092789	-1.497110	3.086849
H	1.112622	-1.796173	2.691438
H	2.028375	-1.493686	4.186077
H	2.817350	-2.270238	2.802705
C	2.346005	-1.380483	0.942672
C	4.728681	-0.753530	1.056284
C	6.049834	-1.201997	1.029896
C	4.442008	0.488494	1.621530
C	7.073506	-0.417153	1.547312
H	6.276109	-2.175651	0.591269
C	5.465218	1.272224	2.144431
H	3.413474	0.850015	1.639055
C	6.781782	0.824825	2.105057
H	8.100291	-0.777935	1.519764
H	5.230948	2.241399	2.581298
H	7.580892	1.441488	2.512772
C	3.671470	-1.592972	0.379224
H	3.913398	-2.658269	0.527333
N	1.272817	-1.191647	1.353943

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SCF done: -1541.072409

Pd	0.453808	-1.490149	-0.950312
C	-1.637473	-1.317494	1.258769
C	-2.767469	-2.172477	1.045074
C	-1.901493	0.068000	1.621434
C	-4.022863	-1.811846	1.649335
H	-2.545570	-3.236717	0.943555
C	-3.207322	0.449001	2.021563
C	-4.242664	-0.546949	2.079326
H	-4.822092	-2.553052	1.675127
H	-5.215288	-0.254868	2.477520
C	-3.468437	1.787478	2.355709
C	-2.473321	2.745481	2.295286
H	-4.481308	2.061565	2.654308
C	-0.906203	1.056469	1.581374
C	-1.182255	2.372659	1.903534
H	-2.693783	3.781918	2.545615
H	0.093281	0.787043	1.245085
H	-0.388619	3.117806	1.833417
C	-0.333527	-1.817795	1.138211
H	0.465746	-1.310157	1.679285
H	-0.221458	-2.905354	1.095664
P	2.300027	-0.107799	-0.489060
C	1.988497	1.718643	-0.630133
C	0.778392	2.109543	-1.213344
C	2.896227	2.715340	-0.245359
C	0.482856	3.454752	-1.412836
H	0.060085	1.339703	-1.504421
C	2.596279	4.060306	-0.433610
H	3.845380	2.444708	0.214637
C	1.389931	4.432804	-1.020553
H	-0.464761	3.738527	-1.867764
H	3.311062	4.820403	-0.122048
H	1.158304	5.486096	-1.170664
C	2.981179	-0.361196	1.220826
C	3.328874	-1.671778	1.580888

C	3.020326	0.627861	2.208511	H	3.117743	4.671739	1.251228
C	3.762434	-1.968870	2.866837	H	1.236286	5.605733	-0.078099
H	3.219085	-2.476830	0.854118	C	2.662789	-0.676557	1.270413
C	3.439389	0.325797	3.502072	C	2.958293	-2.043429	1.390172
H	2.700208	1.643600	1.982114	C	2.454166	0.055076	2.444098
C	3.825542	-0.967389	3.831979	C	3.089799	-2.642630	2.636253
H	4.032107	-2.992770	3.120824	H	3.039762	-2.655599	0.491960
H	3.456423	1.110992	4.256263	C	2.561700	-0.551764	3.693867
H	4.153383	-1.200892	4.843450	H	2.175405	1.106408	2.393967
C	3.768576	-0.387048	-1.692655	C	2.891809	-1.897242	3.796265
C	3.272661	0.059112	-3.067542	H	3.325261	-3.703883	2.701072
H	4.050169	-0.145497	-3.819310	H	2.379245	0.036912	4.591725
H	2.364622	-0.486121	-3.364920	H	2.978271	-2.368908	4.773705
H	3.051251	1.134294	-3.098214	C	4.071974	-0.043865	-1.307179
C	5.030200	0.377113	-1.313026	C	3.891568	0.707018	-2.625142
H	5.353454	0.150959	-0.286975	H	4.822526	0.649832	-3.210120
H	5.848723	0.087707	-1.990531	H	3.082514	0.266910	-3.226100
H	4.899950	1.461994	-1.409986	H	3.660624	1.768972	-2.465957
C	4.078618	-1.882147	-1.739765	C	5.181707	0.594120	-0.481581
H	3.175950	-2.480912	-1.930056	H	5.253700	0.149399	0.521621
H	4.792478	-2.075177	-2.555230	H	6.149103	0.439542	-0.984880
H	4.544647	-2.235051	-0.810254	H	5.043897	1.677224	-0.374412
C	-2.178305	-2.436030	-1.605577	C	4.439829	-1.494550	-1.613353
C	-3.855588	-0.688723	-1.249637	H	3.622275	-2.018648	-2.129493
C	-5.195894	-0.365858	-1.003496	H	5.326081	-1.511973	-2.266606
C	-2.971799	0.346913	-1.591593	H	4.696042	-2.054982	-0.704264
C	-5.637414	0.950457	-1.079849	C	-1.997413	-2.036165	-2.017170
H	-5.894482	-1.162059	-0.742705	C	-3.550604	-0.240431	-1.405325
C	-3.413256	1.658301	-1.661276	C	-4.879820	0.162844	-1.523443
H	-1.922462	0.110771	-1.785271	C	-2.553368	0.726674	-1.278094
C	-4.747569	1.969582	-1.400857	C	-5.212138	1.512993	-1.490530
H	-6.684242	1.179694	-0.884552	H	-5.662610	-0.589992	-1.627009
H	-2.706503	2.448662	-1.913468	C	-2.886131	2.074525	-1.226528
H	-5.090516	3.001532	-1.452929	H	-1.507165	0.415578	-1.193241
C	-3.380939	-2.057004	-1.024820	C	-4.216048	2.471132	-1.331461
H	-4.142862	-2.832965	-0.933550	H	-6.253909	1.815556	-1.583046
N	-1.053582	-2.627681	-1.910953	H	-2.098498	2.812613	-1.074142
				H	-4.477059	3.527417	-1.290493
				C	-3.226323	-1.717602	-1.306176
				H	-4.047046	-2.295133	-1.760481
				N	-0.954795	-2.248667	-2.496920

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SCF done: -1541.088190

Pd	0.690783	-1.217103	-1.499239
C	-1.929947	-1.654604	0.934980
C	-3.100105	-2.248492	0.194874
C	-2.151081	-0.358911	1.591590
C	-4.396846	-1.992080	0.903179
H	-2.936348	-3.332217	0.091356
C	-3.456989	-0.020395	2.003463
C	-4.544666	-0.951432	1.733572
H	-5.238660	-2.647552	0.675325
H	-5.509426	-0.754367	2.203785
C	-3.684731	1.209119	2.624896
C	-2.646436	2.111764	2.817316
H	-4.697426	1.461156	2.942342
C	-1.116019	0.555779	1.793560
C	-1.359136	1.784173	2.394012
H	-2.840771	3.074187	3.287905
H	-0.119599	0.314989	1.421671
H	-0.543911	2.497367	2.518314
C	-0.743577	-2.283435	0.959835
H	0.106280	-1.894669	1.519260
H	-0.603000	-3.250611	0.476816
P	2.352944	-0.029007	-0.448974
C	2.035862	1.793187	-0.224631
C	0.980087	2.334624	-0.965922
C	2.802751	2.657724	0.568392
C	0.696238	3.696768	-0.919555
H	0.390008	1.666426	-1.598786
C	2.512418	4.017571	0.625252
H	3.632876	2.270331	1.157394
C	1.458689	4.540542	-0.119005
H	-0.118905	4.100493	-1.519658

TS₄₋₈

SCF done: -1541.044489

Pd	-0.245585	-1.290721	-0.074195
C	1.241511	-0.952474	-1.805428
C	1.474289	-2.225827	-1.170697
C	2.287118	0.013722	-1.877762
C	2.755342	-2.485091	-0.435642
H	0.944524	-3.090252	-1.582415
C	3.616185	-0.485204	-1.633509
C	3.826183	-1.760986	-1.109517
H	2.940206	-3.565718	-0.388278
H	4.843889	-2.154859	-1.078523
C	4.699941	0.387350	-1.961404
C	4.483712	1.672837	-2.376169
H	5.716618	0.017547	-1.817455
C	2.100836	1.341965	-2.321836
C	3.168786	2.175981	-2.543424
H	5.334781	2.322378	-2.580706
H	1.088869	1.708188	-2.504164
H	3.011725	3.198657	-2.882370
C	-0.142106	-0.747977	-2.098869
H	-0.507165	0.234996	-2.404970
H	-0.709643	-1.582383	-2.524215
P	-2.145305	0.061145	0.481384
C	-1.705581	1.860031	0.362882
C	-0.372362	2.153944	0.056989
C	-2.588920	2.929650	0.569502
C	0.071287	3.468985	-0.051400
H	0.336405	1.340900	-0.108206

C	-2.145950	4.244244	0.469029
H	-3.635446	2.743555	0.801296
C	-0.816186	4.517735	0.157944
H	1.114354	3.654663	-0.308442
H	-2.848289	5.060169	0.632117
H	-0.476516	5.548978	0.076937
C	-3.517000	-0.225091	-0.731315
C	-3.797570	-1.559732	-1.054647
C	-4.236403	0.785458	-1.373759
C	-4.798004	-1.874481	-1.966233
H	-3.209980	-2.358959	-0.599612
C	-5.228940	0.468893	-2.297567
H	-4.011254	1.831446	-1.174738
C	-5.518377	-0.858973	-2.589480
H	-5.005767	-2.917187	-2.201063
H	-5.774288	1.269640	-2.794645
H	-6.295201	-1.103252	-3.311976
C	-2.920121	-0.199481	2.204324
C	-1.844275	0.170645	3.224262
H	-2.251682	0.047110	4.239286
H	-0.964787	-0.482278	3.138371
H	-1.519261	1.215808	3.119692
C	-4.183942	0.618834	2.441632
H	-4.920464	0.487352	1.635667
H	-4.655332	0.285257	3.378882
H	-3.968924	1.688457	2.555324
C	-3.250719	-1.686992	2.326711
H	-2.376647	-2.320317	2.122344
H	-3.580706	-1.893439	3.356206
H	-4.070322	-1.977749	1.655023
C	1.374606	-2.339368	1.727003
C	3.206130	-0.727035	1.549487
C	4.584879	-0.503046	1.569486
C	2.350418	0.365369	1.699087
C	5.095562	0.782060	1.711690
H	5.263145	-1.350090	1.461306
C	2.858023	1.651394	1.845460
H	1.268159	0.213227	1.693849
C	4.233212	1.865396	1.844564
H	6.173436	0.937144	1.715890
H	2.169353	2.487743	1.963858
H	4.632254	2.872449	1.954211
C	2.710957	-2.110630	1.257170
H	3.391346	-2.854548	1.692140
N	0.227707	-2.493034	1.935745

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SCF done: -1541.096099

Pd	-0.362316	-1.321535	0.319739
C	0.631592	-2.075065	-1.524332
C	0.846333	-3.170656	-0.641331
C	1.772857	-1.241186	-1.869927
C	2.126603	-3.462525	-0.121992
H	0.026471	-3.871080	-0.475890
C	3.033489	-1.522018	-1.276949
C	3.179874	-2.633742	-0.393408
H	2.248699	-4.316611	0.541024
H	4.165495	-2.819499	0.033181
C	4.127277	-0.677497	-1.555767
C	3.993599	0.403041	-2.398078
H	5.080703	-0.882195	-1.070041
C	1.669901	-0.150302	-2.753397
C	2.757337	0.659747	-3.011247
H	4.843382	1.057969	-2.581838
H	0.718070	0.058865	-3.239875
H	2.654006	1.498830	-3.698256
C	-0.728074	-1.693590	-1.748637
H	-0.964434	-0.827570	-2.368213
H	-1.493793	-2.473082	-1.764986
P	-2.039538	0.342819	0.534376
C	-1.523097	1.889142	-0.341804

