

Supporting Information

Molecular Recognition in Mn-Catalyzed C-H Oxidation. Reaction Mechanism and Origin of Selectivity from a DFT Perspective.

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Optimized geometries and absolute gas phase energies with basis sets I, E(I), and II, E(II), of all stationary points.

Toluene E(I) = -271.506978332 / E(II) = -271.572910754

C	-2.429814	0.001093	0.007798
H	-2.817810	-0.181869	1.019258
H	-2.837835	-0.782162	-0.641265
H	-2.833911	0.961531	-0.328548
C	-0.916081	0.002293	-0.009107
C	-0.193872	1.207339	-0.007453
C	1.205877	1.207968	0.001734
C	1.909158	-0.001500	0.007005
C	1.201862	-1.210059	0.001749
C	-0.196635	-1.206013	-0.007387
H	-0.733177	2.150791	-0.014908
H	1.744561	2.150816	0.001435
H	2.994642	-0.003331	0.011739
H	1.738628	-2.154031	0.001335
H	-0.738069	-2.148469	-0.015080

AFD E(I) = -2229.85364025 / E(II) = -2230.29974164

Mn	-0.849912	0.000015	0.211223
Mn	1.756749	0.000014	-0.882085
O	-1.617836	0.000038	1.840904
O	0.110555	0.000011	-1.510733
O	2.669053	0.000038	-2.434451
O	0.855300	0.000017	0.788762
S	-3.303466	0.000021	2.259868
O	-3.816175	1.262489	1.611176
O	-3.816133	-1.262495	1.611238
O	-3.238913	0.000059	3.746063
N	3.438766	-0.000015	0.234613
C	5.407746	-0.000070	2.126252
C	4.908523	1.217255	1.646449
H	5.291714	2.154523	2.028773
C	3.896596	1.187974	0.679802
C	3.896576	-1.188030	0.679755
C	4.908504	-1.217367	1.646399

H	5.291680	-2.154658	2.028684
C	1.549916	-2.933104	-1.509067
N	2.171478	-1.999688	-0.764716
C	3.235401	-2.335892	0.029841
C	3.660260	-3.662779	0.120352
C	3.004800	-4.642427	-0.634623
C	1.945668	-4.273020	-1.468132
H	0.741397	-2.579303	-2.134334
H	4.503888	-3.926634	0.746008
H	3.331253	-5.674671	-0.584140
H	1.434115	-5.003106	-2.082516
C	3.235447	2.335872	0.029926
C	3.660330	3.662748	0.120490
C	3.004901	4.642435	-0.634462
C	1.945777	4.273077	-1.468002
C	1.549999	2.933170	-1.508990
N	2.171529	1.999716	-0.764659
H	4.503954	3.926565	0.746167
H	3.331372	5.674671	-0.583936
H	1.434249	5.003195	-2.082369
H	0.741486	2.579406	-2.134287
H	6.184739	-0.000091	2.881586
N	-2.524043	-0.000022	-0.884054
C	-4.667271	-0.000073	-2.573450
C	-4.130719	-1.216649	-2.135980
H	-4.565961	-2.154469	-2.455222
C	-3.038535	-1.186442	-1.263750
C	-3.038555	1.186374	-1.263796
C	-4.130739	1.216529	-2.136029
H	-4.565995	2.154330	-2.455309
C	-0.687271	2.890429	0.936471
N	-1.273397	1.988368	0.126149
C	-2.374014	2.327122	-0.611554
C	-2.846609	3.640236	-0.615502
C	-2.220830	4.590850	0.195227
C	-1.138393	4.209330	0.994553
H	0.125129	2.519376	1.546797
H	-3.724081	3.902882	-1.192347
H	-2.597730	5.606536	0.229367
H	-0.665388	4.910732	1.670298
C	-2.373971	-2.327152	-0.611464
C	-2.846543	-3.640274	-0.615355
C	-2.220740	-4.590844	0.195406
C	-1.138304	-4.209274	0.994708
C	-0.687207	-2.890367	0.936573
N	-1.273356	-1.988349	0.126219

