

30

4-1 scf done: -692.373320

C	-2.394420	-0.113774	2.902986
C	-1.222147	-0.070405	3.588646
C	-2.434870	0.118581	1.496457
C	0.012491	0.070871	2.892163
C	-1.252586	0.430337	0.789338
C	0.011202	0.252994	1.476198
C	-3.683322	0.032585	0.812447
C	-3.771577	0.275537	-0.521510
C	-2.640175	0.758135	-1.240080
C	-1.386522	0.905683	-0.573150
H	-3.332380	-0.300610	3.420498
H	-1.201391	-0.205187	4.667377
H	-4.562474	-0.259937	1.381674
H	-4.717221	0.166821	-1.047054
C	-2.773814	1.161995	-2.586645
C	-0.371586	1.611318	-1.265409
C	-0.537282	2.027140	-2.569078
C	-1.735516	1.767766	-3.255101
H	-3.732208	1.011290	-3.078458
H	0.536476	1.887074	-0.743269
H	0.260034	2.578546	-3.060103
H	-1.854540	2.082492	-4.288130
C	2.437392	-0.060831	2.915823
C	1.236655	-0.045102	3.586542
C	2.439142	-0.004533	1.512086
C	1.259363	0.143654	0.814881
H	3.371710	-0.160284	3.461286
H	1.208592	-0.154008	4.668421
H	3.374374	-0.099541	0.966944
H	1.287903	0.114331	-0.267515

30

4TS scf done: -692.365335

C	-2.499595	-0.011235	1.204495
C	-1.897504	-0.008050	2.415102
C	-1.738908	-0.008143	-0.000101
C	-0.479980	-0.001482	2.500839
C	-0.317715	-0.001590	-0.000022
C	0.332558	0.001867	1.316924
C	-2.499456	-0.012069	-1.204783
C	-1.897226	-0.009724	-2.415323
C	-0.479692	-0.003224	-2.500901
C	0.332710	0.000943	-1.316895
H	-3.583596	-0.016260	1.123014
H	-2.478915	-0.010419	3.333670
H	-3.583467	-0.017034	-1.123423
H	-2.478531	-0.012728	-3.333955
C	0.097616	-0.001026	-3.790461

C	1.729780	0.007298	-1.568773
C	2.273896	0.009351	-2.835608
C	1.457412	0.005176	-3.973229
H	-0.573576	-0.004426	-4.646281
H	3.355493	0.014302	-2.941223
H	1.888778	0.006807	-4.970071
C	1.456954	0.007964	3.973385
C	0.097179	0.001620	3.790464
C	2.273569	0.011357	2.835855
C	1.729599	0.008413	1.568960
H	1.888205	0.010294	4.970275
H	-0.574111	-0.001191	4.646209
H	3.355154	0.016395	2.941591
H	2.442303	0.010877	-0.766602
H	2.442215	0.011442	0.766867

36

5-1 scf done: -845.837861

C	-2.369180	-0.206576	2.854286
C	-1.198630	-0.047483	3.532847
C	-2.414277	-0.018379	1.447430
C	0.024662	0.103925	2.827633
C	-1.232074	0.296527	0.732300
C	0.031747	0.131792	1.410822
C	-3.664605	-0.111111	0.764764
C	-3.769797	0.184921	-0.556668
C	-2.656058	0.735040	-1.256941
C	-1.396572	0.850750	-0.601317
H	-3.296222	-0.415955	3.382327
H	-1.171824	-0.097568	4.618595
H	-4.534955	-0.432129	1.332176
H	-4.719465	0.086575	-1.076931
C	-2.817892	1.248876	-2.563210
C	-0.401186	1.626096	-1.242520
C	-0.594702	2.152239	-2.500438
C	-1.802159	1.934436	-3.187332
H	-3.780091	1.120905	-3.054005
H	0.529180	1.825583	-0.724131
H	0.189776	2.749329	-2.957234
H	-1.943096	2.336427	-4.186862
C	2.448782	0.208678	2.916141
C	1.250176	0.189531	3.554777
C	2.511635	-0.002290	1.507251
C	1.306875	-0.102253	0.753524
C	3.757099	-0.203743	0.871017
C	3.826982	-0.576376	-0.450909
C	2.637644	-0.788993	-1.170272
C	1.413940	-0.559824	-0.581491
H	3.377322	0.300951	3.474275
H	1.198838	0.244904	4.639588

H	4.663763	-0.091761	1.461360
H	4.790309	-0.741293	-0.925593
H	0.510865	-0.751492	-1.148782
H	2.679635	-1.147866	-2.194982

36

5TS scf done: -845.796919

C	3.171188	-0.700447	-0.614485
C	3.151188	-0.666836	0.741722
C	1.984280	-0.444954	-1.338753
C	1.943637	-0.376664	1.417157
C	0.700322	-0.463948	-0.712551
C	0.678678	-0.427587	0.755097
C	2.170722	-0.009855	-2.688150
C	1.143281	0.502244	-3.401631
C	-0.185443	0.336301	-2.915905
C	-0.420231	-0.311547	-1.659387
H	4.105401	-0.805427	-1.160140
H	4.068838	-0.743980	1.319201
H	3.185048	0.005259	-3.078737
H	1.296784	0.952681	-4.378858
C	-1.259325	0.677612	-3.764130
C	-1.721926	-0.834225	-1.514079
C	-2.759131	-0.544148	-2.379818
C	-2.548655	0.284191	-3.486629
H	-1.033150	1.217242	-4.680964
H	-1.907482	-1.577709	-0.763486
H	-3.734536	-0.990131	-2.205659
H	-3.366303	0.544201	-4.152839
C	1.042885	0.670874	3.404930
C	2.090541	0.124851	2.748264
C	-0.271066	0.480086	2.889074
C	-0.469182	-0.229340	1.659793
C	-1.369237	0.862148	3.687353
C	-2.650106	0.454494	3.391796
C	-2.828457	-0.427771	2.321618
C	-1.766395	-0.759553	1.502236
H	1.167842	1.169250	4.362759
H	3.092927	0.160043	3.167344
H	-1.169801	1.446669	4.582619
H	-3.486847	0.746539	4.019937
H	-1.930271	-1.539414	0.784216
H	-3.798620	-0.882566	2.141082

42

6-1 scf done: -999.304861

C	-2.403586	-0.246876	2.864410
C	-1.222897	-0.135184	3.534020
C	-2.454208	-0.018637	1.462507
C	-0.000061	-0.000115	2.822767
C	-1.264996	0.242873	0.740906

C	-0.000076	-0.000142	1.400442
C	-3.716629	-0.005243	0.795034
C	-3.816440	0.344884	-0.513562
C	-2.674114	0.831311	-1.216117
C	-1.402124	0.839386	-0.575386
H	-3.333423	-0.427860	3.397943
H	-1.188832	-0.188697	4.619422
H	-4.599967	-0.286251	1.363599
H	-4.776827	0.329014	-1.023175
C	-2.809053	1.368449	-2.515270
C	-0.347107	1.512937	-1.231718
C	-0.510119	2.059445	-2.485181
C	-1.743304	1.961070	-3.151953
H	-3.785434	1.329104	-2.993074
H	0.607367	1.620001	-0.730534
H	0.322430	2.574358	-2.956410
H	-1.861093	2.378234	-4.148281
C	2.403436	0.246879	2.864345
C	1.222782	0.135038	3.533989
C	2.454045	0.018697	1.462433
C	1.264858	-0.243014	0.740856
C	3.716445	0.005608	0.794924
C	3.816290	-0.344411	-0.513696
C	2.674057	-0.831070	-1.216235
C	1.402083	-0.839477	-0.575466
H	3.333261	0.428005	3.397849
H	1.188737	0.188591	4.619389
H	4.599739	0.286783	1.363476
H	4.776658	-0.328307	-1.023335
C	2.809109	-1.368155	-2.515399
C	0.347282	-1.513443	-1.231732
C	0.510411	-2.059898	-2.485202
C	1.743520	-1.961096	-3.152046
H	3.785465	-1.328529	-2.993232
H	-0.607106	-1.620914	-0.730486
H	-0.321981	-2.575117	-2.956374
H	1.861402	-2.378231	-4.148375

42

6TS scf done: -999.243667

C	-2.131931	0.015300	3.349275
C	-0.899773	0.392011	3.777208
C	-2.492480	0.204199	1.991527
C	0.090372	0.737726	2.817240
C	-1.673300	0.977580	1.128709
C	-0.246262	1.068750	1.465091
C	-3.670890	-0.439468	1.495811
C	-4.072841	-0.282994	0.209485
C	-3.497218	0.770671	-0.561263
C	-2.387842	1.495745	-0.031598

H	-2.846833	-0.450319	4.023069
H	-0.596461	0.247188	4.810792
H	-4.196391	-1.113681	2.167893
H	-4.914038	-0.840619	-0.194129
C	-4.141353	1.230199	-1.728876
C	-2.215417	2.804206	-0.517663
C	-2.913119	3.282816	-1.607940
C	-3.833301	2.459256	-2.271120
H	-4.944734	0.628493	-2.147633
H	-1.589178	3.477602	0.048609
H	-2.758693	4.306197	-1.938543
H	-4.356074	2.817652	-3.153589
C	2.343932	0.137718	2.264925
C	1.426300	0.455631	3.213679
C	2.033307	0.327980	0.895082
C	0.871510	1.047180	0.512187
C	2.886004	-0.260137	-0.092702
C	2.646473	-0.099224	-1.418377
C	1.728539	0.913590	-1.827289
C	0.948452	1.586990	-0.839872
H	3.310812	-0.281903	2.531280
H	1.637208	0.308280	4.269649
H	3.694724	-0.897858	0.256145
H	3.237477	-0.617680	-2.168965
C	1.742664	1.391118	-3.154377
C	0.505516	2.878619	-1.176861
C	0.601582	3.378936	-2.459442
C	1.157727	2.595751	-3.480284
H	2.295446	0.826501	-3.901685
H	0.173759	3.525815	-0.378503
H	0.260446	4.388761	-2.669990
H	1.199740	2.969591	-4.499582

48

7-1 scf done: -1152.772227

C	3.491223	-0.488915	1.694744
C	2.807187	-0.329051	2.861908
C	2.792815	-0.733701	0.479860
C	1.390262	-0.205042	2.855509
C	1.379365	-0.759242	0.469265
C	0.683087	-0.242734	1.625075
C	3.520286	-0.965345	-0.726408
C	2.879059	-1.270800	-1.885161
C	1.474434	-1.517794	-1.886483
C	0.727996	-1.337171	-0.688496
H	4.578406	-0.501298	1.682852
H	3.331692	-0.248818	3.810881
H	4.603389	-0.871519	-0.699040
H	3.434203	-1.404153	-2.810538
C	0.831130	-2.008382	-3.044001

C	-0.602815	-1.812202	-0.669376
C	-1.201693	-2.316229	-1.802593
C	-0.492133	-2.382980	-3.014313
H	1.413074	-2.109071	-3.957329
H	-1.159432	-1.796507	0.259866
H	-2.227956	-2.669240	-1.753371
H	-0.975649	-2.762638	-3.910229
C	-0.679188	0.047801	4.077591
C	0.679361	-0.048070	4.077559
C	-1.390141	0.204852	2.855581
C	-0.683020	0.242618	1.625118
C	-2.807065	0.328867	2.862050
C	-3.491150	0.488811	1.694926
C	-2.792794	0.733676	0.480028
C	-1.379345	0.759207	0.469373
H	-1.237984	0.065495	5.010056
H	1.238197	-0.065822	5.009999
H	-3.331529	0.248576	3.811040
H	-4.578334	0.501202	1.683083
C	-3.520317	0.965407	-0.726192
C	-0.728022	1.337207	-0.688379
C	-1.474512	1.517914	-1.886322
C	-2.879139	1.270935	-1.884953
H	-4.603419	0.871589	-0.698782
H	-3.434324	1.404357	-2.810295
C	-0.831253	2.008566	-3.043838
C	0.602794	1.812226	-0.669288
C	0.492016	2.383146	-3.014186
C	1.201628	2.316315	-1.802502
H	-1.413236	2.109318	-3.957134
H	0.975496	2.762853	-3.910101
H	2.227897	2.669312	-1.753302
H	1.159451	1.796471	0.259928

48

7TS scf done: -1152.702386

C	3.950066	0.945850	0.678905
C	3.950066	0.945850	-0.678905
C	2.828502	0.418225	1.373379
C	2.828502	0.418225	-1.373379
C	1.559117	0.305713	0.734649
C	1.559117	0.305713	-0.734649
C	3.087032	-0.218918	2.622512
C	2.182737	-1.100297	3.128357
C	0.853636	-1.096808	2.623057
C	0.493315	-0.183235	1.606186
H	4.849177	1.188348	1.239853
H	4.849177	1.188348	-1.239853
H	4.076927	-0.115469	3.059325
H	2.426024	-1.742683	3.970793

C	-0.147707	-1.929815	3.212565
C	-0.878037	0.265560	1.656927
C	-1.871145	-0.546590	2.278854
C	-1.469128	-1.735115	2.956406
H	0.179418	-2.722356	3.881601
H	-2.227020	-2.384751	3.386958
C	2.182737	-1.100297	-3.128357
C	3.087032	-0.218918	-2.622512
C	0.853636	-1.096808	-2.623057
C	0.493315	-0.183235	-1.606186
C	-0.147707	-1.929815	-3.212565
C	-1.469128	-1.735115	-2.956406
C	-1.871145	-0.546590	-2.278854
C	-0.878037	0.265560	-1.656927
H	2.426024	-1.742683	-3.970793
H	4.076927	-0.115469	-3.059325
H	0.179418	-2.722356	-3.881601
H	-2.227020	-2.384751	-3.386958
C	-1.207279	1.609645	-1.392136
C	-3.193160	-0.066578	-2.385149
C	-1.207279	1.609645	1.392136
C	-3.193160	-0.066578	2.385149
C	-2.479639	2.092906	-1.608112
C	-3.498478	1.234733	-2.050901
C	-2.479639	2.092906	1.608112
C	-3.498478	1.234733	2.050901
H	-0.413366	2.281152	-1.082507
H	-2.695331	3.142333	-1.427266
H	-4.509573	1.610527	-2.181484
H	-3.950628	-0.717517	-2.815834
H	-0.413366	2.281152	1.082507
H	-2.695331	3.142333	1.427266
H	-4.509573	1.610527	2.181484
H	-3.950628	-0.717517	2.815834

54

8-1 scf done: -1306.240613

C	-3.394732	-2.382970	-0.407152
C	-4.076386	-1.218274	-0.219575
C	-1.983070	-2.373380	-0.594724
C	-3.372501	-0.000155	-0.000024
C	-1.280304	-1.142095	-0.577243
C	-1.956046	-0.000085	-0.000014
C	-1.269757	-3.588712	-0.784581
C	0.084006	-3.575518	-0.942715
C	0.775738	-2.347201	-1.129257
C	0.066150	-1.126296	-1.093570
H	-3.920668	-3.332499	-0.471113
H	-5.162622	-1.207473	-0.174080
H	-1.819380	-4.526267	-0.749614

H	0.647142	-4.503869	-0.998828
C	2.182505	-2.346024	-1.371338
C	0.720840	0.048909	-1.629751
C	2.128232	0.024585	-1.836258
C	2.847207	-1.192397	-1.643186
H	2.714060	-3.292836	-1.314434
H	3.924897	-1.191348	-1.787565
C	-3.394975	2.382656	0.407118
C	-4.076511	1.217893	0.219519
C	-1.983316	2.373203	0.594721
C	-1.280428	1.141985	0.577241
C	-1.270125	3.588600	0.784614
C	0.083637	3.575537	0.942778
C	0.775485	2.347285	1.129315
C	0.066015	1.126312	1.093598
H	-3.921008	3.332132	0.471079
H	-5.162745	1.206984	0.174009
H	-1.819837	4.526103	0.749643
H	0.646680	4.503943	0.998912
C	2.182249	2.346240	1.371408
C	0.720818	-0.048844	1.629756
C	2.128208	-0.024388	1.836261
C	2.847063	1.192671	1.643227
H	2.713714	3.293104	1.314533
H	3.924752	1.191724	1.787608
C	2.785721	-1.184939	2.300964
C	0.015436	-1.197790	2.056320
C	2.077352	-2.317012	2.630107
C	0.673985	-2.305732	2.539892
H	3.866528	-1.155881	2.419921
H	2.593902	-3.201535	2.992915
H	0.101760	-3.173458	2.855848
H	-1.067541	-1.199869	2.017875
C	2.785631	1.185186	-2.300998
C	0.015346	1.197778	-2.056338
C	2.077152	2.317183	-2.630167
C	0.673786	2.305770	-2.539942
H	3.866440	1.156227	-2.419958
H	2.593615	3.201746	-2.993002
H	0.101474	3.173436	-2.855908
H	-1.067632	1.199758	-2.017879

54

scf done: -1306.176536

C	-2.738646	-3.112491	0.589990
C	-3.274914	-2.642385	-0.568006
C	-1.573559	-2.498775	1.130161
C	-2.885165	-1.354198	-1.042746
C	-0.911945	-1.489516	0.385569
C	-1.743279	-0.689324	-0.512994

C	-1.046228	-2.898272	2.390659
C	0.128481	-2.375844	2.848345
C	0.974177	-1.683771	1.939300
C	0.499179	-1.376308	0.642941
H	-3.160547	-3.975198	1.099442
H	-4.131666	-3.128577	-1.027348
H	-1.624777	-3.593091	2.994498
H	0.496677	-2.605935	3.844876
C	2.343750	-1.443886	2.260956
C	1.478534	-1.295901	-0.416208
C	2.857803	-1.189688	-0.083287
C	3.247923	-1.150166	1.288154
H	2.657378	-1.553692	3.296409
H	4.295111	-0.988017	1.531021
C	-3.920980	0.701585	-1.710250
C	-3.843010	-0.651051	-1.823694
C	-2.987770	1.394348	-0.893799
C	-1.763363	0.774154	-0.518653
C	-3.389609	2.625494	-0.296339
C	-2.663885	3.153496	0.728240
C	-1.334505	2.694395	0.946302
C	-0.814054	1.664814	0.131378
H	-4.758006	1.251668	-2.133281
H	-4.614205	-1.213967	-2.343538
H	-4.352971	3.043649	-0.576874
H	-3.035442	3.992488	1.311113
C	-0.473591	3.351354	1.878341
C	0.599786	1.734632	-0.132100
C	1.452637	2.443911	0.760651
C	0.872990	3.151727	1.854479
H	-0.921810	4.036369	2.594342
H	1.524249	3.646561	2.570810
C	2.819802	2.591879	0.440496
C	1.112364	1.381176	-1.399623
C	3.298376	2.203290	-0.790596
C	2.422482	1.639915	-1.734794
H	3.470050	3.095896	1.152025
H	4.341021	2.368032	-1.048696
H	0.433262	0.959094	-2.132456
H	2.782247	1.390158	-2.727517
C	1.136921	-1.522475	-1.769351
H	0.093442	-1.667287	-2.031362
C	3.823403	-1.217617	-1.111053
H	4.871699	-1.111497	-0.840993
C	3.459604	-1.426236	-2.423270
C	2.103471	-1.599564	-2.748566
H	1.813265	-1.801616	-3.776209
H	4.217950	-1.477244	-3.200055

8TS scf done: -1306.169084

C	3.554004	2.279154	-0.848468
C	3.799857	1.206005	-1.646550
C	2.432361	2.272750	0.023929
C	3.077306	0.000195	-1.415389
C	1.424800	1.284849	-0.133125
C	1.850871	0.000098	-0.689570
C	2.361062	3.193759	1.109629
C	1.332192	3.129393	2.002137
C	0.161872	2.401514	1.648426
C	0.152127	1.639096	0.458921
H	4.226484	3.133318	-0.831239
H	4.670196	1.179852	-2.297159
H	3.192472	3.878347	1.257910
H	1.327296	3.736165	2.903956
C	-1.054523	2.576915	2.377430
C	-1.108031	1.555819	-0.237093
C	-2.315570	1.857412	0.455051
C	-2.253497	2.245540	1.826544
H	-1.002274	3.032018	3.363780
H	-3.180177	2.398840	2.374274
C	3.554224	-2.278779	-0.848688
C	3.799955	-1.205533	-1.646679
C	2.432625	-2.272541	0.023768
C	1.424968	-1.284726	-0.133174
C	2.361469	-3.193595	1.109439
C	1.332648	-3.129349	2.002020
C	0.162240	-2.401557	1.648409
C	0.152365	-1.639112	0.458929
H	4.226767	-3.132896	-0.831579
H	4.670269	-1.179249	-2.297316
H	3.192944	-3.878118	1.257648
H	1.327864	-3.736152	2.903819
C	-1.054107	-2.577044	2.377476
C	-1.107824	-1.555922	-0.237030
C	-2.315307	-1.857615	0.455162
C	-2.253134	-2.245737	1.826655
H	-1.001781	-3.032144	3.363823
H	-3.179776	-2.399087	2.374435
C	-3.529188	-1.914851	-0.260034
C	-1.156404	-1.451122	-1.643867
C	-3.545889	-1.797901	-1.632112
C	-2.342316	-1.598864	-2.327953
H	-4.447440	-2.114876	0.287601
H	-4.481754	-1.884970	-2.177266
H	-0.228534	-1.298864	-2.187250
H	-2.347054	-1.545118	-3.413257
C	-1.156552	1.451012	-1.643931
H	-0.228646	1.298830	-2.187276

C	-3.529427	1.914551	-0.260190
H	-4.447714	2.114516	0.287409
C	-3.546069	1.797577	-1.632265
C	-2.342454	1.598632	-2.328058
H	-2.347146	1.544887	-3.413363
H	-4.481921	1.884563	-2.177457

60

9-1 scf done: -1459.709618

C	-2.932815	1.746375	-1.915634
C	-2.379320	2.931052	-1.530462
C	-2.198931	0.531811	-1.802465
C	-1.153034	2.947384	-0.807996
C	-0.886478	0.552451	-1.269379
C	-0.496944	1.726663	-0.523931
C	-2.771177	-0.702811	-2.213962
C	-2.058660	-1.859736	-2.113980
C	-0.674517	-1.829219	-1.788313
C	-0.046245	-0.599221	-1.489143
H	-3.921016	1.714635	-2.367885
H	-2.893861	3.872369	-1.707778
H	-3.800815	-0.708904	-2.562549
H	-2.517100	-2.817449	-2.347610
C	0.086408	-3.036966	-1.790321
C	1.403300	-0.561244	-1.506097
C	2.129578	-1.784691	-1.479689
C	1.427652	-3.023083	-1.574275
H	-0.440250	-3.974675	-1.950353
H	1.996005	-3.949584	-1.539988
C	0.586327	4.171391	0.348362
C	-0.584932	4.171532	-0.348671
C	1.154032	2.947124	0.807863
C	0.497590	1.726567	0.523907
C	2.380238	2.930517	1.530461
C	2.933300	1.745724	1.915898
C	2.199039	0.531376	1.802838
C	0.886656	0.552340	1.269581
H	1.077358	5.104408	0.614079
H	-1.075692	5.104668	-0.614472
H	2.895050	3.871700	1.707699
H	3.921438	1.713736	2.368268
C	2.770854	-0.703352	2.214609
C	0.046058	-0.599073	1.489352
C	0.673955	-1.829216	1.788725
C	2.058023	-1.860084	2.114655
H	3.800445	-0.709702	2.563331
H	2.516161	-2.817905	2.348441
C	-0.087269	-3.036775	1.790632
C	-1.403492	-0.560744	1.506008
C	-1.428454	-3.022579	1.574264

C	-2.130056	-1.784021	1.479460
H	0.439129	-3.974606	1.950806
H	-1.997021	-3.948945	1.539877
C	3.540880	-1.759746	-1.434987
C	2.144828	0.634370	-1.647437
C	4.231828	-0.571440	-1.489525
C	3.522009	0.633154	-1.633829
H	4.074249	-2.706398	-1.382905
H	5.318103	-0.565677	-1.459957
H	4.058722	1.571624	-1.741091
H	1.619044	1.570646	-1.790039
C	-3.541341	-1.758755	1.434407
C	-2.144791	0.635034	1.647186
C	-4.232031	-0.570293	1.488759
C	-3.521970	0.634134	1.633239
H	-4.074914	-2.705286	1.382222
H	-5.318298	-0.564283	1.458941
H	-4.058491	1.572729	1.740367
H	-1.618844	1.571190	1.789938

60

9-2 scf done: -1459.643110

C	2.607141	-3.242581	0.246426
C	2.253569	-3.140943	1.556561
C	2.478871	-2.093749	-0.590422
C	1.472271	-2.035581	1.995051
C	1.666790	-0.989256	-0.205077
C	0.901375	-1.167376	1.029579
C	3.415660	-1.981957	-1.652660
C	3.843074	-0.745909	-2.025814
C	3.252183	0.409142	-1.451126
C	2.008533	0.312111	-0.767115
H	3.176103	-4.094244	-0.117063
H	2.546932	-3.895299	2.282363
H	3.915735	-2.878499	-2.010127
H	4.698568	-0.624247	-2.685690
C	3.997586	1.624459	-1.422899
C	1.375061	1.588163	-0.485680
C	2.211264	2.698098	-0.229893
C	3.562395	2.677314	-0.677244
H	4.971869	1.641136	-1.904807
H	4.183971	3.555438	-0.521686
C	0.504686	-0.714680	3.769214
C	1.265736	-1.776922	3.380849
C	-0.368671	-0.109470	2.821584
C	-0.317995	-0.518299	1.461247
C	-1.391066	0.779793	3.244855
C	-2.432282	1.068308	2.415120
C	-2.594642	0.344641	1.202654
C	-1.559014	-0.497620	0.724145

H	0.439665	-0.414535	4.811749
H	1.793280	-2.391389	4.105984
H	-1.344295	1.188820	4.251104
H	-3.218403	1.752852	2.723182
C	-1.888400	-1.440720	-0.335194
C	-3.848157	0.407438	0.530562
C	-0.019833	1.876733	-0.686850
C	1.650225	3.886553	0.327033
C	-3.161555	-1.348563	-0.976749
C	-4.116277	-0.388909	-0.535875
C	-0.558789	3.112307	-0.228670
C	0.301806	4.055480	0.404066
H	-5.074282	-0.332064	-1.047460
H	-4.593979	1.105511	0.902684
H	-0.124077	4.967247	0.815895
H	2.328757	4.673507	0.648068
C	-1.066121	-2.528173	-0.714565
C	-3.490764	-2.230452	-2.029325
C	-0.796427	1.098316	-1.576077
C	-1.886602	3.458068	-0.564446
C	-2.611959	2.686081	-1.441335
C	-2.044375	1.515819	-1.977215
C	-1.417004	-3.389027	-1.732564
C	-2.627299	-3.225294	-2.424669
H	-0.148596	-2.724470	-0.178468
H	-0.751214	-4.209740	-1.985202
H	-2.893258	-3.897740	-3.235632
H	-4.458994	-2.116515	-2.512206
H	-0.366158	0.192368	-1.991501
H	-2.599508	0.924690	-2.698619
H	-3.612908	2.987278	-1.737991
H	-2.295188	4.389826	-0.179459

60

9-3 scf done: -1459.646623

C	3.661686	-1.202926	-2.031185
C	3.552372	-2.251235	-1.170495
C	3.028857	0.027504	-1.699909
C	2.700960	-2.148530	-0.038135
C	1.946480	0.067109	-0.776446
C	1.699401	-1.141440	0.004802
C	3.717774	1.217977	-2.075863
C	3.565302	2.335292	-1.314701
C	2.509104	2.411146	-0.364456
C	1.520269	1.394925	-0.342255
H	4.378756	-1.223325	-2.847948
H	4.184475	-3.129799	-1.274173
H	4.500296	1.154047	-2.827492
H	4.231261	3.187539	-1.425135
C	2.433234	3.483974	0.568892

C	0.242169	1.804076	0.182737
C	0.224520	2.785960	1.200335
C	1.388316	3.566872	1.442237
H	3.254404	4.195579	0.604977
H	1.365573	4.322850	2.223048
C	2.353381	-2.646507	2.295998
C	2.972954	-2.937698	1.118678
C	1.182607	-1.834436	2.287951
C	0.710171	-1.312702	1.056705
C	0.410396	-1.640858	3.464826
C	-0.844147	-1.111026	3.385707
C	-1.470184	-0.979813	2.116900
C	-0.713798	-1.164639	0.932260
H	2.666320	-3.106578	3.229747
H	3.779584	-3.664677	1.070225
H	0.835976	-1.935251	4.421079
H	-1.430900	-0.927379	4.282242
C	-1.429996	-1.494236	-0.286941
C	-2.883522	-0.811915	2.046028
C	-1.005915	1.534777	-0.495509
C	-1.008352	3.105171	1.844631
C	-2.853514	-1.428336	-0.290267
C	-3.550889	-1.005876	0.878779
C	-2.222578	2.005095	0.072907
C	-2.193601	2.682611	1.327763
H	-4.632134	-0.903220	0.831066
H	-3.420712	-0.574784	2.961207
H	-3.134989	2.955860	1.798336
H	-0.981613	3.748690	2.720951
C	-0.801838	-2.028148	-1.437563
C	-3.571283	-1.824854	-1.438409
C	-1.040870	1.032441	-1.816550
C	-3.422177	1.901469	-0.663330
C	-3.420813	1.420864	-1.952709
C	-2.214946	0.995140	-2.535006
C	-1.527560	-2.433711	-2.536007
C	-2.927102	-2.319698	-2.548779
H	0.274295	-2.148295	-1.452095
H	-1.008304	-2.853242	-3.393599
H	-3.495488	-2.634748	-3.419792
H	-4.656008	-1.746543	-1.420136
H	-0.115728	0.708300	-2.281512
H	-2.207497	0.621666	-3.554482
H	-4.345102	1.375447	-2.522189
H	-4.343671	2.254937	-0.206053

60

9TS scf done: -1459.638978

C	-3.673859	-0.680353	-2.277729
C	-3.673817	0.681049	-2.277579

C	-2.932442	-1.374940	-1.286509
C	-2.932346	1.375373	-1.286215
C	-1.867110	-0.730335	-0.597294
C	-1.867049	0.730548	-0.597155
C	-3.457068	-2.618297	-0.818041
C	-3.094634	-3.071713	0.411607
C	-1.940985	-2.531268	1.052075
C	-1.158604	-1.566831	0.368082
H	-4.359337	-1.238635	-2.910502
H	-4.359264	1.239512	-2.910226
H	-4.271852	-3.078588	-1.370843
H	-3.621283	-3.893741	0.889738
C	-1.513097	-3.002486	2.322620
C	0.246814	-1.586303	0.671240
C	0.646598	-2.017635	1.959740
C	-0.298382	-2.631163	2.823479
H	-2.179169	-3.650973	2.886436
H	0.015319	-2.936863	3.818412
C	-3.094402	3.071782	0.412280
C	-3.456889	2.618660	-0.817460
C	-1.940755	2.531144	1.052591
C	-1.158456	1.566807	0.368365
C	-1.512767	3.002100	2.323199
C	-0.298038	2.630626	2.823914
C	0.646859	2.017213	1.960004
C	0.246977	1.586153	0.671445
H	-3.620992	3.893735	0.890604
H	-4.271659	3.079119	-1.370143
H	-2.178769	3.650522	2.887172
H	0.015742	2.936135	3.818881
C	1.262574	1.535612	-0.361965
C	2.027774	1.991306	2.320549
C	1.262474	-1.535608	-0.362100
C	2.027492	-1.991888	2.320368
C	2.632594	1.668101	0.004973
C	2.988040	1.790257	1.381148
C	2.632465	-1.668264	0.004890
C	2.987823	-1.790723	1.381059
H	4.041619	1.807478	1.649693
H	2.295020	2.201070	3.353588
H	4.041386	-1.808078	1.649661
H	2.294668	-2.201880	3.353379
C	0.946176	1.566037	-1.738583
C	3.619248	1.760902	-0.998368
C	0.946157	-1.565702	-1.738743
C	3.619171	-1.760933	-0.998413
C	3.277631	-1.786976	-2.330803
C	1.924895	-1.703568	-2.697612
C	1.924867	1.704033	-2.697481

C	3.277632	1.787245	-2.330733
H	-0.092254	1.509982	-2.046219
H	1.644036	1.743128	-3.746536
H	4.046273	1.880777	-3.093029
H	4.660533	1.842463	-0.694467
H	-0.092249	-1.509487	-2.046430
H	1.644122	-1.742412	-3.746692
H	4.046308	-1.880409	-3.093074
H	4.660432	-1.842630	-0.694467

66

10-1 scf done: -1613.177602

C	-1.843728	3.129628	-1.566224
C	-0.938885	3.818919	-0.814072
C	-1.728763	1.717957	-1.723958
C	0.000307	3.122173	-0.000084
C	-0.676009	1.030608	-1.077455
C	0.000190	1.709263	0.000007
C	-2.660251	0.986428	-2.512824
C	-2.542076	-0.365263	-2.637198
C	-1.380862	-1.039775	-2.163855
C	-0.352618	-0.304322	-1.523173
H	-2.632311	3.649651	-2.104455
H	-0.959046	4.905366	-0.773931
H	-3.497678	1.517908	-2.957632
H	-3.305629	-0.945626	-3.149153
C	-1.242059	-2.444719	-2.331533
C	0.938226	-0.933627	-1.371242
C	0.998180	-2.344301	-1.427674
C	-0.125538	-3.085724	-1.886589
H	-2.064764	-2.999051	-2.776066
H	-0.048446	-4.169150	-1.937317
C	1.844278	3.129526	1.566142
C	0.939619	3.818867	0.813835
C	1.729039	1.717884	1.724105
C	0.676222	1.030621	1.077612
C	2.660265	0.986348	2.513247
C	2.541815	-0.365307	2.637852
C	1.380585	-1.039690	2.164412
C	0.352545	-0.304167	1.523479
H	2.632904	3.649480	2.104375
H	0.959952	4.905306	0.773550
H	3.497733	1.517742	2.958078
H	3.305200	-0.945723	3.150000
C	1.241613	-2.444624	2.332137
C	-0.938347	-0.933378	1.371332
C	-0.998391	-2.344040	1.427724
C	0.125166	-3.085553	1.886931
H	2.064193	-2.998991	2.776858
H	0.047974	-4.168971	1.937629