C	-0.187702	1.976301	-0.746789
C	-2.365942	2.984886	-0.574665
C	0.295169	3.119191	-1.378180
H	0.488937	1.138911	-0.564204
C	-1.882604	4.128672	-1.201049
H	-3.413163	2.944379	-0.278776
C	-0.551273	4.198034	-1.604983
H	1.337707	3.148474	-1.694713
H	-2.551910	4.969271	-1.376818
H	-0.177607	5.094489	-2.097176
C	-3.582956	-0.236285	-0.313386
C	-4.150624	-1.439167	0.130972
C	-4.141162	0.393512	-1.428454
C	-5.274963	-1.966829	-0.491206
H	-3.689597	-1.983519	0.955766
C	-5.260640	-0.144339	-2.059003
H	-3.695074	1.303190	-1.826385
C	-5.837412	-1.317042	-1.587060
H	-5.704734	-2.898362	-0.126279
H	-5.680053	0.359566	-2.928481
H	-6.713921	-1.734233	-2.079841
C	-2.552295	0.910551	2.283480
C	-1.361363	1.680086	2.856058
H	-1.601830	1.989521	3.884699
H	-0.462393	1.050373	2.898328
H	-1.134426	2.587061	2.279067
C	-3.802885	1.781150	2.284966
H	-4.653351	1.288303	1.793169
H	-4.093307	1.984084	3.327409
H	-3.632844	2.753260	1.804938
C	-2.793214	-0.338194	3.131423
H	-1.926425	-1.011552	3.112681
H	-2.957873	-0.028808	4.174902
H	-3.691067	-0.884473	2.812422
C	1.665507	-1.087336	2.254026
C	3.662410	0.193948	1.636875
C	5.065847	0.252203	1.542175
C	2.935994	1.297194	1.143525
C	5.707266	1.347503	0.979282
H	5.651609	-0.588300	1.920234
C	3.581182	2.387422	0.581499
H	1.846475	1.288514	1.217651
C	4.972701	2.424478	0.486928
H	6.795949	1.360784	0.925096
H	2.987372	3.229061	0.221804
H	5.476181	3.284615	0.048496
C	3.015611	-0.980619	2.168853
H	3.622805	-1.822384	2.497741
N	0.469640	-1.134791	2.321286

TS₄₋₉

SCF done: -1541.052522

Pd	-0.459938	-1.257837	0.362348
C	0.432234	-2.627388	-1.208358
C	0.402790	-3.892651	-0.537162
C	1.721567	-1.965011	-1.390549
C	1.526617	-4.432753	0.034916
H	-0.554808	-4.412477	-0.482946
C	2.821911	-2.458387	-0.590018
C	2.715137	-3.675440	0.051992
H	1.484212	-5.396548	0.537168
H	3.578126	-4.044486	0.610408
C	3.993630	-1.610422	-0.415392
C	4.238926	-0.649551	-1.452884
H	4.867926	-2.122587	-0.004755
C	1.945112	-0.893261	-2.240222
C	3.223420	-0.290972	-2.299636
H	5.207098	-0.155841	-1.511314
H	1.158928	-0.550678	-2.912410
H	3.404407	0.472457	-3.057702
C	-0.799314	-2.012866	-1.582883

H	-0.815141	-1.187584	-2.296572	H	4.478544	0.043539	-2.097376
H	-1.701780	-2.629333	-1.596256	H	0.428948	-1.210688	-2.822109
P	-2.058222	0.473785	0.407668	H	2.448887	0.077900	-3.459391
C	-1.519598	1.863254	-0.698080	C	-1.107834	-2.686615	-1.107096
C	-0.245650	1.740213	-1.263638	H	-1.319129	-2.081507	-1.989181
C	-2.246524	3.034890	-0.952347	H	-1.897852	-3.396219	-0.852165
C	0.287043	2.743143	-2.067806	P	-2.183991	0.522665	0.476454
H	0.345272	0.842316	-1.066069	C	-1.366837	1.963411	-0.372470
C	-1.716760	4.037377	-1.758333	C	-0.123691	1.704930	-0.963394
H	-3.235478	3.178316	-0.520112	C	-1.872738	3.268486	-0.443761
C	-0.450327	3.894826	-2.319606	C	0.592766	2.712622	-1.603399
H	1.284525	2.612264	-2.488436	H	0.287428	0.692974	-0.923150
H	-2.298605	4.938164	-1.947503	C	-1.156502	4.277469	-1.080042
H	-0.041548	4.682488	-2.950440	H	-2.839256	3.510966	-0.005237
C	-3.749380	-0.052836	-0.138024	C	0.079828	4.003773	-1.659099
C	-4.200428	-1.278512	0.370652	H	1.558174	2.475740	-2.052607
C	-4.567444	0.641454	-1.032719	H	-1.569383	5.284306	-1.123238
C	-5.453607	-1.773135	0.030239	H	0.636957	4.796379	-2.156602
H	-3.545683	-1.860701	1.021683	C	-3.772152	0.235272	-0.439938
C	-5.816452	0.137177	-1.385785	C	-4.349429	-1.031603	-0.295066
H	-4.225946	1.571599	-1.482245	C	-4.415840	1.178601	-1.245364
C	-6.267461	-1.062868	-0.847900	C	-5.557057	-1.337837	-0.912748
H	-5.789053	-2.724651	0.439790	H	-3.826566	-1.787457	0.293829
H	-6.438064	0.688471	-2.089670	C	-5.616951	0.866934	-1.875935
H	-7.245246	-1.453263	-1.125035	H	-3.971347	2.161170	-1.398830
C	-2.305925	1.279522	2.123065	C	-6.193766	-0.387485	-1.705108
C	-0.971650	1.923113	2.495643	H	-5.994533	-2.327126	-0.786270
H	-1.034011	2.322536	3.519356	H	-6.102543	1.610137	-2.506721
H	-0.146929	1.196044	2.467768	H	-7.133640	-0.628271	-2.199459
H	-0.716930	2.756498	1.826342	C	-2.760367	1.141222	2.194411
C	-3.427405	2.310039	2.160863	C	-1.530341	1.702374	2.903245
H	-4.375740	1.901919	1.782792	H	-1.798356	1.983945	3.933494
H	-3.593814	2.628865	3.201629	H	-0.718070	0.964688	2.954028
H	-3.178175	3.210836	1.586518	H	-1.142587	2.598651	2.399880
C	-2.619533	0.150341	3.103105	C	-3.881855	2.172963	2.177413
H	-1.846202	-0.631032	3.084101	H	-4.736896	1.849168	1.568406
H	-2.662860	0.559655	4.123911	H	-4.246634	2.326235	3.205404
H	-3.593190	-0.314422	2.893708	H	-3.543671	3.151580	1.815708
C	2.349157	-0.843568	1.689471	C	-3.250589	-0.105572	2.932811
C	3.975841	0.858218	1.025213	H	-2.481317	-0.890637	2.959557
C	5.289335	1.332474	1.125485	H	-3.505202	0.161416	3.970196
C	2.994130	1.723326	0.524520	H	-4.154054	-0.525941	2.468194
C	5.609591	2.631886	0.752352	C	2.341418	-0.425708	1.222952
H	6.066005	0.664227	1.502061	C	4.426250	0.753722	0.608048
C	3.313033	3.024526	0.159972	C	5.813858	0.796793	0.735895
H	1.966042	1.367751	0.424746	C	3.736421	1.916068	0.262483
C	4.621975	3.487509	0.270899	C	6.504358	1.985304	0.523101
H	6.637183	2.981606	0.843858	H	6.357373	-0.111180	1.003421
H	2.527296	3.681732	-0.214076	C	4.425448	3.104823	0.051783
H	4.870933	4.508141	-0.015081	H	2.650227	1.889467	0.159040
C	3.679398	-0.549019	1.323378	C	5.810704	3.142499	0.180166
H	4.414141	-1.039258	1.969126	H	7.587630	2.008582	0.629414
N	1.222464	-1.136742	1.825726	H	3.872311	4.004899	-0.214406

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SCF done: -1541.061642

Pd	-0.670675	-1.322707	0.484646
C	0.216857	-3.000953	-0.720688
C	0.453015	-4.115306	0.170549
C	1.385494	-2.258422	-1.220572
C	1.694266	-4.417269	0.629839
H	-0.411979	-4.713180	0.461460
C	2.646422	-2.482152	-0.520702
C	2.789048	-3.553421	0.306973
H	1.853727	-5.265943	1.291527
H	3.758594	-3.730883	0.780109
C	3.727908	-1.428992	-0.606284
C	3.619359	-0.569359	-1.828785
H	4.720150	-1.911824	-0.584242
C	1.343538	-1.351003	-2.247913
C	2.495854	-0.556546	-2.572660

TS₄₋₁₀

SCF done: -1541.043792

Pd	0.175439	0.948530	-0.010238
C	0.174457	2.875731	-1.357299
C	0.656942	4.092551	-0.897365
C	-1.183628	2.447947	-1.032997
C	-0.193864	4.924416	-0.136604
H	1.699115	4.357782	-1.071581
C	-2.026027	3.295018	-0.185637
C	-1.461259	4.549454	0.222900
H	0.183126	5.890562	0.201522
H	-2.083654	5.216416	0.820535
C	-3.308128	2.898876	0.114444

C	-3.825440	1.566857	-0.256283	C	-1.523461	4.581378	0.267913
H	-3.948354	3.562517	0.698310	H	0.089420	5.960737	0.280564
C	-1.876503	1.401670	-1.771263	H	-2.169044	5.228893	0.862320
C	-3.128729	1.016053	-1.448080	C	-3.327428	2.884681	0.122554
H	-4.916593	1.572015	-0.418664	C	-3.803052	1.542995	-0.265736
H	-1.387562	0.959482	-2.639944	H	-3.991488	3.525501	0.705238
H	-3.635248	0.250561	-2.035973	C	-1.833147	1.443030	-1.758367
C	1.017602	1.765562	-1.759707	C	-3.078650	1.021609	-1.453794
H	0.702131	1.113576	-2.579803	H	-4.892050	1.517603	-0.439119
H	2.098266	1.930085	-1.738897	H	-1.321291	1.022014	-2.624285
P	1.844170	-0.697251	0.397949	H	-3.558023	0.248872	-2.054903
C	1.535130	-2.200337	-0.644725	C	1.047318	1.870403	-1.699047
C	0.378241	-2.178618	-1.432477	H	0.760638	1.220018	-2.530831
C	2.316067	-3.364083	-0.644791	H	2.124254	2.053778	-1.655076
C	0.010030	-3.281968	-2.196684	P	1.817567	-0.672202	0.412401
H	-0.243890	-1.279982	-1.438738	C	1.392714	-2.195909	-0.557690
C	1.950368	-4.465724	-1.410516	C	0.208625	-2.158640	-1.302970
H	3.219261	-3.423869	-0.040414	C	2.128593	-3.388695	-0.538186
C	0.795784	-4.428508	-2.187164	C	-0.231391	-3.277720	-2.005275
H	-0.897075	-3.241629	-2.797942	H	-0.382318	-1.239207	-1.326790
H	2.570782	-5.360404	-1.396063	C	1.691198	-4.505734	-1.241448
H	0.510440	-5.294331	-2.782457	H	3.054646	-3.455099	0.030723
C	3.537454	-0.072849	-0.011883	C	0.508997	-4.453882	-1.975111
C	3.825404	1.244588	0.368854	H	-1.158328	-3.223796	-2.575177
C	4.524773	-0.817143	-0.661027	H	2.277299	-5.422904	-1.213120
C	5.083426	1.789713	0.139134	H	0.168532	-5.330854	-2.523216
H	3.043408	1.858420	0.821514	C	3.514074	-0.153968	-0.115002
C	5.779822	-0.265435	-0.901239	C	3.937611	1.118064	0.292457
H	4.315076	-1.829181	-1.002280	C	4.372159	-0.934006	-0.892446
C	6.065532	1.033288	-0.494053	C	5.205939	1.580082	-0.038649
H	5.290665	2.814633	0.442113	H	3.254036	1.762759	0.848528
H	6.537350	-0.855949	-1.414210	C	5.636325	-0.462644	-1.236405
H	7.048694	1.461555	-0.681805	H	4.050475	-1.909361	-1.253430
C	1.996567	-1.325596	2.198671	C	6.059523	0.788402	-0.802520
C	0.789531	-2.219959	2.475250	H	5.522184	2.569276	0.288051
H	0.782548	-2.498206	3.540236	H	6.290897	-1.079282	-1.850471
H	-0.156691	-1.704385	2.261484	H	7.048954	1.154247	-1.071533
H	0.821296	-3.146719	1.886758	C	2.034553	-1.246584	2.227331
C	3.291444	-2.078099	2.484142	C	0.842918	-2.136414	2.576178
H	4.180712	-1.477132	2.251850	H	0.866228	-2.361977	3.653232
H	3.328171	-2.325594	3.556425	H	-0.113109	-1.638949	2.363347
H	3.359430	-3.026823	1.937699	H	0.867624	-3.090351	2.033471
C	1.939154	-0.084782	3.091056	C	3.342626	-1.985234	2.487504
H	1.013776	0.484755	2.939878	H	4.221068	-1.382640	2.221725
H	1.979296	-0.398879	4.145305	H	3.410990	-2.216731	3.561836
H	2.795768	0.581131	2.915267	H	3.403180	-2.940937	1.952770
C	-2.382601	0.492242	1.487239	C	1.997601	0.016157	3.090307
C	-4.247249	-0.866579	0.662362	H	1.063147	0.574894	2.955048
C	-5.625175	-1.092300	0.637727	H	2.073650	-0.272801	4.149867
C	-3.386850	-1.889398	0.253820	H	2.842752	0.684427	2.874460
C	-6.135332	-2.316623	0.221730	C	-2.357083	0.504609	1.502588
H	-6.302357	-0.296562	0.952738	C	-4.141655	-0.917604	0.618034
C	-3.897606	-3.115966	-0.155968	C	-5.506835	-1.200906	0.539571
H	-2.307027	-1.725792	0.266249	C	-3.225208	-1.897528	0.225866
C	-5.272150	-3.333823	-0.174792	C	-5.948503	-2.438059	0.084957
H	-7.212059	-2.478461	0.213048	H	-6.228696	-0.440359	0.842080
H	-3.214313	-3.908295	-0.458860	C	-3.666996	-3.136515	-0.223330
H	-5.670089	-4.294815	-0.496217	H	-2.154008	-1.691649	0.280539
C	-3.744176	0.501673	1.022388	C	-5.029453	-3.411221	-0.297656
H	-4.379255	0.971022	1.786197	H	-7.016364	-2.644928	0.034580
N	-1.242277	0.483110	1.734778	H	-2.935401	-3.890490	-0.513352
10				H	-5.375576	-4.381624	-0.649427
SCF done: -1541.043884				C	-3.706884	0.465768	1.007035
Pd	0.191960	1.019582	0.027405	H	-4.379428	0.901903	1.758025
C	0.175101	2.959626	-1.300813	N	-1.222108	0.529094	1.773978
C	0.621998	4.183398	-0.823895	TS₄₋₁₁			
C	-1.178256	2.500139	-1.002021	SCF done: -1541.051148			
C	-0.259960	4.988830	-0.070385	Pd	0.080877	-1.202922	0.175024
H	1.659388	4.475886	-0.981002	C	1.010887	-2.679955	-1.241857
C	-2.052100	3.317381	-0.158072	C	0.751099	-4.004932	-0.761400