H	-3.724016	-3.902958	-1.192182
H	-2.597622	-5.606536	0.229590
H	-0.665280	-4.910641	1.670477
H	0.125190	-2.519273	1.546878
H	-5.517651	-0.000093	-3.245165

FS E(I) = -2229.85068066 / E(II) = -2230.29677306

Mn	-0.846458	0.000064	0.216744
Mn	1.751819	0.000146	-0.885692
O	-1.616866	0.000098	1.843140
O	0.108898	0.000156	-1.523056
O	2.670889	0.000240	-2.432802
O	0.861146	0.000037	0.806120
S	-3.304671	-0.000094	2.260111
O	-3.814750	1.262451	1.609887
O	-3.814398	-1.262878	1.610075
O	-3.242822	0.000028	3.746117
N	3.435143	0.000110	0.231014
C	5.398444	0.000057	2.128321
C	4.900006	1.217364	1.647666
H	5.281369	2.154654	2.031782
C	3.890540	1.188017	0.678449
C	3.890553	-1.187821	0.678377
C	4.900012	-1.217227	1.647596
H	5.281383	-2.154536	2.031655
C	1.541708	-2.932639	-1.508798
N	2.163931	-1.999514	-0.764577
C	3.228338	-2.335597	0.029411
C	3.652625	-3.662685	0.119932
C	2.996533	-4.642137	-0.634740
C	1.937204	-4.272575	-1.468015
H	0.733205	-2.578059	-2.133737
H	4.496565	-3.926703	0.745093
H	3.322802	-5.674452	-0.584393
H	1.425451	-5.002577	-2.082326
C	3.228276	2.335831	0.029607
C	3.652554	3.662915	0.120231
C	2.996413	4.642438	-0.634298
C	1.937032	4.272954	-1.467534
C	1.541539	2.933017	-1.508422
N	2.163826	1.999815	-0.764347
H	4.496531	3.926873	0.745369
H	3.322683	5.674749	-0.583870
H	1.425228	5.003013	-2.081734
H	0.732988	2.578511	-2.133342
H	6.173501	0.000037	2.885636

N	-2.519493	-0.000232	-0.881084
C	-4.655246	-0.000607	-2.579957
C	-4.119954	-1.217079	-2.140650
H	-4.552989	-2.155051	-2.462477
C	-3.031295	-1.186647	-1.264040
C	-3.031594	1.186009	-1.264188
C	-4.120259	1.216055	-2.140804
H	-4.553530	2.153877	-2.462751
C	-0.680735	2.889749	0.936859
N	-1.267067	1.987935	0.126241
C	-2.367326	2.326849	-0.611938
C	-2.839374	3.640167	-0.616237
C	-2.213551	4.590530	0.194782
C	-1.131570	4.208716	0.994704
H	0.131320	2.517774	1.547224
H	-3.716566	3.903064	-1.193405
H	-2.590192	5.606320	0.228822
H	-0.658856	4.910002	1.670771
C	-2.366734	-2.327225	-0.611640
C	-2.838443	-3.640664	-0.615736
C	-2.212366	-4.590740	0.195423
C	-1.130472	-4.208525	0.995273
C	-0.679974	-2.889452	0.937223
N	-1.266552	-1.987915	0.126472
H	-3.715576	-3.903874	-1.192851
H	-2.588748	-5.606621	0.229626
H	-0.657575	-4.909588	1.671443
H	0.131997	-2.517159	1.547508
H	-5.502864	-0.000756	-3.255147

AFD2 E(I) = -2229.84576008 / E(II) = -2230.29072169

Mn	-1.736233	0.001481	-0.801540
Mn	0.868240	0.001193	0.245225
O	1.664598	0.003013	1.856564
O	-0.135531	0.000455	-1.496892
O	-2.571714	0.003621	-2.481786
O	-0.824130	0.002636	0.856897
S	3.367142	0.002225	2.234117
O	3.863194	-1.261989	1.579915
O	3.865521	1.263034	1.575144
O	3.319468	0.005085	3.721583
N	-3.471271	-0.001518	0.231026
C	-5.529815	-0.005995	2.028963
C	-5.007978	-1.222153	1.570612
H	-5.408828	-2.160382	1.931955
C	-3.951664	-1.190089	0.652973