C	-2.196310	-3.023443	1.052133
C	-2.192273	-0.214002	1.253166
C	-3.314621	-2.335888	0.702540
C	-3.361075	-0.917606	0.847232
H	-2.184410	-4.110639	1.033583
H	-4.212345	-2.858302	0.380409
C	2.196157	-3.023761	-1.052351
C	2.192218	-0.214317	-1.253314
C	3.314568	-2.336265	-0.702968
C	3.361062	-0.917974	-0.847626
H	2.184218	-4.110958	-1.033823
H	4.212323	-2.858725	-0.380997
C	-4.574460	-0.216489	0.670969
C	-2.345656	1.141315	1.627675
C	-4.667522	1.124879	0.961154
C	-3.547651	1.797139	1.481264
H	-5.446421	-0.768825	0.327532
H	-5.608539	1.651891	0.828360
H	-3.627379	2.839593	1.776581
H	-1.504933	1.670164	2.059692
C	4.574491	-0.216886	-0.671572
C	2.345529	1.141013	-1.627802
C	3.547567	1.796807	-1.481607
C	4.667512	1.124493	-0.961729
H	1.504692	1.669881	-2.059585
H	3.627280	2.839272	-1.776887
H	5.608565	1.651482	-0.829083
H	5.446514	-0.769232	-0.328310

66

10-2 scf done: -1613.099277

C	0.751202	1.301531	3.677760
C	-0.314778	0.481010	3.890224
C	1.267503	1.476895	2.364012
C	-0.705283	-0.429617	2.871056
C	0.646622	0.822401	1.266330
C	-0.076467	-0.386905	1.595589
C	2.427975	2.273624	2.149449
C	2.884283	2.469954	0.884607
C	2.005769	2.214484	-0.209484
C	0.787479	1.504217	-0.024531
H	1.187589	1.882359	4.486614
H	-0.797273	0.419213	4.862164
H	2.960672	2.663790	3.013027
H	3.812900	3.001139	0.694137
C	2.232681	2.981796	-1.384080
C	-0.338366	1.922087	-0.853055
C	-0.145001	3.059167	-1.685479
C	1.163005	3.430450	-2.093716
H	3.233353	3.358588	-1.579701

H	1.280547	4.177942	-2.874420
C	-1.873300	-2.458126	2.283137
C	-1.658113	-1.443425	3.161503
C	-1.030705	-2.612166	1.148257
C	-0.055430	-1.622845	0.831527
C	-1.150800	-3.785559	0.362289
C	-0.378305	-3.961405	-0.745841
C	0.666520	-3.050025	-1.038600
C	0.939214	-1.976011	-0.156873
H	-2.627674	-3.216255	2.476662
H	-2.202843	-1.388832	4.100804
H	-1.911965	-4.512979	0.632154
H	-0.529693	-4.813432	-1.404603
C	2.271635	-1.405695	-0.252403
C	1.444982	-3.215397	-2.226956
C	-1.732062	1.544763	-0.672847
C	-1.216402	3.970605	-1.926806
C	3.012736	-1.558404	-1.457307
C	2.516806	-2.421126	-2.482009
C	-2.690962	2.579903	-0.637819
C	-2.394831	3.826636	-1.259683
H	3.077373	-2.515367	-3.408812
H	1.139191	-3.982268	-2.935129
H	-3.161629	4.596479	-1.292027
H	-1.015029	4.853566	-2.528078
C	2.949264	-0.867304	0.862819
C	4.296420	-0.980915	-1.566849
C	-2.257593	0.210078	-0.766769
C	-3.997030	2.305339	-0.129152
C	-4.407172	1.026909	0.097449
C	-3.597521	-0.052231	-0.363633
C	4.232534	-0.376465	0.755016
C	4.897051	-0.382117	-0.482883
H	2.466113	-0.883740	1.831667
H	4.728971	0.016508	1.637367
H	5.896601	0.035356	-0.569580
H	4.827457	-1.072011	-2.511797
H	-5.405151	0.818482	0.475368
H	-4.670838	3.143254	0.034403
C	-4.165345	-1.318371	-0.628016
C	-1.596912	-0.752775	-1.564326
C	-3.506588	-2.226958	-1.423305
C	-2.233827	-1.914331	-1.934429
H	-5.175005	-1.520688	-0.277248
H	-3.980615	-3.168766	-1.686692
H	-1.743685	-2.597677	-2.619776
H	-0.614697	-0.516707	-1.961533

66

10-3 scf done: -1613.103680

C	-2.431253	2.884887	1.914134
C	-2.152697	2.071154	2.969879
C	-2.181570	2.424073	0.587529
C	-1.283396	0.957562	2.784800
C	-1.490430	1.199386	0.367261
C	-0.710896	0.728815	1.506158
C	-2.761082	3.125172	-0.500529
C	-2.991061	2.477507	-1.673984
C	-2.769323	1.075430	-1.731436
C	-1.906285	0.429488	-0.800134
H	-2.983089	3.812045	2.045436
H	-2.505848	2.298909	3.972308
H	-3.112587	4.141700	-0.341606
H	-3.526446	2.961988	-2.486417
C	-3.684002	0.327391	-2.530493
C	-1.916485	-1.030813	-0.831373
C	-3.121624	-1.641309	-1.261592
C	-3.963587	-0.956543	-2.182390
H	-4.287332	0.854701	-3.264804
H	-4.806193	-1.489435	-2.615877
C	0.061797	-0.817340	3.716238
C	-0.914155	0.121158	3.874043
C	0.909520	-0.758241	2.576339
C	0.615837	0.149398	1.518409
C	2.115402	-1.505766	2.557887
C	3.062762	-1.261330	1.611568
C	2.915579	-0.172161	0.713505
C	1.720512	0.591680	0.695703
H	0.299628	-1.521056	4.509750
H	-1.445648	0.230319	4.816150
H	2.272716	-2.257097	3.327576
H	3.979543	-1.844282	1.575704
C	1.769922	1.867464	-0.003891
C	4.002356	0.162457	-0.145310
C	-0.868865	-1.947589	-0.460090
C	-3.461658	-2.938300	-0.785047
C	2.836791	2.126390	-0.914990
C	3.937877	1.226329	-0.986210
C	-1.240025	-3.203269	0.077791
C	-2.592548	-3.634474	0.001597
H	4.752720	1.447733	-1.671600
H	4.877581	-0.481978	-0.132866
H	-2.867475	-4.593737	0.432778
H	-4.441548	-3.338814	-1.032972
C	0.909019	2.950429	0.281501
C	2.855821	3.328934	-1.655705
C	0.484543	-1.806887	-0.952731
C	-0.232693	-4.118021	0.505077
C	1.066587	-3.929976	0.153238

C	1.426887	-2.841391	-0.693381
C	0.968150	4.134518	-0.421072
C	1.917055	4.311474	-1.441139
H	0.217489	2.873649	1.108422
H	0.284136	4.939325	-0.165944
H	1.946013	5.236132	-2.011163
H	3.659191	3.480058	-2.373562
H	1.828381	-4.656849	0.424913
H	-0.540180	-5.012601	1.041658
C	2.674037	-2.834327	-1.356266
C	0.847384	-0.800102	-1.879305
C	2.973160	-1.872234	-2.291264
C	2.047838	-0.846098	-2.550241
H	3.377868	-3.636248	-1.143466
H	3.921744	-1.896052	-2.820677
H	2.282903	-0.073975	-3.276870
H	0.145226	-0.003962	-2.101398

66

10-4 scf done: -1613.113211

C	3.487845	-0.483134	-2.683578
C	3.349663	-1.725706	-2.145749
C	2.917926	0.637797	-2.025779
C	2.752756	-1.855567	-0.863014
C	1.915799	0.447561	-1.035458
C	1.922828	-0.827440	-0.333644
C	3.486192	1.929610	-2.231443
C	3.148904	2.951451	-1.398510
C	1.974581	2.843733	-0.598165
C	1.200551	1.654745	-0.648390
H	4.116316	-0.316213	-3.554934
H	3.856271	-2.583357	-2.580893
H	4.286729	2.033363	-2.959302
H	3.688446	3.894958	-1.410839
C	1.496553	3.957978	0.139556
C	-0.221126	1.807700	-0.485475
C	-0.685241	2.951250	0.215110
C	0.225821	3.957177	0.632712
H	2.152815	4.813996	0.276192
H	-0.149313	4.796220	1.213344
C	3.216971	-2.734126	1.321524
C	3.245659	-2.902484	-0.029100
C	2.427145	-1.696954	1.891418
C	1.524277	-0.983242	1.062508
C	2.535916	-1.351687	3.269013
C	1.761477	-0.354064	3.782758
C	0.614115	0.075218	3.057504
C	0.379119	-0.432413	1.751113
H	3.781636	-3.385425	1.984046
H	3.817590	-3.707945	-0.482220

H	3.299580	-1.841682	3.867657
H	1.914735	0.018886	4.792106
C	-0.375511	0.881096	3.678944
C	-0.996382	-0.595742	1.341759
C	-1.979619	0.160733	2.028097
C	-1.615256	0.988379	3.124978
H	-0.135832	1.371718	4.619165
H	-2.381386	1.604848	3.588378
C	-3.358849	0.032200	1.698328
C	-1.454337	-1.647398	0.446422
C	-3.776975	-0.867129	0.771669
C	-2.847324	-1.747288	0.150161
H	-4.071491	0.666868	2.219038
C	-1.191833	1.040781	-1.254209
C	-2.082209	3.193883	0.362045
H	-2.396664	4.032027	0.979525
C	-2.991872	2.454214	-0.320763
C	-2.566602	1.413629	-1.196347
C	-3.509795	0.772261	-2.027840
C	-0.839729	0.032548	-2.182987
C	-0.624327	-2.676191	-0.061728
C	-3.316061	-2.753638	-0.721944
C	-2.464155	-3.689467	-1.258210
C	-1.777390	-0.573242	-2.989516
C	-1.108686	-3.661749	-0.893382
C	-3.129816	-0.205419	-2.915961
H	-4.054972	2.670274	-0.247486
H	-4.551153	1.078316	-1.955162
H	-3.865155	-0.689472	-3.552738
H	-1.460919	-1.345481	-3.684546
H	0.193752	-0.270343	-2.282185
H	0.413362	-2.729243	0.234117
H	-0.431352	-4.432093	-1.252228
H	-2.839614	-4.460828	-1.925233
H	-4.379366	-2.780563	-0.949295
H	-4.830032	-0.958008	0.516936

66

10TS scf done: -1613.106029

C	-3.022258	-3.060944	-0.875196
C	-3.084836	-2.269344	-1.980510
C	-2.376789	-2.589751	0.299008
C	-2.728512	-0.896663	-1.853750
C	-1.549285	-1.438055	0.228396
C	-1.925937	-0.441754	-0.768922
C	-2.641081	-3.194645	1.562733
C	-2.127134	-2.639164	2.694972
C	-1.029059	-1.737292	2.585138
C	-0.570508	-1.340985	1.299660
H	-3.500272	-4.037234	-0.853611

H	-3.598638	-2.600041	-2.879310
H	-3.346093	-4.020873	1.604323
H	-2.433498	-2.974403	3.682370
C	-0.282071	-1.374566	3.736066
C	0.853009	-1.151374	1.150432
C	1.604145	-0.885213	2.325396
C	0.974175	-0.866678	3.598620
H	-0.711246	-1.558417	4.717955
H	1.562600	-0.589409	4.469686
C	-3.708421	1.265428	-2.186112
C	-3.452013	0.019307	-2.669652
C	-3.053252	1.718341	-1.009879
C	-1.942015	0.992999	-0.505817
C	-3.548766	2.844607	-0.290303
C	-2.972590	3.205182	0.890502
C	-1.677589	2.707238	1.211625
C	-1.061771	1.758864	0.351717
H	-4.439335	1.914574	-2.662026
H	-3.961789	-0.354188	-3.553931
H	-4.450168	3.332685	-0.652129
H	-3.417097	3.963928	1.529342
C	-0.933824	3.254260	2.289595
C	0.370511	1.804816	0.243721
C	1.094107	2.394375	1.311005
C	0.405754	3.018834	2.384944
H	-1.445885	3.886572	3.010778
H	0.984553	3.420713	3.212948
C	2.516038	2.463260	1.266668
C	1.085965	1.521845	-0.991007
C	3.200057	2.082226	0.158530
C	2.505563	1.658806	-1.011039
H	3.039910	2.851907	2.136736
C	1.591439	-1.502504	-0.057004
C	3.023658	-0.775591	2.278905
H	3.547329	-0.504454	3.192569
C	3.709733	-1.062564	1.145335
C	3.019780	-1.480081	-0.027756
C	3.761799	-1.903079	-1.151162
C	0.991948	-2.002353	-1.236607
C	0.452624	1.255113	-2.228055
C	3.221919	1.424959	-2.204120
C	2.574066	1.120256	-3.377375
C	1.738615	-2.422009	-2.315958
C	1.171909	1.062624	-3.386761
C	3.140031	-2.366877	-2.285312
H	4.795786	-1.012566	1.121978
H	4.847452	-1.862696	-1.094013
H	3.723095	-2.692926	-3.142273
H	1.227878	-2.801195	-3.196914

H	-0.083676	-2.080176	-1.305036
H	-0.626778	1.228114	-2.288606
H	0.641409	0.868357	-4.315015
H	3.138045	0.945862	-4.289530
H	4.306185	1.506805	-2.177860
H	4.285426	2.137938	0.127551

72

11-1 scf done: -1766.645668

C	-2.335197	-1.261516	2.612717
C	-1.935762	-2.445380	2.067722
C	-1.622456	-0.058261	2.337268
C	-0.935366	-2.470881	1.053614
C	-0.513165	-0.092682	1.460813
C	-0.361706	-1.255296	0.621921
C	-2.007092	1.176732	2.930363
C	-1.322397	2.319483	2.645054
C	-0.096778	2.271256	1.921868
C	0.404237	1.024791	1.470704
C	0.630837	3.462759	1.653438
C	1.790800	0.960562	1.070581
C	2.428794	2.164115	0.694108
C	1.808563	3.413541	0.970645
C	0.493550	-3.693321	-0.470930
C	-0.493543	-3.693321	0.470935
C	0.935370	-2.470881	-1.053611
C	0.361707	-1.255296	-0.621920
C	1.935766	-2.445380	-2.067719
C	2.335198	-1.261515	-2.612716
C	1.622456	-0.058262	-2.337269
C	0.513164	-0.092684	-1.460814
C	2.007090	1.176731	-2.930365
C	-0.404238	1.024789	-1.470704
C	0.096775	2.271255	-1.921869
C	1.322394	2.319483	-2.645056
C	-0.630840	3.462757	-1.653439
C	-1.790801	0.960559	-1.070580
C	-1.808566	3.413538	-0.970645
C	-2.428795	2.164112	-0.694108
C	3.712633	2.126855	0.070503
C	2.606418	-0.237746	1.126211
C	4.376791	0.954526	-0.102501
C	3.870448	-0.248983	0.472495
C	-3.712635	2.126851	-0.070504
C	-2.606417	-0.237749	-1.126210
C	-4.376793	0.954522	0.102500
C	-3.870448	-0.248987	-0.472496
C	4.647726	-1.428139	0.472420
C	2.261859	-1.372113	1.897222
C	3.052637	-2.499411	1.912375

C	4.240731	-2.546456	1.162385
C	-2.261858	-1.372115	-1.897222
C	-4.647726	-1.428143	-0.472423
C	-3.052635	-2.499413	-1.912376
C	-4.240729	-2.546460	-1.162387
H	-3.167954	-1.223080	3.310535
H	-2.414082	-3.379448	2.351456
H	-2.892151	1.198551	3.561174
H	-1.669898	3.282492	3.011305
H	0.202248	4.413665	1.960127
H	2.328193	4.326358	0.689344
H	0.912778	-4.626705	-0.838652
H	-0.912769	-4.626705	0.838659
H	2.414087	-3.379447	-2.351452
H	3.167956	-1.223079	-3.310534
H	2.892149	1.198551	-3.561176
H	1.669894	3.282491	-3.011307
H	-0.202252	4.413663	-1.960128
H	-2.328197	4.326355	-0.689345
H	4.139420	3.063847	-0.279477
H	5.337754	0.927470	-0.610845
H	-4.139424	3.063843	0.279475
H	-5.337757	0.927465	0.610843
H	4.851351	-3.445394	1.161098
H	5.594955	-1.423841	-0.062511
H	-5.594956	-1.423846	0.062507
H	-4.851348	-3.445399	-1.161101
H	-2.754400	-3.353558	-2.513838
H	-1.366450	-1.346823	-2.506173
H	1.366453	-1.346821	2.506175
H	2.754404	-3.353556	2.513837

72

11-2 scf done: -1766.568930

C	1.021682	0.801964	3.497017
C	0.057051	-0.118268	3.777714
C	1.264576	1.199532	2.154113
C	-0.483774	-0.898062	2.720325
C	0.460130	0.680552	1.107088
C	-0.136812	-0.606354	1.372304
C	2.341875	2.078829	1.846568
C	2.534973	2.479751	0.563997
C	1.468670	2.337148	-0.372827
C	0.328435	1.543805	-0.070454
H	1.588381	1.285678	4.288697
H	-0.216028	-0.358732	4.801970
H	3.033556	2.353543	2.637887
H	3.401358	3.071487	0.282033
C	1.447254	3.265272	-1.448666
C	-0.947075	2.014194	-0.600795

C	-0.945341	3.257533	-1.291977
C	0.250800	3.744584	-1.882114
H	2.382602	3.715477	-1.771073
H	0.197917	4.592151	-2.561067
C	-1.606155	-2.926977	2.042473
C	-1.284825	-2.034519	3.016984
C	-1.016157	-2.821576	0.752920
C	-0.199172	-1.703478	0.426005
C	-1.229182	-3.857314	-0.192873
C	-0.733671	-3.749657	-1.456733
C	0.147105	-2.689607	-1.793975
C	0.584797	-1.786933	-0.787705
H	-2.248443	-3.778307	2.252206
H	-1.625101	-2.175552	4.039966
H	-1.857513	-4.697589	0.090793
H	-0.989670	-4.477351	-2.223416
C	1.821466	-1.083074	-1.066922
C	0.571968	-2.507742	-3.140428
C	-2.267807	1.555291	-0.199367
C	-2.063001	4.139867	-1.198903
C	2.149184	-0.838571	-2.419926
C	1.444124	-1.511311	-3.458256
C	-3.219471	2.533089	0.161855
C	-3.081799	3.858756	-0.339847
H	1.711541	-1.307161	-4.491948
H	0.148452	-3.149797	-3.909170
H	-3.855058	4.590370	-0.119577
H	-2.003766	5.100216	-1.704884
C	2.844839	-0.811005	-0.076097
C	3.269301	-0.018311	-2.749509
C	-2.775516	0.218784	-0.351270
C	-4.382879	2.138938	0.891061
C	-4.706095	0.824740	1.041234
C	-3.990017	-0.154087	0.291355
C	4.001392	-0.066753	-0.451499
C	4.142214	0.393441	-1.793385
H	5.002579	1.007108	-2.050085
H	3.428003	0.237915	-3.794375
H	-5.594955	0.526699	1.591987
H	-5.024615	2.919299	1.293701
C	2.832689	-1.383109	1.217195
C	5.029630	0.157130	0.489427
C	3.859479	-1.171464	2.110052
C	4.961620	-0.374658	1.756090
C	-4.570926	-1.407771	-0.000887
C	-2.288467	-0.603966	-1.392537
C	-4.082212	-2.181726	-1.028211
C	-2.965783	-1.742999	-1.762358
H	-5.473427	-1.701268	0.530867

H	-4.580375	-3.108676	-1.299714
H	-2.629224	-2.309302	-2.624009
H	-1.427841	-0.268883	-1.962962
H	2.006331	-2.020453	1.508187
H	5.892882	0.743810	0.182479
H	5.764798	-0.204145	2.468037
H	3.812892	-1.629984	3.093941

72

11-3 scf done: -1766.566827

C	2.643938	2.293209	1.803627
C	1.806913	2.085656	2.856918
C	2.218859	1.958739	0.484863
C	0.698520	1.203613	2.700688
C	0.965844	1.324162	0.280472
C	0.449304	0.607772	1.436904
C	2.971896	2.413518	-0.630160
C	2.360722	2.591686	-1.832146
C	0.942422	2.491253	-1.886476
C	0.224962	1.759096	-0.899635
H	3.581069	2.830890	1.921488
H	2.023538	2.487085	3.843460
H	4.010606	2.693686	-0.477935
H	2.895758	3.019558	-2.675995
C	0.278241	3.428244	-2.732331
C	-1.217285	1.973553	-0.864373
C	-1.685577	3.218411	-1.350263
C	-0.950167	3.887253	-2.368297
H	0.847035	3.915988	-3.519830
H	-1.390134	4.759517	-2.845424
C	-1.031830	-0.155216	3.700877
C	-0.105817	0.838106	3.815035
C	-1.028294	-0.996000	2.554578
C	-0.174991	-0.695811	1.456847
C	-1.807604	-2.184073	2.550017
C	-1.697242	-3.081450	1.533651
C	-0.704732	-2.916198	0.530183
C	0.144690	-1.775158	0.543656
H	-1.699499	-0.396961	4.523927
H	0.023800	1.380473	4.748475
H	-2.499524	-2.352155	3.371513
H	-2.330348	-3.964077	1.495485
C	1.322254	-1.837999	-0.294712
C	-0.562934	-3.900769	-0.482517
C	-2.238591	1.111821	-0.327037
C	-2.871390	3.782435	-0.796060
C	1.301681	-2.695338	-1.418638
C	0.334550	-3.731075	-1.493967
C	-3.346690	1.709198	0.314979
C	-3.587561	3.101815	0.144642

H	0.373418	-4.424376	-2.330940
H	-1.242301	-4.748754	-0.476521
H	-4.439840	3.557273	0.642473
H	-3.153467	4.788082	-1.098185
C	2.606989	-1.251993	0.033069
C	2.310329	-2.571457	-2.425000
C	-2.382790	-0.260371	-0.756782
C	-4.323211	0.879613	0.942803
C	-4.366610	-0.455780	0.684954
C	-3.489987	-1.020128	-0.287991
C	3.608818	-1.156168	-0.972375
C	3.381067	-1.753885	-2.249346
H	4.133762	-1.641282	-3.025824
H	2.199113	-3.155766	-3.335659
H	-5.144782	-1.080787	1.116604
H	-5.081946	1.350987	1.563248
C	2.979925	-0.946764	1.361035
C	4.864545	-0.594758	-0.654408
C	4.236048	-0.466397	1.660322
C	5.176915	-0.244989	0.640179
C	-3.787746	-2.262702	-0.890221
C	-1.631583	-0.775025	-1.840629
C	-3.077303	-2.706692	-1.980694
C	-1.996055	-1.946840	-2.461723
H	-4.635208	-2.831669	-0.513656
H	-3.348854	-3.638108	-2.470423
H	-1.433528	-2.291532	-3.324298
H	-0.797257	-0.200081	-2.228100
H	2.272810	-1.124284	2.162893
H	5.603688	-0.495138	-1.446337
H	6.157433	0.158685	0.878488
H	4.494002	-0.253965	2.693958

72

11-4 scf done: -1766.568220

C	-3.811209	-1.647275	-0.161951
C	-3.589716	-2.003716	1.131736
C	-2.687498	-1.426895	-1.011164
C	-2.308271	-1.796072	1.715703
C	-1.383051	-1.265156	-0.470590
C	-1.305379	-1.108621	0.981533
C	-2.870872	-1.728968	-2.389029
C	-1.856364	-2.330352	-3.068360
C	-0.611613	-2.542561	-2.418145
C	-0.277817	-1.780002	-1.267037
H	-4.797400	-1.732351	-0.610217
H	-4.386240	-2.407540	1.751817
H	-3.870121	-1.669622	-2.812715
H	-2.021236	-2.770381	-4.048823
C	0.183912	-3.669011	-2.785228

C	1.107240	-1.905517	-0.835582
C	1.676664	-3.197916	-0.957088
C	1.175555	-4.088616	-1.951683
H	-0.123502	-4.263114	-3.641948
H	1.673526	-5.043626	-2.098074
C	-0.812819	-2.007764	3.596470
C	-2.032610	-2.244383	3.037174
C	0.056081	-1.052467	3.001088
C	-0.299787	-0.435815	1.769843
C	1.237091	-0.645612	3.678360
C	1.949771	0.422625	3.231691
C	1.426074	1.256842	2.205374
C	0.235579	0.891774	1.513745
H	-0.534158	-2.444534	4.551977
H	-2.786235	-2.834652	3.552539
H	1.551853	-1.204570	4.556195
H	2.877617	0.717800	3.714922
C	-0.406581	1.917276	0.719951
C	2.077437	2.484919	1.929029
C	2.010101	-0.844341	-0.480383
C	2.825353	-3.524494	-0.188002
C	0.346380	3.061432	0.355960
C	1.591436	3.327096	0.976377
C	3.182092	-1.187677	0.240822
C	3.490634	-2.550925	0.496999
H	2.126940	4.232367	0.702748
H	2.992701	2.717531	2.466763
H	4.362561	-2.788276	1.101335
H	3.173792	-4.554434	-0.181891
C	-1.821908	1.960901	0.384998
C	-0.153119	3.974701	-0.622786
C	1.966475	0.457067	-1.131713
C	4.161876	-0.196650	0.540765
C	4.111668	1.026648	-0.045783
C	3.066502	1.346631	-0.960168
C	-2.273062	2.837334	-0.642387
C	-1.376778	3.807090	-1.183778
H	-1.731998	4.472768	-1.966876
H	0.497215	4.787188	-0.935790
H	4.894752	1.760917	0.128080
H	4.997182	-0.473903	1.179606
C	-2.813031	1.321968	1.161398
C	-3.638072	2.851647	-1.003561
C	-4.150206	1.402827	0.836300
C	-4.567235	2.127718	-0.292018
C	3.141188	2.532414	-1.722998
C	0.982780	0.824537	-2.080975
C	2.181469	2.841616	-2.657463
C	1.091810	1.973616	-2.831412

H	3.994293	3.190009	-1.569257
H	2.262287	3.747369	-3.252612
H	0.318760	2.209880	-3.556760
H	0.130118	0.180390	-2.248627
H	-2.520695	0.798936	2.062225
H	-3.949909	3.496417	-1.822423
H	-5.618880	2.163462	-0.563557
H	-4.882252	0.904736	1.465184

72

11-5 scf done: -1766.567117

C	-3.259555	2.339793	-1.324116
C	-3.742114	2.220269	-0.058477
C	-2.463965	1.285550	-1.844095
C	-3.298429	1.160012	0.771356
C	-1.800706	0.363762	-0.982558
C	-2.125804	0.422664	0.434408
C	-2.622317	1.011884	-3.235000
C	-2.499567	-0.274127	-3.662153
C	-1.915765	-1.249772	-2.808213
C	-1.252416	-0.826208	-1.628239
H	-3.636748	3.101968	-2.000822
H	-4.526005	2.878129	0.309029
H	-3.050793	1.778413	-3.875215
H	-2.844487	-0.579409	-4.646906
C	-2.024658	-2.642285	-3.089710
C	-0.203265	-1.720775	-1.183968
C	-0.486346	-3.108792	-1.308090
C	-1.478940	-3.548269	-2.230642
H	-2.625047	-2.954226	-3.940425
H	-1.661960	-4.614291	-2.336791
C	-3.795273	-0.354805	2.573109
C	-4.094602	0.782100	1.889723
C	-2.512238	-0.950286	2.410680
C	-1.566659	-0.372040	1.519653
C	-2.145331	-2.067078	3.206682
C	-0.856378	-2.501992	3.216429
C	0.162186	-1.698453	2.638630
C	-0.170002	-0.538388	1.875561
H	-4.472172	-0.767488	3.316593
H	-5.003578	1.342913	2.091678
H	-2.914407	-2.563200	3.793443
H	-0.566601	-3.389648	3.772932
C	0.870571	0.455984	1.690641
C	1.513582	-2.007810	2.937786
C	1.173528	-1.348297	-0.937339
C	0.347861	-4.053629	-0.657632
C	2.210739	0.089782	1.976711
C	2.511908	-1.161338	2.573464
C	2.029806	-2.349400	-0.409212

C	1.544910	-3.658444	-0.144136
H	3.552251	-1.402413	2.775466
H	1.727088	-2.927994	3.476021
H	2.207377	-4.371264	0.340349
H	0.042112	-5.096775	-0.636506
C	0.644974	1.858404	1.372817
C	3.289404	0.976668	1.688029
C	1.796674	-0.132922	-1.455318
C	3.425834	-2.114815	-0.251543
C	4.000545	-0.972907	-0.703883
C	3.212576	0.023104	-1.345155
C	1.742671	2.671715	0.965933
C	3.072236	2.186236	1.113814
H	3.899985	2.828786	0.826026
H	4.299503	0.631727	1.892983
H	5.071969	-0.811425	-0.611090
H	4.027949	-2.898945	0.201287
C	1.518926	4.002108	0.547688
C	-0.580598	2.525209	1.592119
C	3.851739	1.159905	-1.885846
C	1.116305	0.866648	-2.191188
C	3.143736	2.133487	-2.548267
C	1.760549	1.967394	-2.711867
C	-0.771430	3.840106	1.226851
C	0.271995	4.574636	0.639085
H	2.368807	4.578080	0.188794
H	0.110982	5.601406	0.321771
H	-1.733272	4.309907	1.412415
H	-1.374963	2.009165	2.110738
H	0.059989	0.773976	-2.382699
H	1.182776	2.704860	-3.261956
H	3.648077	3.004751	-2.957447
H	4.929799	1.245462	-1.766795

72

11TS scf done: -1766.557686

C	3.029564	-2.880254	0.680212
C	3.029564	-2.880254	-0.680212
C	1.830384	-2.576966	1.366641
C	1.830384	-2.576966	-1.366641
C	0.772230	-1.862436	0.726958
C	0.772230	-1.862436	-0.726958
C	1.632589	-3.212439	2.630035
C	0.367424	-3.354064	3.104686
C	-0.679304	-2.554075	2.560620
C	-0.368171	-1.559556	1.595582
H	3.875521	-3.267603	1.242323
H	3.875521	-3.267603	-1.242323
H	2.470371	-3.731928	3.087477
H	0.140981	-4.013162	3.938836

C	-2.015193	-2.694055	3.024079
C	-1.208270	-0.380772	1.653740
C	-2.571409	-0.589318	2.018012
C	-2.971938	-1.812050	2.619247
H	-2.254915	-3.534724	3.670285
H	-4.017133	-1.950135	2.883661
C	0.367424	-3.354064	-3.104686
C	1.632589	-3.212439	-2.630035
C	-0.679304	-2.554075	-2.560620
C	-0.368171	-1.559556	-1.595582
C	-2.015193	-2.694055	-3.024079
C	-2.971938	-1.812050	-2.619247
C	-2.571409	-0.589318	-2.018012
C	-1.208270	-0.380772	-1.653740
H	0.140981	-4.013162	-3.938836
H	2.470371	-3.731928	-3.087477
H	-2.254915	-3.534724	-3.670285
H	-4.017133	-1.950135	-2.883661
C	-0.726601	0.984176	-1.646413
C	-3.504005	0.476291	-1.930800
C	-0.726601	0.984176	1.646413
C	-3.504005	0.476291	1.930800
C	-1.686821	2.028943	-1.619952
C	-3.075987	1.741796	-1.679072
C	-1.686821	2.028943	1.619952
C	-3.075987	1.741796	1.679072
H	-3.781507	2.566179	-1.610818
H	-4.554690	0.264555	-2.113289
H	-3.781507	2.566179	1.610818
H	-4.554690	0.264555	2.113289
C	0.658957	1.371909	-1.870703
C	-1.280646	3.393958	-1.592153
C	0.658957	1.371909	1.870703
C	-1.280646	3.393958	1.592153
C	0.030316	3.740413	1.594477
C	1.033090	2.743889	1.749153
C	1.033090	2.743889	-1.749153
C	0.030316	3.740413	-1.594477
H	0.333891	4.782347	-1.526767
H	-2.055249	4.155443	-1.541068
H	0.333891	4.782347	1.526767
H	-2.055249	4.155443	1.541068
C	2.386376	3.124403	-1.883595
C	1.654493	0.495765	-2.359202
C	2.386376	3.124403	1.883595
C	1.654493	0.495765	2.359202
C	3.352280	2.209761	2.230141
C	2.963526	0.892493	2.522579
C	2.963526	0.892493	-2.522579

C	3.352280	2.209761	-2.230141
H	2.643268	4.171151	-1.736652
H	4.390517	2.513573	-2.331785
H	3.691401	0.178559	-2.898460
H	1.380232	-0.501137	-2.669428
H	1.380232	-0.501137	2.669428
H	3.691401	0.178559	2.898460
H	4.390517	2.513573	2.331785
H	2.643268	4.171151	1.736652