C	2.333609	-2.091059	-0.999225	SCF done: -1541.065781		
C	1.706457	-4.759333	-0.138214	Pd	0.015370	-1.152802
H	-0.248053	-4.408375	-0.933884	C	1.606567	-2.041387
C	3.309625	-2.931615	-0.318807	C	1.228051	-3.443009
C	2.992347	-4.215965	0.064050	C	2.839947	-1.622639
H	1.481004	-5.767993	0.201281	C	1.914656	-4.336317
H	3.759446	-4.814547	0.557285	H	0.351555	-3.749805
C	4.619885	-2.394382	-0.080676	C	3.518891	-2.633762
C	4.904514	-1.100805	-0.340565	C	3.070422	-3.917608
H	5.378502	-3.066263	0.322867	H	1.596818	-5.375863
C	2.689881	-0.792852	-1.336081	H	3.612982	-4.648551
C	3.865757	-0.193473	-0.800612	C	4.712606	-2.229409
H	5.898983	-0.700414	-0.141655	C	5.143994	-0.960982
H	1.980646	-0.148322	-1.857072	H	5.264729	-3.009072
H	4.203229	0.730855	-1.276000	C	3.331372	-0.361859
C	-0.060324	-1.953945	-1.828926	C	4.375800	0.141215
H	0.150508	-1.123182	-2.504533	H	6.041783	-0.689136
H	-0.976256	-2.498046	-2.066609	H	2.853112	0.387389
P	-1.796590	0.210945	0.477476	H	5.059536	0.838198
C	-1.793162	1.795841	-0.495744	C	0.819535	-1.170048
C	-1.271532	1.690700	-1.791488	H	1.145072	-0.157823
C	-2.277359	3.038515	-0.075012	H	0.056299	-1.583677
C	-1.247334	2.785260	-2.646465	P	-1.865219	0.017869
H	-0.875999	0.730768	-2.125915	C	-2.161419	1.623588
C	-2.248676	4.138949	-0.930104	C	-1.850009	1.604612
H	-2.684662	3.167733	0.924827	C	-2.665025	2.806725
C	-1.738270	4.015429	-2.217262	C	-2.048232	2.726795
H	-0.835882	2.678405	-3.648670	H	-1.439783	0.688992
H	-2.630480	5.097301	-0.581344	C	-2.846463	3.938088
H	-1.716617	4.876856	-2.882595	H	-2.918341	2.864217
C	-3.321395	-0.622976	-0.177054	C	-2.542447	3.901496
C	-3.376202	-2.019762	-0.130177	H	-1.803965	2.687426
C	-4.415924	0.080214	-0.688478	H	-3.232262	4.851964
C	-4.508856	-2.699571	-0.566287	H	-2.688164	4.786123
H	-2.506967	-2.572556	0.235136	C	-3.431590	-0.907821
C	-5.543778	-0.600764	-1.135529	C	-3.381778	-2.305238
H	-4.387403	1.168810	-0.744858	C	-4.646637	-0.274380
C	-5.594435	-1.990177	-1.070973	C	-4.527809	-3.055555
H	-4.538944	-3.787098	-0.521057	C	-2.425983	-2.801795
H	-6.387341	-0.041790	-1.537802	C	-5.789403	-1.024883
H	-6.478273	-2.520776	-1.421616	H	-4.700658	0.814478
C	-2.244528	0.577246	2.295490	C	-5.733298	-2.415654
C	-1.211808	1.550678	2.864116	H	-4.474535	-4.143101
H	-1.408153	1.694555	3.937821	H	-6.729191	-0.519977
H	-0.192297	1.155016	2.763019	H	-6.628792	-3.000803
H	-1.243456	2.538613	2.386617	C	-1.987833	0.317897
C	-3.668029	1.088265	2.498085	C	-0.984667	1.398117
H	-4.412770	0.366629	2.137688	H	-1.015154	1.521815
H	-3.842644	1.237639	3.574898	H	0.041669	1.110565
H	-3.866931	2.045792	2.001598	H	-1.193687	2.376379
C	-2.107476	-0.765042	3.019405	C	-3.392634	0.656057
H	-1.090339	-1.170465	2.935899	H	-4.105968	-0.146842
H	-2.329223	-0.620040	4.087972	H	-3.367096	0.779050
H	-2.816894	-1.511150	2.633391	H	-3.796198	1.585710
C	2.404920	0.107195	1.546403	C	-1.556339	-1.006949
C	3.126257	2.214514	0.542638	H	-0.516835	-1.258182
C	4.159266	3.151819	0.408400	H	-1.620890	-0.918218
C	1.824041	2.604452	0.198760	H	-2.209564	-1.838554
C	3.897532	4.442702	-0.033022	C	2.767343	0.226842
H	5.178911	2.857330	0.663608	C	3.041263	2.280430
C	1.564315	3.896498	-0.239434	C	3.805957	3.437668
H	1.007586	1.883548	0.277693	C	1.708984	2.284676
C	2.597571	4.823585	-0.355294	C	3.251348	4.585958
H	4.713928	5.158487	-0.121649	H	4.847151	3.437451
H	0.541930	4.177235	-0.493841	C	1.151343	3.436034
H	2.391228	5.836887	-0.696028	H	1.100338	1.378994
C	3.442347	0.829844	0.926948	C	1.920474	4.587459
H	4.422163	0.691715	1.389270	H	3.857979	5.484072
N	1.451811	-0.466215	1.931051	H	0.107688	3.430174
				H	1.480943	5.488245
				C	3.701337	1.041554
						1.046674

H	4.509215	1.352057	1.730018
N	2.003661	-0.426762	2.405006

TS₄₋₁₂

SCF done: -1541.029899

Pd	0.340271	-1.079538	-0.600886
C	-0.890327	-2.377625	0.883900
C	-0.501717	-3.679306	0.463752
C	-2.254491	-1.977380	0.732314
C	-1.430551	-4.569348	-0.060876
H	0.537370	-3.979282	0.604576
C	-3.228755	-2.962352	0.364456
C	-2.771467	-4.219513	-0.080868
H	-1.115243	-5.553418	-0.402205
H	-3.513093	-4.942196	-0.425681
C	-4.605524	-2.680590	0.539038
C	-4.945222	-1.564724	1.309641
H	-5.341682	-3.438336	0.274244
C	-2.760489	-0.604336	0.844870
C	-4.012569	-0.581094	1.585870
H	-5.955602	-1.480488	1.713480
H	-2.023102	0.142975	1.164327
H	-4.250662	0.266313	2.224983
C	0.172925	-1.543742	1.404911
H	-0.079314	-0.645281	1.974156
H	1.058770	-2.059752	1.786243
P	2.087026	0.439644	-0.309203
C	1.645766	1.653551	1.016727
C	0.381720	2.250624	0.912351
C	2.420774	1.923117	2.147059
C	-0.080010	3.125720	1.886468
H	-0.270283	2.002334	0.075193
C	1.953636	2.794483	3.128855
H	3.384209	1.437448	2.287144
C	0.710929	3.404021	2.998495
H	-1.068177	3.571549	1.774738
H	2.567921	2.990665	4.006247
H	0.350717	4.081588	3.770706
C	3.673768	-0.370911	0.193673
C	3.724334	-1.766477	0.115180
C	4.828739	0.320589	0.583900
C	4.892568	-2.456660	0.423142
H	2.828476	-2.309427	-0.195720
C	5.993932	-0.369873	0.899307
H	4.823908	1.407107	0.646868
C	6.028368	-1.758936	0.818759
H	4.913232	-3.542818	0.353937
H	6.880795	0.182642	1.205196
H	6.942356	-2.297004	1.064505
C	2.528363	1.445024	-1.874078
C	1.269115	2.160821	-2.357672
H	1.485950	2.646743	-3.320962
H	0.436796	1.460650	-2.518702
H	0.948570	2.947075	-1.659438
C	3.638043	2.463886	-1.646005
H	4.604170	1.985195	-1.443462
H	3.761003	3.069436	-2.556996
H	3.404066	3.152898	-0.821608
C	2.954601	0.414109	-2.918638
H	2.155231	-0.315711	-3.113684
H	3.178842	0.926126	-3.866478
H	3.856361	-0.134061	-2.612108
C	-2.091247	-0.328708	-1.737858
C	-3.478518	1.438212	-0.770155
C	-4.703540	1.856281	-0.233282
C	-2.540697	2.421551	-1.114758
C	-4.957027	3.206589	-0.011074
H	-5.459270	1.110129	0.006593
C	-2.793992	3.768610	-0.892022
H	-1.605988	2.121999	-1.591578
C	-4.003395	4.169452	-0.326833

H	-5.916345	3.509370	0.407091
H	-2.043273	4.508704	-1.170869
H	-4.208018	5.224738	-0.153524
C	-3.159824	-0.006728	-0.859135
H	-4.025862	-0.656118	-1.047401
N	-1.121430	-0.616820	-2.339641

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SCF done: -1541.030485

Pd	0.395654	-1.155028	-0.599833
C	-0.893285	-2.397695	0.875542
C	-0.502333	-3.689463	0.413503
C	-2.244530	-1.979932	0.701587
C	-1.428985	-4.542998	-0.171825
H	0.527602	-4.008966	0.576561
C	-3.228154	-2.941912	0.289661
C	-2.767783	-4.179332	-0.205099
H	-1.116571	-5.514763	-0.549480
H	-3.505749	-4.881599	-0.597518
C	-4.599868	-2.652323	0.472647
C	-4.911137	-1.585325	1.335590
H	-5.345954	-3.390830	0.182750
C	-2.746841	-0.585720	0.806203
C	-3.973580	-0.624596	1.639438
H	-5.898305	-1.546145	1.800571
H	-1.996226	0.122257	1.186055
H	-4.147093	0.140101	2.393588
C	0.171316	-1.585872	1.417060
H	-0.069350	-0.676873	1.974118
H	1.048249	-2.112869	1.803074
P	2.088612	0.436458	-0.320896
C	1.577564	1.644087	0.986437
C	0.299427	2.202619	0.846949
C	2.307232	1.929647	2.142730
C	-0.222723	3.052237	1.812876
H	-0.316666	1.943478	-0.013738
C	1.781497	2.777989	3.115127
H	3.281073	1.473803	2.309440
C	0.523604	3.346768	2.951641
H	-1.222081	3.465044	1.673884
H	2.362007	2.987416	4.012324
H	0.117549	4.005092	3.717669
C	3.692750	-0.309213	0.226458
C	3.793027	-1.703320	0.170105
C	4.812632	0.427187	0.636145
C	4.976795	-2.348100	0.514752
H	2.922533	-2.281211	-0.150216
C	5.993476	-0.217747	0.987282
H	4.765959	1.513286	0.689636
C	6.078324	-1.605837	0.925591
H	5.036455	-3.433788	0.462570
H	6.853030	0.368933	1.307214
H	7.004715	-2.108175	1.199000
C	2.525759	1.449033	-1.882538
C	1.254015	2.126157	-2.390008
H	1.468917	2.603958	-3.357859
H	0.440113	1.403833	-2.549369
H	0.906456	2.913477	-1.706134
C	3.600616	2.501849	-1.642596
H	4.576954	2.052284	-1.422982
H	3.719618	3.108223	-2.553621
H	3.333330	3.185779	-0.824048
C	2.998929	0.427317	-2.915441
H	2.221901	-0.322701	-3.124466
H	3.230868	0.941973	-3.859997
H	3.906915	-0.098047	-2.588111
C	-2.105787	-0.349702	-1.656586
C	-3.454625	1.450530	-0.683739
C	-4.628711	1.897524	-0.066882
C	-2.567203	2.405040	-1.191957
C	-4.877823	3.258626	0.077812