C	-3.953558	1.184978	0.656727
C	-5.009772	1.212453	1.574583
H	-5.411975	2.148889	1.939051
C	-1.532537	2.930164	-1.445823
N	-2.171180	1.998056	-0.713435
C	-3.269266	2.333905	0.033590
C	-3.709126	3.657682	0.094168
C	-3.033342	4.635825	-0.644249
C	-1.941188	4.266469	-1.434180
H	-0.703039	2.575678	-2.042261
H	-4.580065	3.919277	0.682227
H	-3.370187	5.665605	-0.617123
H	-1.414846	4.994083	-2.038956
C	-3.265060	-2.335852	0.026776
C	-3.702870	-3.660525	0.082634
C	-3.024551	-4.635296	-0.657885
C	-1.931757	-4.261786	-1.444977
C	-1.525207	-2.924830	-1.451902
N	-2.166559	-1.995898	-0.717798
H	-4.574193	-3.925302	0.668696
H	-3.359839	-5.665676	-0.634466
H	-1.403322	-4.986713	-2.051156
H	-0.695239	-2.567107	-2.045768
H	-6.341856	-0.007760	2.746539
N	2.513965	-0.001956	-0.891481
C	4.603692	-0.006474	-2.646383
C	4.081041	1.211333	-2.195557
H	4.505638	2.148293	-2.531234
C	3.015809	1.183630	-1.290664
C	3.014278	-1.189631	-1.286393
C	4.079531	-1.221979	-2.191111
H	4.502980	-2.160690	-2.523337
C	0.717352	-2.888657	0.975498
N	1.285577	-1.988029	0.150856
C	2.365614	-2.329172	-0.615950
C	2.834681	-3.643221	-0.632232
C	2.227444	-4.592501	0.194573
C	1.166748	-4.208820	1.021398
H	-0.079699	-2.516345	1.605112
H	3.695793	-3.908291	-1.232210
H	2.602350	-5.609211	0.218513
H	0.708672	-4.909560	1.707986
C	2.368972	2.326405	-0.623992
C	2.839971	3.639690	-0.645084
C	2.234828	4.592666	0.179009
C	1.174307	4.213311	1.008026

C	0.722848	2.893681	0.966854
N	1.288976	1.989457	0.144731
H	3.700975	3.901463	-1.246663
H	2.611254	5.608895	0.199200
H	0.717894	4.916991	1.692711
H	-0.074217	2.524778	1.598453
H	5.432949	-0.008262	-3.343975

FO E(I) = -2229.84255390 / E(II) = -2230.28248776

Mn	0.890008	0.006287	0.230433
Mn	-1.732549	0.006078	-0.755950
O	1.693562	0.015208	1.844716
O	-0.101431	0.003359	-1.459444
O	-2.780970	0.029655	-2.347954
O	-0.822493	0.017405	0.874324
S	3.384932	0.007851	2.234750
O	3.874172	-1.264443	1.586223
O	3.890743	1.260646	1.561544
O	3.354415	0.022537	3.721301
N	-3.430035	-0.004431	0.327563
C	-5.544916	-0.026143	2.044475
C	-5.016054	-1.239197	1.584181
H	-5.442092	-2.179380	1.910318
C	-3.931840	-1.197141	0.698496
C	-3.938606	1.177909	0.720142
C	-5.021909	1.198139	1.607089
H	-5.452518	2.129906	1.950782
C	-1.608428	2.894336	-1.517517
N	-2.218808	1.973795	-0.744948
C	-3.275902	2.320162	0.060142
C	-3.697376	3.648328	0.132383
C	-3.054592	4.614404	-0.651557
C	-2.008941	4.232989	-1.496739
H	-0.806306	2.526438	-2.143426
H	-4.529262	3.924571	0.768187
H	-3.381448	5.647112	-0.613408
H	-1.510518	4.952952	-2.133329
C	-3.260224	-2.325217	0.022127
C	-3.677793	-3.655903	0.068767
C	-3.024310	-4.607471	-0.723789
C	-1.970139	-4.209859	-1.550917
C	-1.573732	-2.870051	-1.546697
N	-2.196716	-1.962719	-0.768237
H	-4.514716	-3.944846	0.692187
H	-3.348450	-5.641574	-0.705501
H	-1.461872	-4.918541	-2.192378