78

12-1 scf done: -1920.114010

C	0.743243	3.277659	-0.997832
C	1.453667	2.587888	-1.935701
C	0.000007	2.584424	0.000007
C	1.292714	1.178948	-2.073560
C	0.000003	1.173848	0.000003
C	0.422875	0.495093	-1.195976
C	-0.743226	3.277658	0.997850
C	-1.453656	2.587884	1.935714
C	-1.292711	1.178943	2.073565
C	-0.422875	0.495088	1.195978
H	0.782781	4.363147	-0.956666
H	2.106265	3.107766	-2.632784
H	-0.782759	4.363145	0.956690
H	-2.106251	3.107762	2.632799
C	-1.973019	0.446811	3.088845
C	0.032764	-0.820899	1.574394
C	-0.777071	-1.564999	2.463188
C	-1.794018	-0.899180	3.207573
H	-2.681401	0.972891	3.723870
H	-2.384729	-1.479172	3.912495
C	1.794012	-0.899171	-3.207579
C	1.973018	0.446818	-3.088845
C	0.777064	-1.564990	-2.463195
C	-0.032768	-0.820891	-1.574397
C	0.561312	-2.964696	-2.601986
C	-0.407280	-3.587078	-1.873445
C	-1.354700	-2.828611	-1.129292
C	-1.271853	-1.413606	-1.122607
H	2.384720	-1.479163	-3.912504
H	2.681402	0.972899	-3.723868
H	1.224912	-3.532325	-3.249567
H	-0.511174	-4.669253	-1.894134
C	-2.436949	-0.673923	-0.694137
C	-2.390679	-3.477563	-0.403104
C	1.271850	-1.413614	1.122606
C	-0.561323	-2.964705	2.601975
C	-3.379362	-1.336864	0.124171
C	-3.313143	-2.748567	0.284588

C	1.354695	-2.828619	1.129287
C	0.407271	-3.587088	1.873435
H	-4.059429	-3.237557	0.906140
H	-2.401283	-4.564294	-0.372182
H	0.511163	-4.669263	1.894121
H	-1.224925	-3.532335	3.249553
C	-2.762330	0.669600	-1.133907
C	-4.422286	-0.595546	0.757130
C	2.436948	-0.673932	0.694140
C	2.390675	-3.477572	0.403101
C	3.313140	-2.748576	-0.284589
C	3.379360	-1.336873	-0.124170
C	-3.792491	1.389301	-0.465486
C	-4.578573	0.734419	0.528557
H	-5.352800	1.301261	1.040325
H	-5.081799	-1.122461	1.442709
H	4.059426	-3.237565	-0.906142
H	2.401276	-4.564302	0.372176
C	4.422283	-0.595555	-0.757131
C	2.762331	0.669591	1.133909
C	4.578569	0.734410	-0.528560
C	3.792490	1.389293	0.465484
H	5.081794	-1.122470	-1.442711
H	5.352796	1.301252	-1.040330
C	4.081082	2.717346	0.849349
C	2.183301	1.271641	2.275101
C	-2.183295	1.271649	-2.275096
C	-4.081083	2.717354	-0.849354
C	3.435887	3.305037	1.912661
C	2.504813	2.556237	2.653139
C	-2.504805	2.556244	-2.653137
C	-3.435883	3.305044	-1.912664
H	1.486399	0.703106	2.878539
H	2.036305	2.987205	3.533494
H	3.671773	4.325385	2.202840
H	4.849586	3.258980	0.302101
H	-1.486388	0.703113	-2.878530
H	-2.036294	2.987212	-3.533490
H	-3.671768	4.325391	-2.202844
H	-4.849588	3.258989	-0.302108

78

12-2 scf done: -1920.034779

C	0.451214	-2.661780	-2.380637
C	0.850626	-3.355259	-1.280099
C	-0.054393	-1.339181	-2.257636
C	0.598393	-2.834886	0.018737
C	-0.003628	-0.677549	-1.001501
C	0.087062	-1.516750	0.172769
C	-0.700303	-0.716644	-3.359689

C	-1.368072	0.453172	-3.163029
C	-1.165333	1.205817	-1.972552
C	-0.251905	0.743725	-0.989675
H	0.504710	-3.105346	-3.371797
H	1.274822	-4.352081	-1.368782
H	-0.755686	-1.248492	-4.305748
H	-2.019105	0.866233	-3.929114
C	-1.880550	2.416413	-1.760861
C	0.375649	1.784859	-0.170282
C	-0.424489	2.935716	0.073018
C	-1.627172	3.163269	-0.655010
H	-2.664570	2.689206	-2.461338
H	-2.216493	4.046890	-0.424986
C	0.568652	-3.185930	2.408103
C	0.791411	-3.665921	1.152403
C	-0.019184	-1.907416	2.592184
C	-0.456859	-1.165894	1.464372
C	-0.137980	-1.343996	3.895415
C	-0.698904	-0.114721	4.058602
C	-1.437204	0.473288	2.990059
C	-1.478414	-0.163928	1.721902
H	0.822971	-3.774004	3.286817
H	1.183574	-4.668068	1.000074
H	0.286545	-1.886007	4.737131
H	-0.699696	0.379886	5.026608
C	-2.606086	0.127058	0.865169
C	-2.215784	1.635707	3.227816
C	1.819543	1.968600	-0.052747
C	0.098001	4.054311	0.779334
C	-3.358306	1.299289	1.130441
C	-3.095516	2.079139	2.288007
C	2.290507	3.289426	0.183310
C	1.442820	4.249259	0.798019
H	-3.675083	2.984892	2.449381
H	-2.101485	2.153585	4.176952
H	1.870795	5.186101	1.146373
H	-0.586448	4.830521	1.112210
C	-3.125713	-0.777207	-0.150543
C	-4.417586	1.695270	0.260203
C	2.852413	1.040641	-0.487629
C	3.516358	3.735392	-0.394727
C	4.185749	2.937255	-1.272417
C	3.884657	1.545973	-1.307722
C	-4.148863	-0.322227	-1.033786
C	-4.756888	0.949571	-0.821031
H	-5.542111	1.273899	-1.500096
H	-4.934127	2.627793	0.475814
H	5.023849	3.312428	-1.854207
H	3.813535	4.768939	-0.235678

C	4.718486	0.633215	-2.023043
C	3.066306	-0.278574	0.041212
C	4.700677	-0.699191	-1.743749
C	3.986227	-1.156834	-0.597970
H	5.401316	1.036874	-2.767159
H	5.345390	-1.391709	-2.279489
C	4.333330	-2.373752	0.029939
C	2.649280	-0.586555	1.357256
C	-2.764521	-2.140980	-0.245690
C	-4.620958	-1.165622	-2.062327
C	3.933673	-2.633569	1.320097
C	3.124528	-1.705465	2.000665
C	-3.261829	-2.958049	-1.238027
C	-4.168416	-2.458910	-2.186333
H	2.023976	0.125376	1.887329
H	2.862682	-1.875664	3.039947
H	4.266881	-3.536253	1.825311
H	5.005926	-3.054160	-0.487874
H	-2.105711	-2.571645	0.495901
H	-2.950112	-3.998121	-1.275064
H	-4.542186	-3.100176	-2.979971
H	-5.378398	-0.778350	-2.740461

78

12-3 scf done: -1920.034779

C	0.451214	-2.661781	-2.380636
C	0.850625	-3.355259	-1.280097
C	-0.054393	-1.339181	-2.257635
C	0.598392	-2.834886	0.018739
C	-0.003628	-0.677549	-1.001501
C	0.087062	-1.516750	0.172770
C	-0.700302	-0.716645	-3.359689
C	-1.368072	0.453171	-3.163029
C	-1.165333	1.205816	-1.972553
C	-0.251905	0.743725	-0.989676
H	0.504710	-3.105347	-3.371795
H	1.274821	-4.352081	-1.368780
H	-0.755686	-1.248493	-4.305748
H	-2.019104	0.866232	-3.929114
C	-1.880549	2.416413	-1.760862
C	0.375649	1.784859	-0.170283
C	-0.424489	2.935716	0.073017
C	-1.627172	3.163269	-0.655012
H	-2.664569	2.689205	-2.461339
H	-2.216493	4.046890	-0.424987
C	0.568652	-3.185929	2.408104
C	0.791411	-3.665921	1.152404
C	-0.019184	-1.907415	2.592185
C	-0.456859	-1.165893	1.464373
C	-0.137980	-1.343993	3.895416

C	-0.698904	-0.114719	4.058602
C	-1.437204	0.473290	2.990059
C	-1.478414	-0.163927	1.721902
H	0.822970	-3.774002	3.286819
H	1.183574	-4.668068	1.000076
H	0.286545	-1.886004	4.737131
H	-0.699696	0.379889	5.026607
C	-2.606086	0.127059	0.865169
C	-2.215784	1.635709	3.227815
C	1.819543	1.968600	-0.052747
C	0.098001	4.054311	0.779333
C	-3.358306	1.299290	1.130440
C	-3.095516	2.079140	2.288005
C	2.290507	3.289425	0.183309
C	1.442820	4.249259	0.798018
H	-3.675082	2.984893	2.449379
H	-2.101485	2.153588	4.176950
H	1.870795	5.186101	1.146373
H	-0.586448	4.830521	1.112209
C	-3.125713	-0.777207	-0.150542
C	-4.417586	1.695270	0.260202
C	2.852413	1.040641	-0.487630
C	3.516358	3.735392	-0.394727
C	4.185750	2.937254	-1.272417
C	3.884657	1.545973	-1.307722
C	-4.148863	-0.322228	-1.033786
C	-4.756887	0.949570	-0.821032
H	-5.542111	1.273898	-1.500097
H	-4.934127	2.627794	0.475812
H	5.023849	3.312428	-1.854207
H	3.813535	4.768938	-0.235678
C	4.718486	0.633215	-2.023043
C	3.066306	-0.278575	0.041211
C	4.700676	-0.699192	-1.743750
C	3.986226	-1.156834	-0.597970
H	5.401316	1.036874	-2.767159
H	5.345390	-1.391710	-2.279490
C	4.333329	-2.373752	0.029939
C	2.649280	-0.586555	1.357256
C	-2.764521	-2.140980	-0.245689
C	-4.620957	-1.165623	-2.062326
C	3.933673	-2.633569	1.320097
C	3.124529	-1.705465	2.000665
C	-3.261829	-2.958050	-1.238025
C	-4.168416	-2.458912	-2.186331
H	2.023977	0.125376	1.887329
H	2.862683	-1.875664	3.039947
H	4.266881	-3.536254	1.825311
H	5.005926	-3.054161	-0.487875

H	-2.105711	-2.571645	0.495903
H	-2.950112	-3.998122	-1.275060
H	-4.542186	-3.100178	-2.979969
H	-5.378397	-0.778352	-2.740461

78

12-4 scf done: -1920.036568

C	2.017162	2.308014	2.574140
C	0.992291	1.884129	3.366884
C	2.044236	1.964010	1.194513
C	0.132429	0.851874	2.901079
C	0.984366	1.202288	0.642145
C	0.262318	0.371679	1.570182
C	3.133702	2.350943	0.363592
C	3.092130	2.094309	-0.970750
C	1.836535	1.786309	-1.572421
C	0.713761	1.439506	-0.774337
H	2.796202	2.961055	2.959399
H	0.891014	2.228791	4.392849
H	4.009703	2.796346	0.826456
H	3.941540	2.311679	-1.612521
C	1.667808	2.180799	-2.928640
C	-0.590423	1.869740	-1.258891
C	-0.609734	2.724644	-2.393039
C	0.467700	2.691708	-3.318591
H	2.544637	2.263235	-3.565833
H	0.358168	3.198557	-4.274271
C	-1.438210	-0.910547	3.411904
C	-0.788266	0.225448	3.784968
C	-1.075538	-1.586065	2.213098
C	-0.143359	-0.997297	1.316091
C	-1.612326	-2.873003	1.949834
C	-1.284002	-3.536807	0.807478
C	-0.274194	-3.033497	-0.052027
C	0.428423	-1.847329	0.293988
H	-2.174678	-1.372925	4.064111
H	-0.956606	0.672105	4.761951
H	-2.332205	-3.287690	2.650471
H	-1.766953	-4.474457	0.545821
C	1.713310	-1.660731	-0.353697
C	0.039023	-3.721860	-1.256854
C	-1.836134	1.825033	-0.507721
C	-1.574620	3.772563	-2.480901
C	1.906457	-2.249208	-1.624290
C	1.011488	-3.254292	-2.085728
C	-2.535781	3.051994	-0.394319
C	-2.375705	4.038432	-1.411778
H	1.195505	-3.715690	-3.052990
H	-0.563941	-4.583757	-1.528667
H	-2.981797	4.939644	-1.367755

H	-1.537064	4.440447	-3.337682
C	2.889919	-1.121856	0.300866
C	3.072119	-1.937474	-2.387296
C	-2.520696	0.658168	-0.021627
C	-3.480137	3.214715	0.654715
C	-3.851587	2.145387	1.416086
C	-3.491412	0.836315	0.996082
C	4.072519	-0.892059	-0.460466
C	4.096994	-1.228822	-1.845769
H	4.985958	-0.997088	-2.427738
H	3.132728	-2.312287	-3.406512
H	-4.557382	2.259927	2.234965
H	-3.911707	4.198947	0.819936
C	-4.257451	-0.272223	1.462022
C	-2.540081	-0.589207	-0.771584
C	-4.249044	-1.452031	0.789576
C	-3.467913	-1.602499	-0.393011
H	-4.914981	-0.122633	2.315262
H	-4.884359	-2.276953	1.103427
C	-3.647298	-2.736660	-1.214246
C	-1.834451	-0.779309	-1.983434
C	2.982238	-0.972047	1.704382
C	5.236469	-0.411614	0.177659
C	-2.967507	-2.872179	-2.401800
C	-2.053411	-1.877463	-2.784256
C	4.140023	-0.536867	2.309364
C	5.273866	-0.223846	1.539977
H	-1.122859	-0.033946	-2.313268
H	-1.502509	-1.974395	-3.715264
H	-3.135166	-3.737693	-3.037488
H	-4.361698	-3.493742	-0.897483
H	2.129458	-1.227704	2.321830
H	4.171605	-0.438058	3.390881
H	6.180974	0.131865	2.021413
H	6.118389	-0.220839	-0.430204

78

12-5 scf done: -1920.033349

C	3.548166	-2.373075	-0.491677
C	2.840719	-2.948791	-1.501495
C	2.900412	-1.494934	0.423630
C	1.569676	-2.411914	-1.853733
C	1.528045	-1.171060	0.252300
C	1.021433	-1.343462	-1.096703
C	3.603590	-1.029076	1.565057
C	2.918868	-0.542844	2.634342
C	1.508757	-0.719138	2.669136
C	0.767680	-0.964138	1.478196
H	4.581075	-2.648946	-0.295535
H	3.268628	-3.734125	-2.119245

H	4.686262	-1.117264	1.581121
H	3.435753	-0.227632	3.536917
C	0.942737	-0.976737	3.952795
C	-0.581192	-1.490886	1.661156
C	-0.806739	-2.216552	2.857392
C	-0.110509	-1.835234	4.036845
H	1.494673	-0.677806	4.840081
H	-0.417842	-2.261502	4.988611
C	-0.206069	-2.207199	-3.479825
C	0.893627	-2.865845	-3.019162
C	-0.560335	-0.945280	-2.930583
C	0.135561	-0.443116	-1.796076
C	-1.551768	-0.153402	-3.568747
C	-1.840463	1.095294	-3.111647
C	-1.059417	1.686842	-2.082421
C	0.030954	0.973286	-1.517349
H	-0.761354	-2.576847	-4.338283
H	1.271462	-3.750079	-3.526751
H	-2.090851	-0.578021	-4.412128
H	-2.646471	1.678394	-3.548538
C	0.994731	1.752925	-0.772328
C	-1.366592	2.996076	-1.623014
C	-1.690056	-1.535553	0.727592
C	-1.653572	-3.364290	2.828460
C	0.560958	2.959001	-0.179835
C	-0.651413	3.559225	-0.609953
C	-2.321909	-2.800711	0.592922
C	-2.224860	-3.750142	1.652769
H	-0.953903	4.504840	-0.169835
H	-2.232996	3.500466	-2.042056
H	-2.746187	-4.698969	1.557704
H	-1.734852	-3.971201	3.726550
C	2.422294	1.502814	-0.753102
C	1.388891	3.616418	0.782124
C	-2.402370	-0.392292	0.200035
C	-3.202802	-3.024633	-0.496293
C	-3.649682	-1.969446	-1.232990
C	-3.386065	-0.645092	-0.790509
C	3.239945	2.194109	0.183673
C	2.658583	3.195859	1.019204
H	3.280859	3.685067	1.764756
H	0.972908	4.467639	1.315787
H	-4.342898	-2.117495	-2.057161
H	-3.560197	-4.034215	-0.683801
C	-4.247750	0.391632	-1.252618
C	-2.410515	0.920733	0.840502
C	-4.268264	1.604841	-0.647441
C	-3.393219	1.879500	0.441627
H	-4.939159	0.160768	-2.059623

H	-4.969018	2.374803	-0.962186
C	-3.512818	3.108699	1.124176
C	-1.590006	1.285197	1.932890
C	3.070109	0.734434	-1.746849
C	4.633194	1.966624	0.195200
C	-2.693275	3.423434	2.182338
C	-1.721812	2.494650	2.582464
C	4.437877	0.572117	-1.750859
C	5.228660	1.161231	-0.749317
H	-0.833328	0.606512	2.293226
H	-1.062518	2.717906	3.416849
H	-2.799060	4.371770	2.702583
H	-4.276748	3.807945	0.790501
H	2.479199	0.284133	-2.536083
H	4.903346	-0.019070	-2.534520
H	6.305310	1.012827	-0.744369
H	5.235936	2.479517	0.941647

78

12-6 scf done: -1920.020024

C	4.204199	0.244999	0.745368
C	4.400150	-0.865984	-0.010996
C	2.908834	0.484073	1.292441
C	3.278064	-1.547858	-0.562421
C	1.771338	-0.241622	0.838643
C	1.971832	-1.016860	-0.388875
C	2.881241	1.198414	2.518577
C	2.000837	0.804494	3.477367
C	1.084676	-0.236507	3.185521
C	0.757028	-0.552450	1.835403
H	5.039585	0.837141	1.108938
H	5.398627	-1.216743	-0.259334
H	3.687965	1.890636	2.744648
H	2.081460	1.165647	4.499645
C	0.663715	-1.087082	4.251612
C	-0.355989	-1.489741	1.691111
C	-0.392441	-2.537129	2.647948
C	0.119279	-2.299970	3.957450
H	0.947402	-0.825227	5.267603
H	-0.016960	-3.063693	4.718742
C	2.405431	-3.327372	-1.937706
C	3.466593	-2.731178	-1.327310
C	1.184111	-2.612681	-2.063667
C	1.020762	-1.351997	-1.423306
C	0.170332	-3.113503	-2.923466
C	-0.894530	-2.337913	-3.255387
C	-0.939387	-0.972332	-2.863849
C	0.054701	-0.432689	-1.998569
H	2.507432	-4.284583	-2.442514
H	4.461066	-3.168811	-1.366656

H	0.276922	-4.120246	-3.320110
H	-1.688331	-2.720428	-3.891993
C	0.094063	1.007181	-1.865537
C	-1.964070	-0.145976	-3.391927
C	-1.482575	-1.459342	0.780442
C	-1.015970	-3.769681	2.308762
C	-1.055042	1.752118	-2.219164
C	-2.066295	1.157621	-3.013931
C	-2.023848	-2.721716	0.398003
C	-1.680564	-3.894568	1.125569
H	-2.898297	1.773659	-3.343362
H	-2.695268	-0.592238	-4.061354
H	-2.093197	-4.848573	0.807836
H	-0.923847	-4.605533	2.997818
C	1.277478	1.795582	-1.565205
C	-1.174537	3.119714	-1.817716
C	-2.267333	-0.280237	0.471830
C	-3.033614	-2.793778	-0.595275
C	-3.615530	-1.657951	-1.067505
C	-3.301499	-0.400415	-0.490846
C	1.128824	3.141688	-1.130451
C	-0.158467	3.757838	-1.184161
H	-0.272182	4.777188	-0.824333
H	-2.118917	3.623445	-2.006262
H	-4.390065	-1.702876	-1.829171
H	-3.358664	-3.773778	-0.935630
C	-4.083688	0.731934	-0.866571
C	-2.239576	0.958405	1.241174
C	-3.880757	1.950744	-0.306893
C	-2.973910	2.091352	0.781577
H	-4.838121	0.594167	-1.637420
H	-4.456621	2.816934	-0.625198
C	-2.894775	3.317386	1.477135
C	-1.668961	1.068719	2.527945
C	2.274013	3.904405	-0.815078
C	2.580327	1.358952	-1.888254
C	-2.204980	3.419936	2.662466
C	-1.636144	2.261975	3.216205
C	3.683126	2.151957	-1.653076
C	3.538095	3.415624	-1.056903
H	-3.428721	4.174437	1.072179
H	-2.155304	4.366802	3.193273
H	-1.182623	2.293554	4.203169
H	-1.298295	0.182071	3.019524
H	2.709900	0.399443	-2.373291
H	4.668947	1.790380	-1.930541
H	4.413009	4.022728	-0.839963
H	2.135688	4.915029	-0.437254

12TS scf done: -1920.008673

C	-2.620214	2.605370	2.206792
C	-3.325745	2.039865	1.193493
C	-1.200547	2.562444	2.189075
C	-2.619870	1.709832	0.000000
C	-0.528204	1.698215	1.279581
C	-1.213008	1.493857	0.000000
C	-0.455982	3.413475	3.052963
C	0.903185	3.435249	2.973727
C	1.573077	2.364327	2.319009
C	0.821048	1.338472	1.680566
H	-3.117672	3.117028	3.027235
H	-4.411660	2.072023	1.174563
H	-0.999528	4.110799	3.685511
H	1.493684	4.180494	3.500015
C	2.987548	2.257047	2.400974
C	1.413642	0.012949	1.683630
C	2.836581	-0.057988	1.761045
C	3.607371	1.107079	2.024003
H	3.552453	3.106421	2.777051
H	4.690965	1.021745	2.041456
C	-2.620214	2.605370	-2.206792
C	-3.325745	2.039865	-1.193493
C	-1.200547	2.562444	-2.189075
C	-0.528204	1.698215	-1.279581
C	-0.455982	3.413475	-3.052963
C	0.903185	3.435249	-2.973727
C	1.573077	2.364327	-2.319009
C	0.821048	1.338472	-1.680566
H	-3.117672	3.117028	-3.027235
H	-4.411660	2.072023	-1.174563
H	-0.999528	4.110799	-3.685511
H	1.493684	4.180494	-3.500015
C	2.987548	2.257047	-2.400974
C	1.413642	0.012949	-1.683630
C	2.836581	-0.057988	-1.761045
C	3.607371	1.107079	-2.024003
H	3.552453	3.106421	-2.777051
H	4.690965	1.021745	-2.041456
C	3.506557	-1.303996	-1.680228
C	0.683815	-1.233611	-1.810463
C	2.804120	-2.461422	-1.560089
C	1.389286	-2.451272	-1.638747
H	4.593476	-1.309815	-1.704899
C	0.683815	-1.233611	1.810463
C	3.506557	-1.303996	1.680228
H	4.593476	-1.309815	1.704899
C	2.804120	-2.461422	1.560089
C	1.389286	-2.451272	1.638747

C	0.690835	-3.694697	1.573536
C	-0.688861	-1.363001	2.278319
C	-0.688861	-1.363001	-2.278319
C	0.690835	-3.694697	-1.573536
C	-0.657965	-3.754643	-1.696145
C	-1.380560	-2.596620	2.102642
C	-1.380560	-2.596620	-2.102642
C	-0.657965	-3.754643	1.696145
H	3.313511	-3.415619	1.450064
H	1.271348	-4.593260	1.379103
H	-1.191857	-4.694688	1.580106
H	-1.191857	-4.694688	-1.580106
H	1.271348	-4.593260	-1.379103
H	3.313511	-3.415619	-1.450064
C	-2.734799	-2.707219	2.486940
C	-1.326265	-0.394144	3.082449
C	-1.326265	-0.394144	-3.082449
C	-2.734799	-2.707219	-2.486940
C	-3.368355	-1.683789	-3.153011
C	-3.368355	-1.683789	3.153011
C	-2.629747	-0.542751	-3.505363
C	-2.629747	-0.542751	3.505363
H	-3.251531	-3.644678	2.293437
H	-4.406029	-1.783687	3.459632
H	-3.078684	0.226628	4.126941
H	-0.758771	0.459509	3.424564
H	-0.758771	0.459509	-3.424564
H	-3.078684	0.226628	-4.126941
H	-4.406029	-1.783687	-3.459632
H	-3.251531	-3.644678	-2.293437

84

13-1 scf done: -2073.582123

C	-1.277819	-0.808794	3.267790
C	-1.079342	-1.992099	2.619571
C	-0.724126	0.399231	2.754365
C	-0.506188	-2.016339	1.316064
C	0.002872	0.364513	1.544088
C	-0.129491	-0.800135	0.707542
C	-0.867049	1.636681	3.445872
C	-0.317392	2.777665	2.941893
C	0.583720	2.721438	1.839294
C	0.882049	1.470836	1.249966
C	1.196870	3.899962	1.328752
C	2.066401	1.374079	0.425322
C	2.531509	2.565350	-0.185938
C	2.061272	3.826618	0.278305
C	0.292002	-3.238484	-0.615911
C	-0.292008	-3.238484	0.615907
C	0.506183	-2.016338	-1.316066

C	0.129488	-0.800135	-0.707544
C	1.079337	-1.992098	-2.619573
C	1.277816	-0.808794	-3.267791
C	0.724126	0.399232	-2.754365
C	-0.002872	0.364514	-1.544088
C	0.867051	1.636682	-3.445872
C	-0.882047	1.470838	-1.249965
C	-0.583717	2.721440	-1.839293
C	0.317394	2.777666	-2.941892
C	-1.196866	3.899965	-1.328751
C	-2.066400	1.374082	-0.425323
C	-2.061268	3.826621	-0.278304
C	-2.531506	2.565353	0.185938
C	3.475473	2.491366	-1.246412
C	2.826502	0.164940	0.207063
C	3.947728	1.285217	-1.668149
C	3.663421	0.103297	-0.930113
C	-3.475470	2.491369	1.246414
C	-2.826501	0.164943	-0.207063
C	-3.947726	1.285221	1.668150
C	-3.663419	0.103300	0.930114
C	4.254808	-1.137749	-1.315132
C	2.875475	-0.950989	1.132622
C	3.448486	-2.182356	0.707061
C	4.091190	-2.257940	-0.564275
C	-2.875475	-0.950986	-1.132622
C	-4.254807	-1.137745	1.315134
C	-3.448487	-2.182353	-0.707060
C	-4.091191	-2.257937	0.564275
C	2.484661	-0.849273	2.487909
C	3.450687	-3.292121	1.580356
C	2.979657	-3.182771	2.868221
C	2.528637	-1.935394	3.333474
C	-3.450689	-3.292118	-1.580356
C	-2.484662	-0.849271	-2.487909
C	-2.979660	-3.182768	-2.868221
C	-2.528639	-1.935391	-3.333474
H	-1.807934	-0.776085	4.216661
H	-1.411728	-2.929414	3.058357
H	-1.473885	1.661581	4.347639
H	-0.507996	3.741277	3.408172
H	0.914859	4.859769	1.754495
H	2.456135	4.728778	-0.182691
H	0.547884	-4.172284	-1.109878
H	-0.547890	-4.172284	1.109875
H	1.411722	-2.929413	-3.058360
H	1.807930	-0.776084	-4.216662
H	1.473886	1.661581	-4.347638
H	0.507999	3.741278	-3.408171

H	-0.914855	4.859771	-1.754494
H	-2.456130	4.728781	0.182693
H	3.775078	3.412394	-1.740396
H	4.608149	1.215237	-2.529188
H	-3.775073	3.412398	1.740398
H	-4.608145	1.215240	2.529190
H	4.513149	-3.208749	-0.881367
H	4.827844	-1.167193	-2.238935
H	-4.827842	-1.167190	2.238937
H	-4.513150	-3.208746	0.881368
H	2.163784	0.109326	2.876640
H	2.215957	-1.820434	4.367520
H	2.993282	-4.042215	3.533159
H	3.862789	-4.232676	1.221244
H	-2.163786	0.109328	-2.876641
H	-2.215959	-1.820432	-4.367520
H	-2.993286	-4.042212	-3.533159
H	-3.862792	-4.232673	-1.221244

84

13-2 scf done: -2073.498774

C	0.350425	-3.192924	-1.204630
C	0.421258	-2.416900	-2.320310
C	0.340713	-2.592450	0.083845
C	0.309910	-1.002154	-2.229888
C	0.275736	-1.178821	0.204916
C	0.008536	-0.396401	-0.980223
C	0.442821	-3.402538	1.244024
C	0.395784	-2.842605	2.486493
C	0.441820	-1.432203	2.637456
C	0.600020	-0.613749	1.490368
H	0.390387	-4.276738	-1.273314
H	0.562759	-2.862314	-3.301899
H	0.488479	-4.481175	1.120241
H	0.353567	-3.462075	3.379527
C	0.338458	-0.821723	3.922234
C	1.183622	0.695063	1.715243
C	0.920719	1.314681	2.961564
C	0.435799	0.530773	4.050901
H	0.125520	-1.452994	4.781814
H	0.258214	1.018483	5.006052
C	0.660916	1.162086	-3.209462
C	0.574819	-0.188293	-3.363443
C	0.206825	1.782056	-2.012907
C	-0.375063	0.994093	-0.986855
C	0.354365	3.185671	-1.829385
C	-0.114796	3.769155	-0.696232
C	-1.069407	3.068838	0.096218
C	-1.345800	1.693544	-0.136545
H	1.029580	1.797350	-4.010972

H	0.823465	-0.666440	-4.307196
H	0.908184	3.753520	-2.571596
H	0.068498	4.819258	-0.484554
C	-2.740285	1.288007	0.016695
C	-1.961119	3.874388	0.857541
C	2.118622	1.348692	0.823547
C	1.223398	2.691335	3.144674
C	-3.687780	2.306292	0.312375
C	-3.268063	3.510613	0.938484
C	2.334728	2.742337	0.999372
C	1.834808	3.401354	2.156130
H	-4.018073	4.190684	1.334894
H	-1.630426	4.856967	1.184771
H	2.016495	4.467808	2.266010
H	0.944115	3.165020	4.082636
C	-3.334063	0.045904	-0.455279
C	-5.005665	2.250309	-0.232145
C	2.917880	0.678902	-0.180512
C	3.061909	3.479924	0.025933
C	3.523531	2.871495	-1.101043
C	3.474633	1.456112	-1.221536
C	-4.495770	0.136971	-1.251519
C	-5.324136	1.290487	-1.144911
H	-6.255271	1.327139	-1.704654
H	-5.683640	3.074097	-0.023407
H	4.001319	3.446080	-1.891197
H	3.185491	4.550193	0.172976
C	-4.907392	-0.997339	-2.016495
C	-3.003928	-1.272564	0.011473
C	4.039183	0.817171	-2.367620
C	3.316462	-0.714399	-0.126897
C	4.140371	-0.535460	-2.439679
C	3.853351	-1.332046	-1.291245
C	-3.503658	-2.413411	-0.677724
C	-4.353674	-2.223489	-1.806874
H	-5.705571	-0.863906	-2.743165
H	-4.675045	-3.088376	-2.382141
H	4.533313	-1.020433	-3.330067
H	4.372344	1.444659	-3.191077
C	3.348825	-1.454841	1.076230
C	4.206828	-2.698609	-1.257108
C	-2.506741	-1.445504	1.323564
C	-3.337541	-3.694509	-0.106670
C	-2.507414	-2.687230	1.915171
C	-2.873136	-3.830113	1.181265
C	4.140234	-3.418692	-0.086416
C	3.750171	-2.772063	1.098907
H	3.083846	-0.965328	2.005242
H	3.764483	-3.309765	2.042626

H	4.430709	-4.465698	-0.068246
H	4.576996	-3.161127	-2.169456
H	-2.220266	-0.567142	1.893219
H	-2.213614	-2.784473	2.954977
H	-2.824143	-4.811942	1.644753
H	-3.683985	-4.562667	-0.663227

84

13-3 scf done: -2073.500526

C	0.284385	-1.706135	-2.957561
C	0.887477	-0.531788	-3.295223
C	-0.072203	-1.951143	-1.604106
C	0.934738	0.548495	-2.371571
C	0.060350	-0.913359	-0.642841
C	0.269224	0.428303	-1.124753
C	-0.464660	-3.253225	-1.193492
C	-0.642635	-3.541363	0.125244
C	-0.292471	-2.591185	1.121542
C	0.171943	-1.303102	0.742735
H	0.181529	-2.511924	-3.679657
H	1.324818	-0.389563	-4.280266
H	-0.626813	-4.009625	-1.957155
H	-0.998471	-4.518306	0.442202
C	-0.366917	-2.943803	2.496017
C	0.867940	-0.539474	1.756904
C	0.529922	-0.789686	3.110744
C	-0.081620	-2.024142	3.460243
H	-0.741704	-3.929393	2.757901
H	-0.258083	-2.239064	4.511514
C	1.812512	2.679828	-1.695810
C	1.695099	1.718701	-2.651707
C	0.909887	2.703032	-0.594621
C	-0.053896	1.671747	-0.442167
C	0.859630	3.851999	0.239811
C	-0.284002	4.154092	0.908934
C	-1.457225	3.410251	0.599276
C	-1.369024	2.111348	0.026010
H	2.503214	3.510665	-1.812907
H	2.257508	1.770044	-3.579762
H	1.716195	4.520008	0.257407
H	-0.373360	5.072959	1.482740
C	-2.607524	1.577644	-0.532402
C	-2.669431	4.160341	0.542841
C	1.985277	0.359970	1.532690
C	0.858355	0.173152	4.107604
C	-3.558043	2.525033	-0.986088
C	-3.623769	3.799391	-0.357102
C	2.208824	1.368467	2.507941
C	1.569010	1.286150	3.778235
H	-4.449913	4.462623	-0.601243