H	-5.342039	1.163925	0.303199
C	-2.818046	3.765329	-1.051254
H	-1.676206	2.078297	-1.730243
C	-3.972167	4.198944	-0.403900
H	-5.795910	3.586489	0.563608
H	-2.109878	4.487077	-1.458167
H	-4.173870	5.263312	-0.293938
C	-3.147129	-0.017647	-0.715680
H	-4.034158	-0.626316	-0.959885
N	-1.182993	-0.640889	-2.316504

TS₄₋₁₃

SCF done: -1541.028729

Pd	0.027937	-0.742694	0.029711
C	-3.155206	0.015979	-0.703633
C	-2.810421	1.158856	0.027604
C	-4.431024	-0.607577	-0.456795
C	-3.695015	1.750191	0.930337
H	-1.830345	1.606608	-0.139285
C	-5.327806	0.010314	0.464983
C	-4.937686	1.191024	1.140807
H	-3.394572	2.655378	1.456106
H	-5.638450	1.641848	1.844058
C	-6.594446	-0.577293	0.698727
C	-6.960354	-1.736384	0.062626
H	-7.270828	-0.089693	1.401369
C	-4.827489	-1.810467	-1.079321
C	-6.063260	-2.360881	-0.826880
H	-7.935777	-2.181751	0.250684
H	-4.127916	-2.327915	-1.732203
H	-6.346711	-3.293731	-1.311188
C	-2.268423	-0.436196	-1.712297
H	-2.599845	-1.091801	-2.505358
H	-1.392148	0.169587	-1.939090
P	1.265421	1.188279	0.375372
C	2.934503	1.163003	-0.426715
C	3.510674	-0.083218	-0.695256
C	3.644665	2.326115	-0.741393
C	4.781599	-0.164485	-1.255417
H	2.955904	-0.996301	-0.466035
C	4.909579	2.242233	-1.313817
H	3.198448	3.303196	-0.551780
C	5.480847	0.997423	-1.567087
H	5.217474	-1.143663	-1.450824
H	5.451380	3.153120	-1.564792
H	6.472070	0.934715	-2.013935
C	0.512753	2.744956	-0.313302
C	-0.126694	3.740359	0.431980
C	0.391247	2.787656	-1.711504
C	-0.874202	4.735845	-0.195981
H	-0.058904	3.748151	1.516800
C	-0.345906	3.783405	-2.337666
H	0.873356	2.014536	-2.313227
C	-0.991613	4.758662	-1.579486
H	-1.366376	5.497245	0.407575
H	-0.424117	3.794579	-3.423687
H	-1.580465	5.532557	-2.068554
C	1.665706	1.460859	2.221702
C	2.505636	0.255464	2.649811
H	2.676650	0.305352	3.736092
H	1.993716	-0.691901	2.425585
H	3.485717	0.238342	2.155211
C	2.451039	2.736987	2.501391
H	1.920416	3.647761	2.196458
H	2.649048	2.815470	3.581900
H	3.422863	2.727133	1.989574
C	0.350247	1.420443	3.001999
H	-0.194075	0.487128	2.795714
H	0.562180	1.465054	4.081546
H	-0.325997	2.251716	2.764210
C	-0.810578	-2.752851	-0.260769

C	1.546905	-3.359869	0.345116
C	2.467795	-3.609490	1.375959
C	1.988138	-3.503803	-0.981939
C	3.781564	-3.955655	1.093783
H	2.140099	-3.502478	2.411407
C	3.300829	-3.859303	-1.258907
H	1.285946	-3.322667	-1.796820
C	4.211118	-4.081221	-0.225928
H	4.477924	-4.132894	1.912538
H	3.618411	-3.962821	-2.296162
H	5.240636	-4.357818	-0.447075
C	0.197509	-2.918589	0.685632
H	-0.132229	-3.064088	1.714839
N	-1.680473	-2.609309	-1.078445

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SCF done: -1541.098520

Pd	-0.006367	0.768906	0.439794
C	3.095741	-0.031373	-1.022867
C	2.572377	-1.266800	-0.719266
C	4.286181	0.409617	-0.371650
C	3.187576	-2.112688	0.228194
H	1.663355	-1.601752	-1.220178
C	4.905577	-0.446886	0.587506
C	4.327617	-1.709112	0.871383
H	2.748362	-3.088954	0.432684
H	4.815074	-2.352911	1.604317
C	6.093256	-0.021358	1.229372
C	6.654752	1.196475	0.941063
H	6.553676	-0.687494	1.959984
C	4.889661	1.663471	-0.643903
C	6.044104	2.045625	-0.005819
H	7.568894	1.511356	1.441827
H	4.415370	2.338808	-1.354377
H	6.490526	3.013518	-0.228494
C	2.419970	0.831158	-2.055352
H	3.104324	1.038271	-2.889843
H	1.553800	0.291505	-2.467910
P	-1.268363	-1.252248	0.551711
C	-3.025869	-0.908315	0.069809
C	-3.489530	0.406087	0.184720
C	-3.895007	-1.898641	-0.400901
C	-4.803550	0.723406	-0.145889
H	-2.803350	1.185847	0.525521
C	-5.206770	-1.579715	-0.734181
H	-3.536738	-2.920931	-0.527020
C	-5.663007	-0.269778	-0.603945
H	-5.142446	1.754743	-0.058337
H	-5.875357	-2.355907	-1.103817
H	-6.689885	-0.023351	-0.870365
C	-0.774597	-2.508396	-0.722258
C	-0.160659	-3.736887	-0.468407
C	-0.907017	-2.091979	-2.055664
C	0.309546	-4.526662	-1.517150
H	-0.034283	-4.094358	0.551521
C	-0.444360	-2.881232	-3.099685
H	-1.372254	-1.127889	-2.269881
C	0.172098	-4.102647	-2.832511
H	0.786873	-5.480562	-1.297532
H	-0.558702	-2.538376	-4.126834
H	0.543814	-4.719031	-3.649044
C	-1.417722	-2.082794	2.258207
C	-2.074478	-1.034070	3.159294
H	-2.114201	-1.418102	4.190023
H	-1.501662	-0.094906	3.170370
H	-3.101473	-0.804301	2.845839
C	-2.262395	-3.350871	2.270714
H	-1.869789	-4.135196	1.610795
H	-2.292385	-3.761480	3.292042
H	-3.298290	-3.143921	1.970107
C	-0.005089	-2.341303	2.783312

H	0.603884	-1.426473	2.748131
H	-0.060325	-2.676859	3.830451
H	0.529979	-3.115093	2.219280
C	1.144549	2.243045	-0.632560
C	-0.964284	3.460691	-0.001487
C	-1.693918	4.067002	1.029795
C	-1.542908	3.397469	-1.278486
C	-2.962870	4.584767	0.796769
H	-1.253550	4.124165	2.026079
C	-2.809742	3.913858	-1.507354
H	-0.987540	2.927886	-2.090955
C	-3.530427	4.509004	-0.472001
H	-3.509943	5.053690	1.613693
H	-3.241471	3.851616	-2.505482
H	-4.522999	4.917366	-0.655872
C	0.373577	2.918784	0.280805
H	0.866029	3.237205	1.203144
N	1.969528	2.131742	-1.546245

TS₄₋₁₄

SCF done: -1541.049267

Pd	0.571028	-1.267806	-0.756147
C	-2.753053	0.169987	-2.219233
C	-4.022792	-0.401752	-2.445496
C	-2.630499	1.174745	-1.177290
C	-5.174724	0.065371	-1.798682
H	-4.109476	-1.167342	-3.216853
C	-3.802925	1.599087	-0.493555
C	-5.064655	1.032124	-0.831921
H	-6.142989	-0.374384	-2.031851
H	-5.946591	1.378962	-0.292363
C	-3.698050	2.549662	0.544129
C	-2.472878	3.056062	0.914524
H	-4.608000	2.859628	1.058907
C	-1.392928	1.709467	-0.778550
C	-1.312320	2.626598	0.250304
H	-2.400767	3.782441	1.722275
H	-0.472748	1.377527	-1.257787
H	-0.334283	3.010172	0.544324
C	-1.661940	-0.372284	-2.888598
H	-0.654447	0.025832	-2.801361
H	-1.821204	-1.076701	-3.700595
P	2.265401	-0.186241	0.328288
C	3.996832	-0.719753	-0.092867
C	4.190118	-2.045139	-0.494306
C	5.102092	0.133678	-0.019292
C	5.465539	-2.515128	-0.792013
H	3.321682	-2.700445	-0.586699
C	6.375061	-0.333369	-0.328416
H	4.968501	1.175962	0.273122
C	6.559774	-1.659465	-0.709983
H	5.601940	-3.550012	-1.102572
H	7.227318	0.342606	-0.273275
H	7.557023	-2.023205	-0.953312
C	2.350897	1.636474	-0.064447
C	2.471013	2.698928	0.835928
C	2.246583	1.938304	-1.429959
C	2.476866	4.019149	0.386745
H	2.553605	2.512869	1.904057
C	2.262395	3.251780	-1.880633
H	2.136734	1.117497	-2.143037
C	2.371967	4.300337	-0.969958
H	2.566508	4.829895	1.108639
H	2.180653	3.458669	-2.946624
H	2.373484	5.331890	-1.317958
C	2.215210	-0.399428	2.229281
C	2.102116	-1.908128	2.461332
H	2.028415	-2.105312	3.542250
H	1.212195	-2.325077	1.969157
H	2.983475	-2.445274	2.083365
C	3.451563	0.103184	2.969052

H	3.633226	1.178127	2.848926
H	3.330714	-0.088479	4.046996
H	4.356931	-0.423568	2.639929
C	0.941272	0.264988	2.749849
H	0.058865	-0.116562	2.215702
H	0.816053	0.035326	3.819797
H	0.948646	1.357038	2.639782
C	-2.244257	-2.407774	-1.059526
C	-3.803758	-1.713370	0.689781
C	-5.140756	-1.570325	1.096100
C	-2.803132	-1.105266	1.474393
C	-5.468692	-0.849831	2.240418
H	-5.926512	-2.037904	0.500379
C	-3.136361	-0.381821	2.604790
H	-1.755611	-1.198207	1.171910
C	-4.471183	-0.247021	2.997316
H	-6.512719	-0.759946	2.538346
H	-2.346732	0.088428	3.190812
H	-4.726075	0.320440	3.890890
C	-3.499792	-2.413745	-0.539662
H	-4.263620	-3.037324	-1.002179
N	-1.175729	-2.194117	-1.543144

14

SCF done: -1541.090051

Pd	0.020163	-0.1951950	-1.279921
C	-3.110391	1.6212110	-1.452894
C	-4.414410	1.3387850	-1.108493
C	-2.266170	2.3140970	-0.533385
C	-4.940777	1.7123530	0.144793
H	-5.044825	0.7957740	-1.813820
C	-2.798456	2.6772810	0.741661
C	-4.143512	2.3600250	1.052341
H	-5.973957	1.4724990	0.388702
H	-4.531568	2.6443950	2.030992
C	-1.966303	3.3385400	1.678479
C	-0.663159	3.6406560	1.370904
H	-2.386759	3.6025970	2.649372
C	-0.913785	2.6420210	-0.816367
C	-0.136590	3.2989670	0.108612
H	-0.028296	4.1477770	2.096922
H	-0.478103	2.3816640	-1.781357
H	0.898704	3.5413090	-0.128985
C	-2.567342	1.0797010	-2.742642
H	-1.889575	1.7763300	-3.246067
H	-3.387815	0.8471050	-3.433878
P	1.790567	-0.3032050	0.180658
C	3.198567	-1.4338350	-0.258432
C	2.916052	-2.5328940	-1.074582
C	4.509613	-1.2400270	0.188346
C	3.919428	-3.4322110	-1.422272
H	1.897101	-2.6632840	-1.445151
C	5.514677	-2.1334550	-0.167820
H	4.750688	-0.3770830	0.810430
C	5.219917	-3.2327220	-0.970020
H	3.685545	-4.2850230	-2.057973
H	6.533093	-1.9696710	0.181951
H	6.008357	-3.9299770	-1.249901
C	2.678281	1.3291790	0.315229
C	2.846447	2.1108000	1.460274
C	3.133700	1.8422560	-0.908508
C	3.445385	3.3683470	1.385258
H	2.497551	1.7592970	2.428130
C	3.742232	3.0877010	-0.983529
H	2.989907	1.2536230	-1.816638
C	3.895181	3.8608030	0.166836
H	3.558084	3.9626510	2.291221
H	4.090533	3.4625570	-1.944895
H	4.361457	4.8430810	0.109279
C	1.292373	-0.8972450	1.925756
C	0.677310	-2.2846500	1.719593