H	-0.764256	-2.490039	-2.155816
H	-6.377418	-0.034622	2.738029
N	2.542323	-0.011883	-0.885540
C	4.672165	-0.037134	-2.591667
C	4.143684	1.185635	-2.162152
H	4.579867	2.118649	-2.493811
C	3.058410	1.168858	-1.281212
C	3.047528	-1.204273	-1.259764
C	4.132822	-1.247063	-2.139765
H	4.560842	-2.189875	-2.453940
C	0.686921	-2.878221	0.953821
N	1.286455	-1.983012	0.145446
C	2.377051	-2.336333	-0.599868
C	2.829070	-3.656639	-0.609394
C	2.190219	-4.600084	0.199461
C	1.115672	-4.204908	1.003149
H	-0.115602	-2.495620	1.570583
H	3.699611	-3.931404	-1.191039
H	2.550563	-5.621916	0.228244
H	0.632909	-4.901887	1.676554
C	2.399953	2.319054	-0.640682
C	2.865511	3.634228	-0.674656
C	2.238764	4.598364	0.119160
C	1.162799	4.228329	0.932765
C	0.720033	2.905507	0.907641
N	1.307855	1.990068	0.113571
H	3.736923	3.889789	-1.263705
H	2.609494	5.616827	0.128744
H	0.689221	4.941857	1.595277
H	-0.084703	2.542741	1.533398
H	5.517782	-0.047133	-3.269247

AFD-1 E(I) = -2501.36666773 / E(II) = -2501.87827623

Mn	-1.728553	-0.198396	0.218492
Mn	0.848720	0.672337	-0.547980
O	-2.670825	-0.397579	1.741665
O	-0.594052	0.075666	-1.368641
O	1.913804	0.957712	-1.979497
O	-0.223908	0.418985	0.992921
H	4.460144	0.976636	-2.151548
C	5.547574	1.124554	-2.093652
H	5.919904	1.160086	-3.123935
H	5.730203	2.105333	-1.641646
C	6.223883	0.023355	-1.305586
C	6.738727	0.257877	-0.017929
C	7.369751	-0.762681	0.707081

C	7.498563	-2.042009	0.152761
C	6.992929	-2.289448	-1.131179
C	6.362540	-1.267948	-1.849642
H	6.670877	1.256362	0.406370
H	7.787291	-0.550851	1.687347
H	8.010042	-2.827190	0.700605
H	7.110757	-3.270952	-1.580669
H	5.990039	-1.464601	-2.851318
S	-4.297236	-0.961219	1.965258
O	-5.112347	0.021039	1.159961
O	-4.263502	-2.347701	1.369709
O	-4.438132	-0.881046	3.444109
N	2.265491	1.286873	0.751115
C	3.856315	2.008705	2.848116
C	3.030739	2.966074	2.243964
H	3.012580	3.983830	2.612040
C	2.225457	2.568398	1.171199
C	3.047336	0.342954	1.312718
C	3.878512	0.687540	2.385653
H	4.518214	-0.047919	2.854980
C	1.702628	-2.167389	-0.975843
N	1.883700	-1.053274	-0.242631
C	2.905234	-0.975683	0.668289
C	3.754775	-2.062826	0.874446
C	3.560636	-3.230469	0.127909
C	2.527108	-3.283596	-0.810446
H	0.892886	-2.135650	-1.692259
H	4.587923	-1.986039	1.560553
H	4.226112	-4.074385	0.263892
H	2.364065	-4.165390	-1.417216
C	1.304936	3.402025	0.373875
C	1.229471	4.795175	0.430267
C	0.390132	5.469818	-0.463998
C	-0.348357	4.738848	-1.398819
C	-0.248580	3.344655	-1.401086
N	0.544820	2.701688	-0.524506
H	1.832998	5.348717	1.138818
H	0.330247	6.551747	-0.440172
H	-0.988001	5.233192	-2.118989
H	-0.788931	2.717894	-2.097788
H	4.481698	2.293626	3.686033
N	-3.132842	-0.834047	-1.057038
C	-4.893321	-1.660611	-2.971662
C	-4.042278	-2.592031	-2.365708
H	-4.084804	-3.636745	-2.644348
C	-3.157145	-2.142144	-1.381423