H	-2.713826	5.119949	1.051564
H	1.757007	2.069337	4.508323
H	0.501005	0.013270	5.122111
C	-2.986303	0.202748	-0.737955
C	-4.424337	2.184319	-2.064984
C	2.962893	0.225783	0.475682
C	3.137618	2.411695	2.254772
C	3.868988	2.425086	1.105736
C	3.827048	1.318327	0.217128
C	-3.767884	-0.113770	-1.872438
C	-4.400900	0.931081	-2.602523
H	-4.992895	0.682442	-3.479662
H	-5.062039	2.961874	-2.478443
H	4.548634	3.245285	0.885918
H	3.244415	3.201683	2.994208
C	-4.095627	-1.475649	-2.142862
C	-2.961243	-0.760823	0.339384
C	4.683061	1.306827	-0.925658
C	3.231296	-1.005318	-0.249516
C	4.722458	0.240969	-1.764955
C	4.039406	-0.963472	-1.421882
C	-3.497191	-2.060080	0.119110
C	-3.929393	-2.430241	-1.188112
H	-4.562604	-1.716839	-3.095018
H	-4.234672	-3.458130	-1.369129
H	5.340832	0.255655	-2.659455
H	5.282637	2.192434	-1.123749
C	2.849480	-2.282183	0.220659
C	4.249873	-2.140250	-2.172455
C	-2.680503	-0.373835	1.671925
C	-3.711899	-2.921432	1.217941
C	-2.972733	-1.204469	2.728649
C	-3.487028	-2.494174	2.505467
C	3.766427	-3.354021	-1.740331
C	3.100975	-3.425898	-0.505681
H	2.380623	-2.371850	1.191792
H	2.785253	-4.387390	-0.110875
H	3.941564	-4.254927	-2.322180
H	4.838778	-2.073575	-3.084718
H	-2.288454	0.619039	1.864459
H	-2.791851	-0.861508	3.743200
H	-3.703930	-3.147418	3.346542
H	-4.119174	-3.912306	1.027774

84

13-4 scf done: -2073.503406

C	1.524570	0.313066	-3.378912
C	2.241615	1.269817	-2.726703
C	0.610652	-0.493486	-2.646669
C	1.866065	1.680364	-1.416605

C	0.375849	-0.221048	-1.273382
C	0.742639	1.084476	-0.789182
C	0.003771	-1.629110	-3.247876
C	-0.681774	-2.528756	-2.489823
C	-0.634979	-2.450314	-1.070425
C	-0.022199	-1.334354	-0.440694
H	1.723706	0.068143	-4.418784
H	3.068443	1.782348	-3.211396
H	0.102270	-1.762296	-4.322443
H	-1.185320	-3.376978	-2.946709
C	-1.127966	-3.530989	-0.292695
C	0.328678	-1.469592	0.954571
C	-0.352088	-2.451185	1.721631
C	-1.063710	-3.490007	1.067333
H	-1.602753	-4.363776	-0.804584
H	-1.528747	-4.262144	1.674332
C	2.168490	3.141090	0.474161
C	2.601778	2.686122	-0.731926
C	0.823168	2.884181	0.863581
C	0.030651	1.932245	0.165850
C	0.217518	3.850658	1.715124
C	-1.078736	4.197754	1.492023
C	-1.818945	3.514821	0.489398
C	-1.389862	2.235857	0.044398
H	2.751378	3.856962	1.047650
H	3.533154	3.037621	-1.166144
H	0.848898	4.438171	2.376886
H	-1.515735	5.072875	1.966796
C	-2.353777	1.533542	-0.791741
C	-2.839187	4.214892	-0.220768
C	1.406310	-0.766770	1.631401
C	-0.312642	-2.394933	3.143548
C	-3.080753	2.337903	-1.705559
C	-3.300443	3.712921	-1.399971
C	1.267546	-0.578983	3.031823
C	0.361309	-1.393243	3.769510
H	-3.930456	4.302799	-2.060670
H	-3.109526	5.213616	0.112409
H	0.306040	-1.265124	4.847831
H	-0.899918	-3.115907	3.705172
C	-2.788638	0.168852	-0.666407
C	-3.698767	1.725381	-2.828502
C	2.670869	-0.388045	1.040347
C	2.109825	0.340040	3.711601
C	3.134448	0.951255	3.055318
C	3.482192	0.539142	1.740967
C	-3.455330	-0.417798	-1.772125
C	-3.772292	0.366419	-2.913945
H	-4.229488	-0.116620	-3.773862

H	-4.133153	2.361309	-3.596074
H	3.763272	1.682634	3.557283
H	1.922194	0.536120	4.764591
C	-3.990702	-1.735482	-1.676383
C	-2.909484	-0.486655	0.628232
C	4.688695	1.030952	1.159484
C	3.252899	-1.022109	-0.133372
C	5.121560	0.587560	-0.047799
C	4.442374	-0.480498	-0.703973
C	-3.624424	-1.717089	0.710672
C	-4.078946	-2.362894	-0.475566
H	-4.405840	-2.189495	-2.573242
H	-4.548168	-3.340234	-0.390105
H	6.027995	0.986062	-0.497871
H	5.248849	1.785612	1.706952
C	2.780758	-2.237907	-0.679922
C	4.992509	-1.056736	-1.868990
C	-2.526361	0.118755	1.848679
C	-3.917108	-2.280372	1.971636
C	-2.851802	-0.434704	3.066612
C	-3.554066	-1.648159	3.137482
C	4.445334	-2.187305	-2.430525
C	3.352065	-2.802080	-1.800091
H	1.969762	-2.762257	-0.192847
H	2.951257	-3.734308	-2.188192
H	4.880706	-2.624417	-3.325113
H	5.882402	-0.602010	-2.299076
H	-1.985557	1.055524	1.837518
H	-2.550214	0.073100	3.978171
H	-3.807070	-2.081119	4.101761
H	-4.463302	-3.220986	2.000661

84

13-5 scf done: -2073.502302

C	-2.919621	2.839482	-0.027170
C	-3.286879	2.040171	-1.063689
C	-1.757370	2.511596	0.726514
C	-2.357568	1.110240	-1.612645
C	-0.971563	1.390049	0.355589
C	-1.075394	0.945165	-1.022292
C	-1.436893	3.234262	1.906905
C	-0.464332	2.785549	2.748702
C	0.076614	1.483940	2.572250
C	-0.262408	0.724257	1.418659
H	-3.552139	3.655040	0.312544
H	-4.244358	2.166093	-1.561807
H	-1.982796	4.150525	2.117889
H	-0.175254	3.357162	3.627171
C	0.864271	0.904619	3.603218
C	-0.064842	-0.707756	1.479113

C	0.832840	-1.219614	2.452335
C	1.285498	-0.385849	3.510980
H	1.136870	1.521526	4.456075
H	1.943131	-0.815521	4.261690
C	-1.692976	-0.115477	-3.575022
C	-2.677808	0.444295	-2.823531
C	-0.342394	0.171000	-3.239715
C	0.013686	0.636802	-1.941864
C	0.556633	0.297970	-4.340330
C	1.554151	1.220223	-4.260374
C	1.870919	1.809571	-3.005987
C	1.339758	1.236717	-1.822924
H	-1.912996	-0.582072	-4.531709
H	-3.711237	0.441181	-3.157596
H	0.293679	-0.163130	-5.288769
H	2.104405	1.537052	-5.142891
C	2.144735	1.479442	-0.641416
C	2.642020	3.005983	-2.918815
C	-0.783660	-1.683208	0.682384
C	1.277011	-2.567408	2.372190
C	2.685801	2.788709	-0.529889
C	2.857548	3.581305	-1.702371
C	-0.138645	-2.926237	0.454987
C	0.903330	-3.349182	1.322774
H	3.306951	4.566480	-1.609892
H	2.951572	3.491279	-3.840873
H	1.346317	-4.328233	1.166217
H	1.992387	-2.921957	3.109071
C	2.707051	0.465228	0.224603
C	3.231598	3.213184	0.708772
C	-2.147045	-1.567075	0.208444
C	-0.585715	-3.774435	-0.595005
C	-1.703463	-3.459531	-1.303967
C	-2.550756	-2.407472	-0.856601
C	3.377795	0.912119	1.392337
C	3.485643	2.298379	1.685077
H	3.924518	2.599928	2.632793
H	3.500425	4.259343	0.832956
H	-2.027978	-4.072123	-2.141479
H	-0.004357	-4.664180	-0.822957
C	4.090723	0.002091	2.225173
C	2.906795	-0.925101	-0.177493
C	-3.847973	-2.270765	-1.433289
C	-3.179992	-0.789765	0.873164
C	-4.762825	-1.410889	-0.915921
C	-4.473366	-0.690743	0.279052
C	3.739996	-1.765917	0.624294
C	4.280768	-1.287256	1.850920
H	4.534475	0.386702	3.140466

H	4.871268	-1.965842	2.462276
H	-5.748632	-1.307647	-1.363846
H	-4.090846	-2.885710	-2.296806
C	-3.020490	-0.218934	2.157485
C	-5.482977	0.069402	0.907931
C	2.436446	-1.485456	-1.387839
C	4.043658	-3.079714	0.208298
C	2.744061	-2.773056	-1.773470
C	3.554849	-3.589213	-0.971439
C	-5.265033	0.675525	2.123199
C	-4.028264	0.498190	2.764282
H	-2.093329	-0.367520	2.695198
H	-3.859084	0.922644	3.750004
H	-6.051949	1.254498	2.599159
H	-6.451357	0.146945	0.418056
H	1.822599	-0.900672	-2.053807
H	2.352762	-3.147430	-2.715467
H	3.800005	-4.601448	-1.282073
H	4.681294	-3.685390	0.848982

84

13-6 scf done: -2073.481439

C	1.386642	-2.875681	-2.080933
C	2.510870	-2.111056	-2.111017
C	0.128934	-2.209219	-2.107156
C	2.394299	-0.699608	-2.008633
C	-0.002641	-0.882422	-1.616326
C	1.230841	-0.127136	-1.429944
C	-0.827506	-2.757624	-3.012994
C	-1.665319	-1.905369	-3.661842
C	-1.853920	-0.584763	-3.164354
C	-1.269645	-0.213743	-1.924023
H	1.426831	-3.943467	-2.279709
H	3.484170	-2.542071	-2.328325
H	-0.713155	-3.789675	-3.333392
H	-2.233270	-2.221916	-4.533186
C	-2.641661	0.357281	-3.881870
C	-1.944065	0.843008	-1.209179
C	-2.558506	1.852071	-2.002471
C	-2.844801	1.605016	-3.373039
H	-3.009673	0.081058	-4.866953
H	-3.335403	2.381333	-3.954388
C	3.074264	1.453436	-2.851483
C	3.339687	0.129285	-2.680832
C	2.087716	2.072885	-2.029195
C	1.357561	1.287354	-1.099791
C	1.898716	3.481804	-2.051055
C	1.126850	4.088244	-1.105539
C	0.718361	3.358083	0.043075
C	0.945515	1.954460	0.112793

H	3.672778	2.074317	-3.512895
H	4.186133	-0.347499	-3.167966
H	2.373516	4.056739	-2.842464
H	0.924698	5.155587	-1.146075
C	0.958219	1.342786	1.427836
C	0.190401	4.054028	1.163454
C	-2.234755	0.851885	0.215867
C	-2.980879	3.066243	-1.398149
C	0.369436	2.055471	2.506897
C	-0.032133	3.407926	2.339304
C	-2.672995	2.083239	0.782656
C	-2.951736	3.204655	-0.046161
H	-0.472061	3.926543	3.187389
H	-0.027406	5.114091	1.058243
H	-3.244413	4.138416	0.427220
H	-3.337734	3.869278	-2.038416
C	1.638840	0.111235	1.770435
C	0.194671	1.427238	3.769509
C	-2.278555	-0.318325	1.069538
C	-2.916092	2.195688	2.175039
C	-2.709293	1.135992	3.002891
C	-2.379327	-0.133826	2.469028
C	1.237047	-0.577397	2.935594
C	0.509108	0.112855	3.938811
H	0.286140	-0.403210	4.868945
H	-0.258574	2.001142	4.573525
H	-2.833729	1.232470	4.078537
H	-3.244148	3.155251	2.566579
C	1.657944	-1.928144	3.143970
C	2.861401	-0.364919	1.153512
C	-2.173775	-1.232446	3.361459
C	-2.416487	-1.695559	0.614856
C	-1.932002	-2.483234	2.896397
C	-2.126537	-2.763336	1.510293
C	3.293721	-1.698551	1.395137
C	2.584537	-2.505910	2.336515
H	1.214493	-2.478378	3.970239
H	2.886222	-3.540782	2.477990
H	-1.719989	-3.305854	3.575208
H	-2.184909	-1.027373	4.428822
C	-3.035404	-2.038209	-0.605672
C	-2.220074	-4.099404	1.065538
C	3.756399	0.505440	0.493372
C	4.496808	-2.156412	0.816384
C	4.963639	0.055427	0.004063
C	5.321936	-1.297780	0.124184
C	-2.727155	-4.396998	-0.178973
C	-3.194190	-3.352531	-0.992231
H	-3.444425	-1.252984	-1.227199

H	-3.688642	-3.574124	-1.933363
H	-2.821687	-5.429941	-0.503052
H	-1.944871	-4.894824	1.754708
H	3.501009	1.554639	0.399313
H	5.635733	0.755186	-0.484560
H	6.262559	-1.653472	-0.288094
H	4.790334	-3.191077	0.980050

84

13-7 scf done: -2073.481439

C	-2.510872	-2.111054	-2.111017
C	-1.386643	-2.875679	-2.080935
C	-2.394301	-0.699606	-2.008632
C	-0.128935	-2.209216	-2.107159
C	-1.230843	-0.127134	-1.429943
C	0.002639	-0.882419	-1.616327
C	-3.339690	0.129288	-2.680829
C	-3.074268	1.453439	-2.851478
C	-2.087719	2.072887	-2.029190
C	-1.357563	1.287355	-1.099788
H	-3.484171	-2.542068	-2.328325
H	-1.426833	-3.943464	-2.279713
H	-4.186136	-0.347495	-3.167963
H	-3.672782	2.074321	-3.512889
C	-1.898719	3.481807	-2.051048
C	-0.945516	1.954459	0.112796
C	-0.718363	3.358083	0.043081
C	-1.126854	4.088246	-1.105532
H	-2.373521	4.056743	-2.842456
H	-0.924701	5.155588	-1.146066
C	1.665316	-1.905363	-3.661846
C	0.827504	-2.757620	-3.012998
C	1.853917	-0.584758	-3.164356
C	1.269642	-0.213739	-1.924024
C	2.641657	0.357288	-3.881872
C	2.844796	1.605022	-3.373040
C	2.558503	1.852075	-2.002471
C	1.944062	0.843011	-1.209179
H	2.233267	-2.221909	-4.533190
H	0.713154	-3.789670	-3.333397
H	3.009668	0.081066	-4.866956
H	3.335398	2.381340	-3.954388
C	2.234753	0.851886	0.215867
C	2.980876	3.066246	-1.398148
C	-0.958218	1.342783	1.427839
C	-0.190403	4.054026	1.163460
C	2.672993	2.083240	0.782656
C	2.951733	3.204657	-0.046159
C	-0.369435	2.055468	2.506900
C	0.032132	3.407923	2.339309

H	3.244411	4.138417	0.427222
H	3.337729	3.869283	-2.038414
H	0.472060	3.926539	3.187395
H	0.027403	5.114090	1.058251
C	2.278555	-0.318326	1.069535
C	2.916092	2.195686	2.175039
C	-1.638837	0.111232	1.770436
C	-0.194668	1.427232	3.769511
C	-0.509103	0.112848	3.938811
C	-1.237042	-0.577403	2.935593
C	2.379329	-0.133828	2.469025
C	2.709295	1.135989	3.002890
H	2.833732	1.232466	4.078536
H	3.244147	3.155250	2.566580
H	-0.286134	-0.403218	4.868944
H	0.258577	2.001135	4.573528
C	2.173779	-1.232449	3.361455
C	2.416489	-1.695558	0.614851
C	-1.657938	-1.928151	3.143967
C	-2.861399	-0.364923	1.153514
C	-2.584531	-2.505916	2.336513
C	-3.293717	-1.698556	1.395137
C	2.126540	-2.763337	1.510287
C	1.932007	-2.483237	2.896392
H	2.184915	-1.027378	4.428818
H	1.719995	-3.305858	3.575202
H	-2.886215	-3.540788	2.477986
H	-1.214485	-2.478386	3.970235
C	-3.756398	0.505436	0.493377
C	-4.496805	-2.156416	0.816385
C	3.035404	-2.038206	-0.605678
C	2.220079	-4.099404	1.065531
C	3.194190	-3.352527	-0.992239
C	2.727157	-4.396997	-0.178982
C	-5.321934	-1.297784	0.124187
C	-4.963638	0.055424	0.004069
H	-3.501010	1.554636	0.399319
H	-5.635734	0.755183	-0.484553
H	-6.262557	-1.653476	-0.288091
H	-4.790329	-3.191082	0.980049
H	3.444422	-1.252980	-1.227205
H	3.688642	-3.574119	-1.933372
H	2.821691	-5.429939	-0.503061
H	1.944877	-4.894826	1.754700

84

13TS scf done: -2073.474152

C	3.401207	-1.560525	0.680524
C	3.401207	-1.560525	-0.680524
C	2.168824	-1.759858	1.355993

C	2.168824	-1.759858	-1.355993
C	0.939795	-1.416609	0.729239
C	0.939795	-1.416609	-0.729239
C	2.187983	-2.625065	2.492490
C	1.047947	-3.274766	2.847758
C	-0.208111	-2.779167	2.386450
C	-0.244718	-1.619866	1.568382
H	4.328071	-1.611540	1.245825
H	4.328071	-1.611540	-1.245825
H	3.149577	-2.889405	2.923860
H	1.058694	-4.101566	3.553170
C	-1.426345	-3.378814	2.806147
C	-1.424657	-0.800198	1.697534
C	-2.643558	-1.462361	2.016780
C	-2.621284	-2.797997	2.497944
H	-1.380661	-4.322586	3.344136
H	-3.563050	-3.287246	2.733197
C	1.047947	-3.274766	-2.847758
C	2.187983	-2.625065	-2.492490
C	-0.208111	-2.779167	-2.386450
C	-0.244718	-1.619866	-1.568382
C	-1.426345	-3.378814	-2.806147
C	-2.621284	-2.797997	-2.497944
C	-2.643558	-1.462361	-2.016780
C	-1.424657	-0.800198	-1.697534
H	1.058694	-4.101566	-3.553170
H	3.149577	-2.889405	-2.923860
H	-1.380661	-4.322586	-3.344136
H	-3.563050	-3.287246	-2.733197
C	-1.422647	0.650129	-1.750853
C	-3.874892	-0.754239	-1.955600
C	-1.422647	0.650129	1.750853
C	-3.874892	-0.754239	1.955600
C	-2.675580	1.321061	-1.671022
C	-3.890949	0.583727	-1.717964
C	-2.675580	1.321061	1.671022
C	-3.890949	0.583727	1.717964
H	-4.830171	1.125231	-1.636349
H	-4.798385	-1.306470	-2.111862
H	-4.830171	1.125231	1.636349
H	-4.798385	-1.306470	2.111862
C	-0.262640	1.470810	-2.018791
C	-2.728722	2.735887	-1.592949
C	-0.262640	1.470810	2.018791
C	-2.728722	2.735887	1.592949
C	-1.584614	3.470665	1.521551
C	-0.326282	2.851501	1.719935
C	-0.326282	2.851501	-1.719935
C	-1.584614	3.470665	-1.521551

H	-1.619249	4.545773	-1.363225
H	-3.702853	3.214055	-1.526716
H	-1.619249	4.545773	1.363225
H	-3.702853	3.214055	1.526716
C	0.872806	3.630750	-1.683434
C	0.909641	1.049541	-2.765618
C	0.872806	3.630750	1.683434
C	0.909641	1.049541	2.765618
C	2.066381	3.103177	2.055558
C	2.096754	1.831240	2.705325
C	2.096754	1.831240	-2.705325
C	2.066381	3.103177	-2.055558
H	0.802422	4.657792	-1.333504
H	2.983624	3.682541	-1.985225
H	2.983624	3.682541	1.985225
H	0.802422	4.657792	1.333504
C	0.858689	0.018221	3.727685
C	3.238297	1.424563	3.428553
C	0.858689	0.018221	-3.727685
C	3.238297	1.424563	-3.428553
C	1.960458	-0.307982	-4.489620
C	3.180407	0.362346	-4.303219
C	3.180407	0.362346	4.303219
C	1.960458	-0.307982	4.489620
H	-0.078096	-0.497776	3.899732
H	1.879894	-1.095285	5.233556
H	4.055571	0.078460	4.881716
H	4.149480	2.011012	3.332353
H	-0.078096	-0.497776	-3.899732
H	1.879894	-1.095285	-5.233556
H	4.055571	0.078460	-4.881716
H	4.149480	2.011012	-3.332353

90

14-1 scf done: -2227.050358

C	-0.737878	-1.180072	3.594062
C	-0.572013	0.173378	3.620154
C	-0.993201	-1.852264	2.364416
C	-0.427896	0.909113	2.409151
C	-1.032431	-1.105031	1.166441
C	-0.475105	0.223004	1.177178
C	-1.239961	-3.254943	2.318004
C	-1.511876	-3.870697	1.132763
C	-1.766044	-3.102091	-0.040425
C	-1.696124	-1.691176	0.025967
C	-2.101941	-3.728810	-1.273139
C	-2.329299	-0.929033	-1.027407
C	-2.487394	-1.564154	-2.284650
C	-2.349554	-2.977799	-2.382715
C	-0.144903	3.008141	1.235423

C	-0.251461	2.322743	2.409100
C	0.000001	2.313728	-0.000002
C	0.000001	0.902221	-0.000001
C	0.144905	3.008140	-1.235427
C	0.251463	2.322741	-2.409103
C	0.427898	0.909111	-2.409153
C	0.475106	0.223003	-1.177179
C	0.572015	0.173375	-3.620155
C	1.032432	-1.105032	-1.166440
C	0.993203	-1.852266	-2.364415
C	0.737880	-1.180075	-3.594062
C	1.239964	-3.254945	-2.318002
C	1.696125	-1.691176	-0.025966
C	1.511879	-3.870698	-1.132760
C	1.766047	-3.102091	0.040427
C	-2.796282	-0.785679	-3.433559
C	-2.842620	0.413941	-0.883903
C	-2.955269	0.563392	-3.331734
C	-3.018450	1.185787	-2.054542
C	2.101944	-3.728808	1.273142
C	2.329299	-0.929031	1.027408
C	2.349556	-2.977796	2.382717
C	2.487395	-1.564151	2.284652
C	-3.300971	2.581497	-1.953599
C	-3.297881	0.988058	0.367910
C	-3.549655	2.387034	0.440256
C	-3.485686	3.176350	-0.746328
C	2.842619	0.413943	0.883903
C	2.796282	-0.785675	3.433560
C	3.018448	1.185790	2.054542
C	2.955267	0.563395	3.331734
C	-3.622176	0.208840	1.502612
C	-3.942978	2.964651	1.667367
C	-4.165800	2.185966	2.779335
C	-4.039460	0.789572	2.679503
C	3.300966	2.581501	1.953598
C	3.297878	0.988060	-0.367910
C	3.485681	3.176353	0.746326
C	3.549651	2.387036	-0.440257
C	3.942975	2.964653	-1.667368
C	3.622175	0.208843	-1.502612
C	4.165797	2.185968	-2.779335
C	4.039459	0.789575	-2.679503
H	-0.743398	-1.758652	4.514774
H	-0.483888	0.705030	4.564272
H	-1.149376	-3.829479	3.236612
H	-1.602788	-4.952667	1.074633
H	-2.097497	-4.814865	-1.323201
H	-2.508020	-3.448255	-3.350158

H	-0.108312	4.094472	1.227878
H	-0.265107	2.848200	3.360653
H	0.108314	4.094470	-1.227884
H	0.265110	2.848197	-3.360656
H	0.483890	0.705025	-4.564273
H	0.743401	-1.758657	-4.514773
H	1.149380	-3.829482	-3.236609
H	1.602792	-4.952668	-1.074629
H	-2.855366	-1.283982	-4.398076
H	-3.111362	1.174794	-4.217312
H	2.097501	-4.814864	1.323205
H	2.508022	-3.448252	3.350161
H	-3.665407	4.246389	-0.673212
H	-3.348702	3.162063	-2.871905
H	2.855365	-1.283978	4.398077
H	3.111359	1.174799	4.217312
H	-3.562216	-0.870696	1.439011
H	-4.275634	0.158998	3.532046
H	-4.475837	2.641515	3.716017
H	-4.096445	4.040903	1.707287
H	3.665401	4.246392	0.673211
H	3.348696	3.162067	2.871904
H	4.096440	4.040906	-1.707288
H	4.475834	2.641517	-3.716017
H	4.275633	0.159000	-3.532046
H	3.562215	-0.870694	-1.439011

90

14-2 scf done: -2226.967774

C	-1.230924	-2.757716	-1.790633
C	-1.184464	-3.152615	-0.486740
C	-0.939280	-1.413708	-2.141206
C	-0.663191	-2.289616	0.512416
C	-0.681113	-0.471924	-1.116163
C	-0.281159	-0.963585	0.177621
C	-0.901600	-0.989215	-3.502014
C	-0.670005	0.317524	-3.811846
C	-0.752051	1.311627	-2.791458
C	-0.937912	0.912458	-1.447083
H	-1.526421	-3.449208	-2.575619
H	-1.482143	-4.157437	-0.199430
H	-1.009583	-1.739112	-4.282021
H	-0.540144	0.635828	-4.843204
C	-0.753587	2.695981	-3.119356
C	-1.533475	1.866413	-0.540244
C	-1.445249	3.243467	-0.867481
C	-1.008752	3.634694	-2.164441
H	-0.534442	2.987922	-4.143573
H	-0.953553	4.695531	-2.396887
C	-0.195445	-1.873865	2.842535

C	-0.551072	-2.740853	1.855583
C	0.230150	-0.553268	2.531650
C	0.398670	-0.167652	1.174417
C	0.410041	0.403498	3.565782
C	0.611013	1.710239	3.238262
C	0.934803	2.076316	1.903029
C	1.092197	1.070375	0.915145
H	-0.228677	-2.173516	3.887200
H	-0.837032	-3.763672	2.085920
H	0.261402	0.096129	4.597661
H	0.578835	2.491510	3.993634
C	2.005230	1.411406	-0.182395
C	1.081651	3.446403	1.545687
C	-2.297742	1.507294	0.636745
C	-1.802855	4.224874	0.098777
C	2.010648	2.781283	-0.562839
C	1.428971	3.776517	0.274866
C	-2.423120	2.483959	1.656737
C	-2.169392	3.851683	1.355641
H	1.453497	4.812440	-0.052846
H	0.840175	4.206790	2.283102
H	-2.336162	4.593522	2.133170
H	-1.701762	5.274817	-0.165192
C	3.206343	0.650959	-0.516270
C	2.880776	3.251053	-1.585029
C	-3.010611	0.264155	0.830946
C	-2.834079	2.093972	2.960930
C	-3.149383	0.795454	3.224613
C	-3.303350	-0.130716	2.156333
C	4.275619	1.357274	-1.133259
C	4.018996	2.557044	-1.849621
H	4.802116	2.978082	-2.475415
H	2.723348	4.247432	-1.990391
H	-3.386916	0.471644	4.234955
H	-2.849515	2.845040	3.746979
C	5.631303	1.028407	-0.832770
C	3.590076	-0.638501	0.039771
C	-3.835061	-1.430020	2.414113
C	-3.600443	-0.515331	-0.241328
C	-4.190176	-2.258652	1.398124
C	-4.153079	-1.795177	0.049778
C	4.883146	-0.752662	0.593766
C	5.909991	0.129851	0.152438
H	6.418273	1.623392	-1.289411
H	6.922173	-0.008014	0.524171
H	-4.582746	-3.252545	1.599775
H	-3.956761	-1.737270	3.450126
C	-3.787930	-0.009508	-1.548924
C	-4.729350	-2.562443	-0.985780

C	2.878543	-1.875535	-0.131323
C	5.177121	-1.852292	1.457440
C	3.235481	-3.011438	0.649031
C	4.325154	-2.909152	1.563226
C	-4.832416	-2.066738	-2.264972
C	-4.384177	-0.762752	-2.535826
H	-3.477658	1.002977	-1.776231
H	-4.509506	-0.338594	-3.528159
H	-5.288285	-2.663272	-3.050746
H	-5.118604	-3.548965	-0.743197
H	4.553541	-3.749142	2.214778
H	6.119886	-1.840734	1.999679
C	2.662064	-4.266164	0.346861
C	2.096990	-2.077623	-1.291611
C	1.687688	-3.341230	-1.649683
C	1.920572	-4.437133	-0.799524
H	2.906728	-5.117369	0.978595
H	1.549539	-5.422375	-1.069399
H	1.172508	-3.489695	-2.592604
H	1.913123	-1.234717	-1.950095

90

14-3 scf done: -2226.966614

C	0.594175	-3.281760	-0.239969
C	0.530407	-2.852403	-1.530872
C	0.592951	-2.347663	0.830399
C	0.308386	-1.481310	-1.830828
C	0.481195	-0.961322	0.553684
C	0.105154	-0.550389	-0.776854
C	0.725129	-2.790886	2.174366
C	0.665016	-1.901084	3.205227
C	0.735632	-0.504939	2.945984
C	0.871719	-0.056367	1.609742
H	0.704349	-4.337122	-0.006360
H	0.634635	-3.552078	-2.356223
H	0.788240	-3.858978	2.361765
H	0.637234	-2.239538	4.238383
C	0.753880	0.447225	4.007008
C	1.546635	1.211482	1.420590
C	1.453445	2.166458	2.463619
C	0.985892	1.764413	3.749187
H	0.549559	0.101930	5.017809
H	0.924203	2.509545	4.538361
C	0.376041	0.319283	-3.430892
C	0.368006	-1.019036	-3.173230
C	0.086179	1.256699	-2.401592
C	-0.309505	0.784975	-1.124540
C	0.257302	2.654547	-2.610997
C	0.100761	3.508780	-1.562981
C	-0.579455	3.076866	-0.389063

C	-1.021174	1.732530	-0.281035
H	0.586875	0.695670	-4.428950
H	0.525134	-1.743212	-3.968416
H	0.622260	3.000437	-3.574170
H	0.373971	4.557676	-1.643710
C	-2.340048	1.561913	0.330511
C	-0.978478	4.033869	0.583591
C	2.411574	1.520440	0.301818
C	1.894459	3.500115	2.244241
C	-2.862799	2.656350	1.072727
C	-2.049853	3.784101	1.381614
C	2.719655	2.884826	0.057228
C	2.431424	3.864832	1.046460
H	-2.421857	4.534467	2.074497
H	-0.464812	4.990786	0.612891
H	2.703438	4.899093	0.848327
H	1.764772	4.227200	3.042241
C	-3.324554	0.639365	-0.224060
C	-4.269785	2.853366	1.201274
C	3.058926	0.542712	-0.546517
C	3.320105	3.267559	-1.174008
C	3.583253	2.337680	-2.133305
C	3.488861	0.951756	-1.828342
C	-4.613603	1.165497	-0.483087
C	-5.103163	2.228977	0.324836
H	-6.145122	2.524232	0.228887
H	-4.628675	3.658820	1.837007
H	3.954338	2.632860	-3.111923
H	3.503222	4.324082	-1.354793
C	-5.381824	0.630560	-1.558323
C	-3.148693	-0.735405	-0.617019
C	3.902639	-0.023774	-2.785940
C	3.449546	-0.785334	-0.117702
C	4.007644	-1.336395	-2.451374
C	3.864562	-1.738196	-1.089826
C	-3.844635	-1.200252	-1.755113
C	-4.915200	-0.425475	-2.284963
H	-6.315647	1.123045	-1.818457
H	-5.445734	-0.783874	-3.163454
H	4.296102	-2.080083	-3.190400
H	4.129171	0.312893	-3.794925
C	3.594902	-1.135631	1.244250
C	4.232704	-3.038288	-0.680449
C	-2.650249	-1.729856	0.305265
C	-3.617996	-2.530384	-2.219437
C	-2.631696	-3.095410	-0.092542
C	-2.988679	-3.441824	-1.428974
C	4.289662	-3.372365	0.653203
C	4.005905	-2.394409	1.622054

H	3.406564	-0.388691	2.005903
H	4.109115	-2.627922	2.677944
H	4.591100	-4.371437	0.956626
H	4.510932	-3.762331	-1.443192
H	-2.865927	-4.471690	-1.755780
H	-4.034885	-2.821843	-3.180752
C	-2.395867	-4.098821	0.873016
C	-2.460860	-1.431128	1.675736
C	-2.320064	-2.434332	2.606036
C	-2.275715	-3.781767	2.205983
H	-2.378049	-5.137093	0.548236
H	-2.150116	-4.566505	2.947390
H	-2.228567	-2.178843	3.657617
H	-2.494792	-0.397342	2.002722