H	0.308609	-2.6649400	2.685328
H	-0.172169	-2.2552400	1.021920
H	1.414866	-3.0034830	1.335958
C	2.448759	-1.0251530	2.912058
H	2.960626	-0.0759940	3.112899
H	2.065762	-1.4015410	3.873865
H	3.201391	-1.7410310	2.555062
C	0.205381	0.0425020	2.448910
H	-0.610389	0.1424320	1.716933
H	-0.215264	-0.3673700	3.380902
H	0.570832	1.0549450	2.664215
C	-2.372922	-1.1819400	-2.077243
C	-3.160539	-2.5282120	-0.192182
C	-3.524390	-3.8084200	0.239685
C	-2.980835	-1.5220140	0.767930
C	-3.691772	-4.0786730	1.592900
H	-3.668954	-4.5983360	-0.498233
C	-3.154986	-1.7935160	2.117182
H	-2.713810	-0.5151500	0.443546
C	-3.508298	-3.0738470	2.538310
H	-3.969499	-5.0829460	1.909937
H	-3.024421	-0.9923510	2.844467
H	-3.649109	-3.2850510	3.597063
C	-2.986200	-2.2580650	-1.621540
H	-3.348513	-2.9898430	-2.344540
N	-1.791551	-0.1732470	-2.496009

4'

SCF done: -1231.670420

Pd	-0.714588	0.462410	-0.929831
C	0.329234	2.315430	-0.321148
C	0.626376	2.336276	-1.710807
C	1.409806	2.007834	0.603473
C	1.922252	2.078095	-2.198260
H	-0.149588	2.671847	-2.400217
C	2.701432	1.723658	0.080649
C	2.922732	1.734919	-1.328767
H	2.103698	2.104081	-3.270815
H	3.925365	1.505558	-1.689559
C	3.752934	1.419617	0.969176
C	3.548316	1.405012	2.329915
H	4.731051	1.175837	0.554261
C	1.227977	1.987659	1.998904
C	2.275465	1.692158	2.846583
H	4.368385	1.157665	3.001463
H	0.250028	2.220080	2.417037
H	2.112275	1.683956	3.923111
C	-1.056576	2.337854	0.038618
H	-1.348944	2.308342	1.087797
H	-1.732879	2.915457	-0.596322
P	-2.459608	-1.039095	-0.429825
C	-4.014845	-0.543069	0.434188
C	-4.280037	0.810442	0.643435
C	-4.950482	-1.493575	0.854940
C	-5.459328	1.210953	1.265665
H	-3.551531	1.549117	0.308747
C	-6.125945	-1.095154	1.479601
H	-4.765713	-2.556339	0.692615
C	-6.380880	0.258768	1.686517
H	-5.656252	2.270019	1.424354
H	-6.846879	-1.842708	1.806756
H	-7.301858	0.570066	2.176800
C	1.350884	-1.249877	-1.825707
C	3.377215	-1.598002	-0.477329
C	4.780563	-1.697533	-0.448709
C	2.685840	-1.811897	0.731016
C	5.457007	-2.011180	0.722425
H	5.336378	-1.530354	-1.373339
C	3.365637	-2.130838	1.896381
H	1.598731	-1.705999	0.745909
C	4.756192	-2.234554	1.906050

H	6.544120	-2.088088	0.709641
H	2.803124	-2.289746	2.816509
H	5.286202	-2.486217	2.823234
C	2.700938	-1.245997	-1.704424
H	3.292506	-1.019599	-2.590459
N	0.155521	-1.286300	-1.912981
C	-3.070206	-1.898435	-1.948689
H	-3.718595	-2.746925	-1.695189
H	-3.625138	-1.190956	-2.573860
H	-2.185482	-2.245757	-2.494845
C	-1.816523	-2.457938	0.566111
H	-0.944449	-2.854397	0.032837
H	-1.500247	-2.106006	1.553908
H	-2.563666	-3.253009	0.681240

TS₄₋₆'

SCF done: -1231.657464

Pd	-0.787982	0.220434	-0.686483
C	0.324045	2.109298	-0.815734
C	0.704348	1.880739	-2.182440
C	1.381610	2.036991	0.193896
C	1.957327	1.449772	-2.538001
H	-0.046314	2.074939	-2.949711
C	2.669597	1.585915	-0.190662
C	2.897492	1.116914	-1.536736
H	2.194662	1.262853	-3.584175
H	3.939560	0.964926	-1.822041
C	3.709725	1.577974	0.756218
C	3.493183	1.987238	2.056650
H	4.696118	1.229920	0.447904
C	1.181016	2.432934	1.527227
C	2.215601	2.406049	2.443619
H	4.309198	1.969056	2.776873
H	0.199677	2.785496	1.839329
H	2.034514	2.726166	3.468719
C	-1.043509	2.346046	-0.513512
H	-1.343223	2.690363	0.475691
H	-1.695243	2.684166	-1.321857
P	-2.632378	-1.158848	-0.144673
C	-4.261185	-0.486246	0.420016
C	-4.439940	0.896664	0.461625
C	-5.318120	-1.320188	0.797368
C	-5.654592	1.440728	0.870883
H	-3.610874	1.542143	0.168611
C	-6.530804	-0.779070	1.207015
H	-5.197660	-2.404377	0.774907
C	-6.700047	0.603463	1.243409
H	-5.782845	2.521694	0.899733
H	-7.348118	-1.436603	1.499605
H	-7.650154	1.026538	1.566099
C	1.424666	-1.442282	-1.260385
C	3.671710	-1.425038	-0.275688
C	5.048033	-1.553938	-0.514120
C	3.213417	-1.519035	1.046802
C	5.935013	-1.773043	0.531851
H	5.417134	-1.480672	-1.538838
C	4.101266	-1.748362	2.088889
H	2.148802	-1.388212	1.253036
C	5.466170	-1.872550	1.839949
H	6.999701	-1.873239	0.324420
H	3.724476	-1.816886	3.108527
H	6.161270	-2.047604	2.659303
C	2.768834	-1.102732	-1.379217
H	3.171599	-1.225682	-2.386640
N	0.282924	-1.734724	-1.142147
C	-3.105831	-2.272216	-1.550067
H	-3.839408	-3.031524	-1.250241
H	-3.518836	-1.672722	-2.368390
H	-2.189885	-2.763401	-1.899375
C	-2.219922	-2.407683	1.161849
H	-1.292900	-2.907326	0.856403

H	-2.049406	-1.898956	2.116711
H	-3.014124	-3.155270	1.284497

6'

SCF done: -1231.680569

Pd	-0.960893	0.286687	-0.479726
C	0.318021	2.012640	-0.859192
C	0.809308	1.776679	-2.215893
C	1.343893	2.020372	0.206373
C	2.033284	1.294289	-2.478177
H	0.127173	2.018353	-3.032848
C	2.632874	1.517028	-0.064399
C	2.944236	0.857028	-1.381196
H	2.356420	1.124493	-3.505795
H	3.993567	1.070788	-1.645405
C	3.632153	1.618142	0.906994
C	3.373137	2.167003	2.154392
H	4.633096	1.249238	0.676650
C	1.097840	2.566416	1.475013
C	2.090721	2.631273	2.438973
H	4.165054	2.235940	2.898035
H	0.109404	2.960327	1.704391
H	1.868518	3.065109	3.412953
C	-1.008675	2.440817	-0.674743
H	-1.342463	2.900966	0.253955
H	-1.601185	2.706197	-1.551802
P	-2.744867	-1.200719	-0.015707
C	-4.460314	-0.585312	0.319172
C	-4.693991	0.789149	0.262093
C	-5.521969	-1.442646	0.622360
C	-5.966556	1.300982	0.501928
H	-3.859722	1.452705	0.025858
C	-6.793031	-0.934035	0.862118
H	-5.359281	-2.520432	0.674359
C	-7.016447	0.439949	0.801443
H	-6.137306	2.375510	0.454403
H	-7.613633	-1.610405	1.097602
H	-8.012650	0.838361	0.988288
C	1.616708	-1.251026	-0.961135
C	3.997387	-1.267806	-0.349650
C	5.310023	-1.369654	-0.811902
C	3.719154	-1.565495	0.983904
C	6.334153	-1.750083	0.047319
H	5.530133	-1.139518	-1.856064
C	4.742153	-1.954057	1.842128
H	2.699028	-1.472663	1.357640
C	6.050825	-2.042310	1.378646
H	7.354472	-1.824194	-0.325124
H	4.514276	-2.181472	2.882062
H	6.850620	-2.342804	2.053327
C	2.938636	-0.738578	-1.288977
H	3.164693	-1.084454	-2.311035
N	0.557181	-1.659946	-0.698630
C	-3.027589	-2.457650	-1.356866
H	-3.762161	-3.221413	-1.069413
H	-3.368476	-1.950920	-2.266147
H	-2.065302	-2.940518	-1.567043
C	-2.442992	-2.337602	1.424031
H	-1.467302	-2.815020	1.271764
H	-2.404471	-1.752874	2.349479
H	-3.216341	-3.111565	1.514775

TS4-7'

SCF done: -1231.659773

Pd	-0.753631	-1.964992	-0.197726
C	0.875106	0.133350	-1.671769
C	2.077969	-0.446340	-2.192350
C	0.992616	1.391067	-0.945373
C	3.229324	0.392976	-2.377116
H	1.945342	-1.281188	-2.882874
C	2.223682	2.096277	-0.963829

C	3.317800	1.586602	-1.744605
H	4.068526	0.009451	-2.957863
H	4.220971	2.193475	-1.820001
C	2.358621	3.286260	-0.230800
C	1.304452	3.795937	0.502335
H	3.319799	3.801812	-0.249458
C	-0.073667	1.948004	-0.219514
C	0.077357	3.122699	0.494991
H	1.423550	4.716275	1.071408
H	-1.038884	1.443596	-0.207203
H	-0.768983	3.524290	1.052989
C	-0.358125	-0.506239	-1.867011
H	-1.270028	0.087091	-1.791507
H	-0.394926	-1.286197	-2.633430
P	-2.391222	-0.871249	1.048911
C	-3.414480	0.443405	0.242714
C	-3.978744	0.137977	-1.000898
C	-3.632063	1.709119	0.791415
C	-4.755485	1.073008	-1.675069
H	-3.795302	-0.843229	-1.445205
C	-4.395449	2.651708	0.107970
H	-3.196655	1.973222	1.754860
C	-4.960137	2.334788	-1.123072
H	-5.191135	0.821232	-2.640580
H	-4.549629	3.638597	0.541871
H	-5.555295	3.073826	-1.656640
C	1.896234	-2.682345	-0.630082
C	3.257766	-0.942049	0.460119
C	4.511356	-0.320920	0.540957
C	2.302332	-0.647560	1.446927
C	4.801410	0.571950	1.566413
H	5.262194	-0.543433	-0.218373
C	2.592257	0.249257	2.463584
H	1.311242	-1.108769	1.389543
C	3.841834	0.865643	2.528827
H	5.783468	1.040878	1.611995
H	1.833635	0.474392	3.212755
H	4.064384	1.569413	3.329204
C	2.944359	-1.775087	-0.702887
H	3.787099	-2.071586	-1.330014
N	0.870512	-3.271212	-0.626114
C	-1.685437	-0.041412	2.551302
H	-1.181139	-0.816342	3.141682
H	-0.931547	0.696290	2.247003
H	-2.453812	0.433823	3.175928
C	-3.729827	-1.901573	1.831059
H	-3.266638	-2.692598	2.432307
H	-4.379466	-1.284157	2.465324
H	-4.331353	-2.372307	1.045389

7'

SCF done: -1231.679383

Pd	-1.350860	0.446790	-0.645083
C	1.696406	-0.988426	1.084524
C	2.821283	0.009039	1.079333
C	1.992000	-2.284067	0.461059
C	4.131318	-0.641288	1.423488
H	2.591777	0.824924	1.781618
C	3.319639	-2.764508	0.515670
C	4.346118	-1.932104	1.131632
H	4.918053	-0.023822	1.854516
H	5.315423	-2.390967	1.332941
C	3.616229	-4.024008	-0.010581
C	2.627810	-4.792257	-0.612252
H	4.639707	-4.396121	0.050763
C	1.011721	-3.057449	-0.164605
C	1.326096	-4.301924	-0.697875
H	2.873102	-5.768969	-1.025758
H	0.002242	-2.653841	-0.261413
H	0.553929	-4.888630	-1.192860
C	0.496590	-0.677513	1.596480