C	-3.961903	0.079317	-1.600215
C	-4.867361	-0.314192	-2.590109
H	-5.546369	0.396942	-3.041941
C	-2.670921	2.591633	0.700332
N	-2.791336	1.508379	-0.090570
C	-3.823879	1.408421	-0.981633
C	-4.709085	2.472215	-1.161156
C	-4.567026	3.616040	-0.371173
C	-3.546964	3.671285	0.583982
H	-1.878521	2.553536	1.435870
H	-5.531552	2.386295	-1.859562
H	-5.267425	4.436728	-0.474872
H	-3.443824	4.521935	1.245836
C	-2.241742	-2.947732	-0.556057
C	-2.234450	-4.341792	-0.492654
C	-1.437430	-4.974797	0.464729
C	-0.666586	-4.202433	1.339700
C	-0.688536	-2.813176	1.212955
N	-1.433287	-2.211930	0.265462
H	-2.884009	-4.921098	-1.136194
H	-1.446747	-6.055374	0.549058
H	-0.076915	-4.662201	2.122758
H	-0.140090	-2.153094	1.871616
H	-5.591420	-1.988425	-3.732953

AFD-TS1 E(I) = -2501.35557729 / E(II) = -2501.86781776

Mn	1.692987	-0.061484	-0.142382
Mn	-1.127203	0.217086	-0.152327
O	3.053340	-0.053249	-1.341604
O	0.154636	-0.053130	1.047236
O	-2.483731	0.193377	1.042171
O	0.373054	0.209919	-1.333250
H	-3.755207	0.422073	0.697457
C	-4.939198	0.677593	0.426933
H	-4.950843	1.771071	0.408184
H	-5.096258	0.254451	-0.568924
C	-5.768940	0.074794	1.483609
C	-6.319180	-1.218793	1.327324
C	-7.085177	-1.796995	2.339249
C	-7.312654	-1.099310	3.534592
C	-6.769050	0.181846	3.709313
C	-6.004675	0.761771	2.697536
H	-6.150327	-1.758266	0.399281
H	-7.510478	-2.785512	2.199705
H	-7.909443	-1.548649	4.321244
H	-6.945796	0.724070	4.632250

H	-5.583515	1.753219	2.835619
S	4.745883	-0.247389	-1.077307
O	5.084345	0.888574	-0.140105
O	4.842492	-1.608082	-0.427258
O	5.288098	-0.141190	-2.459739
N	-2.182880	0.534260	-1.858338
C	-3.059846	0.939944	-4.415161
C	-2.720393	2.039441	-3.616522
H	-2.790893	3.044959	-4.011254
C	-2.266497	1.801262	-2.314033
C	-2.487900	-0.543717	-2.609806
C	-2.946928	-0.365518	-3.920401
H	-3.191453	-1.211976	-4.549351
C	-1.503863	-2.744502	0.134570
N	-1.656033	-1.685103	-0.681063
C	-2.285409	-1.816519	-1.889787
C	-2.737378	-3.065754	-2.320242
C	-2.562475	-4.177646	-1.487663
C	-1.950047	-4.015006	-0.241698
H	-1.026530	-2.543244	1.084193
H	-3.237979	-3.169162	-3.275107
H	-2.915317	-5.152485	-1.804025
H	-1.820483	-4.851731	0.433076
C	-1.845498	2.797100	-1.308618
C	-2.046519	4.175731	-1.406091
C	-1.679269	4.995342	-0.332155
C	-1.128085	4.419548	0.816325
C	-0.935944	3.035382	0.856348
N	-1.274201	2.256564	-0.187979
H	-2.502565	4.602693	-2.290796
H	-1.837340	6.066178	-0.388796
H	-0.852506	5.025407	1.670312
H	-0.518704	2.520946	1.711778
H	-3.401542	1.100544	-5.430950
N	2.799767	-0.361227	1.497940
C	4.119579	-0.765814	3.851638
C	3.678720	-1.866127	3.107414
H	3.866866	-2.873756	3.454028
C	3.014029	-1.628989	1.900445
C	3.240474	0.715981	2.176578
C	3.911156	0.539148	3.390480
H	4.278917	1.385823	3.955054
C	2.096035	2.870724	-0.529874
N	2.236914	1.842099	0.327608
C	2.990772	1.978235	1.460160
C	3.542538	3.214926	1.798322