90

14-4 scf done: -2226.967693

C	0.159801	-2.667363	-2.033034
C	0.592026	-1.708073	-2.897391
C	0.030933	-2.379225	-0.645942
C	0.738842	-0.359653	-2.469804
C	0.224125	-1.052285	-0.182723
C	0.325691	0.005110	-1.161526
C	-0.227611	-3.424590	0.278000
C	-0.341581	-3.159283	1.610611
C	-0.013658	-1.875094	2.115734
C	0.448662	-0.870182	1.228318
H	0.000521	-3.689249	-2.367200
H	0.828234	-1.952718	-3.930054
H	-0.385162	-4.428511	-0.106525
H	-0.644552	-3.931959	2.311894
C	-0.107469	-1.593616	3.509916
C	1.239783	0.192748	1.819399
C	0.956258	0.544377	3.161772
C	0.237736	-0.367697	3.989872
H	-0.532170	-2.352354	4.161361
H	0.067405	-0.103006	5.030648
C	1.649048	1.841112	-2.803666
C	1.358234	0.608225	-3.306257
C	1.081936	2.268582	-1.571107
C	0.195914	1.409375	-0.874281
C	1.393011	3.546111	-1.026675
C	0.769677	3.972653	0.104092
C	-0.432930	3.325247	0.509222
C	-0.821196	2.085604	-0.067014
H	2.269949	2.541481	-3.356659
H	1.696377	0.308174	-4.294546
H	2.171401	4.138286	-1.499196
H	1.045100	4.910432	0.579399
C	-2.249934	1.893575	-0.282223

C	-1.378681	4.131973	1.203228
C	2.391651	0.815923	1.200833
C	1.469590	1.757549	3.697043
C	-3.098111	3.005591	-0.034651
C	-2.697410	4.004086	0.894050
C	2.823312	2.065720	1.721634
C	2.301238	2.541660	2.956121
H	-3.426824	4.737191	1.229785
H	-1.021273	4.970467	1.795718
H	2.647544	3.501257	3.332372
H	1.171016	2.050171	4.700869
C	-2.866078	0.828355	-1.062088
C	-4.218261	3.253371	-0.883303
C	3.201060	0.219634	0.158934
C	3.798865	2.829354	1.025537
C	4.318484	2.383467	-0.151355
C	4.047347	1.061858	-0.598256
C	-3.716536	1.248724	-2.115257
C	-4.385097	2.503754	-2.008488
H	-5.103727	2.782089	-2.774971
H	-4.818748	4.141080	-0.701814
H	5.004835	2.998900	-0.728471
H	4.081224	3.799132	1.428354
C	-4.000188	0.347938	-3.176764
C	-2.871066	-0.579450	-0.771563
C	4.672498	0.570034	-1.784582
C	3.324527	-1.206595	-0.076289
C	4.539732	-0.727482	-2.163264
C	3.923188	-1.666066	-1.283278
C	-3.211483	-1.470147	-1.820877
C	-3.638205	-0.963289	-3.078149
H	-4.533623	0.719968	-4.048155
H	-3.835527	-1.661180	-3.887958
H	4.982756	-1.088403	-3.088476
H	5.244561	1.270117	-2.389187
C	3.019740	-2.175208	0.906610
C	4.004538	-3.052035	-1.539962
C	-2.924475	-1.082091	0.594090
C	-3.330478	-2.868445	-1.570022
C	-3.250702	-2.453313	0.807939
C	-3.359407	-3.344615	-0.298742
C	3.607942	-3.972068	-0.596721
C	3.154943	-3.522586	0.655311
H	2.704958	-1.849596	1.890152
H	2.909785	-4.238003	1.435028
H	3.688478	-5.036653	-0.799596
H	4.429202	-3.379557	-2.486443
H	-3.521895	-4.401975	-0.102951
H	-3.489794	-3.532407	-2.416541

C	-3.495197	-2.924818	2.115595
C	-2.862588	-0.249006	1.735683
C	-3.134032	-0.726722	2.998461
C	-3.454020	-2.078602	3.199160
H	-3.740588	-3.976874	2.245868
H	-3.667464	-2.450569	4.197908
H	-3.087544	-0.047212	3.844559
H	-2.618056	0.798817	1.623385

90

14-5 scf done: -2226.966745

C	1.086106	-2.211832	-2.717312
C	1.791658	-1.123799	-3.132998
C	0.449876	-2.201648	-1.446945
C	1.724330	0.101383	-2.414262
C	0.433484	-1.007413	-0.677149
C	0.839131	0.219729	-1.311650
C	-0.086010	-3.400567	-0.908027
C	-0.611931	-3.422853	0.348553
C	-0.486418	-2.293627	1.201103
C	0.177255	-1.130354	0.735614
H	1.089955	-3.134593	-3.291820
H	2.411377	-1.166402	-4.025212
H	-0.089374	-4.292360	-1.529828
H	-1.091321	-4.316100	0.739145
C	-0.987550	-2.333955	2.533026
C	0.665649	-0.213922	1.744427
C	-0.042832	-0.157235	2.968283
C	-0.882520	-1.243412	3.341480
H	-1.531482	-3.217667	2.854908
H	-1.381770	-1.210480	4.305325
C	2.607886	2.285060	-1.949622
C	2.590941	1.180114	-2.742591
C	1.560319	2.513563	-1.013727
C	0.517213	1.560729	-0.861603
C	1.507549	3.748886	-0.316086
C	0.351492	4.151017	0.273260
C	-0.840948	3.439868	-0.032720
C	-0.799646	2.114952	-0.553526
H	3.359617	3.059544	-2.078294
H	3.302240	1.054166	-3.554290
H	2.393749	4.376911	-0.304418
H	0.280557	5.112222	0.775622
C	-2.022644	1.650068	-1.202560
C	-2.021181	4.235094	-0.129476
C	1.894345	0.552209	1.665632
C	0.140232	0.955618	3.836738
C	-2.861919	2.658780	-1.739860
C	-2.939931	3.915507	-1.081115
C	1.995164	1.706063	2.487763

C	1.055517	1.917450	3.537179
H	-3.718979	4.614908	-1.374198
H	-2.051069	5.195097	0.379263
H	1.152500	2.809893	4.150512
H	-0.489424	1.032095	4.719675
C	-2.447843	0.302638	-1.538869
C	-3.532656	2.425420	-2.977321
C	3.063563	0.171094	0.904504
C	3.068694	2.617659	2.307012
C	4.025531	2.385512	1.365673
C	4.058816	1.149283	0.667288
C	-2.880257	0.120086	-2.880171
C	-3.356295	1.239687	-3.624638
H	-3.721036	1.082249	-4.636170
H	-4.081835	3.246313	-3.431222
H	4.815810	3.109910	1.182032
H	3.093636	3.516561	2.918294
C	-3.037227	-1.194349	-3.388742
C	-2.795838	-0.739131	-0.597051
C	5.120130	0.887490	-0.251818
C	3.365967	-1.184324	0.478745
C	5.233469	-0.314845	-0.871971
C	4.396743	-1.401663	-0.479366
C	-3.104607	-2.017037	-1.131734
C	-3.056832	-2.252697	-2.531578
H	-3.212929	-1.327995	-4.453369
H	-3.204293	-3.265646	-2.897471
H	6.016227	-0.494586	-1.605219
H	5.822785	1.690333	-0.463349
C	2.786393	-2.328216	1.072715
C	4.656194	-2.708569	-0.945893
C	-3.158942	-0.486231	0.795628
C	-3.618944	-3.057232	-0.304508
C	-3.801867	-1.521187	1.544177
C	-3.976522	-2.817071	0.980927
C	3.995246	-3.794329	-0.418689
C	3.085791	-3.599493	0.634092
H	2.118098	-2.206464	1.915440
H	2.615882	-4.453264	1.113913
H	4.210383	-4.796982	-0.778336
H	5.422014	-2.844200	-1.706553
H	-4.424153	-3.597345	1.592330
H	-3.780186	-4.034669	-0.753231
C	-4.273294	-1.273392	2.850912
C	-3.027935	0.762691	1.444573
C	-3.491270	0.980790	2.725401
C	-4.126030	-0.042004	3.444552
H	-4.761345	-2.087691	3.382551
H	-4.497494	0.137005	4.450121

H	-3.361254	1.963400	3.170835
H	-2.555665	1.589513	0.938936

90

14-6 scf done: -2226.955474

C	-2.459733	-1.809374	2.699207
C	-2.959786	-0.545360	2.768719
C	-1.497757	-2.120188	1.701747
C	-2.325055	0.518448	2.070386
C	-0.961408	-1.087395	0.885779
C	-1.143343	0.271513	1.324701
C	-1.158987	-3.474897	1.443297
C	-0.440589	-3.808486	0.337426
C	-0.152287	-2.829020	-0.650968
C	-0.472655	-1.463750	-0.420760
H	-2.872382	-2.615058	3.300709
H	-3.818727	-0.312226	3.392644
H	-1.501397	-4.236987	2.139129
H	-0.154676	-4.839672	0.145712
C	0.379373	-3.239253	-1.902331
C	-0.463874	-0.582070	-1.566307
C	0.319959	-0.957760	-2.686078
C	0.688647	-2.317861	-2.856045
H	0.591838	-4.294367	-2.055401
H	1.196132	-2.605949	-3.772214
C	-2.244851	2.842237	1.467299
C	-2.884829	1.825247	2.098967
C	-0.874571	2.686270	1.111870
C	-0.239842	1.413144	1.165423
C	-0.113792	3.884611	1.053497
C	1.149753	3.871667	1.553018
C	1.690746	2.647880	2.023445
C	1.159139	1.404127	1.575727
H	-2.691112	3.830418	1.395577
H	-3.853140	1.969539	2.569445
H	-0.617038	4.817885	0.814860
H	1.695357	4.794411	1.734522
C	1.957437	0.240965	1.962119
C	2.626376	2.692925	3.099268
C	-1.280843	0.608128	-1.745116
C	0.708461	0.026658	-3.639784
C	2.513964	0.296918	3.267222
C	2.862721	1.562527	3.821409
C	-0.750196	1.623184	-2.584100
C	0.305569	1.316631	-3.490682
H	3.391375	1.591302	4.770625
H	2.993081	3.661876	3.427954
H	0.690419	2.105047	-4.131882
H	1.388045	-0.264291	-4.435742
C	2.358174	-0.915120	1.183941

C	2.792565	-0.914400	3.959305
C	-2.641958	0.770558	-1.285459
C	-1.349864	2.908946	-2.610753
C	-2.509668	3.143334	-1.936542
C	-3.210702	2.069026	-1.327362
C	2.550250	-2.130640	1.904549
C	2.652990	-2.110933	3.323111
H	2.781260	-3.051088	3.853168
H	3.089595	-0.858965	5.003651
H	-2.961793	4.132345	-1.929903
H	-0.870505	3.693426	-3.191165
C	2.811253	-3.339519	1.210961
C	2.855750	-0.867746	-0.177233
C	-4.509523	2.310400	-0.787489
C	-3.530591	-0.327654	-0.935330
C	-5.245570	1.307259	-0.246452
C	-4.794533	-0.042120	-0.339980
C	3.147792	-2.095183	-0.824885
C	3.046747	-3.327010	-0.129326
H	2.859646	-4.264482	1.780219
H	3.246299	-4.248990	-0.669937
H	-6.218312	1.503978	0.198522
H	-4.884913	3.331227	-0.797607
C	-3.273609	-1.678277	-1.265332
C	-5.637077	-1.098646	0.067501
C	3.308776	0.342533	-0.853679
C	3.594028	-2.117254	-2.179928
C	3.674197	0.287887	-2.231198
C	3.779738	-0.973018	-2.884193
C	-5.300817	-2.410795	-0.174124
C	-4.126087	-2.693691	-0.888716
H	-2.404971	-1.925850	-1.860242
H	-3.883708	-3.717851	-1.158222
H	-5.959735	-3.215559	0.140627
H	-6.579838	-0.850310	0.550387
H	4.086564	-0.999991	-3.927506
H	3.761560	-3.086872	-2.642887
C	4.045940	1.466435	-2.913873
C	3.587232	1.554406	-0.185365
C	3.990186	2.687775	-0.857714
C	4.168833	2.664804	-2.250000
H	4.274079	1.396529	-3.975429
H	4.462271	3.564953	-2.783399
H	4.189123	3.596168	-0.295555
H	3.542431	1.585261	0.892596

90

14-7 scf done: -2226.951151

C	-3.062550	0.274491	-2.763707
C	-3.007026	-1.035608	-2.402182

C	-2.192820	1.206402	-2.126179
C	-1.858377	-1.533156	-1.718961
C	-1.264197	0.744044	-1.159605
C	-0.835238	-0.641174	-1.301753
C	-2.313204	2.602023	-2.364530
C	-1.647424	3.495591	-1.579486
C	-1.046347	3.052693	-0.370548
C	-0.955388	1.659977	-0.091193
H	-3.831364	0.647457	-3.434484
H	-3.752579	-1.748297	-2.743311
H	-2.939832	2.934955	-3.188292
H	-1.683401	4.562158	-1.786796
C	-0.665849	4.004842	0.612565
C	-0.821314	1.264056	1.296334
C	-0.382392	2.236937	2.233232
C	-0.289269	3.603842	1.856906
H	-0.690254	5.059423	0.348835
H	0.038950	4.324650	2.601488
C	-0.372493	-3.415425	-1.618362
C	-1.643740	-2.935291	-1.660338
C	0.694891	-2.491691	-1.800036
C	0.532956	-1.116762	-1.481154
C	1.721934	-2.926902	-2.690170
C	2.320565	-2.002846	-3.487663
C	2.216121	-0.619916	-3.166234
C	1.601186	-0.227925	-1.947026
H	-0.171385	-4.480764	-1.696092
H	-2.495970	-3.600147	-1.765995
H	1.837174	-3.991521	-2.875128
H	2.918246	-2.296351	-4.347098
C	2.040969	1.037216	-1.408267
C	2.745166	0.369555	-4.039988
C	-1.229850	-0.019005	1.841377
C	-0.046959	1.853183	3.560662
C	2.386957	2.042842	-2.354188
C	2.676748	1.687091	-3.699720
C	-0.613662	-0.433382	3.050126
C	-0.042309	0.539168	3.913113
H	2.959788	2.469051	-4.399538
H	3.134124	0.053529	-5.004850
H	0.327711	0.216693	4.882716
H	0.283296	2.621665	4.254499
C	2.365347	1.299251	-0.014785
C	2.546487	3.388834	-1.929609
C	-2.316158	-0.855063	1.372857
C	-0.644980	-1.803446	3.428831
C	-1.376465	-2.697310	2.709589
C	-2.303528	-2.221834	1.740759
C	2.534198	2.660679	0.369275

C	2.530735	3.695697	-0.605617
H	2.622175	4.725025	-0.268318
H	2.694081	4.157936	-2.683833
H	-1.365904	-3.757134	2.950895
H	-0.059631	-2.115289	4.289845
C	2.783078	3.008432	1.721267
C	2.693199	0.291614	0.974224
C	-3.293963	-3.114737	1.235301
C	-3.524084	-0.344367	0.746881
C	-4.348253	-2.659636	0.509953
C	-4.525267	-1.260796	0.305118
C	2.786622	0.679054	2.332233
C	2.838371	2.049906	2.684993
H	2.899253	4.059947	1.971281
H	2.965392	2.313918	3.731868
H	-5.106187	-3.344154	0.135609
H	-3.198105	-4.171882	1.472053
C	-3.837893	1.032671	0.671138
C	-5.712417	-0.778599	-0.286839
C	3.125268	-1.069523	0.686973
C	2.858665	-0.308249	3.364494
C	3.110116	-2.045164	1.723347
C	2.895712	-1.632174	3.072690
C	-5.952578	0.570597	-0.403726
C	-5.013076	1.480103	0.108498
H	-3.152028	1.759501	1.086451
H	-5.209864	2.547879	0.068276
H	-6.872775	0.929190	-0.857243
H	-6.447284	-1.502326	-0.633233
H	2.895546	-2.382969	3.859335
H	2.852048	0.035042	4.395831
C	3.490640	-3.375020	1.443243
C	3.769380	-1.428106	-0.515946
C	4.015464	-3.717652	0.217886
C	4.209891	-2.714718	-0.744882
H	3.422633	-4.111754	2.240764
H	4.331806	-4.738217	0.019616
H	4.713678	-2.946111	-1.678648
H	3.971082	-0.662981	-1.253536

90

14-8 scf done: -2226.949874

C	-2.882262	-1.852282	-2.339028
C	-2.225560	-2.771693	-1.583450
C	-2.457819	-0.492916	-2.323721
C	-0.917200	-2.457007	-1.107553
C	-1.442874	-0.093416	-1.419361
C	-0.444070	-1.118323	-1.110189
C	-3.053457	0.473185	-3.180561
C	-2.679335	1.782141	-3.106122

C	-1.946518	2.229607	-1.972904
C	-1.481096	1.286775	-1.016200
H	-3.766369	-2.117185	-2.911709
H	-2.572655	-3.799456	-1.520871
H	-3.764556	0.130809	-3.928264
H	-3.037470	2.515333	-3.824280
C	-1.778249	3.619223	-1.726991
C	-1.324944	1.748420	0.348926
C	-1.168187	3.145443	0.560654
C	-1.321788	4.055755	-0.521464
H	-2.036074	4.321678	-2.515973
H	-1.162719	5.114747	-0.334460
C	1.248558	-3.358192	-1.538564
C	-0.006701	-3.550029	-1.050383
C	1.643917	-2.055333	-1.943865
C	0.965399	-0.920880	-1.426991
C	2.546639	-1.907485	-3.037944
C	2.672904	-0.697183	-3.649385
C	2.240062	0.474589	-2.961379
C	1.632500	0.349291	-1.685354
H	1.911436	-4.194665	-1.742548
H	-0.387184	-4.548915	-0.853194
H	3.001403	-2.802825	-3.453468
H	3.197256	-0.588540	-4.595127
C	2.495918	1.771863	-3.484300
C	1.848183	1.441694	-0.766902
C	2.041957	2.736441	-1.325510
C	2.275639	2.879349	-2.720046
H	2.853525	1.857529	-4.507592
H	2.403445	3.878238	-3.129452
C	2.116338	3.874994	-0.478906
C	2.101661	1.280546	0.652501
C	2.092276	3.735955	0.874070
C	2.120122	2.445114	1.466936
H	2.196487	4.857081	-0.938562
C	-1.480174	0.909280	1.519164
C	-0.924936	3.651974	1.864275
H	-0.810532	4.725670	1.990277
C	-0.780695	2.804047	2.918888
C	-1.025569	1.415214	2.764897
C	-0.823767	0.531387	3.862506
C	-2.171544	-0.366942	1.580096
C	2.477655	0.040049	1.298648
C	2.192143	2.328915	2.881250
C	2.170674	1.105243	3.478851
C	-1.810091	-1.265778	2.608467
C	2.310421	-0.069756	2.696251
C	-1.067404	-0.800435	3.729216
H	-0.507163	3.175295	3.903173

H	-0.418209	0.938272	4.784659
H	-0.825928	-1.500477	4.525017
H	2.131007	1.009604	4.561083
H	2.201164	3.239860	3.474081
H	2.110051	4.606062	1.525578
C	-2.323123	-2.597461	2.609855
C	-3.374509	-0.681368	0.834682
C	3.233161	-1.029598	0.674868
C	2.379338	-1.353526	3.322931
C	2.769383	-2.453366	2.628623
C	-3.314506	-2.967014	1.757675
C	3.315091	-2.296006	1.317674
C	-3.933241	-1.989867	0.924306
H	-1.926922	-3.298263	3.341049
H	-3.713423	-3.978643	1.767936
H	2.794545	-3.434277	3.096912
H	2.109508	-1.422813	4.374017
C	-4.130787	0.302221	0.155367
C	-5.136947	-2.287535	0.249687
C	4.071671	-0.805233	-0.438634
C	4.064212	-3.333030	0.721775
C	-5.320725	-0.003647	-0.466034
C	-5.820859	-1.317071	-0.445183
C	4.822108	-3.101965	-0.404959
C	4.858787	-1.810836	-0.957301
H	-3.777813	1.326546	0.141432
H	-5.873432	0.781438	-0.974609
H	-6.754610	-1.555268	-0.947743
H	-5.529753	-3.300015	0.315125
H	4.121355	0.186942	-0.871751
H	5.504033	-1.599667	-1.805298
H	5.422110	-3.899036	-0.836121
H	4.080825	-4.306310	1.207531

90

14TS scf done: -2226.941137

C	-2.199054	-2.912613	-1.705322
C	-1.197825	-3.438215	-0.951770
C	-2.165141	-1.537654	-2.065049
C	-0.000007	-2.675671	-0.816728
C	-1.272544	-0.662574	-1.394563
C	-0.000005	-1.264649	-0.988154
C	-2.955099	-1.051243	-3.145497
C	-2.844178	0.246858	-3.544349
C	-2.240992	1.186647	-2.660817
C	-1.655092	0.733969	-1.448236
H	-3.023744	-3.524246	-2.059677
H	-1.189613	-4.490993	-0.682294
H	-3.564640	-1.763340	-3.695977
H	-3.318480	0.606300	-4.453746

C	-2.324599	2.583241	-2.916088
C	-1.701079	1.648837	-0.329895
C	-1.767220	3.040521	-0.616007
C	-1.994139	3.482919	-1.948096
H	-2.662657	2.912287	-3.895771
H	-2.013048	4.551518	-2.147377
C	2.199038	-2.912621	-1.705324
C	1.197808	-3.438219	-0.951770
C	2.165129	-1.537662	-2.065051
C	1.272536	-0.662578	-1.394564
C	2.955086	-1.051254	-3.145502
C	2.844167	0.246846	-3.544355
C	2.240987	1.186639	-2.660823
C	1.655089	0.733964	-1.448239
H	3.023726	-3.524256	-2.059680
H	1.189593	-4.490997	-0.682294
H	3.564624	-1.763354	-3.695982
H	3.318468	0.606286	-4.453754
C	2.324597	2.583232	-2.916097
C	1.701084	1.648834	-0.329899
C	1.767229	3.040517	-0.616014
C	1.994144	3.482912	-1.948105
H	2.662652	2.912275	-3.895781
H	2.013056	4.551511	-2.147387
C	1.695595	3.991796	0.435538
C	1.876553	1.242865	1.049438
C	1.573853	3.588671	1.728839
C	1.663588	2.212313	2.066339
H	1.709971	5.048480	0.179758
C	-1.876543	1.242866	1.049442
C	-1.695576	3.991797	0.435547
H	-1.709948	5.048482	0.179769
C	-1.573828	3.588669	1.728846
C	-1.663567	2.212311	2.066344
C	-1.560655	1.808744	3.425054
C	-2.379072	-0.040877	1.495222
C	2.379077	-0.040880	1.495218
C	1.560682	1.808750	3.425050
C	1.625880	0.491721	3.763320
C	-2.067317	-0.460779	2.808135
C	2.067326	-0.460778	2.808133
C	-1.625859	0.491715	3.763322
H	-1.447390	4.312762	2.529977
H	-1.357792	2.568693	4.175382
H	-1.439235	0.164107	4.783051
H	1.439261	0.164116	4.783052
H	1.357827	2.568702	4.175378
H	1.447423	4.312766	2.529969
C	-2.324708	-1.809245	3.205132

C	-3.384009	-0.819035	0.798743
C	3.384006	-0.819045	0.798736
C	2.324711	-1.809244	3.205131
C	3.041330	-2.648274	2.413009
C	-3.041336	-2.648269	2.413013
C	3.682875	-2.137453	1.244831
C	-3.682884	-2.137443	1.244838
H	-1.950011	-2.138550	4.171635
H	-3.231246	-3.676260	2.711967
H	3.231233	-3.676267	2.711963
H	1.950016	-2.138546	4.171635
C	-4.225741	-0.255985	-0.187417
C	-4.691789	-2.882511	0.597310
C	4.225739	-0.256000	-0.187427
C	4.691773	-2.882529	0.597300
C	-5.242927	-0.983141	-0.765147
C	-5.459802	-2.322321	-0.398577
C	5.459787	-2.322343	-0.398590
C	5.242919	-0.983161	-0.765161
H	-4.084600	0.779208	-0.475613
H	-5.876145	-0.513872	-1.512895
H	-6.250834	-2.898149	-0.871822
H	-4.881463	-3.899544	0.933869
H	4.084603	0.779194	-0.475624
H	5.876138	-0.513897	-1.512911
H	6.250814	-2.898176	-0.871838
H	4.881443	-3.899562	0.933858

96

15-1 scf done: -2380.518517

C	-1.765053	3.036782	-0.769643
C	-1.397345	2.466017	-1.951785
C	-1.683257	2.298259	0.445498
C	-0.728443	1.208367	-1.973940
C	-1.198003	0.973409	0.412399
C	-0.477189	0.539835	-0.756455
C	-2.099614	2.854771	1.688878
C	-2.026501	2.121989	2.836654
C	-1.747935	0.725783	2.784114
C	-1.500502	0.119368	1.532561
C	-1.745904	-0.078882	3.959853
C	-1.644705	-1.313850	1.435791
C	-1.469237	-2.073603	2.615772
C	-1.507848	-1.418770	3.881003
C	0.308573	-0.607952	-3.195211
C	-0.308583	0.607510	-3.195296
C	0.728436	-1.208638	-1.973773
C	0.477184	-0.539937	-0.756380
C	1.397338	-2.466285	-1.951445
C	1.765048	-3.036887	-0.769224

C	1.683249	-2.298198	0.445815
C	1.197997	-0.973351	0.412535
C	2.099608	-2.854538	1.689271
C	1.500502	-0.119156	1.532578
C	1.747936	-0.725399	2.784214
C	2.026498	-2.121598	2.836946
C	1.745913	0.079428	3.959842
C	1.644714	1.314048	1.435611
C	1.507864	1.419307	3.880808
C	1.469250	2.073965	2.615486
C	-1.270235	-3.479472	2.519904
C	-2.000292	-2.016848	0.222836
C	-1.242193	-4.089430	1.301998
C	-1.623969	-3.380093	0.128056
C	1.270250	3.479821	2.519425
C	2.000297	2.016878	0.222556
C	1.242205	4.089610	1.301435
C	1.623973	3.380110	0.127590
C	-1.648109	-4.031676	-1.135233
C	-2.743055	-1.447186	-0.877885
C	-2.641534	-2.072692	-2.141189
C	-2.050016	-3.361246	-2.250823
C	2.743056	1.447064	-0.878089
C	1.648105	4.031517	-1.135789
C	2.641530	2.072396	-2.141479
C	2.050009	3.360934	-2.251289
C	-3.680173	-0.346828	-0.751933
C	-3.171083	-1.430277	-3.300850
C	-3.848019	-0.256268	-3.207591
C	-4.172795	0.285139	-1.928395
C	3.171073	1.429821	-3.301054
C	3.680174	0.346725	-0.751989
C	3.848009	0.255825	-3.207635
C	4.172790	-0.285406	-1.928366
C	5.046244	-1.389310	-1.816533
C	4.231120	-0.061743	0.484809
C	5.495196	-1.817918	-0.588843
C	5.110160	-1.118623	0.568013
H	-2.187071	4.038242	-0.742302
H	-1.553970	2.987131	-2.892858
H	-2.420313	3.893289	1.711080
H	-2.246465	2.573335	3.801234
H	-1.880421	0.407431	4.922953
H	-1.406516	-2.020892	4.780746
H	0.545079	-1.111215	-4.129336
H	-0.545087	1.110643	-4.129491
H	1.553959	-2.987530	-2.892446
H	2.187062	-4.038344	-0.741745
H	2.420308	-3.893053	1.711615

H	2.246468	-2.572811	3.801587
H	1.880433	-0.406752	4.923009
H	1.406537	2.021553	4.780469
H	-1.080875	-4.041685	3.431002
H	-0.990139	-5.143338	1.211966
H	1.080894	4.042160	3.430445
H	0.990151	5.143506	1.211258
H	-1.996380	-3.828024	-3.231460
H	-1.296844	-5.058756	-1.196666
H	1.296839	5.058589	-1.197364
H	1.996369	3.827576	-3.231990
H	-4.219383	0.245998	-4.097820
H	-3.004112	-1.899826	-4.267442
H	4.219371	-0.246564	-4.097795
H	3.004100	1.899237	-4.267709
H	5.382612	-1.877625	-2.728627
H	6.173363	-2.664015	-0.516375
H	5.509172	-1.406391	1.536634
H	3.974215	0.482499	1.385179
C	-4.231113	0.061813	0.484811
C	-5.046250	1.389058	-1.816712
C	-5.495196	1.817836	-0.589079
C	-5.110154	1.118703	0.567872
H	-5.382623	1.877245	-2.728872
H	-6.173364	2.663941	-0.516725
H	-5.509161	1.406605	1.536455
H	-3.974202	-0.482304	1.385256

96

15TS scf done: -2380.413407

C	3.531295	-0.622836	0.680440
C	3.531295	-0.622836	-0.680440
C	2.369683	-1.078166	1.358703
C	2.369683	-1.078166	-1.358703
C	1.097849	-1.012919	0.729787
C	1.097849	-1.012919	-0.729787
C	2.569405	-1.906997	2.505214
C	1.601772	-2.791546	2.862336
C	0.272886	-2.602306	2.379395
C	-0.013676	-1.483360	1.558009
H	4.447370	-0.472265	1.245517
H	4.447370	-0.472265	-1.245517
H	3.558927	-1.942254	2.952061
H	1.789177	-3.577429	3.588305
C	-0.782663	-3.466904	2.774766
C	-1.347060	-0.955574	1.670522
C	-2.391907	-1.871170	1.977932
C	-2.074618	-3.172018	2.450190
H	-0.531069	-4.376795	3.314045
H	-2.883656	-3.863868	2.670677

C	1.601772	-2.791546	-2.862336
C	2.569405	-1.906997	-2.505214
C	0.272886	-2.602306	-2.379395
C	-0.013676	-1.483360	-1.558009
C	-0.782663	-3.466904	-2.774766
C	-2.074618	-3.172018	-2.450190
C	-2.391907	-1.871170	-1.977932
C	-1.347060	-0.955574	-1.670522
H	1.789177	-3.577429	-3.588305
H	3.558927	-1.942254	-2.952061
H	-0.531069	-4.376795	-3.314045
H	-2.883656	-3.863868	-2.670677
C	-1.656116	0.457533	-1.755764
C	-3.746419	-1.442531	-1.925264
C	-1.656116	0.457533	1.755764
C	-3.746419	-1.442531	1.925264
C	-3.021251	0.847284	-1.675508
C	-4.049871	-0.134803	-1.707907
C	-3.021251	0.847284	1.675508
C	-4.049871	-0.134803	1.707907
H	-5.083474	0.193467	-1.631240
H	-4.530368	-2.181642	-2.071903
H	-5.083474	0.193467	1.631240
H	-4.530368	-2.181642	2.071903
C	-0.692096	1.496001	-2.059730
C	-3.371364	2.220960	-1.607969
C	-0.692096	1.496001	2.059730
C	-3.371364	2.220960	1.607969
C	-2.404369	3.175301	1.535914
C	-1.042267	2.832957	1.733121
C	-1.042267	2.832957	-1.733121
C	-2.404369	3.175301	-1.535914
H	-2.658480	4.218869	-1.367303
H	-4.423642	2.485330	-1.539426
H	-2.658480	4.218869	1.367303
H	-4.423642	2.485330	1.539426
C	-0.031800	3.830422	-1.642772
C	0.551074	1.337297	-2.791124
C	-0.031800	3.830422	1.642772
C	0.551074	1.337297	2.791124
C	1.262746	3.527787	1.929424
C	1.563337	2.304179	2.590421
C	1.563337	2.304179	-2.590421
C	1.262746	3.527787	-1.929424
H	-0.314590	4.823303	-1.302697
H	2.056578	4.256359	-1.785542
H	2.056578	4.256359	1.785542
H	-0.314590	4.823303	1.302697
C	0.738443	0.405123	3.887597

C	2.853893	2.126521	3.171841
C	0.738443	0.405123	-3.887597
C	2.853893	2.126521	-3.171841
C	2.015173	0.310690	-4.517276
C	3.087886	1.136778	-4.072363
C	3.087886	1.136778	4.072363
C	2.015173	0.310690	4.517276
H	4.068656	1.013801	4.526151
H	3.637163	2.832552	2.905685
H	4.068656	1.013801	-4.526151
H	3.637163	2.832552	-2.905685
C	2.197831	-0.558899	5.613857
C	-0.326797	-0.312910	4.479314
C	-0.129691	-1.137259	5.564738
C	1.149351	-1.286434	6.126788
H	-1.329028	-0.197784	4.085782
H	-0.975960	-1.672103	5.986966
H	1.300873	-1.946567	6.976708
H	3.187558	-0.626174	6.060725
C	2.197831	-0.558899	-5.613857
C	-0.326797	-0.312910	-4.479314
C	-0.129691	-1.137259	-5.564738
C	1.149351	-1.286434	-6.126788
H	-1.329028	-0.197784	-4.085782
H	-0.975960	-1.672103	-5.986966
H	1.300873	-1.946567	-6.976708
H	3.187558	-0.626174	-6.060725

102

16-1 scf done: -2533.986511

C	2.306758	1.013233	2.863156
C	2.166209	-0.339217	2.960623
C	1.964962	1.689606	1.656826
C	1.481125	-1.073659	1.949941
C	1.452877	0.944051	0.573382
C	0.965003	-0.386740	0.829818
C	2.149868	3.093893	1.507813
C	1.830559	3.716000	0.336829
C	1.519572	2.951649	-0.824291
C	1.501207	1.541903	-0.736178
C	1.258538	3.573903	-2.079184
C	1.614456	0.787689	-1.962119
C	1.181819	1.407675	-3.157379
C	0.992160	2.819977	-3.183097
C	0.682894	-3.169593	1.039264
C	1.311764	-2.485127	2.036420
C	0.000000	-2.474630	0.000025
C	0.000000	-1.063338	0.000009
C	-0.682896	-3.169616	-1.039196
C	-1.311769	-2.485171	-2.036366