H	-0.324346	-1.391109	1.621042
H	0.307917	0.294409	2.051284
P	-3.335982	-0.611224	-0.242696
C	1.659867	1.095455	-0.804014
C	2.981633	0.701923	-0.344216
N	0.540200	1.279874	-1.058992
C	-4.007754	-1.682633	-1.609828
H	-4.175410	-1.068831	-2.501103
H	-3.255188	-2.442929	-1.852282
H	-4.945385	-2.180198	-1.327780
C	-4.802960	0.453763	0.155921
C	-6.076955	-0.074067	0.383533
C	-4.618424	1.835129	0.227427
C	-7.145911	0.763928	0.678673
H	-6.242943	-1.151531	0.328596
C	-5.687424	2.676472	0.523788
H	-3.620469	2.239055	0.043582
C	-6.951036	2.141697	0.749711
H	-8.135090	0.342126	0.852159
H	-5.532037	3.753022	0.576825
H	-7.788860	2.797920	0.981097
C	-3.398517	-1.844849	1.155555
H	-3.132290	-1.345322	2.094046
H	-4.390265	-2.304546	1.261662
H	-2.661919	-2.635008	0.960680
C	3.960579	1.850649	-0.291608
C	5.295010	1.644605	-0.640187
C	3.559783	3.106709	0.164886
C	6.217677	2.679907	-0.531657
H	5.610032	0.662256	-0.993771
C	4.480604	4.143046	0.267639
H	2.514804	3.275401	0.431006
C	5.811995	3.931020	-0.078384
H	7.256784	2.508463	-0.807542
H	4.155104	5.120981	0.617958
H	6.533147	4.742446	0.002453
H	3.349788	-0.071791	-1.037178

TS₄-8'

SCF done: -1231.630432

Pd	-0.756894	-0.294652	-0.296481
C	0.423696	1.153758	-1.502296
C	0.890431	-0.085131	-2.035470
C	1.318229	1.972395	-0.707088
C	2.270913	-0.554793	-1.857232
H	0.272498	-0.573310	-2.792144
C	2.701734	1.618004	-0.720293
C	3.148856	0.454750	-1.383747
H	2.656490	-1.164667	-2.676825
H	4.223889	0.311818	-1.481302
C	3.618748	2.484961	-0.061811
C	3.184221	3.600353	0.610849
H	4.673504	2.218122	-0.075847
C	0.902650	3.120530	-0.007475
C	1.811230	3.921438	0.652844
H	3.899764	4.240283	1.121736
H	-0.152429	3.384545	0.013601
H	1.474832	4.801697	1.193526
C	-0.993985	1.391950	-1.582989
H	-1.421727	2.296930	-1.155292
H	-1.526892	1.000212	-2.453075
P	-2.689782	-0.186762	1.088128
C	-4.376601	-0.218204	0.274709
C	-4.443132	-0.385095	-1.109026
C	-5.553933	-0.079747	1.014501
C	-5.679376	-0.410114	-1.751637
H	-3.520191	-0.500906	-1.675813
C	-6.787763	-0.104782	0.370548
H	-5.515394	0.046166	2.095246
C	-6.850196	-0.268629	-1.012305
H	-5.727115	-0.540551	-2.829271

H	-7.701759	0.003733	0.948338
H	-7.814750	-0.287059	-1.512407
C	1.245053	-2.232666	0.102462
C	3.661400	-1.864195	0.122286
C	4.902045	-2.331359	-0.332108
C	3.639959	-0.890617	1.131676
C	6.085849	-1.853685	0.218294
H	4.930578	-3.071894	-1.130156
C	4.824834	-0.422084	1.688359
H	2.682931	-0.484843	1.458844
C	6.053201	-0.895131	1.231707
H	7.039943	-2.228561	-0.144255
H	4.788189	0.337746	2.465274
H	6.978851	-0.521511	1.661458
C	2.433055	-2.194957	-0.609809
H	2.534010	-3.007713	-1.335592
N	0.184524	-2.130252	0.624793
C	-2.744132	1.397435	2.115639
H	-1.810354	1.470264	2.685404
H	-2.810960	2.251154	1.431481
H	-3.598418	1.405700	2.803604
C	-2.794994	-1.523567	2.412214
H	-1.870346	-1.489423	2.999592
H	-3.664715	-1.375146	3.063543
H	-2.852276	-2.498416	1.917014

8'

SCF done: -1231.673343

Pd	-1.287193	-1.151873	-0.367304
C	0.305970	0.067607	-2.144874
C	1.154929	-1.029487	-2.089240
C	0.917293	1.443978	-2.146159
C	2.688642	-0.931777	-1.812872
H	0.723113	-2.001347	-2.216432
C	2.297032	1.567153	-1.936778
C	3.150364	0.427135	-1.757715
H	3.224959	-1.432606	-2.588720
H	4.189212	0.599837	-1.573530
C	2.841003	2.862497	-1.895842
C	2.033990	3.953706	-2.057852
H	3.887491	2.998887	-1.734373
C	0.108620	2.567962	-2.329701
C	0.657737	3.801215	-2.284338
H	2.454731	4.935780	-2.015270
H	-0.941692	2.448685	-2.502888
H	0.036379	4.660791	-2.423503
C	-1.091682	-0.159434	-2.130622
H	-1.644780	0.754055	-2.129259
H	-1.417838	-0.740460	-2.966988
P	-3.169510	-1.300381	0.966696
C	1.628503	-1.846325	-0.023016
C	3.656799	-0.857677	0.586783
C	4.849193	-1.349352	1.132223
C	3.149281	0.373836	1.005066
C	5.505302	-0.637010	2.143850
H	5.254538	-2.273844	0.776679
C	3.796045	1.081659	2.021143
H	2.262276	0.767476	0.550292
C	4.969145	0.572640	2.598640
H	6.413807	-1.020199	2.570310
H	3.389577	2.009938	2.356803
H	5.451742	1.111248	3.385920
C	2.883035	-1.673108	-0.454360
H	3.401523	-2.597223	-0.609858
N	0.512165	-1.772391	0.054076
C	-2.791005	-2.276114	2.455303
H	-1.993424	-1.807374	2.993589
H	-3.659184	-2.329381	3.077463
H	-2.494887	-3.266776	2.170804
C	-3.630796	0.402823	1.413475
C	-3.076223	1.003600	2.548264

C	-4.521836	1.119943	0.606578
C	-3.382003	2.337151	2.854852
H	-2.412651	0.445595	3.179014
C	-4.832438	2.451119	0.915812
H	-4.961310	0.650517	-0.250017
C	-4.257216	3.061575	2.037326
H	-2.942348	2.800596	3.710961
H	-5.506889	3.000869	0.289622
H	-4.487593	4.080173	2.267055
C	-4.522852	-2.097750	0.068124
H	-4.228954	-3.088874	-0.212536
H	-5.385883	-2.145927	0.698019
H	-4.751394	-1.531462	-0.809235

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SCF done: -1231.628679

Pd	1.453589	-1.253276	-0.527198
C	0.602497	-2.559261	1.120425
C	0.566854	-3.839639	0.479782
C	-0.660292	-1.868295	1.369903
C	-0.602191	-4.376450	0.002827
H	1.510809	-4.375260	0.370303
C	-1.827673	-2.375088	0.679959
C	-1.782563	-3.610308	0.064243
H	-0.607587	-5.351822	-0.478400
H	-2.691674	-3.986460	-0.409962
C	-3.003677	-1.525070	0.574660
C	-3.140203	-0.493688	1.560551
H	-3.919416	-2.036971	0.266788
C	-0.798206	-0.753665	2.181193
C	-2.052215	-0.112482	2.301250
H	-4.088751	0.030929	1.661401
H	0.045713	-0.390858	2.766934
H	-2.156098	0.699090	3.022754
C	1.869672	-1.971766	1.413771
H	1.939105	-1.133092	2.109778
H	2.748729	-2.620893	1.412290
P	3.054321	0.458059	-0.670848
C	2.360370	1.965282	0.152285
C	1.097632	1.885499	0.743838
C	3.060978	3.174013	0.207575
C	0.544991	2.989732	1.386973
H	0.539047	0.946191	0.703023
C	2.508191	4.279015	0.845190
H	4.047283	3.261794	-0.251596
C	1.250035	4.187405	1.437627
H	-0.440091	2.902484	1.846359
H	3.061266	5.216376	0.881301
H	0.821117	5.054111	1.938338
C	-1.493646	-0.768225	-1.635696
C	-3.320573	0.784389	-1.059684
C	-4.689977	1.066062	-1.149951
C	-2.459985	1.803256	-0.630138
C	-5.181542	2.325462	-0.831630
H	-5.372979	0.277316	-1.470873
C	-2.951949	3.064714	-0.320118
H	-1.390486	1.599784	-0.543585
C	-4.314535	3.334157	-0.416812
H	-6.249741	2.523374	-0.912123
H	-2.259098	3.842560	0.001828
H	-4.699395	4.322694	-0.171843
C	-2.843298	-0.583180	-1.271564
H	-3.520105	-1.223324	-1.846082
N	-0.356077	-1.003218	-1.786845
C	4.669334	0.222692	0.215559
H	5.287188	1.129526	0.197736
H	4.467082	-0.056008	1.256137
H	5.218907	-0.597034	-0.262629
C	3.638069	1.105530	-2.309495
H	4.311948	1.964903	-2.197274
H	4.165720	0.303156	-2.838302

H	2.767553	1.399201	-2.905682
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SCF done: -1231.639433

Pd	1.885840	-0.991863	-0.348722
C	1.235260	-2.780616	0.804715
C	1.241136	-3.916140	-0.093562
C	-0.070727	-2.240428	1.222936
C	0.098142	-4.412342	-0.629670
H	2.208460	-4.365594	-0.321837
C	-1.231352	-2.662227	0.443511
C	-1.142823	-3.738527	-0.384183
H	0.120515	-5.274243	-1.293139
H	-2.036727	-4.071106	-0.918509
C	-2.478038	-1.806441	0.459647
C	-2.585740	-0.940891	1.679053
H	-3.370985	-2.451971	0.393278
C	-0.244492	-1.344967	2.244996
C	-1.530052	-0.749944	2.492731
H	-3.547511	-0.473552	1.885508
H	0.594205	-1.061179	2.878695
H	-1.640749	-0.117188	3.374517
C	2.460922	-2.268604	1.288572
H	2.502713	-1.646581	2.181729
H	3.372005	-2.833921	1.086909
P	2.870143	1.151264	-0.603492
C	1.776339	2.429685	0.186724
C	0.649764	2.014221	0.900702
C	2.035281	3.798928	0.073261
C	-0.203025	2.947588	1.485853
H	0.437177	0.945693	0.995012
C	1.185083	4.732230	0.656025
H	2.909566	4.148877	-0.478426
C	0.061968	4.307451	1.362135
H	-1.079314	2.603605	2.036356
H	1.398711	5.795754	0.558444
H	-0.604169	5.038934	1.817632
C	-1.185721	-0.573409	-1.299640
C	-3.478972	0.213968	-0.817385
C	-4.845383	0.000513	-0.996256
C	-3.027165	1.488898	-0.475928
C	-5.749211	1.044910	-0.834698
H	-5.203009	-0.995890	-1.262153
C	-3.930063	2.534213	-0.317679
H	-1.960315	1.667467	-0.330641
C	-5.292861	2.315307	-0.494486
H	-6.813537	0.866957	-0.979758
H	-3.561082	3.524384	-0.052506
H	-6.000355	3.133297	-0.369833
C	-2.536166	-0.960466	-0.894134
H	-2.885509	-1.660270	-1.671294
N	-0.088869	-0.323471	-1.592807
C	4.552772	1.636457	0.021703
H	4.777278	2.692990	-0.174976
H	4.607524	1.450052	1.099667
H	5.304630	1.012609	-0.476067
C	2.962909	1.772978	-2.352797
H	3.263182	2.827279	-2.407600
H	3.685636	1.163613	-2.908311
H	1.976232	1.646936	-2.812324

TS_{4-10'}

SCF done: -1231.621000

Pd	-0.539678	0.202477	0.276191
C	-0.838365	2.349499	1.184352
C	-1.591427	3.332165	0.551930
C	0.552210	2.132889	0.799921
C	-0.996141	4.129983	-0.445142
H	-2.645548	3.442037	0.804853
C	1.118939	2.912010	-0.295369
C	0.290958	3.924745	-0.871625