C	3.369635	4.296827	0.931527
C	2.652282	4.120525	-0.256211
H	1.554322	2.653598	-1.440695
H	4.147673	3.317246	2.689910
H	3.821023	5.254639	1.163497
H	2.544912	4.926386	-0.971372
C	2.547007	-2.622401	0.918833
C	2.849423	-3.984558	0.951387
C	2.494677	-4.786439	-0.136145
C	1.848289	-4.210528	-1.234661
C	1.543682	-2.849467	-1.201867
N	1.857324	-2.090151	-0.134930
H	3.405491	-4.400400	1.781717
H	2.753069	-5.839121	-0.140634
H	1.605913	-4.795618	-2.112918
H	1.072999	-2.331854	-2.026923
H	4.642916	-0.926425	4.786916

AFD-2 E(I) = -2501.38062671 / E(II) = -2501.90043321

Mn	-1.702141	-0.158397	0.211647
Mn	0.950926	0.515092	-0.468072
O	-2.698083	-0.309055	1.713878
O	-0.520875	0.041440	-1.325119
O	2.037551	0.701638	-1.948777
O	-0.171204	0.324865	1.037305
H	3.007495	0.825002	-1.853266
C	5.314007	1.218387	-2.282408
H	4.907700	1.048501	-3.274127
H	5.310386	2.237854	-1.909807
C	5.954640	0.181957	-1.565453
C	6.566589	0.422621	-0.293763
C	7.215232	-0.596710	0.394933
C	7.281147	-1.893215	-0.147311
C	6.685187	-2.157040	-1.394103
C	6.032576	-1.147033	-2.091927
H	6.541354	1.428363	0.116502
H	7.695337	-0.385163	1.345609
H	7.808614	-2.679529	0.382618
H	6.750702	-3.151883	-1.823389
H	5.588001	-1.351644	-3.061311
S	-4.362936	-0.739985	1.888189
O	-5.078299	0.320999	1.086214
O	-4.430966	-2.113240	1.262774
O	-4.540327	-0.680587	3.364736
N	2.365763	1.028365	0.898822
C	3.834281	1.630940	3.122481

C	3.129612	2.645930	2.462085
H	3.152650	3.661324	2.836754
C	2.380400	2.306925	1.329441
C	3.024225	0.029498	1.521054
C	3.791188	0.310485	2.658027
H	4.326199	-0.471808	3.180608
C	1.668972	-2.366017	-0.881346
N	1.877568	-1.273702	-0.123212
C	2.825973	-1.278025	0.865111
C	3.560825	-2.433552	1.135512
C	3.331692	-3.581564	0.368352
C	2.383634	-3.546409	-0.657873
H	0.928668	-2.262444	-1.663444
H	4.323070	-2.430854	1.903965
H	3.901554	-4.483336	0.559841
H	2.200182	-4.411822	-1.282188
C	1.564568	3.201583	0.484365
C	1.587560	4.597140	0.532589
C	0.842396	5.324022	-0.403489
C	0.100786	4.641627	-1.372212
C	0.100775	3.243678	-1.366817
N	0.800717	2.552784	-0.448324
H	2.194452	5.110592	1.268139
H	0.857691	6.407661	-0.384910
H	-0.465694	5.176258	-2.124219
H	-0.442649	2.649515	-2.089261
H	4.410391	1.868726	4.009084
N	-3.124011	-0.657107	-1.101851
C	-4.907837	-1.309580	-3.061076
C	-4.146267	-2.315702	-2.455517
H	-4.267471	-3.349245	-2.752078
C	-3.246957	-1.953645	-1.448305
C	-3.866093	0.328304	-1.644256
C	-4.780884	0.024354	-2.656921
H	-5.391396	0.795055	-3.108727
C	-2.424274	2.693928	0.721010
N	-2.616415	1.634546	-0.087627
C	-3.633590	1.632461	-1.001370
C	-4.424449	2.767906	-1.183128
C	-4.206010	3.885517	-0.373580
C	-3.205671	3.843691	0.602911
H	-1.654049	2.581383	1.472170
H	-5.235373	2.759202	-1.900028
H	-4.833968	4.762635	-0.479494
H	-3.046861	4.674299	1.279063
C	-2.414015	-2.842649	-0.621339