C	-1.481130	-1.073702	-1.949917
C	-0.965002	-0.386758	-0.829811
C	-2.166215	-0.339281	-2.960615
C	-1.452873	0.944042	-0.573405
C	-1.964957	1.689572	-1.656866
C	-2.306758	1.013170	-2.863179
C	-2.149862	3.093862	-1.507885
C	-1.501201	1.541923	0.736141
C	-1.830551	3.715995	-0.336916
C	-1.519563	2.951672	0.824221
C	0.959099	0.613399	-4.316891
C	2.186685	-0.537435	-2.054377
C	1.160694	-0.733459	-4.278199
C	1.797842	-1.337994	-3.157717
C	-1.258527	3.573955	2.079099
C	-1.614451	0.787738	1.962101
C	-0.992151	2.820054	3.183029
C	-1.181813	1.407752	3.157345
C	2.064119	-2.734369	-3.144199
C	3.156138	-1.087378	-1.134505
C	3.299357	-2.492460	-1.082219
C	2.707385	-3.305153	-2.087846
C	-2.186685	-0.537382	2.054390
C	-0.959099	0.613504	4.316879
C	-1.797845	-1.337915	3.157750
C	-1.160698	-0.733353	4.278219
C	4.080447	-0.294141	-0.346074
C	4.074255	-3.093465	-0.044701
C	4.750045	-2.335833	0.857767
C	4.821266	-0.920351	0.695613
C	-2.064122	-2.734291	3.144266
C	-3.156139	-1.087346	1.134531
C	-2.707386	-3.305099	2.087925
C	-3.299357	-2.492430	1.082280
C	-4.074256	-3.093461	0.044778
C	-4.080448	-0.294129	0.346080
C	-4.750050	-2.335852	-0.857708
C	-4.821271	-0.920366	-0.695588
H	2.744879	1.587627	3.675509
H	2.524487	-0.873309	3.837077
H	2.494793	3.665776	2.365631
H	1.873911	4.799211	0.251168
H	1.218111	4.659551	-2.122756
H	0.693507	3.286962	-4.118540
H	0.639600	-4.255855	1.052365
H	1.751353	-3.010500	2.880550
H	-0.639604	-4.255878	-1.052274
H	-1.751361	-3.010562	-2.880482
H	-2.524497	-0.873393	-3.837056

H	-2.744880	1.587548	-3.675545
H	-2.494788	3.665726	-2.365716
H	-1.873902	4.799208	-0.251280
H	0.570041	1.094835	-5.210685
H	0.898588	-1.361029	-5.126607
H	-1.218099	4.659604	2.122647
H	-0.693498	3.287060	4.118462
H	2.844844	-4.382530	-2.034605
H	1.703760	-3.339680	-3.972349
H	-0.570045	1.094961	5.210663
H	-0.898598	-1.360905	5.126642
H	5.310287	-2.798622	1.666876
H	4.096392	-4.179164	0.014216
H	-2.844845	-4.382477	2.034709
H	-1.703762	-3.339581	3.972431
H	-4.096391	-4.179161	-0.014113
H	-5.310294	-2.798661	-1.666803
C	4.381290	1.056996	-0.635705
C	5.685916	-0.147935	1.501710
C	5.888669	1.188713	1.247172
C	5.256409	1.782892	0.141378
H	6.215201	-0.641789	2.313798
H	6.562818	1.770738	1.869924
H	5.459157	2.820262	-0.109620
H	3.931322	1.526398	-1.501727
C	-4.381289	1.057017	0.635674
C	-5.685925	-0.147972	-1.501701
C	-5.888678	1.188682	-1.247198
C	-5.256412	1.782892	-0.141423
H	-6.215214	-0.641847	-2.313774
H	-6.562831	1.770690	-1.869962
H	-5.459158	2.820269	0.109548
H	-3.931317	1.526441	1.501681

102

16TS scf done: -2533.877590

C	2.920510	-1.714010	2.198538
C	3.490920	-1.002264	1.192552
C	1.522551	-1.963867	2.182739
C	2.732664	-0.814207	0.000000
C	0.688691	-1.253602	1.279162
C	1.312315	-0.895421	0.000000
C	0.974296	-2.992310	3.001415
C	-0.339973	-3.327856	2.889947
C	-1.227168	-2.419187	2.248635
C	-0.712323	-1.237363	1.651799
H	3.513390	-2.117562	3.013538
H	4.561534	-0.816055	1.172751
H	1.650523	-3.558489	3.636234
H	-0.750278	-4.199151	3.392776

C	-2.633237	-2.619197	2.305006
C	-1.580684	-0.085109	1.668366
C	-2.984230	-0.310350	1.722862
C	-3.487034	-1.620857	1.946454
H	-3.006346	-3.580480	2.649710
H	-4.563215	-1.775517	1.947579
C	2.920510	-1.714010	-2.198538
C	3.490920	-1.002264	-1.192552
C	1.522551	-1.963867	-2.182739
C	0.688691	-1.253602	-1.279162
C	0.974296	-2.992310	-3.001415
C	-0.339973	-3.327856	-2.889947
C	-1.227168	-2.419187	-2.248635
C	-0.712323	-1.237363	-1.651799
H	3.513390	-2.117562	-3.013538
H	4.561534	-0.816055	-1.172751
H	1.650523	-3.558489	-3.636234
H	-0.750278	-4.199151	-3.392776
C	-2.633237	-2.619197	-2.305006
C	-1.580684	-0.085109	-1.668366
C	-2.984230	-0.310350	-1.722862
C	-3.487034	-1.620857	-1.946454
H	-3.006346	-3.580480	-2.649710
H	-4.563215	-1.775517	-1.947579
C	-3.888441	0.782602	-1.668815
C	-1.118956	1.271212	-1.874677
C	-3.429286	2.059414	-1.570864
C	-2.039388	2.333019	-1.666933
H	-4.955357	0.573177	-1.679625
C	-1.118956	1.271212	1.874677
C	-3.888441	0.782602	1.668815
H	-4.955357	0.573177	1.679625
C	-3.429286	2.059414	1.570864
C	-2.039388	2.333019	1.666933
C	-1.573496	3.673284	1.572180
C	0.177424	1.651596	2.410388
C	0.177424	1.651596	-2.410388
C	-1.573496	3.673284	-1.572180
C	-0.240916	3.939046	-1.619666
C	0.667388	2.935591	2.051699
C	0.667388	2.935591	-2.051699
C	-0.240916	3.939046	1.619666
H	-4.116576	2.894018	1.456462
H	-2.296701	4.460253	1.374384
H	0.142563	4.935832	1.416751
H	0.142563	4.935832	-1.416751
H	-2.296701	4.460253	-1.374384
H	-4.116576	2.894018	-1.456462
C	2.041706	3.247072	2.230897

C	0.938894	0.931407	3.408377
C	0.938894	0.931407	-3.408377
C	2.041706	3.247072	-2.230897
C	2.863105	2.378861	-2.881746
C	2.863105	2.378861	2.881746
C	2.307417	1.263252	-3.565170
C	2.307417	1.263252	3.565170
H	2.414817	4.191653	1.842304
H	3.924497	2.585947	2.992848
H	3.924497	2.585947	-2.992848
H	2.414817	4.191653	-1.842304
C	0.354483	0.036827	4.396057
C	3.130251	0.536196	4.475362
C	0.354483	0.036827	-4.396057
C	3.130251	0.536196	-4.475362
C	1.208698	-0.668845	5.295514
C	2.613115	-0.428367	5.278350
C	2.613115	-0.428367	-5.278350
C	1.208698	-0.668845	-5.295514
H	3.248101	-0.984854	5.964127
H	4.189218	0.781174	4.513845
H	3.248101	-0.984854	-5.964127
H	4.189218	0.781174	-4.513845
C	0.657846	-1.554594	6.246092
C	-0.703439	-1.708895	6.370989
C	-1.554443	-0.934243	5.567305
C	-1.037475	-0.082493	4.615204
H	1.337349	-2.098317	6.899087
H	-1.115540	-2.391765	7.109106
C	-1.037475	-0.082493	-4.615204
C	-1.554443	-0.934243	-5.567305
C	-0.703439	-1.708895	-6.370989
C	0.657846	-1.554594	-6.246092
H	-1.115540	-2.391765	-7.109106
H	1.337349	-2.098317	-6.899087
H	-1.722069	0.530033	4.044427
H	-2.631681	-0.996835	5.693992
H	-1.722069	0.530033	-4.044427
H	-2.631681	-0.996835	-5.693992

108

17-1 scf done: -2687.454515

C	-1.888876	1.068675	2.960177
C	-1.479896	2.249919	2.416537
C	-1.803222	-0.140199	2.211517
C	-0.768407	2.274533	1.182398
C	-1.256780	-0.105386	0.910357
C	-0.500854	1.058000	0.518236
C	-2.266313	-1.380429	2.737821
C	-2.166044	-2.527175	2.007225

C	-1.796879	-2.477335	0.632403
C	-1.511197	-1.226941	0.043531
C	-1.731456	-3.653253	-0.168611
C	-1.549286	-1.137996	-1.393757
C	-1.312438	-2.313865	-2.139820
C	-1.389249	-3.577533	-1.486596
C	0.325881	3.495977	-0.598706
C	-0.325879	3.495984	0.598668
C	0.768409	2.274518	-1.182420
C	0.500857	1.057994	-0.518243
C	1.479895	2.249888	-2.416561
C	1.888872	1.068636	-2.960187
C	1.803219	-0.140228	-2.211511
C	1.256781	-0.105397	-0.910351
C	2.266307	-1.380466	-2.737802
C	1.511196	-1.226944	-0.043511
C	1.796871	-2.477345	-0.632369
C	2.166036	-2.527202	-2.007192
C	1.731444	-3.653254	0.168657
C	1.549286	-1.137982	1.393776
C	1.389238	-3.577516	1.486642
C	1.312434	-2.313841	2.139851
C	-1.038259	-2.209624	-3.534013
C	-1.900190	0.060903	-2.117655
C	-1.008502	-0.991078	-4.144296
C	-1.459457	0.173064	-3.456934
C	1.038254	-2.209582	3.534044
C	1.900196	0.060925	2.117658
C	1.008504	-0.991029	4.144311
C	1.459464	0.173105	3.456936
C	-1.489865	1.442279	-4.099741
C	-2.717850	1.126809	-1.581463
C	-2.582034	2.409556	-2.169264
C	-1.939242	2.541903	-3.432624
C	2.717857	1.126822	1.581450
C	1.489878	1.442326	4.099730
C	2.582046	2.409576	2.169239
C	1.939258	2.541940	3.432598
C	-3.694638	0.972460	-0.527471
C	-3.105216	3.550241	-1.501256
C	-3.752734	3.417326	-0.310228
C	-4.094659	2.127645	0.181708
C	3.105226	3.550253	1.501217
C	3.694641	0.972460	0.527457
C	3.752743	3.417325	0.310188
C	4.094664	2.127638	-0.181733
C	4.880152	2.001655	-1.367172
C	4.387418	-0.266302	0.226529
C	5.326441	0.790462	-1.790277

C	5.145524	-0.365458	-0.974112
H	-2.349636	1.038847	3.944372
H	-1.639009	3.188287	2.942142
H	-2.649672	-1.401500	3.754878
H	-2.431382	-3.488398	2.440199
H	-1.901058	-4.615594	0.307842
H	-1.237755	-4.478714	-2.076057
H	0.575942	4.429819	-1.096141
H	-0.575939	4.429832	1.096093
H	1.639007	3.188248	-2.942179
H	2.349629	1.038795	-3.944384
H	2.649665	-1.401550	-3.754859
H	2.431370	-3.488432	-2.440154
H	1.901041	-4.615601	-0.307784
H	1.237741	-4.478691	2.076113
H	-0.797593	-3.115172	-4.085556
H	-0.703212	-0.895240	-5.183487
H	0.797585	-3.115122	4.085598
H	0.703215	-0.895175	5.183502
H	-1.873723	3.530836	-3.879978
H	-1.093322	1.524143	-5.108753
H	1.093338	1.524202	5.108742
H	1.873744	3.530880	3.879939
H	-4.085809	4.291497	0.244184
H	-2.936961	4.531002	-1.939360
H	4.085818	4.291490	-0.244234
H	2.936972	4.531019	1.939311
H	5.100026	2.903522	-1.933750
H	5.895193	0.696118	-2.712409
C	-4.387418	-0.266299	-0.226533
C	-4.880146	2.001674	1.367149
C	-5.326438	0.790486	1.790263
C	-5.145525	-0.365441	0.974107
H	-5.100016	2.903547	1.933719
H	-5.895190	0.696149	2.712397
C	4.453207	-1.353629	1.128394
C	5.783111	-1.582250	-1.300982
C	5.752924	-2.653664	-0.438593
C	5.112199	-2.518904	0.805129
H	6.327929	-1.644963	-2.240545
H	6.254327	-3.582308	-0.697984
H	5.137438	-3.334636	1.522192
H	3.994745	-1.260652	2.105124
C	-5.783118	-1.582228	1.300986
C	-4.453211	-1.353631	-1.128392
C	-5.752939	-2.653646	0.438604
C	-5.112210	-2.518899	-0.805119
H	-6.327937	-1.644933	2.240549
H	-6.254344	-3.582287	0.698000

H	-5.137456	-3.334638	-1.522174
H	-3.994743	-1.260664	-2.105119
108			
17TS scf done: -2687.343208			
C	-0.679308	-3.715197	-0.881417
C	0.679309	-3.715204	-0.881426
C	-1.353368	-2.512960	-1.229065
C	1.353375	-2.512973	-1.229084
C	-0.732025	-1.251268	-1.024378
C	0.732043	-1.251274	-1.024392
C	-2.478671	-2.636518	-2.096218
C	-2.849240	-1.579282	-2.865437
C	-2.402783	-0.274463	-2.510118
C	-1.576577	-0.104912	-1.369531
H	-1.247066	-4.639887	-0.819312
H	1.247059	-4.639898	-0.819329
H	-2.901328	-3.624899	-2.254698
H	-3.559995	-1.688909	-3.679270
C	-2.825312	0.865652	-3.246574
C	-1.688585	1.167787	-0.709120
C	-2.006520	2.301845	-1.505886
C	-2.506269	2.120978	-2.821915
H	-3.380770	0.707991	-4.167583
H	-2.750865	2.996934	-3.417005
C	2.849254	-1.579305	-2.865458
C	2.478675	-2.636539	-2.096240
C	2.402806	-0.274483	-2.510138
C	1.576601	-0.104926	-1.369551
C	2.825346	0.865631	-3.246592
C	2.506323	2.120960	-2.821926
C	2.006574	2.301829	-1.505898
C	1.688614	1.167773	-0.709140
H	3.560010	-1.688936	-3.679289
H	2.901324	-3.624923	-2.254720
H	3.380794	0.707966	-4.167606
H	2.750931	2.996915	-3.417013
C	1.738594	1.335085	0.724668
C	1.928557	3.604737	-0.944581
C	-1.738597	1.335103	0.724688
C	-1.928496	3.604754	-0.944574
C	1.637407	2.651199	1.252075
C	1.673943	3.774095	0.380966
C	-1.637424	2.651221	1.252094
C	-1.673921	3.774115	0.380980
H	1.577454	4.768760	0.809363
H	2.085739	4.460055	-1.597155
H	-1.577429	4.768780	0.809376
H	-2.085641	4.460072	-1.597158
C	2.080053	0.282683	1.657389

C	1.581080	2.854957	2.656037
C	-2.080085	0.282708	1.657406
C	-1.581147	2.854988	2.656056
C	-1.532630	1.793116	3.507054
C	-1.748701	0.477287	3.022389
C	1.748629	0.477252	3.022362
C	1.532537	1.793079	3.507026
H	1.369279	1.934849	4.572510
H	1.503762	3.872952	3.029869
H	-1.369409	1.934892	4.572543
H	-1.503846	3.872986	3.029883
C	1.674180	-0.643027	3.899224
C	2.868853	-0.905608	1.369716
C	-1.674263	-0.642988	3.899257
C	-2.868874	-0.905590	1.369722
C	-1.973633	-1.888550	3.444545
C	-2.645318	-2.038826	2.196739
C	2.645292	-2.038850	2.196724
C	1.973578	-1.888584	3.444515
H	1.323645	-0.482870	4.915559
H	1.824605	-2.767310	4.066805
H	-1.824663	-2.767272	4.066840
H	-1.323760	-0.482821	4.915603
C	-3.971413	-0.974185	0.436999
C	-3.195777	-3.298388	1.845642
C	3.971404	-0.974193	0.437006
C	3.195762	-3.298407	1.845625
C	4.486417	-2.251586	0.098808
C	4.035869	-3.412860	0.779648
C	-4.035876	-3.412851	0.779661
C	-4.486423	-2.251583	0.098810
H	-4.438788	-4.379649	0.486820
H	-2.941824	-4.163445	2.453521
H	4.438784	-4.379655	0.486802
H	2.941808	-4.163469	2.453496
C	-5.480862	-2.386939	-0.916221
C	-4.704944	0.179990	-0.060023
C	-5.640899	0.010030	-1.121535
C	-5.980151	-1.303347	-1.562228
H	-6.704947	-1.414990	-2.365392
H	-5.806042	-3.390401	-1.181655
C	5.480862	-2.386927	-0.916220
C	4.704949	0.179989	-0.059979
C	5.640915	0.010046	-1.121483
C	5.980160	-1.303324	-1.562204
H	6.704962	-1.414955	-2.365364
H	5.806043	-3.390384	-1.181668
C	-4.649147	1.457724	0.541723
C	-5.338829	2.533929	0.026047

C	-6.141589	2.385283	-1.115939
C	-6.307681	1.131730	-1.658974
H	-6.988432	0.977360	-2.493442
H	-6.665294	3.240642	-1.534267
H	-5.260863	3.499723	0.517280
H	-4.083035	1.592124	1.453564
C	4.649160	1.457707	0.541804
C	5.338867	2.533916	0.026171
C	6.141639	2.385292	-1.115810
C	6.307718	1.131754	-1.658883
H	6.988473	0.977399	-2.493351
H	6.665360	3.240657	-1.534106
H	4.083033	1.592087	1.453639
H	5.260914	3.499696	0.517434

114

18-1 scf done: -2840.922520

C	1.008391	2.832939	-2.201586
C	0.525489	3.520052	-1.127806
C	1.199937	1.423026	-2.132142
C	0.000001	2.826405	0.000010
C	0.851472	0.738986	-0.947553
C	0.000000	1.414505	0.000006
C	1.742734	0.687252	-3.224528
C	1.913832	-0.662495	-3.137720
C	1.753832	-1.333187	-1.891483
C	1.382891	-0.586617	-0.752114
C	1.968374	-2.735854	-1.763459
C	1.584983	-1.188435	0.540704
C	1.613469	-2.596864	0.626138
C	1.797133	-3.359070	-0.563116
C	-1.008391	2.832927	2.201606
C	-0.525485	3.520045	1.127832
C	-1.199940	1.423015	2.132153
C	-0.851475	0.738981	0.947560
C	-1.742742	0.687235	3.224532
C	-1.913845	-0.662510	3.137716
C	-1.753843	-1.333195	1.891475
C	-1.382896	-0.586619	0.752111
C	-1.968387	-2.735862	1.763443
C	-1.584984	-1.188431	-0.540710
C	-1.613469	-2.596859	-0.626152
C	-1.797139	-3.359071	0.563097
C	-1.485119	-3.217805	-1.901449
C	-1.823293	-0.438516	-1.747267
C	-1.334480	-2.464881	-3.028591
C	-1.526450	-1.054118	-2.983658
C	1.485125	-3.217815	1.901433
C	1.823295	-0.438525	1.747263
C	1.334489	-2.464896	3.028580

C	1.526456	-1.054132	2.983652
C	-1.462360	-0.254709	-4.161208
C	-2.433551	0.869812	-1.774741
C	-1.687615	1.088269	-4.099456
C	-2.198869	1.681680	-2.908912
C	1.462367	-0.254728	4.161205
C	2.433549	0.869803	1.774740
C	2.198867	1.681668	2.908914
C	1.687617	1.088251	4.099457
C	-3.314643	1.380580	-0.747419
C	-2.493518	3.072517	-2.847225
C	-3.439587	2.788393	-0.638574
C	-2.997412	3.620139	-1.706052
C	3.314638	1.380578	0.747418
C	2.493512	3.072507	2.847229
C	2.997402	3.620133	1.706057
C	3.439579	2.788391	0.638576
C	-4.024340	3.356309	0.526131
C	-4.113885	0.566381	0.139719
C	-4.485421	2.557034	1.528151
C	-4.576959	1.150410	1.340511
C	-5.178143	0.334717	2.346131
C	-4.580997	-0.771207	-0.173202
C	-5.392717	-0.990928	2.141762
C	-5.157632	-1.565757	0.857512
H	1.319285	3.355530	-3.102867
H	0.476240	4.606139	-1.138412
H	1.964218	1.217252	-4.147658
H	2.240733	-1.238656	-3.999714
H	2.215946	-3.306174	-2.655223
H	1.867003	-4.440894	-0.482154
H	-1.319284	3.355512	3.102890
H	-0.476233	4.606133	1.138446
H	-1.964228	1.217230	4.147665
H	-2.240751	-1.238676	3.999705
H	-2.215962	-3.306186	2.655203
H	-1.867009	-4.440896	0.482130
H	-1.451634	-4.303383	-1.948801
H	-1.135381	-2.933322	-3.989554
H	1.451641	-4.303394	1.948780
H	1.135394	-2.933342	3.989541
H	-1.174410	-0.728979	-5.096264
H	-1.543848	1.718612	-4.973739
H	1.543851	1.718590	4.973743
H	1.174421	-0.729002	5.096260
H	-2.252803	3.693912	-3.706305
H	-3.131865	4.695385	-1.615575
H	3.131852	4.695380	1.615583
H	2.252796	3.693898	3.706312

H	-4.862195	2.984698	2.454231
H	-4.053992	4.439387	0.616765
H	-5.447544	0.801812	3.290580
H	-5.819894	-1.614325	2.923828
C	4.113884	0.566383	-0.139720
C	4.024331	3.356311	-0.526127
C	4.485416	2.557040	-1.528148
C	4.576959	1.150416	-1.340510
H	4.053981	4.439389	-0.616758
H	4.862191	2.984707	-2.454226
C	-4.608571	-1.292303	-1.487611
C	-5.571268	-2.886037	0.575266
C	-5.501690	-3.394337	-0.701195
C	-5.050664	-2.570588	-1.746882
H	-5.977176	-3.485908	1.387022
H	-5.830492	-4.409474	-0.907256
H	-5.052493	-2.937808	-2.769321
H	-4.296635	-0.664801	-2.313282
C	5.178149	0.334726	-2.346129
C	5.392729	-0.990919	-2.141760
C	5.157644	-1.565750	-0.857512
C	4.581001	-0.771203	0.173201
C	5.571286	-2.886028	-0.575265
C	5.501706	-3.394328	0.701196
C	5.050670	-2.570582	1.746882
C	4.608569	-1.292301	1.487610
H	5.447551	0.801822	-3.290577
H	5.819910	-1.614312	-2.923826
H	5.977200	-3.485896	-1.387019
H	5.830513	-4.409463	0.907258
H	5.052496	-2.937804	2.769320
H	4.296623	-0.664801	2.313279

114

18TS scf done: -2840.803827

C	3.464040	-1.366655	2.169256
C	3.941087	-0.559003	1.188393
C	2.102180	-1.773100	2.149885
C	3.160011	-0.438877	0.000000
C	1.186226	-1.123890	1.281006
C	1.759949	-0.681932	0.000000
C	1.676058	-2.887236	2.925950
C	0.395678	-3.341608	2.833591
C	-0.590507	-2.496189	2.255402
C	-0.201427	-1.257281	1.679075
H	4.104979	-1.728037	2.967458
H	4.982579	-0.248718	1.171449
H	2.420449	-3.413151	3.518255
H	0.085042	-4.268113	3.308403
C	-1.971545	-2.826247	2.336612

C	-1.182309	-0.202668	1.712332
C	-2.556114	-0.562719	1.758414
C	-2.923987	-1.914910	1.994928
H	-2.246063	-3.819730	2.682450
H	-3.979455	-2.174104	2.013463
C	3.464040	-1.366655	-2.169256
C	3.941087	-0.559003	-1.188393
C	2.102180	-1.773100	-2.149885
C	1.186226	-1.123890	-1.281006
C	1.676058	-2.887236	-2.925950
C	0.395678	-3.341608	-2.833591
C	-0.590507	-2.496189	-2.255402
C	-0.201427	-1.257281	-1.679075
H	4.104979	-1.728037	-2.967458
H	4.982579	-0.248718	-1.171449
H	2.420449	-3.413151	-3.518255
H	0.085042	-4.268113	-3.308403
C	-1.971545	-2.826247	-2.336612
C	-1.182309	-0.202668	-1.712332
C	-2.556114	-0.562719	-1.758414
C	-2.923987	-1.914910	-1.994928
H	-2.246063	-3.819730	-2.682450
H	-3.979455	-2.174104	-2.013463
C	-3.557281	0.437825	-1.660422
C	-0.858670	1.190536	-1.901680
C	-3.218613	1.749095	-1.521440
C	-1.864702	2.157086	-1.642291
H	-4.599704	0.129204	-1.665890
C	-0.858670	1.190536	1.901680
C	-3.557281	0.437825	1.660422
H	-4.599704	0.129204	1.665890
C	-3.218613	1.749095	1.521440
C	-1.864702	2.157086	1.642291
C	-1.516710	3.534759	1.559319
C	0.362680	1.690652	2.504140
C	0.362680	1.690652	-2.504140
C	-1.516710	3.534759	-1.559319
C	-0.219066	3.926460	-1.682704
C	0.753233	3.013269	2.176710
C	0.753233	3.013269	-2.176710
C	-0.219066	3.926460	1.682704
H	-3.979849	2.510098	1.367898
H	-2.297492	4.252532	1.320930
H	0.078781	4.955224	1.495993
H	0.078781	4.955224	-1.495993
H	-2.297492	4.252532	-1.320930
H	-3.979849	2.510098	-1.367898
C	2.084685	3.442469	2.435862
C	1.129996	1.028678	3.542036

C	1.129996	1.028678	-3.542036
C	2.084685	3.442469	-2.435862
C	2.952783	2.628717	-3.096260
C	2.952783	2.628717	3.096260
C	2.477042	1.444133	-3.725542
C	2.477042	1.444133	3.725542
H	2.392262	4.423058	2.080578
H	3.990688	2.916612	3.243535
H	3.990688	2.916612	-3.243535
H	2.392262	4.423058	-2.080578
C	0.598358	0.072038	4.489170
C	3.339735	0.713342	4.584560
C	0.598358	0.072038	-4.489170
C	3.339735	0.713342	-4.584560
C	1.507750	-0.713749	5.236810
C	2.888974	-0.384929	5.252010
C	2.888974	-0.384929	-5.252010
C	1.507750	-0.713749	-5.236810
H	3.562165	-0.985340	5.859845
H	4.375742	1.032292	4.670555
H	3.562165	-0.985340	-5.859845
H	4.375742	1.032292	-4.670555
C	1.037421	-1.818777	6.010042
C	-0.287542	-2.099888	6.102064
C	-1.246682	-1.180004	5.582974
C	-0.802994	-0.040989	4.852611
H	1.774956	-2.447347	6.504022
H	-0.638811	-2.968612	6.653912
C	-0.802994	-0.040989	-4.852611
C	-1.246682	-1.180004	-5.582974
C	-0.287542	-2.099888	-6.102064
C	1.037421	-1.818777	-6.010042
H	-0.638811	-2.968612	-6.653912
H	1.774956	-2.447347	-6.504022
C	-2.616027	-1.322418	-5.894586
C	-3.518056	-0.326196	-5.598053
C	-3.056660	0.867460	-5.018844
C	-1.733582	1.004412	-4.659947
H	-3.742075	1.693695	-4.853202
H	-1.391601	1.949200	-4.257156
H	-4.567672	-0.440345	-5.855479
H	-2.937508	-2.220845	-6.417028
C	-1.733582	1.004412	4.659947
C	-3.056660	0.867460	5.018844
C	-3.518056	-0.326196	5.598053
C	-2.616027	-1.322418	5.894586
H	-2.937508	-2.220845	6.417028
H	-4.567672	-0.440345	5.855479
H	-3.742075	1.693695	4.853202

H	-1.391601	1.949200	4.257156
120			
19-1 scf done: -2994.390445			
C	0.184497	3.799098	-0.656148
C	-0.184500	3.799098	0.656153
C	0.487024	2.577324	-1.323704
C	-0.487025	2.577323	1.323708
C	0.376607	1.361205	-0.614965
C	-0.376607	1.361204	0.614968
C	0.899951	2.550750	-2.686612
C	1.169446	1.367122	-3.307172
C	1.255706	0.159601	-2.556630
C	1.026955	0.197650	-1.164214
C	1.575422	-1.083946	-3.173731
C	1.476689	-0.922689	-0.376497
C	1.617145	-2.174636	-1.013497
C	1.647470	-2.228383	-2.436476
C	-1.169448	1.367118	3.307173
C	-0.899954	2.550747	2.686615
C	-1.255706	0.159597	2.556631
C	-1.026955	0.197647	1.164215
C	-1.575421	-1.083950	3.173729
C	-1.647469	-2.228387	2.436472
C	-1.617145	-2.174637	1.013493
C	-1.476689	-0.922689	0.376496
C	-1.738506	-3.349474	0.216810
C	-1.824610	-0.835795	-1.018276
C	-1.761837	-2.010311	-1.798491
C	-1.703335	-3.274097	-1.144010
C	-1.786362	-1.902739	-3.218396
C	-2.299586	0.366749	-1.653544
C	-1.866825	-0.682112	-3.821372
C	-2.151636	0.483440	-3.053684
C	1.738506	-3.349474	-0.216816
C	1.824610	-0.835797	1.018274
C	1.703335	-3.274099	1.144005
C	1.761838	-2.010315	1.798488
C	-2.327465	1.756578	-3.668423
C	-3.003389	1.420364	-0.960647
C	-2.638110	2.850916	-2.917513
C	-3.004717	2.707162	-1.547881
C	1.786364	-1.902746	3.218393
C	2.299586	0.366745	1.653544
C	2.151640	0.483434	3.053685
C	1.866828	-0.682119	3.821371
C	-3.757305	1.233243	0.259841
C	-3.390666	3.832711	-0.767415
C	-3.972280	2.374252	1.073132
C	-3.758413	3.674725	0.534792

C	3.003388	1.420362	0.960649
C	2.327470	1.756570	3.668426
C	2.638115	2.850909	2.917519
C	3.004719	2.707158	1.547886
C	-4.420528	2.211526	2.412349
C	-4.351589	-0.013874	0.684949
C	-4.666288	0.968829	2.913018
C	-4.676089	-0.163146	2.052443
C	-5.058145	-1.441317	2.560779
C	-4.756882	-1.077803	-0.214586
C	-5.198253	-2.512903	1.737903
C	-5.112274	-2.346755	0.323701
H	0.317135	4.732860	-1.197108
H	-0.317139	4.732858	1.197113
H	0.936026	3.488050	-3.236452
H	1.389677	1.334034	-4.371355
H	1.703702	-1.109222	-4.253099
H	1.798979	-3.191630	-2.917107
H	-1.389681	1.334028	4.371355
H	-0.936031	3.488045	3.236456
H	-1.703703	-1.109229	4.253098
H	-1.798979	-3.191634	2.917102
H	-1.804171	-4.311697	0.718403
H	-1.701583	-4.175339	-1.751900
H	-1.681357	-2.809327	-3.809118
H	-1.784845	-0.587268	-4.901590
H	1.804171	-4.311696	-0.718410
H	1.701585	-4.175342	1.751893
H	-2.152115	1.845954	-4.737758
H	-2.676368	3.841492	-3.364367
H	1.784850	-0.587278	4.901589
H	1.681360	-2.809334	3.809113
H	-3.329075	4.821728	-1.214795
H	-3.959192	4.536894	1.166272
H	2.676376	3.841484	3.364375
H	2.152123	1.845943	4.737762
H	-4.934245	0.831265	3.957898
H	-4.519299	3.095501	3.037642
H	-5.220171	-1.538529	3.631785
H	-5.456211	-3.491892	2.135092
C	3.757302	1.233243	-0.259841
C	3.390666	3.832710	0.767421
C	3.758409	3.674726	-0.534788
C	3.972275	2.374253	-1.073130
H	3.329075	4.821726	1.214803
H	3.959186	4.536895	-1.166267
C	-4.940504	-0.887124	-1.603795
C	-5.461593	-3.403168	-0.545673
C	-5.544459	-3.206465	-1.904727

C	-5.318135	-1.922502	-2.429669
H	-5.695558	-4.373535	-0.112996
H	-5.822262	-4.025557	-2.562749
H	-5.444538	-1.738442	-3.492862
H	-4.803996	0.100766	-2.025863
C	4.420521	2.211529	-2.412349
C	4.666281	0.968832	-2.913019
C	4.676085	-0.163143	-2.052445
C	4.351586	-0.013873	-0.684950
C	5.058143	-1.441313	-2.560781
C	5.198254	-2.512899	-1.737905
C	5.112277	-2.346752	-0.323703
C	4.756882	-1.077800	0.214585
H	4.519291	3.095504	-3.037641
H	4.934237	0.831269	-3.957900
H	5.220168	-1.538524	-3.631787
H	5.456214	-3.491888	-2.135095
C	4.940505	-0.887121	1.603793
C	5.461598	-3.403164	0.545670
C	5.318137	-1.922499	2.429668
C	5.544463	-3.206461	1.904726
H	4.804002	0.100770	2.025860
H	5.444539	-1.738437	3.492860
H	5.822267	-4.025552	2.562747
H	5.695563	-4.373531	0.112993