H	-1.588702	4.916346	-0.913766
H	0.716224	4.543270	-1.662307
C	2.428486	2.690975	-0.678421
C	3.214821	1.608933	-0.126725
H	2.856184	3.304209	-1.473397
C	1.492183	1.379930	1.609251
C	2.766822	1.172315	1.198348
H	4.302283	1.754492	-0.185970
H	1.176131	1.021252	2.588229
H	3.461821	0.625431	1.834508
C	-1.416298	1.223493	1.895959
H	-0.919408	0.838573	2.791117
H	-2.507990	1.202273	1.973594
P	-1.959207	-1.659380	0.259400
C	-3.687011	-1.253686	-0.244197
C	-3.991551	0.058050	-0.614144
C	-4.694332	-2.223141	-0.263300
C	-5.286955	0.395832	-0.996365
H	-3.204595	0.815610	-0.600586
C	-5.986857	-1.884774	-0.644616
H	-4.473707	-3.253127	0.021305
C	-6.283530	-0.573543	-1.010722
H	-5.515479	1.420944	-1.282664
H	-6.766074	-2.645146	-0.657020
H	-7.297079	-0.309215	-1.307965
C	1.864832	-0.220259	-1.423464
C	4.123241	-0.886829	-0.738061
C	5.491088	-0.818847	-1.023406
C	3.668773	-1.885819	0.132021
C	6.380269	-1.731035	-0.468088
H	5.855332	-0.040642	-1.696375
C	4.558962	-2.797930	0.684478
H	2.605524	-1.945242	0.373109
C	5.917712	-2.726574	0.387567
H	7.440367	-1.666420	-0.708907
H	4.188332	-3.572135	1.355114
H	6.612576	-3.444221	0.820258
C	3.218338	0.165427	-1.262851
H	3.601059	0.657042	-2.163644
N	0.727891	-0.508279	-1.441933
C	-1.470230	-3.048834	-0.859088
H	-2.173103	-3.889696	-0.809103
H	-1.414651	-2.669849	-1.884831
H	-0.468279	-3.388396	-0.569722
C	-2.187298	-2.515958	1.886081
H	-2.584678	-1.798166	2.613116
H	-2.872366	-3.369989	1.811355
H	-1.211967	-2.868640	2.241503

10'

SCF done: -1231.621510

Pd	-0.541598	0.147547	0.272755
C	-0.851151	2.305306	1.200282
C	-1.605883	3.300152	0.600699
C	0.531046	2.068660	0.786938
C	-1.017147	4.102967	-0.404132
H	-2.658845	3.406089	0.860177
C	1.094620	2.863306	-0.308107
C	0.254967	3.890339	-0.858892
H	-1.609297	4.902421	-0.851366
H	0.673531	4.521751	-1.643285
C	2.394673	2.659166	-0.699321
C	3.220410	1.566428	-0.151466
H	2.824527	3.298362	-1.472707
C	1.497687	1.360233	1.614065
C	2.771186	1.165473	1.207154
H	4.294015	1.820829	-0.144311
H	1.193812	1.028534	2.607066
H	3.483073	0.666406	1.864150
C	-1.416229	1.160684	1.895373
H	-0.910535	0.767866	2.782627

H	-2.507458	1.124928	1.977113
P	-2.002673	-1.693976	0.213478
C	-3.725386	-1.224422	-0.255430
C	-3.988827	0.098113	-0.618385
C	-4.767861	-2.156204	-0.255606
C	-5.278023	0.483476	-0.975586
H	-3.175185	0.827015	-0.618277
C	-6.054246	-1.770524	-0.611528
H	-4.578836	-3.193521	0.025277
C	-6.309669	-0.448781	-0.970922
H	-5.474402	1.516843	-1.256066
H	-6.861113	-2.501642	-0.608049
H	-7.318477	-0.147228	-1.248268
C	1.921626	-0.197980	-1.386219
C	4.195325	-0.813020	-0.688781
C	5.550413	-0.745888	-1.018711
C	3.759171	-1.816228	0.180902
C	6.452825	-1.667174	-0.500056
H	5.896846	0.039047	-1.693122
C	4.661658	-2.738510	0.697645
H	2.703972	-1.871873	0.453923
C	6.010080	-2.668287	0.359237
H	7.505315	-1.605678	-0.772083
H	4.308580	-3.517998	1.371217
H	6.714584	-3.392857	0.764051
C	3.270781	0.259684	-1.185324
H	3.640812	0.693076	-2.124819
N	0.803511	-0.529648	-1.434314
C	-1.586578	-3.072868	-0.950303
H	-2.334702	-3.875072	-0.926014
H	-1.513743	-2.666448	-1.964752
H	-0.605621	-3.478900	-0.675452
C	-2.240262	-2.589463	1.818407
H	-2.613836	-1.880467	2.566452
H	-2.947346	-3.423834	1.728457
H	-1.271862	-2.975468	2.157787

TS4-11'

SCF done: -1231.626983

Pd	-0.508974	0.739916	-0.176373
C	0.129537	2.470025	1.112324
C	-0.437642	3.685225	0.609830
C	1.526697	2.157328	0.786748
C	0.284433	4.582679	-0.127837
H	-1.482194	3.884257	0.854805
C	2.238683	3.130108	-0.032079
C	1.630223	4.296895	-0.437481
H	-0.173206	5.503495	-0.482967
H	2.210101	5.004676	-1.031486
C	3.606631	2.855822	-0.373379
C	4.186725	1.678506	-0.061925
H	4.165355	3.634967	-0.893683
C	2.187647	1.000853	1.178367
C	3.418740	0.612364	0.567863
H	5.223406	1.482244	-0.337644
H	1.688442	0.277890	1.824842
H	4.001464	-0.144802	1.100516
C	-0.727968	1.553079	1.783068
H	-0.318886	0.805279	2.465451
H	-1.725656	1.903722	2.056179
P	-1.863906	-1.167733	-0.105075
C	-3.682827	-0.835154	-0.129129
C	-4.124693	0.488519	-0.161370
C	-4.624983	-1.867405	-0.086700
C	-5.486619	0.777522	-0.150329
H	-3.384193	1.290824	-0.198305
C	-5.984480	-1.579574	-0.075792
H	-4.301158	-2.909045	-0.060888
C	-6.416327	-0.255639	-0.106735
H	-5.820766	1.813411	-0.177317
H	-6.710824	-2.390140	-0.042143

H	-7.481637	-0.030551	-0.098229
C	1.919055	-0.241332	-1.595582
C	3.114019	-2.014080	-0.422664
C	4.311520	-2.728121	-0.289812
C	1.940548	-2.590571	0.083622
C	4.330236	-3.984223	0.304632
H	5.236177	-2.289515	-0.668720
C	1.958831	-3.848878	0.670714
H	1.007882	-2.028424	0.010007
C	3.154031	-4.555615	0.783048
H	5.271949	-4.525087	0.388559
H	1.029697	-4.282492	1.043078
H	3.169101	-5.543085	1.240650
C	3.119863	-0.647686	-0.973665
H	4.020010	-0.388590	-1.536396
N	0.843042	0.060911	-1.962168
C	-1.644306	-2.479428	-1.396847
H	-1.802962	-2.032235	-2.384170
H	-0.611709	-2.848901	-1.356098
H	-2.334217	-3.321191	-1.256576
C	-1.678961	-2.137877	1.470036
H	-2.033231	-1.517963	2.302135
H	-2.247849	-3.076355	1.452335
H	-0.616659	-2.358967	1.636980

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SCF done: -1231.643723

Pd	-0.417302	-0.341881	1.548657
C	0.493076	1.648089	2.012427
C	-0.723788	2.335002	2.420991
C	1.101067	2.054309	0.719462
C	-1.346381	3.231924	1.617487
H	-1.125852	2.089491	3.403736
C	0.348470	2.987937	-0.122323
C	-0.809255	3.546770	0.326577
H	-2.265323	3.714592	1.943925
H	-1.327828	4.269637	-0.304816
C	0.933920	3.368158	-1.391748
C	2.082094	2.844530	-1.843174
H	0.407168	4.126053	-1.973629
C	2.302969	1.601421	0.297674
C	2.798181	1.764601	-1.098337
H	2.491886	3.153047	-2.805879
H	2.903235	0.969368	0.950127
H	3.887919	1.945947	-1.098197
C	1.041789	0.680370	2.850603
H	2.021424	0.240680	2.667550
H	0.661208	0.579119	3.867251
P	-1.875287	-1.799051	0.371890
C	-3.132362	-0.936678	-0.675347
C	-2.901387	0.396456	-1.022722
C	-4.288409	-1.571102	-1.136391
C	-3.815977	1.085134	-1.812186
H	-1.986941	0.885301	-0.683211
C	-5.204722	-0.880900	-1.922735
H	-4.486310	-2.613672	-0.882372
C	-4.969996	0.449948	-2.259067
H	-3.622401	2.123816	-2.077380
H	-6.105847	-1.382851	-2.272438
H	-5.689231	0.990897	-2.872470
C	1.232303	0.092612	-2.085162
C	3.361144	-0.745515	-1.194470
C	4.698155	-0.998831	-1.495272
C	2.725846	-1.502315	-0.206704
C	5.396214	-1.996051	-0.821478
H	5.195839	-0.409506	-2.267541
C	3.424774	-2.495670	0.468565
H	1.678004	-1.305374	0.050525
C	4.760153	-2.746539	0.162637
H	6.438796	-2.188874	-1.068914
H	2.918187	-3.073126	1.241427

H	5.303947	-3.528577	0.689944
C	2.647974	0.396004	-1.884722
H	3.094611	0.552398	-2.880873
N	0.108695	-0.165364	-2.219340
C	-1.159001	-3.037386	-0.812803
H	-0.635722	-2.492018	-1.606024
H	-0.440653	-3.673894	-0.280905
H	-1.945305	-3.663227	-1.255257
C	-2.910723	-2.911951	1.442706
H	-3.546554	-2.299259	2.091108
H	-3.537346	-3.599108	0.859538
H	-2.239328	-3.502972	2.076661

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SCF done: -1231.603839

Pd	-0.685343	-0.732901	0.574625
C	0.500046	-2.187559	-0.735911
C	0.120309	-3.419486	-0.135123
C	1.861007	-1.759128	-0.631914
C	1.056119	-4.226177	0.501972
H	-0.915524	-3.745397	-0.234017
C	2.841401	-2.673857	-0.129410
C	2.394743	-3.868767	0.470513
H	0.746839	-5.156994	0.973045
H	3.141768	-4.535214	0.905152
C	4.217373	-2.396783	-0.316912
C	4.558437	-1.370191	-1.201868
H	4.958715	-3.102383	0.055461
C	2.346725	-0.403020	-0.906829
C	3.617721	-0.443593	-1.614313
H	5.577466	-1.313250	-1.587752
H	1.601695	0.279083	-1.335935
H	3.862328	0.330404	-2.338695
C	-0.570738	-1.440876	-1.367067
H	-0.316098	-0.636515	-2.061864
H	-1.454125	-2.009807	-1.668971
P	-2.188078	1.010414	0.254655
C	-3.922946	0.548409	-0.171392
C	-4.293457	-0.796239	-0.125079
C	-4.872544	1.508120	-0.535268
C	-5.595198	-1.178726	-0.435925
H	-3.547276	-1.541408	0.158107
C	-6.170795	1.126049	-0.850156
H	-4.601222	2.564034	-0.575264
C	-6.532606	-0.218393	-0.800660
H	-5.875757	-2.229825	-0.396402
H	-6.903850	1.878701	-1.135667
H	-7.550229	-0.515938	-1.048156
C	1.653769	0.207302	1.636118
C	2.921903	1.867446	0.381360
C	4.176844	2.302235	-0.057615
C	1.865295	2.788774	0.394630
C	4.366971	3.618177	-0.468804
H	5.006877	1.596482	-0.068227
C	2.056939	4.102097	-0.011656
H	0.883665	2.459979	0.746271
C	3.311487	4.523916	-0.448949
H	5.353041	3.939693	-0.801740
H	1.223076	4.803511	0.016205
H	3.465074	5.554302	-0.765143
C	2.695184	0.437895	0.697142
H	3.600015	-0.115852	0.980133
N	0.703616	-0.019402	2.293302
C	-1.701533	2.151333	-1.123177
H	-0.672853	2.497976	-0.958100
H	-1.734538	1.602068	-2.070963
H	-2.366322	3.022139	-1.188581
C	-2.377686	2.177879	1.680422
H	-3.036049	3.020683	1.433292
H	-2.787543	1.631423	2.536470
H	-1.386166	2.554139	1.960892