C	-2.515000	-4.234175	-0.586004
C	-1.786800	-4.944836	0.371426
C	-0.975617	-4.250781	1.275098
C	-0.889437	-2.861822	1.176736
N	-1.567504	-2.187159	0.228894
H	-3.194823	-4.749136	-1.252524
H	-1.880505	-6.022923	0.433417
H	-0.438144	-4.769402	2.058992
H	-0.306267	-2.258127	1.859151
H	-5.615268	-1.568437	-3.840125

AFD-TS2 E(I) = -2501.37358495 / E(II) = -2501.89084006

Mn	-1.298474	0.072335	-0.387753
Mn	1.395482	0.814942	-0.014873
O	-2.608512	0.433114	-1.593939
O	0.193976	-0.228225	0.811442
O	2.791719	0.545777	1.235814
O	-0.032463	1.097484	-1.179224
H	3.612882	0.103273	0.944411
C	2.427704	-0.810642	3.138918
H	2.893986	0.004967	3.676484
H	1.387993	-0.706488	2.856292
C	3.099921	-2.046076	2.973717
C	2.434986	-3.167490	2.389007
C	3.087495	-4.387378	2.242680
C	4.421403	-4.533178	2.662338
C	5.098138	-3.442708	3.235895
C	4.454084	-2.219804	3.391671
H	1.398082	-3.053494	2.084987
H	2.562087	-5.236441	1.816187
H	4.924920	-5.487754	2.552773
H	6.124908	-3.558950	3.566815
H	4.975080	-1.382369	3.846674
S	-4.237926	-0.122478	-1.643037
O	-4.091728	-1.625786	-1.704116
O	-4.812906	0.367433	-0.334094
O	-4.753911	0.536572	-2.873830
N	2.454306	2.052847	-1.170474
C	3.563309	3.792895	-2.982229
C	3.629680	2.414085	-3.213187
H	4.109442	2.032843	-4.105828
C	3.053974	1.547507	-2.276758
C	2.376629	3.383732	-0.926236
C	2.936525	4.290290	-1.830675
H	2.880844	5.357642	-1.658190
C	0.579550	2.707746	2.175510

N	1.139293	2.594383	0.955608
C	1.693462	3.686305	0.339662
C	1.641655	4.943558	0.949119
C	1.047681	5.069719	2.208127
C	0.519442	3.936193	2.836036
H	0.184133	1.794692	2.598680
H	2.079566	5.805482	0.461218
H	1.010961	6.036596	2.696645
H	0.068567	3.998121	3.818483
C	3.028628	0.081514	-2.306373
C	3.695094	-0.725025	-3.234367
C	3.668171	-2.113700	-3.082284
C	2.976877	-2.674280	-2.000273
C	2.307343	-1.831115	-1.114064
N	2.326604	-0.488433	-1.268300
H	4.244290	-0.274443	-4.051845
H	4.189924	-2.747704	-3.789737
H	2.954927	-3.745059	-1.842316
H	1.750735	-2.198681	-0.263566
H	3.994771	4.480607	-3.699575
N	-2.372319	-1.140422	0.788539
C	-3.664272	-2.813792	2.513904
C	-3.696643	-1.432234	2.735396
H	-4.240227	-1.024322	3.577460
C	-3.035812	-0.597595	1.828733
C	-2.355824	-2.462819	0.528676
C	-2.999217	-3.344672	1.402601
H	-3.005898	-4.410712	1.217004
C	-0.615145	-1.812205	-2.605215
N	-1.081797	-1.715315	-1.345775
C	-1.688195	-2.783145	-0.744667
C	-1.741426	-4.021108	-1.386889
C	-1.225987	-4.139006	-2.680214
C	-0.670935	-3.017895	-3.305353
H	-0.226965	-0.899354	-3.037192
H	-2.233809	-4.861159	-0.913963
H	-1.292105	-5.084543	-3.206071
H	-0.309633	-3.065372	-4.324915
C	-3.020934	0.874968	1.805238
C	-3.822190	1.697514	2.598502
C	-3.848548	3.071116	2.343624
C	-3.077156	3.593286	1.300385
C	-2.269854	2.729912	0.559138
N	-2.221754	1.412736	0.834995
H	-4.462270	1.267770	3.358292
H	-4.492203	3.718573	2.927915