120

19TS scf done: -2994.271822

C	0.679360	4.158312	0.397756
C	-0.679452	4.158314	0.397735
C	1.350118	3.145629	-0.342924
C	-1.350192	3.145632	-0.342959
C	0.731886	1.885900	-0.561026
C	-0.731953	1.885903	-0.561048
C	2.438999	3.565934	-1.163138
C	2.766703	2.835361	-2.261874
C	2.338717	1.478405	-2.345299
C	1.569156	0.927642	-1.290329
H	1.247080	5.009317	0.765091
H	-1.247179	5.009321	0.765056
H	2.857482	4.555106	-0.997918
H	3.436906	3.223483	-3.023356
C	2.730076	0.648284	-3.430520
C	1.715299	-0.486856	-1.085782
C	2.009191	-1.296518	-2.217028
C	2.445855	-0.685811	-3.421339
H	3.237000	1.108249	-4.275273
H	2.669879	-1.314809	-4.279003
C	-2.766804	2.835324	-2.261881
C	-2.439085	3.565916	-1.163163

C	-2.338797	1.478377	-2.345304
C	-1.569209	0.927634	-1.290343
C	-2.730143	0.648246	-3.430523
C	-2.445880	-0.685840	-3.421349
C	-2.009187	-1.296538	-2.217043
C	-1.715313	-0.486868	-1.085798
H	-3.437025	3.223431	-3.023357
H	-2.857575	4.555086	-0.997949
H	-3.237082	1.108198	-4.275273
H	-2.669886	-1.314842	-4.279015
C	-1.785929	-1.113493	0.211803
C	-1.947963	-2.712347	-2.103174
C	1.785937	-1.113480	0.211818
C	1.948004	-2.712328	-2.103160
C	-1.666383	-2.525462	0.287638
C	-1.705562	-3.303679	-0.901747
C	1.666427	-2.525451	0.287651
C	1.705622	-3.303667	-0.901734
H	-1.618708	-4.383957	-0.818786
H	-2.101964	-3.310669	-2.997808
H	1.618795	-4.383947	-0.818772
H	2.102020	-3.310645	-2.997794
C	-2.119702	-0.418887	1.432322
C	-1.565964	-3.160401	1.552873
C	2.119721	-0.418872	1.432334
C	1.566021	-3.160394	1.552886
C	1.500875	-2.420949	2.694929
C	1.754255	-1.025630	2.659444
C	-1.754198	-1.025633	2.659426
C	-1.500827	-2.420954	2.694915
H	-1.306490	-2.890401	3.656071
H	-1.472456	-4.242936	1.583288
H	1.306545	-2.890400	3.656085
H	1.472525	-4.242931	1.583300
C	-1.705854	-0.236354	3.845883
C	-2.944090	0.772412	1.537833
C	1.706000	-0.236379	3.845924
C	2.944106	0.772427	1.537823
C	2.067059	1.074894	3.815799
C	2.759021	1.590993	2.680238
C	-2.758944	1.590996	2.680227
C	-2.066897	1.074923	3.815749
H	-1.330135	-0.694424	4.757419
H	-1.943919	1.712975	4.687188
H	1.944173	1.712918	4.687272
H	1.330357	-0.694472	4.757480
C	4.042973	1.101103	0.653696
C	3.349796	2.882252	2.732668
C	-4.042990	1.101074	0.653749

C	-3.349739	2.882243	2.732686
C	-4.553870	2.427366	0.689504
C	-4.158352	3.315945	1.726000
C	4.158348	3.315971	1.725940
C	4.553832	2.427401	0.689429
H	4.568287	4.323279	1.732941
H	3.133269	3.517235	3.588417
H	-4.568317	4.323242	1.733026
H	-3.133180	3.517233	3.588422
C	5.461075	2.870305	-0.311915
C	4.734420	0.160223	-0.203218
C	5.479321	0.666851	-1.291500
C	5.816941	2.047315	-1.336193
H	6.433313	2.407879	-2.156448
H	5.806763	3.900791	-0.277605
C	-5.461139	2.870268	-0.311819
C	-4.734438	0.160195	-0.203168
C	-5.479380	0.666823	-1.291420
C	-5.817036	2.047277	-1.336084
H	-6.433454	2.407834	-2.156307
H	-5.806852	3.900744	-0.277479
C	4.861339	-1.258821	0.063987
C	5.335398	-2.123589	-0.962218
C	5.809561	-1.565532	-2.186789
C	5.956417	-0.220146	-2.304441
H	6.435562	0.212878	-3.179523
H	6.144441	-2.235949	-2.974733
C	-4.861325	-1.258855	0.064022
C	-5.335392	-2.123619	-0.962184
C	-5.809585	-1.565553	-2.186740
C	-5.956476	-0.220170	-2.304366
H	-6.435632	0.212858	-3.179439
H	-6.144459	-2.235966	-2.974690
C	4.702377	-1.807008	1.356832
C	5.444385	-3.508902	-0.712809
C	5.201071	-4.024755	0.539544
C	4.870391	-3.153514	1.591562
H	4.475445	-1.147903	2.185848
H	4.743838	-3.539548	2.599015
H	5.307052	-5.090423	0.724600
H	5.770339	-4.157292	-1.523237
C	-4.702332	-1.807052	1.356859
C	-5.444361	-3.508936	-0.712786
C	-5.201026	-4.024798	0.539560
C	-4.870334	-3.153562	1.591580
H	-4.743746	-3.539606	2.599025
H	-5.306996	-5.090468	0.724611
H	-4.475386	-1.147951	2.185875
H	-5.770325	-4.157322	-1.523214

126

20-1 scf done: -3147.858326

C	-0.410140	3.016062	2.386502
C	-0.223162	3.703446	1.224122
C	-0.603656	1.604794	2.370534
C	0.000000	3.009846	0.000001
C	-0.577444	0.921522	1.135159
C	0.000000	1.597964	0.000000
C	-0.824451	0.865014	3.567527
C	-0.991085	-0.487395	3.526757
C	-1.168076	-1.157273	2.282247
C	-1.135516	-0.406999	1.087045
C	-1.388134	-2.563009	2.213236
C	-1.685708	-1.008943	-0.101540
C	-1.731014	-2.417968	-0.178235
C	-1.557655	-3.182645	1.010773
C	0.410141	3.016063	-2.386500
C	0.223164	3.703447	-1.224120
C	0.603657	1.604795	-2.370533
C	0.577445	0.921522	-1.135158
C	0.824452	0.865016	-3.567526
C	0.991086	-0.487393	-3.526756
C	1.168077	-1.157273	-2.282246
C	1.135517	-0.406999	-1.087044
C	1.388135	-2.563008	-2.213236
C	1.685708	-1.008944	0.101541
C	1.731013	-2.417969	0.178235
C	1.557655	-3.182645	-1.010773
C	1.963789	-3.037844	1.439635
C	2.228443	-0.258430	1.204456
C	2.123949	-2.286142	2.565679
C	2.275659	-0.872865	2.474327
C	-1.963791	-3.037842	-1.439636
C	-2.228442	-0.258428	-1.204455
C	-2.123951	-2.286139	-2.565679
C	-2.275658	-0.872861	-2.474326
C	2.502129	-0.067921	3.627211
C	2.793705	1.060633	1.077428
C	2.669417	1.280571	3.511121
C	2.846077	1.876628	2.229527
C	-2.502128	-0.067917	-3.627209
C	-2.793704	1.060635	-1.077426
C	-2.846075	1.876632	-2.229523
C	-2.669415	1.280575	-3.511118
C	3.399689	1.565081	-0.132478
C	3.112877	3.268615	2.085022
C	3.492581	2.968100	-0.286458
C	3.321777	3.809144	0.851245
C	-3.399689	1.565081	0.132480

C	-3.112875	3.268618	-2.085017
C	-3.321776	3.809146	-0.851240
C	-3.492580	2.968099	0.286462
C	3.774904	3.514694	-1.569598
C	3.974668	0.731966	-1.166117
C	3.957085	2.695518	-2.642761
C	4.083600	1.288679	-2.465269
C	4.339725	0.440478	-3.576970
C	4.495711	-0.601054	-0.963399
C	4.503397	-0.900173	-3.400474
C	4.625073	-1.442455	-2.091603
H	-0.479020	3.538773	3.337404
H	-0.176623	4.789719	1.221234
H	-0.794944	1.393610	4.517192
H	-1.060795	-1.067641	4.443542
H	-1.361864	-3.137708	3.135797
H	-1.633891	-4.265280	0.948335
H	0.479022	3.538775	-3.337401
H	0.176626	4.789719	-1.221231
H	0.794945	1.393612	-4.517191
H	1.060796	-1.067639	-4.443542
H	1.361864	-3.137707	-3.135798
H	1.633890	-4.265280	-0.948336
H	1.956325	-4.123619	1.492953
H	2.208975	-2.756604	3.542031
H	-1.956327	-4.123617	-1.492954
H	-2.208976	-2.756600	-3.542032
H	2.480569	-0.543905	4.604392
H	2.741851	1.911702	4.393745
H	-2.741850	1.911706	-4.393742
H	-2.480569	-0.543900	-4.604391
H	3.089927	3.896909	2.972123
H	3.428295	4.883746	0.723686
H	-3.428293	4.883748	-0.723679
H	-3.089925	3.896914	-2.972117
H	4.075056	3.104711	-3.643297
H	3.783903	4.595888	-1.683867
H	4.357351	0.879454	-4.571539
H	4.621908	-1.564843	-4.252922
C	-3.974668	0.731964	1.166117
C	-3.774905	3.514691	1.569603
C	-3.957087	2.695514	2.642764
C	-4.083602	1.288676	2.465269
H	-3.783904	4.595885	1.683873
H	-4.075059	3.104705	3.643301
C	5.017703	-1.094640	0.297248
C	4.924421	-2.827642	-1.919340
C	5.173274	-3.346317	-0.688852
C	5.288118	-2.484691	0.442232

H	4.933848	-3.462792	-2.802095
H	5.367707	-4.408487	-0.559566
C	-4.339726	0.440472	3.576969
C	-4.503398	-0.900178	3.400472
C	-4.625073	-1.442459	2.091599
C	-4.495711	-0.601056	0.963396
C	-4.924423	-2.827645	1.919334
C	-5.173278	-3.346317	0.688845
C	-5.288121	-2.484690	-0.442238
C	-5.017704	-1.094638	-0.297251
H	-4.357353	0.879447	4.571538
H	-4.621910	-1.564850	4.252918
H	-4.933853	-3.462796	2.802088
H	-5.367713	-4.408487	0.559558
C	-5.395902	-0.244924	-1.362577
C	-5.751934	-2.982495	-1.679531
C	-5.881888	-0.748655	-2.548657
C	-6.026521	-2.135113	-2.727927
H	-5.324199	0.828162	-1.235797
H	-6.157574	-0.064386	-3.346158
H	-6.390948	-2.529703	-3.672697
H	-5.918345	-4.053194	-1.776904
C	5.751930	-2.982500	1.679525
C	5.395904	-0.244928	1.362575
C	5.881889	-0.748661	2.548654
C	6.026520	-2.135120	2.727922
H	5.324204	0.828159	1.235796
H	6.157577	-0.064394	3.346156
H	6.390947	-2.529711	3.672691
H	5.918338	-4.053200	1.776896

126

20TS scf done: -3147.738680

C	4.102625	0.112034	2.162495
C	4.191154	1.055965	1.190407
C	3.042751	-0.835781	2.133717
C	3.431792	0.842775	0.000000
C	1.933478	-0.617565	1.276385
C	2.264430	0.034773	0.000000
C	3.134857	-2.049514	2.871185
C	2.167687	-3.002040	2.753263
C	0.909504	-2.636302	2.199872
C	0.734628	-1.332846	1.665399
H	4.838241	0.048144	2.958537
H	5.004127	1.777258	1.178921
H	4.036844	-2.229544	3.450650
H	2.284707	-3.988139	3.194258
C	-0.206529	-3.515908	2.265527
C	-0.596894	-0.787941	1.721946
C	-1.694215	-1.688891	1.755395

C	-1.457653	-3.076422	1.952403
H	-0.036836	-4.544059	2.576140
H	-2.306818	-3.755036	1.960985
C	4.102625	0.112034	-2.162495
C	4.191154	1.055965	-1.190407
C	3.042751	-0.835781	-2.133717
C	1.933478	-0.617565	-1.276385
C	3.134857	-2.049514	-2.871185
C	2.167687	-3.002040	-2.753263
C	0.909504	-2.636302	-2.199872
C	0.734628	-1.332846	-1.665399
H	4.838241	0.048144	-2.958537
H	5.004127	1.777258	-1.178921
H	4.036844	-2.229544	-3.450650
H	2.284707	-3.988139	-3.194258
C	-0.206529	-3.515908	-2.265527
C	-0.596894	-0.787941	-1.721946
C	-1.694215	-1.688891	-1.755395
C	-1.457653	-3.076422	-1.952403
H	-0.036836	-4.544059	-2.576140
H	-2.306818	-3.755036	-1.960985
C	-3.020651	-1.190537	-1.666879
C	-0.883982	0.610806	-1.918532
C	-3.257111	0.143975	-1.534086
C	-2.194090	1.077373	-1.651817
H	-3.842590	-1.902028	-1.674562
C	-0.883982	0.610806	1.918532
C	-3.020651	-1.190537	1.666879
H	-3.842590	-1.902028	1.674562
C	-3.257111	0.143975	1.534086
C	-2.194090	1.077373	1.651817
C	-2.432256	2.476644	1.545932
C	0.022049	1.568395	2.513996
C	0.022049	1.568395	-2.513996
C	-2.432256	2.476644	-1.545932
C	-1.407098	3.364786	-1.665756
C	-0.153900	2.933307	2.182721
C	-0.153900	2.933307	-2.182721
C	-1.407098	3.364786	1.665756
H	-4.266647	0.520638	1.393315
H	-3.436554	2.812072	1.301042
H	-1.553647	4.423260	1.465153
H	-1.553647	4.423260	-1.465153
H	-3.436554	2.812072	-1.301042
H	-4.266647	0.520638	-1.393315
C	0.881891	3.865378	2.476926
C	0.966062	1.273668	3.570742
C	0.966062	1.273668	-3.570742
C	0.881891	3.865378	-2.476926

C	1.989091	3.473484	-3.166828
C	1.989091	3.473484	3.166828
C	2.025093	2.191715	-3.786991
C	2.025093	2.191715	3.786991
H	0.774560	4.888519	2.124411
H	2.814331	4.159931	3.339071
H	2.814331	4.159931	-3.339071
H	0.774560	4.888519	-2.124411
C	0.832500	0.175417	4.505673
C	3.093256	1.849214	4.660676
C	0.832500	0.175417	-4.505673
C	3.093256	1.849214	-4.660676
C	1.986360	-0.221863	5.230029
C	3.116555	0.639503	5.286110
C	3.116555	0.639503	-5.286110
C	1.986360	-0.221863	-5.230029
H	3.971810	0.336356	5.885884
H	3.912960	2.554001	4.778185
H	3.971810	0.336356	-5.885884
H	3.912960	2.554001	-4.778185
C	2.002216	-1.470890	5.910099
C	0.913309	-2.287807	5.879007
C	-0.327760	-1.799040	5.385232
C	-0.404720	-0.499044	4.837056
H	2.919786	-1.779948	6.405094
H	0.945578	-3.281301	6.319801
C	-0.404720	-0.499044	-4.837056
C	-0.327760	-1.799040	-5.385232
C	0.913309	-2.287807	-5.879007
C	2.002216	-1.470890	-5.910099
H	0.945578	-3.281301	-6.319801
H	2.919786	-1.779948	-6.405094
C	-1.511648	-2.583924	-5.530044
C	-2.738582	-2.058499	-5.277194
C	-2.874529	-0.665711	-5.000678
C	-1.709433	0.133526	-4.825388
H	-3.636493	-2.664502	-5.372691
H	-1.405065	-3.615922	-5.856132
C	-1.709433	0.133526	4.825388
C	-2.874529	-0.665711	5.000678
C	-2.738582	-2.058499	5.277194
C	-1.511648	-2.583924	5.530044
H	-1.405065	-3.615922	5.856132
H	-3.636493	-2.664502	5.372691
C	-1.878906	1.537470	-4.812545
C	-4.148280	-0.057142	-4.994075
C	-4.281950	1.309574	-4.907059
C	-3.129722	2.112271	-4.852973
H	-5.025777	-0.692144	-5.096045

H	-5.267724	1.767130	-4.919105
H	-3.219697	3.194871	-4.842620
H	-1.004697	2.176776	-4.797765
C	-4.148280	-0.057142	4.994075
C	-1.878906	1.537470	4.812545
C	-4.281950	1.309574	4.907059
C	-3.129722	2.112271	4.852973
H	-5.025777	-0.692144	5.096045
H	-5.267724	1.767130	4.919105
H	-3.219697	3.194871	4.842620
H	-1.004697	2.176776	4.797765

132

21-1

C	-0.022002	-0.681383	3.820895
C	0.021991	0.681443	3.820882
C	-0.155007	-1.402116	2.599523
C	0.154998	1.402154	2.599497
C	-0.217379	-0.687288	1.383592
C	0.217370	0.687303	1.383579
C	-0.226252	-2.824683	2.571761
C	-0.327382	-3.490934	1.386675
C	-0.586026	-2.783086	0.177706
C	-0.713484	-1.377584	0.218743
C	-0.724173	-3.455219	-1.070440
C	-1.341959	-0.724115	-0.902082
C	-1.299852	-1.369856	-2.156630
C	-0.964852	-2.753043	-2.214027
C	0.327380	3.490948	1.386611
C	0.226247	2.824720	2.571710
C	0.586023	2.783078	0.177656
C	0.713478	1.377577	0.218719
C	0.724172	3.455188	-1.070503
C	0.964849	2.752990	-2.214077
C	1.299847	1.369803	-2.156653
C	1.341954	0.724087	-0.902093
C	1.604736	0.624078	-3.331473
C	2.037003	-0.535896	-0.815632
C	2.168916	-1.309345	-1.989433
C	1.925184	-0.698688	-3.252806
C	2.556554	-2.675955	-1.881052
C	2.643311	-1.038519	0.390415
C	2.782122	-3.240908	-0.661017
C	2.846732	-2.430249	0.508316
C	-1.604738	-0.624151	-3.331465
C	-2.037001	0.535873	-0.815645
C	-1.925185	0.698616	-3.252823
C	-2.168915	1.309299	-1.989461
C	3.141053	-2.983188	1.787387
C	3.124577	-0.199165	1.458039

C	3.226235	-2.182166	2.887838
C	3.247428	-0.764897	2.746751
C	-2.556549	2.675912	-1.881107
C	-2.643300	1.038524	0.390394
C	-2.846717	2.430256	0.508267
C	-2.782112	3.240891	-0.661082
C	3.584527	1.157137	1.272218
C	3.430060	0.093229	3.869226
C	3.591937	2.010225	2.400492
C	3.491330	1.444991	3.704793
C	-3.124564	0.199192	1.458035
C	-3.141031	2.983221	1.787330
C	-3.226212	2.182221	2.887796
C	-3.247413	0.764949	2.746736
C	3.720240	3.415312	2.215223
C	4.098647	1.681234	0.025584
C	3.837318	3.937341	0.962370
C	4.051797	3.086046	-0.158351
C	4.241653	3.634121	-1.456226
C	4.706503	0.889375	-1.019856
C	4.492215	2.821294	-2.520106
C	4.770197	1.441265	-2.319452
H	-0.021047	-1.238148	4.754815
H	0.021038	1.238225	4.754792
H	-0.132036	-3.367489	3.509122
H	-0.278294	-4.576539	1.352306
H	-0.573599	-4.531599	-1.099682
H	-0.974268	-3.250110	-3.180910
H	0.278295	4.576553	1.352222
H	0.132032	3.367544	3.509061
H	0.573599	4.531567	-1.099764
H	0.974267	3.250039	-3.180969
H	1.521670	1.119336	-4.295816
H	2.068975	-1.291137	-4.152904
H	2.614880	-3.271783	-2.788484
H	2.986914	-4.304572	-0.568822
H	-1.521670	-1.119426	-4.295799
H	-2.068973	1.291050	-4.152931
H	3.239333	-4.062300	1.875628
H	3.351261	-2.609012	3.880197
H	-2.986902	4.304557	-0.568908
H	-2.614878	3.271721	-2.788551
H	3.462296	-0.349467	4.861811
H	3.531860	2.110273	4.563956
H	-3.351236	2.609085	3.880147
H	-3.239308	4.062336	1.875548
H	3.836102	5.013113	0.803825
H	3.663761	4.062211	3.087264
H	4.138841	4.708723	-1.585954

H	4.561716	3.225761	-3.527119
C	-3.584521	-1.157109	1.272236
C	-3.430051	-0.093156	3.869226
C	-3.491333	-1.444921	3.704817
C	-3.591942	-2.010177	2.400525
H	-3.462287	0.349558	4.861803
H	-3.531869	-2.110187	4.563991
C	5.374258	-0.380544	-0.803270
C	5.159584	0.625085	-3.424095
C	5.555100	-0.661767	-3.243596
C	5.732558	-1.178977	-1.926048
H	5.117224	1.058564	-4.420618
H	5.818716	-1.289080	-4.091968
C	-3.720254	-3.415266	2.215278
C	-3.837330	-3.937316	0.962434
C	-4.051799	-3.086038	-0.158303
C	-4.098637	-1.681222	0.025608
C	-4.241658	-3.634133	-1.456168
C	-4.492217	-2.821322	-2.520062
C	-4.770192	-1.441288	-2.319430
C	-4.706491	-0.889377	-1.019844
H	-3.663780	-4.062151	3.087331
H	-3.836122	-5.013090	0.803908
H	-4.138857	-4.708738	-1.585879
H	-4.561726	-3.225806	-3.527067
C	-5.374250	0.380541	-0.803273
C	-5.159587	-0.625125	-3.424083
C	-5.732565	1.178954	-1.926059
C	-5.555109	0.661727	-3.243601
H	-5.818731	1.289027	-4.091981
H	-5.117227	-1.058618	-4.420601
C	6.340506	-2.437467	-1.725074
C	5.807429	-0.818712	0.469683
C	6.432695	-2.034025	0.639399
C	6.669027	-2.873871	-0.462455
H	5.665963	-0.174484	1.328548
H	6.746927	-2.338392	1.633819
H	7.144124	-3.841082	-0.321409
H	6.573334	-3.044812	-2.597144
C	-6.340528	2.437441	-1.725101
C	-5.807417	0.818724	0.469676
C	-6.432696	2.034026	0.639377
C	-6.669048	2.873857	-0.462486
H	-6.573369	3.044771	-2.597178
H	-7.144159	3.841062	-0.321448
H	-6.746928	2.338407	1.633794
H	-5.665933	0.174511	1.328549

132

21TS

C	3.893518	2.060722	0.679558
C	3.893518	2.060722	-0.679558
C	3.326165	0.942606	1.351074
C	3.326165	0.942606	-1.351074
C	2.304451	0.174938	0.731685
C	2.304451	0.174938	-0.731685
C	4.068675	0.405713	2.444910
C	3.918868	-0.905499	2.771495
C	2.753467	-1.600985	2.335314
C	1.782047	-0.911194	1.567472
H	4.485860	2.774026	1.246837
H	4.485860	2.774026	-1.246837
H	4.871777	1.004170	2.866599
H	4.609493	-1.406436	3.443777
C	2.515317	-2.950993	2.709724
C	0.430694	-1.379452	1.707255
C	0.232858	-2.759968	1.982763
C	1.328447	-3.553778	2.410948
H	3.311033	-3.495452	3.212358
H	1.164639	-4.608038	2.619059
C	3.918868	-0.905499	-2.771495
C	4.068675	0.405713	-2.444910
C	2.753467	-1.600985	-2.335314
C	1.782047	-0.911194	-1.567472
C	2.515317	-2.950993	-2.709724
C	1.328447	-3.553778	-2.410948
C	0.232858	-2.759968	-1.982763
C	0.430694	-1.379452	-1.707255
H	4.609493	-1.406436	-3.443777
H	4.871777	1.004170	-2.866599
H	3.311033	-3.495452	-3.212358
H	1.164639	-4.608038	-2.619059
C	-0.722773	-0.515514	-1.786137
C	-1.076656	-3.309172	-1.913012
C	-0.722773	-0.515514	1.786137
C	-1.076656	-3.309172	1.913012
C	-2.011972	-1.096057	-1.667571
C	-2.154853	-2.510513	-1.686102
C	-2.011972	-1.096057	1.667571
C	-2.154853	-2.510513	1.686102
H	-3.152368	-2.932598	-1.595296
H	-1.195908	-4.381620	-2.047360
H	-3.152368	-2.932598	1.595296
H	-1.195908	-4.381620	2.047360
C	-0.665362	0.890529	-2.103903
C	-3.157005	-0.261437	-1.577183
C	-0.665362	0.890529	2.103903
C	-3.157005	-0.261437	1.577183
C	-3.025811	1.092105	1.507754

C	-1.766320	1.701496	1.741059
C	-1.766320	1.701496	-1.741059
C	-3.025811	1.092105	-1.507754
H	-3.887882	1.729594	-1.331591
H	-4.134617	-0.729750	-1.497755
H	-3.887882	1.729594	1.331591
H	-4.134617	-0.729750	1.497755
C	-1.601245	3.115677	-1.671668
C	0.354181	1.538217	-2.902683
C	-1.601245	3.115677	1.671668
C	0.354181	1.538217	2.902683
C	-0.414455	3.690804	2.007633
C	0.566802	2.923767	2.702365
C	0.566802	2.923767	-2.702365
C	-0.414455	3.690804	-2.007633
H	-2.429884	3.714711	-1.303067
H	-0.244844	4.755441	-1.867521
H	-0.244844	4.755441	1.867521
H	-2.429884	3.714711	1.303067
C	1.025508	0.918570	4.022283
C	1.689795	3.559307	3.299802
C	1.025508	0.918570	-4.022283
C	1.689795	3.559307	-3.299802
C	2.189149	1.545718	-4.538469
C	2.521757	2.866403	-4.127999
C	2.521757	2.866403	4.127999
C	2.189149	1.545718	4.538469
H	3.413049	3.332053	4.542165
H	1.873641	4.607051	3.074027
H	3.413049	3.332053	-4.542165
H	1.873641	4.607051	-3.074027
C	3.018145	0.851086	5.463534
C	0.535490	-0.247559	4.731185
C	1.482609	-1.013437	5.456781
C	2.734360	-0.434083	5.809757
H	3.420061	-1.014171	6.422906
H	3.922269	1.339702	5.818877
C	3.018145	0.851086	-5.463534
C	0.535490	-0.247559	-4.731185
C	1.482609	-1.013437	-5.456781
C	2.734360	-0.434083	-5.809757
H	3.420061	-1.014171	-6.422906
H	3.922269	1.339702	-5.818877
C	-0.850586	-0.644676	4.846381
C	-1.128009	-1.991041	5.178976
C	-0.084099	-2.843496	5.631738
C	1.155555	-2.333039	5.871602
H	1.925092	-2.932025	6.352512
H	-0.322286	-3.874923	5.879851

C	-0.850586	-0.644676	-4.846381
C	-1.128009	-1.991041	-5.178976
C	-0.084099	-2.843496	-5.631738
C	1.155555	-2.333039	-5.871602
H	1.925092	-2.932025	-6.352512
H	-0.322286	-3.874923	-5.879851
C	-1.969703	0.281041	4.835028
C	-2.470097	-2.475645	5.146375
C	-3.515561	-1.637876	4.925242
C	-3.299224	-0.231010	4.837500
H	-4.535434	-2.014080	4.891760
H	-2.634713	-3.537483	5.313949
C	-1.969703	0.281041	-4.835028
C	-2.470097	-2.475645	-5.146375
C	-3.515561	-1.637876	-4.925242
C	-3.299224	-0.231010	-4.837500
H	-4.535434	-2.014080	-4.891760
H	-2.634713	-3.537483	-5.313949
C	-1.816379	1.680498	-4.970610
C	-4.395216	0.658479	-4.829477
C	-4.206950	2.020005	-4.889439
C	-2.901643	2.528629	-4.993612
H	-0.823888	2.097924	-5.084490
H	-2.739531	3.597956	-5.096793
H	-5.059699	2.693833	-4.892780
H	-5.399498	0.240791	-4.802792
C	-4.395216	0.658479	4.829477
C	-1.816379	1.680498	4.970610
C	-2.901643	2.528629	4.993612
C	-4.206950	2.020005	4.889439
H	-0.823888	2.097924	5.084490
H	-2.739531	3.597956	5.096793
H	-5.059699	2.693833	4.892780
H	-5.399498	0.240791	4.802792

138

22-1 scf done: -3454.794100

C	0.001426	2.421478	2.883837
C	0.012621	1.244429	3.571767
C	0.198897	2.437826	1.473313
C	-0.000003	0.000000	2.878763
C	0.381807	1.215252	0.791154
C	0.000001	0.000000	1.466773
C	0.219256	3.654584	0.732794
C	0.393503	3.640811	-0.619264
C	0.776430	2.442570	-1.287718
C	0.946029	1.259923	-0.535085
C	0.997098	2.406791	-2.694335
C	1.686368	0.178514	-1.136181
C	1.728099	0.104131	-2.545267

C	1.355243	1.245261	-3.311655
C	-0.001429	-2.421478	2.883840
C	-0.012629	-1.244429	3.571769
C	-0.198897	-2.437828	1.473314
C	-0.381804	-1.215255	0.791153
C	-0.219261	-3.654587	0.732798
C	-0.393513	-3.640816	-0.619261
C	-0.776436	-2.442575	-1.287714
C	-0.946028	-1.259926	-0.535084
C	-0.997105	-2.406795	-2.694333
C	-1.686365	-0.178514	-1.136179
C	-1.728095	-0.104130	-2.545266
C	-1.355242	-1.245263	-3.311653
C	-2.153829	1.106207	-3.164130
C	-2.415003	0.815564	-0.388221
C	-2.509345	2.185595	-2.411186
C	-2.668392	2.061855	-1.001310
C	2.153833	-1.106207	-3.164134
C	2.415005	-0.815568	-0.388221
C	2.509346	-2.185596	-2.411191
C	2.668392	-2.061859	-1.001313
C	-3.092751	3.158458	-0.196965
C	-2.940740	0.600772	0.935592
C	-3.239628	3.017403	1.151022
C	-3.183494	1.726931	1.751210
C	3.092756	-3.158461	-0.196972
C	2.940743	-0.600778	0.935590
C	3.183503	-1.726938	1.751205
C	3.239638	-3.017407	1.151015
C	-3.306992	-0.692478	1.454496
C	-3.396967	1.540732	3.146945
C	-3.349190	-0.860407	2.856666
C	-3.367846	0.291779	3.693869
C	3.306991	0.692474	1.454498
C	3.396974	-1.540741	3.146942
C	3.367847	-0.291790	3.693868
C	3.349188	0.860399	2.856668
C	-3.412554	-2.176481	3.398554
C	-3.732430	-1.800512	0.631589
C	-3.437630	-3.263367	2.576392
C	-3.620382	-3.102816	1.172259
C	-3.712927	-4.230095	0.308766
C	-4.326164	-1.662763	-0.680615
C	-3.911917	-4.059594	-1.028077
C	-4.246140	-2.778582	-1.551469
H	-0.092679	3.370529	3.405949
H	-0.034695	1.234101	4.657980
H	0.029181	4.586243	1.260073
H	0.308581	4.555487	-1.200883

H	0.814990	3.310233	-3.271206
H	1.430021	1.190567	-4.394931
H	0.092674	-3.370529	3.405953
H	0.034683	-1.234099	4.657981
H	-0.029187	-4.586246	1.260077
H	-0.308594	-4.555494	-1.200878
H	-0.815000	-3.310238	-3.271203
H	-1.430021	-1.190568	-4.394929
H	-2.135187	1.167623	-4.249510
H	-2.746521	3.137543	-2.879582
H	2.135190	-1.167622	-4.249513
H	2.746521	-3.137544	-2.879587
H	-3.244193	4.123342	-0.674366
H	-3.473259	3.873670	1.778756
H	3.473272	-3.873676	1.778746
H	3.244199	-4.123345	-0.674374
H	-3.526414	2.419754	3.773434
H	-3.430591	0.152616	4.770584
H	3.430591	-0.152629	4.770583
H	3.526423	-2.419765	3.773428
H	-3.386456	-4.271017	2.981884
H	-3.382795	-2.295464	4.478927
H	-3.563850	-5.221369	0.729802
H	-3.885672	-4.907254	-1.708674
C	3.732428	1.800509	0.631595
C	3.412555	2.176469	3.398560
C	3.437632	3.263358	2.576402
C	3.620384	3.102811	1.172270
H	3.382796	2.295449	4.478934
H	3.386461	4.271007	2.981898
C	-5.043538	-0.498520	-1.149120
C	-4.522817	-2.614093	-2.936098
C	-4.887244	-1.397623	-3.428718
C	-5.193975	-0.327470	-2.544058
H	-4.394500	-3.468628	-3.596013
H	-5.025251	-1.246642	-4.496742
C	3.712924	4.230093	0.308778
C	3.911907	4.059598	-1.028064
C	4.246132	2.778587	-1.551463
C	4.326160	1.662765	-0.680613
C	4.522811	2.614104	-2.936090
C	4.887244	1.397636	-3.428714
C	5.193977	0.327482	-2.544059
C	5.043536	0.498527	-1.149120
H	3.563846	5.221366	0.729819
H	3.885660	4.907259	-1.708660
H	4.394496	3.468641	-3.596004
H	5.025254	1.246661	-4.496739
C	5.734891	-0.441187	-0.286185