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SCF done: -1231.604448

Pd	-0.732449	-0.814552	0.506321
C	0.572558	-2.194223	-0.764970
C	0.180436	-3.416276	-0.139875
C	1.912484	-1.736052	-0.600727
C	1.097267	-4.168956	0.584272
H	-0.837406	-3.775323	-0.293251
C	2.892240	-2.614110	-0.027599
C	2.430612	-3.784514	0.608007
H	0.783087	-5.084562	1.081498
H	3.162653	-4.415119	1.116003
C	4.265729	-2.318824	-0.184188
C	4.602661	-1.345448	-1.142646
H	5.010077	-2.997041	0.230471
C	2.390727	-0.354574	-0.854860
C	3.665684	-0.450466	-1.606646
H	5.614855	-1.328940	-1.551304
H	1.641704	0.275242	-1.356698
H	3.875831	0.240251	-2.420476
C	-0.484587	-1.482146	-1.447770
H	-0.226843	-0.658729	-2.118144
H	-1.339156	-2.072105	-1.788119
P	-2.224491	0.963557	0.248316
C	-3.985186	0.556959	-0.129368
C	-4.346977	-0.779119	-0.307789
C	-4.957490	1.552525	-0.263868
C	-5.660528	-1.117252	-0.621454
H	-3.585272	-1.552959	-0.193376
C	-6.268818	1.215252	-0.575727
H	-4.695746	2.602543	-0.124802
C	-6.620497	-0.120682	-0.756916
H	-5.933078	-2.162236	-0.758991
H	-7.020360	1.996198	-0.679852
H	-7.648300	-0.383039	-1.002271
C	1.646727	0.211456	1.545381
C	2.945681	1.879918	0.319411
C	4.218315	2.315827	-0.054755
C	1.894003	2.801693	0.327674
C	4.431883	3.644593	-0.409882
H	5.040401	1.601327	-0.066050
C	2.107368	4.128850	-0.022952
H	0.897704	2.466916	0.628116
C	3.380218	4.554866	-0.395608
H	5.430829	3.971038	-0.695469
H	1.277538	4.834621	-0.002814
H	3.551915	5.594913	-0.668091
C	2.700725	0.427004	0.584964
H	3.603161	-0.089032	0.950188
N	0.722206	-0.000381	2.232698
C	-1.771213	2.120363	-1.131264
H	-0.726560	2.437790	-1.012320
H	-1.866729	1.592642	-2.086956
H	-2.416931	3.007673	-1.147293
C	-2.334320	2.120341	1.692267
H	-3.030363	2.948374	1.506273
H	-2.657676	1.560939	2.576535
H	-1.334957	2.525291	1.894135

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SCF done: -1231.639450

Pd	0.069132	0.629416	-0.116028
C	-1.999500	-1.215647	1.127448
C	-0.711943	-1.425492	0.563312
C	-3.160913	-1.317925	0.260104
C	-0.605441	-2.058951	-0.721527
H	0.121777	-1.548952	1.259715
C	-3.008149	-1.869808	-1.040568
C	-1.708853	-2.275213	-1.487516
H	0.380371	-2.377718	-1.064231

H	-1.622969	-2.747209	-2.466869
C	-4.136978	-2.009922	-1.869180
C	-5.385479	-1.601212	-1.447266
H	-4.003421	-2.444202	-2.861026
C	-4.441415	-0.891275	0.658674
C	-5.534105	-1.030654	-0.176289
H	-6.248570	-1.711427	-2.101770
H	-4.568054	-0.417074	1.631062
H	-6.512825	-0.687000	0.155072
C	-2.128853	-0.824185	2.468713
H	-3.055105	-1.016623	3.001496
H	-1.236535	-0.828882	3.093307
P	2.297921	0.012523	-0.641914
C	2.993594	-1.569962	0.016811
C	3.540931	-2.572425	-0.786848
C	2.918448	-1.778109	1.399536
C	4.011380	-3.753812	-0.218630
H	3.604340	-2.438622	-1.866544
C	3.397222	-2.952135	1.967390
H	2.477094	-1.006936	2.035541
C	3.943278	-3.944809	1.156880
H	4.434491	-4.527859	-0.857140
H	3.337034	-3.097259	3.044800
H	4.311631	-4.869230	1.598411
C	-2.088169	1.673385	1.569777
C	-0.499178	2.944156	0.114121
C	-0.130191	3.290878	-1.202652
C	0.292740	3.434501	1.174632
C	0.984477	4.089013	-1.445085
H	-0.743721	2.934863	-2.031046
C	1.399459	4.227620	0.922949
H	0.009675	3.187488	2.198354
C	1.753132	4.562666	-0.387065
H	1.243574	4.349731	-2.470543
H	1.992213	4.600020	1.757395
H	2.617114	5.197453	-0.576676
C	-1.651394	2.063853	0.329319
H	-2.403131	2.015766	-0.462722
N	-2.466251	1.139169	2.565947
C	3.592302	1.227592	-0.091026
H	3.565834	1.313357	1.001286
H	4.595887	0.920732	-0.412145
H	3.346515	2.211770	-0.510988
C	2.665516	-0.073791	-2.456924
H	2.033013	-0.832314	-2.933571
H	2.404378	0.901065	-2.887015
H	3.722761	-0.286097	-2.664341

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SCF done: -1231.674049

Pd	0.297272	-0.497685	-0.019191
C	-1.457815	-1.635600	-1.299178
C	-1.537068	-0.312450	-1.735518
C	-2.374120	-2.083579	-0.281866
C	-2.505733	0.585299	-1.210757
H	-0.913522	0.005031	-2.573760
C	-3.333637	-1.168759	0.241865
C	-3.381049	0.164742	-0.251026
H	-2.534546	1.611115	-1.577565
H	-4.127308	0.847376	0.156461
C	-4.235692	-1.615623	1.234126
C	-4.200435	-2.909722	1.694276
H	-4.965941	-0.907301	1.627345
C	-2.363295	-3.409623	0.208902
C	-3.255298	-3.814858	1.174553
H	-4.902548	-3.238729	2.458701
H	-1.623735	-4.111971	-0.174497
H	-3.228796	-4.839904	1.540432
C	-0.612092	-2.649719	-2.055669
H	-1.232797	-3.507026	-2.353419
H	-0.253126	-2.193219	-2.990940

P	0.631851	1.741732	0.808139	C	-1.522652	-2.0494280	0.911516
C	-0.484816	3.078850	0.185324	C	-3.608186	-0.8857160	1.439666
C	-1.520804	3.611283	0.955737	C	-5.011936	-0.9197390	1.459411
C	-0.387139	3.455827	-1.159144	C	-2.971169	0.3481180	1.675869
C	-2.433503	4.502892	0.397567	C	-5.753045	0.2305820	1.710849
H	-1.628933	3.327126	2.002336	H	-5.518638	-1.8682730	1.273624
C	-1.289324	4.355321	-1.714146	C	-3.712803	1.4894050	1.919865
H	0.397061	3.026184	-1.785623	H	-1.881204	0.3995910	1.654473
C	-2.320332	4.878910	-0.936519	C	-5.109538	1.4412000	1.938839
H	-3.236084	4.907844	1.012506	H	-6.840890	0.1760010	1.728226
H	-1.192833	4.644560	-2.759716	H	-3.198874	2.4341320	2.093233
H	-3.032923	5.578459	-1.370286	H	-5.687111	2.3423090	2.138267
C	1.032919	-2.408957	-0.470127	C	-2.864488	-2.0854280	1.119553
C	3.200913	-1.352557	0.269405	H	-3.370278	-3.0498200	1.144737
C	3.970473	-0.924052	1.359909	N	-0.395072	-1.8990000	0.560702
C	3.700513	-1.129418	-1.022392	C	2.800006	2.3561960	-0.300808
C	5.190750	-0.286538	1.167688	H	2.685760	2.1318050	-1.367529
H	3.593030	-1.092835	2.370217	H	1.867289	2.8065950	0.061354
C	4.916094	-0.487629	-1.211026	H	3.616280	3.0784610	-0.167402
H	3.119046	-1.464917	-1.881921	C	3.504734	1.4662540	2.308927
C	5.669883	-0.058377	-0.119491	H	3.823602	0.6487450	2.964297
H	5.772516	0.032807	2.031771	H	4.303496	2.2176210	2.249052
H	5.284612	-0.325243	-2.223335	H	2.606826	1.9232290	2.741682
H	6.624778	0.441581	-0.271702				
C	1.912258	-2.012986	0.511011				
H	1.715609	-2.365050	1.525762				
N	0.561646	-3.162530	-1.348620				
C	2.313822	2.395298	0.358290				
H	2.448462	2.375509	-0.728904				
H	2.468284	3.416171	0.730348				
H	3.064635	1.718977	0.790604				
C	0.661066	2.033876	2.642016				
H	-0.272900	1.696236	3.103998				
H	1.475399	1.422639	3.050765				
H	0.839534	3.088724	2.888631				

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SCF done: -1231.624209

Pd	1.352618	-0.7236570	0.561799
C	-1.931251	-1.1179550	-1.755253
C	-3.026688	-2.0028230	-1.719527
C	-2.195035	0.3064330	-1.673499
C	-4.351213	-1.5446510	-1.750555
H	-2.822774	-3.0729570	-1.758727
C	-3.544772	0.7528340	-1.670484
C	-4.604303	-0.1974320	-1.714443
H	-5.171792	-2.2599080	-1.760626
H	-5.629396	0.1740330	-1.704851
C	-3.822207	2.1335570	-1.580227
C	-2.802347	3.0497400	-1.467329
H	-4.863880	2.4557830	-1.581000
C	-1.171605	1.2629600	-1.542191
C	-1.469883	2.6061340	-1.436278
H	-3.024429	4.1126650	-1.390439
H	-0.132155	0.9380550	-1.479451
H	-0.662822	3.3291560	-1.326387
C	-0.648044	-1.6552160	-1.705243
H	0.253458	-1.0541940	-1.793995
H	-0.509107	-2.7274120	-1.817950
P	3.068381	0.7681400	0.638270
C	4.737399	0.2319690	0.026586
C	4.923473	-1.1120760	-0.300582
C	5.813252	1.1154480	-0.101663
C	6.161062	-1.5668680	-0.747861
H	4.079115	-1.7969680	-0.198615
C	7.047956	0.6647670	-0.553594
H	5.693762	2.1701860	0.151674
C	7.223424	-0.6787330	-0.876952
H	6.294056	-2.6183140	-0.998504
H	7.877408	1.3636420	-0.653452
H	8.190825	-1.0322470	-1.230971

14'

SCF done: -1231.662124

Pd	-1.163166	0.339917	-0.709224
C	2.298142	-1.775754	-1.413207
C	3.512219	-1.797549	-2.060593
C	2.244693	-1.974247	0.000294
C	4.716287	-2.016443	-1.358925
H	3.543229	-1.629598	-3.137806
C	3.466421	-2.174777	0.709613
C	4.691373	-2.196048	-0.001463
H	5.660479	-2.027933	-1.900137
H	5.615167	-2.348445	0.557102
C	3.434748	-2.321703	2.116982
C	2.248355	-2.269138	2.804588
H	4.378280	-2.469952	2.643154
C	1.033793	-1.939470	0.737637
C	1.038385	-2.077540	2.104770
H	2.236634	-2.378076	3.887838
H	0.086224	-1.751149	0.224445
H	0.097240	-2.039822	2.652126
C	1.058895	-1.425805	-2.179368
H	0.207830	-2.071118	-1.939982
H	1.235993	-1.499195	-3.260192
P	-2.883330	0.580574	0.763618
C	-4.603235	0.137183	0.225100
C	-4.817546	-0.214871	-1.107958
C	-5.688777	0.154568	1.105457
C	-6.094630	-0.542913	-1.555517
H	-3.964036	-0.226479	-1.788844
C	-6.963839	-0.175035	0.662065
H	-5.541350	0.427857	2.151707
C	-7.167929	-0.523476	-0.671304
H	-6.251036	-0.814668	-2.598470
H	-7.802584	-0.159772	1.356747
H	-8.167194	-0.780985	-1.019465
C	1.454888	0.880992	-1.863407
C	3.145373	2.114942	-0.590435
C	4.143393	3.094487	-0.631436
C	2.919727	1.432665	0.613861
C	4.900880	3.383130	0.497507
H	4.323663	3.631630	-1.563313
C	3.679375	1.722298	1.737534
H	2.141811	0.668533	0.667900
C	4.674472	2.697157	1.686405
H	5.673347	4.149099	0.445537
H	3.491222	1.176588	2.661251
H	5.269249	2.921787	2.570225

C	2.383377	1.812372	-1.804283
H	2.596196	2.381028	-2.710012
N	0.615983	-0.023852	-1.888614
C	-2.691180	-0.448073	2.305046
H	-2.637198	-1.506280	2.023714
H	-1.743373	-0.166434	2.780903
H	-3.510830	-0.302617	3.021324
C	-3.164057	2.252072	1.534764
H	-3.442180	2.965698	0.751842
H	-3.950197	2.230080	2.301483
H	-2.224503	2.588255	1.988881