C	5.698829	-0.902958	-3.062921
C	6.209298	-1.667739	-0.831124
C	6.121399	-1.894798	-2.236703
H	6.473650	-2.842738	-2.636793
H	5.722767	-1.031511	-4.142590
C	-5.698828	0.902970	-3.062918
C	-5.734891	0.441192	-0.286183
C	-6.209302	1.667745	-0.831120
C	-6.121403	1.894807	-2.236698
H	-6.473657	2.842746	-2.636788
H	-5.722764	1.031525	-4.142587
C	6.841910	-2.609378	0.009617
C	6.079541	-0.149932	1.054085
C	6.730605	-1.068737	1.846975
C	7.083053	-2.329134	1.334732
H	7.164658	-3.554214	-0.422478
H	7.578255	-3.059007	1.969689
C	-6.841911	2.609384	0.009624
C	-6.079534	0.149939	1.054089
C	-6.730594	1.068745	1.846982
C	-7.083047	2.329141	1.334740
H	-7.164663	3.554220	-0.422470
H	-7.578247	3.059013	1.969700
H	-6.974351	0.810138	2.873603
H	-5.847875	-0.826595	1.460732
H	6.974369	-0.810130	2.873594
H	5.847883	0.826602	1.460728

138

22TS scf done: -3454.674108

C	-3.934601	-1.717499	2.160153
C	-3.583037	-2.596219	1.187346
C	-3.415814	-0.394288	2.138524
C	-3.000900	-2.058476	0.000000
C	-2.329914	-0.078821	1.279956
C	-2.329650	-0.806413	0.000000
C	-4.046294	0.635806	2.891279
C	-3.622139	1.924976	2.779288
C	-2.341343	2.178755	2.215570
C	-1.587050	1.102639	1.675624
H	-4.622740	-1.995188	2.952664
H	-3.980864	-3.607557	1.171493
H	-4.926875	0.378595	3.474497
H	-4.173682	2.746697	3.227963
C	-1.762920	3.476394	2.273498
C	-0.152506	1.236031	1.726664
C	0.396895	2.546293	1.749904
C	-0.454684	3.666618	1.946349
H	-2.389318	4.308476	2.585978
H	-0.017101	4.661798	1.944053

C	-3.934601	-1.717499	-2.160153
C	-3.583037	-2.596219	-1.187346
C	-3.415814	-0.394288	-2.138524
C	-2.329914	-0.078821	-1.279956
C	-4.046294	0.635806	-2.891279
C	-3.622139	1.924976	-2.779288
C	-2.341343	2.178755	-2.215570
C	-1.587050	1.102639	-1.675624
H	-4.622740	-1.995188	-2.952664
H	-3.980864	-3.607557	-1.171493
H	-4.926875	0.378595	-3.474497
H	-4.173682	2.746697	-3.227963
C	-1.762920	3.476394	-2.273498
C	-0.152506	1.236031	-1.726664
C	0.396895	2.546293	-1.749904
C	-0.454684	3.666618	-1.946349
H	-2.389318	4.308476	-2.585978
H	-0.017101	4.661798	-1.944053
C	1.800526	2.728970	-1.649509
C	0.759040	0.133447	-1.918075
C	2.635372	1.661266	-1.525726
C	2.136479	0.339638	-1.657654
H	2.190706	3.743828	-1.640542
C	0.759040	0.133447	1.918075
C	1.800526	2.728970	1.649509
H	2.190706	3.743828	1.640542
C	2.635372	1.661266	1.525726
C	2.136479	0.339638	1.657654
C	3.009329	-0.780150	1.553940
C	0.403441	-1.155640	2.468811
C	0.403441	-1.155640	-2.468811
C	3.009329	-0.780150	-1.553940
C	2.523702	-2.048164	-1.641177
C	1.201396	-2.268570	2.114752
C	1.201396	-2.268570	-2.114752
C	2.523702	-2.048164	1.641177
H	3.702884	1.801191	1.379286
H	4.057889	-0.598389	1.334034
H	3.158967	-2.907984	1.445828
H	3.158967	-2.907984	-1.445828
H	4.057889	-0.598389	-1.334034
H	3.702884	1.801191	-1.379286
C	0.707018	-3.584573	2.338632
C	-0.590238	-1.377924	3.491855
C	-0.590238	-1.377924	-3.491855
C	0.707018	-3.584573	-2.338632
C	-0.472809	-3.779985	-2.991321
C	-0.472809	-3.779985	2.991321
C	-1.105837	-2.688400	-3.650958

C	-1.105837	-2.688400	3.650958
H	1.285880	-4.425480	1.964263
H	-0.889720	-4.776959	3.110813
H	-0.889720	-4.776959	-3.110813
H	1.285880	-4.425480	-1.964263
C	-0.963496	-0.391669	4.480953
C	-2.201060	-2.914711	4.529961
C	-0.963496	-0.391669	-4.480953
C	-2.201060	-2.914711	-4.529961
C	-2.164419	-0.594197	5.205334
C	-2.770657	-1.881357	5.212026
C	-2.770657	-1.881357	-5.212026
C	-2.164419	-0.594197	-5.205334
H	-3.661948	-2.033633	5.816574
H	-2.602723	-3.922204	4.608519
H	-3.661948	-2.033633	-5.816574
H	-2.602723	-3.922204	-4.608519
C	-2.742867	0.485969	5.929905
C	-2.153111	1.712634	5.917534
C	-0.829822	1.865326	5.414217
C	-0.151801	0.745807	4.867296
H	-3.695725	0.326249	6.428800
H	-2.638877	2.573295	6.370874
C	-0.151801	0.745807	-4.867296
C	-0.829822	1.865326	-5.414217
C	-2.153111	1.712634	-5.917534
C	-2.742867	0.485969	-5.929905
H	-2.638877	2.573295	-6.370874
H	-3.695725	0.326249	-6.428800
C	-0.160787	3.113875	-5.522114
C	1.152981	3.223802	-5.181282
C	1.918632	2.058570	-4.905639
C	1.293694	0.790167	-4.851135
H	1.658274	4.186243	-5.206748
H	-0.725189	3.977813	-5.864409
C	1.293694	0.790167	4.851135
C	1.918632	2.058570	4.905639
C	1.152981	3.223802	5.181282
C	-0.160787	3.113875	5.522114
H	-0.725189	3.977813	5.864409
H	1.658274	4.186243	5.206748
C	2.152463	-0.378305	-4.959105
C	3.332205	2.172291	-4.745157
C	4.118949	1.072460	-4.626598
C	3.559645	-0.229116	-4.789056
H	3.764136	3.169973	-4.714404
H	5.192991	1.166422	-4.483096
C	3.332205	2.172291	4.745157
C	2.152463	-0.378305	4.959105

C	4.118949	1.072460	4.626598
C	3.559645	-0.229116	4.789056
H	3.764136	3.169973	4.714404
H	5.192991	1.166422	4.483096
C	1.686681	-1.651358	-5.362068
C	4.401933	-1.359354	-4.862578
C	3.899263	-2.602488	-5.170025
C	2.531256	-2.735686	-5.458420
C	1.686681	-1.651358	5.362068
C	4.401933	-1.359354	4.862578
C	3.899263	-2.602488	5.170025
C	2.531256	-2.735686	5.458420
H	0.645719	-1.776638	5.629917
H	2.129388	-3.697090	5.765884
H	4.559034	-3.464011	5.229890
H	5.468373	-1.220332	4.697804
H	0.645719	-1.776638	-5.629917
H	2.129388	-3.697090	-5.765884
H	4.559034	-3.464011	-5.229890
H	5.468373	-1.220332	-4.697804

144

23-1 scf done: -3608.262005

C	0.026130	3.587234	0.681182
C	-0.026124	3.587238	-0.681165
C	-0.059234	2.365822	1.409153
C	0.059241	2.365829	-1.409142
C	-0.172842	1.150246	0.699908
C	0.172851	1.150250	-0.699903
C	-0.035621	2.337507	2.833006
C	-0.104444	1.152956	3.504623
C	-0.419806	-0.052920	2.815339
C	-0.631844	-0.011447	1.419961
C	-0.529125	-1.299281	3.496462
C	-1.304748	-1.129539	0.806018
C	-1.224500	-2.384945	1.447293
C	-0.814812	-2.442160	2.810354
C	0.104445	1.152974	-3.504619
C	0.035624	2.337521	-2.832995
C	0.419810	-0.052905	-2.815342
C	0.631850	-0.011440	-1.419964
C	0.529128	-1.299262	-3.496472
C	0.814814	-2.442146	-2.810371
C	1.224503	-2.384937	-1.447310
C	1.304752	-1.129536	-0.806027
C	1.560683	-3.559887	-0.715836
C	2.071008	-1.043609	0.412444
C	2.227133	-2.215799	1.183430
C	1.943193	-3.479115	0.590167
C	2.678045	-2.105705	2.530234

C	2.717993	0.158059	0.877287
C	2.950694	-0.886511	3.075764
C	2.998014	0.277173	2.256030
C	-1.560684	-3.559888	0.715812
C	-2.071007	-1.043603	-0.412450
C	-1.943196	-3.479107	-0.590190
C	-2.227135	-2.215788	-1.183445
C	3.337412	1.554251	2.788396
C	3.139102	1.230490	0.012772
C	3.378885	2.654889	1.984985
C	3.297123	2.517878	0.569686
C	-2.678046	-2.105684	-2.530248
C	-2.717994	0.158068	-0.877284
C	-2.998014	0.277193	-2.256027
C	-2.950692	-0.886486	-3.075770
C	3.485048	1.055371	-1.374967
C	3.400907	3.642261	-0.298289
C	3.416933	2.181070	-2.226022
C	3.348679	3.482719	-1.651625
C	-3.139106	1.230492	-0.012762
C	-3.337410	1.554275	-2.788383
C	-3.378885	2.654906	-1.984964
C	-3.297124	2.517884	-0.569666
C	3.459920	1.990393	-3.637220
C	3.996575	-0.176250	-1.929337
C	3.572346	0.738176	-4.163789
C	3.866140	-0.374790	-3.323725
C	4.051613	-1.677330	-3.866008
C	4.693029	-1.188524	-1.165368
C	4.356221	-2.726109	-3.051665
C	4.706866	-2.505555	-1.689636
H	0.066376	4.520958	1.236782
H	-0.066372	4.520965	-1.236760
H	0.102106	3.273701	3.368491
H	0.014882	1.117722	4.584742
H	-0.317002	-1.328334	4.562452
H	-0.799676	-3.408825	3.307841
H	-0.014884	1.117745	-4.584738
H	-0.102105	3.273719	-3.368475
H	0.317001	-1.328309	-4.562462
H	0.799677	-3.408809	-3.307863
H	1.447129	-4.524923	-1.203695
H	2.106429	-4.378221	1.179273
H	2.746462	-3.010468	3.129315
H	3.206983	-0.792018	4.128019
H	-1.447131	-4.524928	1.203664
H	-2.106433	-4.378209	-1.179301
H	3.509597	1.640642	3.858328
H	3.546873	3.644150	2.403298

H	-3.206981	-0.791984	-4.128023
H	-2.746465	-3.010442	-3.129336
H	3.464994	4.633729	0.143098
H	3.326883	4.344452	-2.314616
H	-3.546870	3.644171	-2.403270
H	-3.509592	1.640674	-3.858315
H	3.507165	0.576270	-5.237071
H	3.344564	2.857997	-4.282361
H	3.888052	-1.825480	-4.930637
H	4.402806	-3.740101	-3.441669
C	-3.485052	1.055363	1.374977
C	-3.400903	3.642260	0.298318
C	-3.348673	3.482708	1.651652
C	-3.416930	2.181055	2.226040
H	-3.464989	4.633732	-0.143060
H	-3.326872	4.344437	2.314649
C	5.424022	-0.947985	0.058192
C	5.093165	-3.591767	-0.857861
C	5.472574	-3.374126	0.432136
C	5.684749	-2.049718	0.904255
H	5.036376	-4.599908	-1.261127
H	5.694673	-4.205983	1.096376
C	-3.459914	1.990368	3.637236
C	-3.572343	0.738147	4.163796
C	-3.866142	-0.374812	3.323725
C	-3.996580	-0.176261	1.929338
C	-4.051617	-1.677355	3.865999
C	-4.356226	-2.726129	3.051650
C	-4.706870	-2.505565	1.689622
C	-4.693035	-1.188530	1.165363
H	-3.344552	2.857965	4.282384
H	-3.507159	0.576233	5.237077
H	-3.888055	-1.825513	4.930627
H	-4.402810	-3.740124	3.441646
C	-5.424028	-0.947984	-0.058197
C	-5.093167	-3.591772	0.857839
C	-5.684752	-2.049712	-0.904267
C	-5.472576	-3.374123	-0.432156
H	-5.694674	-4.205976	-1.096401
H	-5.036377	-4.599915	1.261099
C	6.206178	-1.835667	2.215900
C	6.024992	0.322802	0.417936
C	6.518669	0.510039	1.739890
C	6.540600	-0.591442	2.646105
H	6.905772	-0.429759	3.657667
H	6.315532	-2.697592	2.870047
C	-6.206180	-1.835654	-2.215912
C	-6.024997	0.322805	-0.417934
C	-6.518674	0.510049	-1.739886

C	-6.540603	-0.591427	-2.646109
H	-6.315529	-2.697576	-2.870064
H	-6.905771	-0.429736	-3.657671
C	-6.266276	1.355499	0.517605
C	-7.063687	1.757854	-2.113637
C	-7.202694	2.775020	-1.197834
C	-6.834112	2.552038	0.139961
C	7.063681	1.757844	2.113645
C	6.266271	1.355500	-0.517599
C	6.834116	2.552033	-0.139952
C	7.202692	2.775012	1.197845
H	7.402380	1.888236	3.139253
H	7.631417	3.728180	1.495811
H	6.999540	3.323598	-0.886655
H	6.021459	1.194202	-1.560066
H	-6.021453	1.194201	1.560069
H	-7.402386	1.888251	-3.139245
H	-7.631417	3.728190	-1.495795
H	-6.999529	3.323602	0.886666

144

23TS scf done: -3608.141628

C	-2.734987	-3.390135	0.679106
C	-2.734987	-3.390135	-0.679106
C	-2.763290	-2.134898	1.348091
C	-2.763290	-2.134898	-1.348091
C	-2.214969	-0.978151	0.732644
C	-2.214969	-0.978151	-0.732644
C	-3.683438	-2.009767	2.430591
C	-4.164196	-0.781089	2.757412
C	-3.449111	0.377088	2.335839
C	-2.262526	0.223163	1.574476
H	-2.921249	-4.297455	1.247770
H	-2.921249	-4.297455	-1.247770
H	-4.120173	-2.915375	2.843068
H	-5.016395	-0.661252	3.420207
C	-3.870869	1.679298	2.717552
C	-1.286866	1.268714	1.724563
C	-1.763259	2.580894	1.997564
C	-3.103228	2.767963	2.425270
H	-4.830983	1.785394	3.216708
H	-3.452431	3.776033	2.633948
C	-4.164196	-0.781089	-2.757412
C	-3.683438	-2.009767	-2.430591
C	-3.449111	0.377088	-2.335839
C	-2.262526	0.223163	-1.574476
C	-3.870869	1.679298	-2.717552
C	-3.103228	2.767963	-2.425270
C	-1.763259	2.580894	-1.997564
C	-1.286866	1.268714	-1.724563

H	-5.016395	-0.661252	-3.420207
H	-4.120173	-2.915375	-2.843068
H	-4.830983	1.785394	-3.216708
H	-3.452431	3.776033	-2.633948
C	0.139422	1.052131	-1.803347
C	-0.870507	3.684277	-1.918636
C	0.139422	1.052131	1.803347
C	-0.870507	3.684277	1.918636
C	0.996931	2.174537	-1.666963
C	0.454415	3.488686	-1.680979
C	0.996931	2.174537	1.666963
C	0.454415	3.488686	1.680979
H	1.133385	4.331199	-1.576744
H	-1.272685	4.686011	-2.049900
H	1.133385	4.331199	1.576744
H	-1.272685	4.686011	2.049900
C	0.761719	-0.210602	-2.126173
C	2.398711	1.984897	-1.558392
C	0.761719	-0.210602	2.126173
C	2.398711	1.984897	1.558392
C	2.927518	0.731848	1.498934
C	2.115415	-0.400375	1.759114
C	2.115415	-0.400375	-1.759114
C	2.927518	0.731848	-1.498934
H	3.986607	0.579931	-1.310429
H	3.033258	2.861620	-1.455810
H	3.986607	0.579931	1.310429
H	3.033258	2.861620	1.455810
C	2.646623	-1.722244	-1.693134
C	0.166610	-1.276158	-2.904547
C	2.646623	-1.722244	1.693134
C	0.166610	-1.276158	2.904547
C	1.876562	-2.795251	2.018208
C	0.636948	-2.594073	2.693254
C	0.636948	-2.594073	-2.693254
C	1.876562	-2.795251	-2.018208
H	3.664304	-1.851856	-1.334258
H	2.240475	-3.810391	-1.883114
H	2.240475	-3.810391	1.883114
H	3.664304	-1.851856	1.334258
C	-0.747307	-1.069546	3.999174
C	-0.071174	-3.693031	3.250806
C	-0.747307	-1.069546	-3.999174
C	-0.071174	-3.693031	-3.250806
C	-1.493348	-2.176295	-4.478037
C	-1.157433	-3.489549	-4.049722
C	-1.157433	-3.489549	4.049722
C	-1.493348	-2.176295	4.478037
H	-1.735803	-4.327901	4.431456

H	0.268194	-4.699415	3.017900
H	-1.735803	-4.327901	-4.431456
H	0.268194	-4.699415	-3.017900
C	-2.552214	-1.964848	5.406949
C	-0.850219	0.164405	4.748917
C	-2.045018	0.396727	5.470899
C	-2.892717	-0.703118	5.789906
H	-3.770403	-0.521355	6.405704
H	-3.131057	-2.823854	5.738116
C	-2.552214	-1.964848	-5.406949
C	-0.850219	0.164405	-4.748917
C	-2.045018	0.396727	-5.470899
C	-2.892717	-0.703118	-5.789906
H	-3.770403	-0.521355	-6.405704
H	-3.131057	-2.823854	-5.738116
C	0.213197	1.134837	4.910922
C	-0.169025	2.466859	5.217694
C	-1.489982	2.738005	5.673995
C	-2.356122	1.714130	5.909914
H	-3.315815	1.889682	6.389816
H	-1.755641	3.763796	5.917297
C	0.213197	1.134837	-4.910922
C	-0.169025	2.466859	-5.217694
C	-1.489982	2.738005	-5.673995
C	-2.356122	1.714130	-5.909914
H	-3.315815	1.889682	-6.389816
H	-1.755641	3.763796	-5.917297
C	1.627627	0.830785	4.903576
C	0.785325	3.515521	5.132161
C	2.083361	3.246062	4.821578
C	2.539501	1.902046	4.751986
H	2.806648	4.049128	4.701098
H	0.450979	4.536160	5.301270
C	1.627627	0.830785	-4.903576
C	0.785325	3.515521	-5.132161
C	2.083361	3.246062	-4.821578
C	2.539501	1.902046	-4.751986
H	2.806648	4.049128	-4.701098
H	0.450979	4.536160	-5.301270
C	2.190031	-0.476713	-5.197662
C	3.931197	1.642585	-4.568086
C	4.421647	0.377007	-4.593253
C	3.575440	-0.710489	-4.961155
H	5.476942	0.182423	-4.415866
H	4.588723	2.489424	-4.384800
C	3.931197	1.642585	4.568086
C	2.190031	-0.476713	5.197662
C	3.575440	-0.710489	4.961155
C	4.421647	0.377007	4.593253

H	5.476942	0.182423	4.415866
H	4.588723	2.489424	4.384800
C	1.466432	-1.506472	5.841916
C	4.121034	-1.992284	5.189426
C	3.357441	-3.005040	5.722701
C	2.028322	-2.739548	6.091286
C	1.466432	-1.506472	-5.841916
C	4.121034	-1.992284	-5.189426
C	3.357441	-3.005040	-5.722701
C	2.028322	-2.739548	-6.091286
H	0.456068	-1.314452	6.178780
H	1.435136	-3.505205	6.583340
H	3.790580	-3.985659	5.900991
H	5.173588	-2.153364	4.966126
H	0.456068	-1.314452	-6.178780
H	1.435136	-3.505205	-6.583340
H	3.790580	-3.985659	-5.900991
H	5.173588	-2.153364	-4.966126

150

24-1

C	0.065102	-2.613785	2.420462
C	0.043104	-3.302464	1.244008
C	0.269839	-1.204232	2.430659
C	0.000000	-2.609988	-0.000002
C	0.419480	-0.523022	1.202941
C	0.000000	-1.198136	-0.000001
C	0.331331	-0.463698	3.645780
C	0.513854	0.887374	3.626696
C	0.863818	1.553663	2.417501
C	0.991656	0.800164	1.230219
C	1.091071	2.959335	2.374339
C	1.699817	1.398272	0.125238
C	1.735552	2.807556	0.045805
C	1.408259	3.575214	1.200249
C	-0.065103	-2.613782	-2.420465
C	-0.043106	-3.302463	-1.244012
C	-0.269839	-1.204229	-2.430661
C	-0.419479	-0.523021	-1.202941
C	-0.331331	-0.463693	-3.645780
C	-0.513853	0.887378	-3.626695
C	-0.863817	1.553667	-2.417499
C	-0.991656	0.800166	-1.230218
C	-1.091072	2.959338	-2.374337
C	-1.699816	1.398273	-0.125237
C	-1.735552	2.807557	-0.045803
C	-1.408261	3.575215	-1.200246
C	-2.104734	3.423352	1.184290
C	-2.392999	0.649014	0.893189
C	-2.411056	2.665999	2.275706

C	-2.583509	1.257559	2.152628
C	2.104736	3.423352	-1.184287
C	2.392999	0.649015	-0.893188
C	2.411057	2.666000	-2.275703
C	2.583509	1.257560	-2.152626
C	-2.957194	0.449394	3.264579
C	-2.937498	-0.671284	0.695243
C	-3.123913	-0.896153	3.122805
C	-3.138508	-1.489538	1.828215
C	2.957192	0.449395	-3.264579
C	2.937498	-0.671285	-0.695244
C	3.138506	-1.489538	-1.828216
C	3.123910	-0.896152	-3.122806
C	-3.334460	-1.193622	-0.587156
C	-3.368177	-2.883777	1.646509
C	-3.380652	-2.594323	-0.755237
C	-3.380306	-3.430502	0.397749
C	3.334460	-1.193623	0.587154
C	3.368175	-2.883776	-1.646511
C	3.380307	-3.430502	-0.397751
C	3.380653	-2.594324	0.755235
C	-3.457985	-3.133870	-2.070994
C	-3.764566	-0.373410	-1.691020
C	-3.488536	-2.311767	-3.158636
C	-3.671359	-0.908662	-2.995251
C	-3.804180	-0.039088	-4.115920
C	-4.383401	0.922771	-1.539411
C	-4.025612	1.293792	-3.935997
C	-4.343288	1.805094	-2.644343
H	-0.005480	-3.135060	3.372004
H	-0.007437	-4.388510	1.235508
H	0.166332	-0.989785	4.582911
H	0.460870	1.469260	4.543639
H	0.943235	3.536933	3.283589
H	1.482994	4.658349	1.141956
H	0.005478	-3.135056	-3.372008
H	0.007435	-4.388509	-1.235513
H	-0.166332	-0.989780	-4.582913
H	-0.460869	1.469265	-4.543638
H	-0.943236	3.536937	-3.283586
H	-1.482996	4.658350	-1.141952
H	-2.078764	4.508380	1.249490
H	-2.599222	3.130188	3.240696
H	2.078766	4.508381	-1.249486
H	2.599224	3.130190	-3.240693
H	-3.052558	0.921496	4.239371
H	-3.320137	-1.527023	3.986151
H	3.320133	-1.527021	-3.986152
H	3.052556	0.921499	-4.239370

H	-3.479478	-3.509907	2.528235
H	-3.463064	-4.505795	0.260911
H	3.463065	-4.505796	-0.260914
H	3.479475	-3.509906	-2.528238
H	-3.447075	-2.718094	-4.166505
H	-3.434612	-4.214205	-2.190449
H	-3.669224	-0.452061	-5.112665
H	-4.030510	1.977760	-4.781327
C	3.764566	-0.373412	1.691020
C	3.457987	-3.133872	2.070992
C	3.488537	-2.311770	3.158634
C	3.671359	-0.908664	2.995250
H	3.434615	-4.214207	2.190446
H	3.447077	-2.718098	4.166503
C	-5.101205	1.352031	-0.358824
C	-4.641762	3.183023	-2.451505
C	-4.967784	3.651175	-1.214401
C	-5.227939	2.747752	-0.145361
H	-4.547147	3.858944	-3.297869
H	-5.100711	4.715878	-1.037809
C	3.804179	-0.039091	4.115919
C	4.025610	1.293789	3.935997
C	4.343286	1.805092	2.644344
C	4.383400	0.922770	1.539411
C	4.641762	3.183021	2.451507
C	4.967785	3.651174	1.214403
C	5.227939	2.747752	0.145363
C	5.101204	1.352031	0.358824
H	3.669224	-0.452065	5.112664
H	4.030509	1.977757	4.781328
H	4.547147	3.858941	3.297871
H	5.100711	4.715877	1.037813
C	5.749031	0.469679	-0.585275
C	5.636625	3.232375	-1.127034
C	6.034055	0.970922	-1.875653
C	5.931281	2.365196	-2.135265
H	6.169585	2.728605	-3.132095
H	5.665850	4.307286	-1.288011
C	-5.636626	3.232374	1.127036
C	-5.749032	0.469679	0.585275
C	-6.034055	0.970921	1.875653
C	-5.931282	2.365194	2.135266
H	-6.169585	2.728603	3.132096
H	-5.665850	4.307285	1.288014
C	6.471982	0.084820	-2.905746
C	6.248564	-0.853532	-0.261008
C	6.660735	-1.719290	-1.313166
C	6.705110	-1.229070	-2.652078
H	6.601115	0.488564	-3.907295

H	7.006663	-1.906423	-3.447701
C	-6.471981	0.084818	2.905746
C	-6.248565	-0.853533	0.261008
C	-6.660734	-1.719291	1.313165
C	-6.705109	-1.229072	2.652077
H	-6.601113	0.488561	3.907295
H	-7.006660	-1.906426	3.447700
C	-6.471221	-1.291577	-1.065073
C	-7.105730	-3.025031	1.011859
C	-7.226838	-3.451182	-0.290596
C	-6.941926	-2.557010	-1.336802
C	6.471222	-1.291576	1.065072
C	7.105732	-3.025030	-1.011860
C	7.226840	-3.451180	0.290595
C	6.941930	-2.557008	1.336801
H	6.290455	-0.609097	1.886169
H	7.095997	-2.859008	2.368940
H	7.578492	-4.455872	0.509816
H	7.382348	-3.680259	-1.835118
H	-6.290454	-0.609098	-1.886169
H	-7.095992	-2.859011	-2.368941
H	-7.578489	-4.455874	-0.509817
H	-7.382342	-3.680263	1.835117

150

24TS

C	-3.108200	-2.885715	2.146181
C	-2.422738	-3.556125	1.185920
C	-3.151737	-1.464469	2.122063
C	-2.089329	-2.833107	0.000000
C	-2.260134	-0.750136	1.279597
C	-1.964532	-1.419241	0.000000
C	-4.147668	-0.761392	2.855682
C	-4.252925	0.592519	2.748373
C	-3.159029	1.324129	2.210036
C	-2.039804	0.624782	1.683694
H	-3.643045	-3.410677	2.931605
H	-2.388427	-4.642357	1.172610
H	-4.871631	-1.342025	3.421983
H	-5.088379	1.134490	3.183094
C	-3.126181	2.744682	2.273386
C	-0.770016	1.303705	1.748402
C	-0.770941	2.724285	1.761633
C	-1.991216	3.426826	1.954167
H	-4.028255	3.269586	2.578613
H	-1.973752	4.513855	1.950625
C	-3.108200	-2.885715	-2.146181
C	-2.422738	-3.556125	-1.185920
C	-3.151737	-1.464469	-2.122063
C	-2.260134	-0.750136	-1.279597

C	-4.147668	-0.761392	-2.855682
C	-4.252925	0.592519	-2.748373
C	-3.159029	1.324129	-2.210036
C	-2.039804	0.624782	-1.683694
H	-3.643045	-3.410677	-2.931605
H	-2.388427	-4.642357	-1.172610
H	-4.871631	-1.342025	-3.421983
H	-5.088379	1.134490	-3.183094
C	-3.126181	2.744682	-2.273386
C	-0.770016	1.303705	-1.748402
C	-0.770941	2.724285	-1.761633
C	-1.991216	3.426826	-1.954167
H	-4.028255	3.269586	-2.578613
H	-1.973752	4.513855	-1.950625
C	0.453342	3.432971	-1.647972
C	0.496350	0.641367	-1.951790
C	1.632662	2.766641	-1.513349
C	1.683592	1.355973	-1.661039
H	0.422966	4.519741	-1.630516
C	0.496350	0.641367	1.951790
C	0.453342	3.432971	1.647972
H	0.422966	4.519741	1.630516
C	1.632662	2.766641	1.513349
C	1.683592	1.355973	1.661039
C	2.914904	0.651981	1.544858
C	0.670232	-0.670171	2.537540
C	0.670232	-0.670171	-2.537540
C	2.914904	0.651981	-1.544858
C	2.956573	-0.702530	-1.672808
C	1.834100	-1.399001	2.198339
C	1.834100	-1.399001	-2.198339
C	2.956573	-0.702530	1.672808
H	2.562060	3.304944	1.348261
H	3.808533	1.215030	1.288649
H	3.869850	-1.257106	1.474244
H	3.869850	-1.257106	-1.474244
H	3.808533	1.215030	-1.288649
H	2.562060	3.304944	-1.348261
C	1.889285	-2.795886	2.470973
C	-0.175138	-1.240950	3.556904
C	-0.175138	-1.240950	-3.556904
C	1.889285	-2.795886	-2.470973
C	0.870408	-3.417169	-3.128314
C	0.870408	-3.417169	3.128314
C	-0.156344	-2.644189	-3.740934
C	-0.156344	-2.644189	3.740934
H	2.755737	-3.355934	2.127763
H	0.878049	-4.492922	3.283736
H	0.878049	-4.492922	-3.283736

H	2.755737	-3.355934	-2.127763
C	-0.936735	-0.460020	4.500081
C	-1.126693	-3.255398	4.582300
C	-0.936735	-0.460020	-4.500081
C	-1.126693	-3.255398	-4.582300
C	-2.004855	-1.086656	5.185021
C	-2.083716	-2.506843	5.201405
C	-2.083716	-2.506843	-5.201405
C	-2.004855	-1.086656	-5.185021
H	-2.881016	-2.978579	5.771640
H	-1.117218	-4.338164	4.680935
H	-2.881016	-2.978579	-5.771640
H	-1.117218	-4.338164	-4.680935
C	-2.954974	-0.286185	5.883181
C	-2.843257	1.071408	5.886362
C	-1.647289	1.692573	5.421899
C	-0.603867	0.889062	4.903949
H	-3.803016	-0.778278	6.353500
H	-3.619061	1.696610	6.321657
C	-0.603867	0.889062	-4.903949
C	-1.647289	1.692573	-5.421899
C	-2.843257	1.071408	-5.886362
C	-2.954974	-0.286185	-5.883181
H	-3.619061	1.696610	-6.321657
H	-3.803016	-0.778278	-6.353500
C	-1.462911	3.098898	-5.531308
C	-0.271724	3.665873	-5.192847
C	0.864564	2.849813	-4.931685
C	0.736285	1.436570	-4.932576
H	-0.146218	4.745913	-5.195487
H	-2.302113	3.709680	-5.854981
C	0.736285	1.436570	4.932576
C	0.864564	2.849813	4.931685
C	-0.271724	3.665873	5.192847
C	-1.462911	3.098898	5.531308
H	-2.302113	3.709680	5.854981
H	-0.146218	4.745913	5.195487
C	1.949411	0.658590	-5.065860
C	2.134688	3.446428	-4.706742
C	3.239078	2.673884	-4.512066
C	3.177276	1.269484	-4.721967
H	2.195605	4.530844	-4.655080
H	4.199423	3.123290	-4.269905
C	2.134688	3.446428	4.706742
C	1.949411	0.658590	5.065860
C	3.239078	2.673884	4.512066
C	3.177276	1.269484	4.721967
H	2.195605	4.530844	4.655080
H	4.199423	3.123290	4.269905

C	2.020664	-0.657135	-5.674993
C	4.367341	0.485499	-4.630667
C	4.365732	-0.835838	-4.943904
C	3.210220	-1.427066	-5.536067
C	2.020664	-0.657135	5.674993
C	4.367341	0.485499	4.630667
C	4.365732	-0.835838	4.943904
C	3.210220	-1.427066	5.536067
H	5.265188	-1.437528	4.835743
H	5.275291	0.973069	4.282877
H	5.265188	-1.437528	-4.835743
H	5.275291	0.973069	-4.282877
C	1.018329	-1.164351	-6.533138
C	3.270619	-2.727356	-6.082576
C	1.116996	-2.418108	-7.095159
C	2.233155	-3.230492	-6.833581
H	4.175630	-3.311480	-5.929880
H	2.296068	-4.228408	-7.259337
H	0.324712	-2.773946	-7.747664
H	0.168318	-0.541189	-6.780803
C	3.270619	-2.727356	6.082576
C	1.018329	-1.164351	6.533138
C	2.233155	-3.230492	6.833581
C	1.116996	-2.418108	7.095159
H	4.175630	-3.311480	5.929880
H	2.296068	-4.228408	7.259337
H	0.324712	-2.773946	7.747664
H	0.168318	-0.541189	6.780803