H	-3.115476	4.645082	1.046311
H	-1.668571	3.058943	-0.277945
H	-4.176752	-3.478394	3.199609

AFD-3 E(I) = -2501.41326391 / E(II) = -2501.93507044

Mn	-1.373992	0.058193	-0.316312
Mn	1.367411	0.658382	-0.214883
O	-2.742178	0.436262	-1.468698
O	0.158890	-0.249805	0.795639
O	2.849546	0.188542	1.184694
O	-0.106592	0.947704	-1.272199
H	3.798314	0.202405	0.958846
C	2.609077	-0.355617	2.565972
H	2.819061	0.459165	3.265620
H	1.542806	-0.581587	2.543927
C	3.465063	-1.558794	2.832375
C	2.966375	-2.854205	2.607447
C	3.773907	-3.972918	2.832835
C	5.090826	-3.808122	3.281507
C	5.595910	-2.522933	3.513386
C	4.785214	-1.404456	3.293991
H	1.938973	-2.977557	2.276554
H	3.377599	-4.969992	2.670894
H	5.715683	-4.676537	3.461269
H	6.610317	-2.394564	3.875700
H	5.171786	-0.409326	3.502168
S	-4.391011	-0.019877	-1.395431
O	-4.341428	-1.531850	-1.378310
O	-4.864536	0.571770	-0.086026
O	-4.948768	0.599876	-2.629685
N	2.482318	1.707240	-1.445056
C	3.630547	3.233690	-3.446863
C	3.587188	1.840983	-3.568226
H	3.992562	1.357623	-4.448451
C	2.997722	1.087831	-2.547036
C	2.512186	3.066351	-1.316783
C	3.090634	3.855924	-2.311592
H	3.112408	4.934802	-2.220801
C	0.781844	2.780228	1.877208
N	1.315373	2.517491	0.664964
C	1.899022	3.521867	-0.065842
C	1.919792	4.834016	0.421897
C	1.365945	5.107288	1.674287
C	0.797519	4.065466	2.418848
H	0.332650	1.936995	2.384415
H	2.376233	5.625214	-0.159785

H	1.383417	6.117389	2.067220
H	0.366887	4.245079	3.395961
C	2.859864	-0.364375	-2.477797
C	3.423515	-1.283749	-3.372268
C	3.287917	-2.649963	-3.127102
C	2.591201	-3.078689	-1.987419
C	2.029819	-2.127456	-1.139334
N	2.153885	-0.800947	-1.379359
H	3.974796	-0.933591	-4.236229
H	3.726473	-3.371273	-3.806902
H	2.480329	-4.132106	-1.763112
H	1.465589	-2.392561	-0.256488
H	4.073748	3.832820	-4.232851
N	-2.456239	-1.028199	0.979755
C	-3.735187	-2.531210	2.864609
C	-3.676273	-1.140611	3.011630
H	-4.144829	-0.658044	3.859340
C	-3.025621	-0.394497	2.023659
C	-2.531701	-2.360259	0.791060
C	-3.170343	-3.156580	1.747089
H	-3.249864	-4.228263	1.619676
C	-0.944216	-1.980228	-2.465999
N	-1.324692	-1.792501	-1.188234
C	-1.962883	-2.785824	-0.499688
C	-2.134806	-4.047120	-1.072721
C	-1.707436	-4.261297	-2.385498
C	-1.120730	-3.211244	-3.098921
H	-0.525357	-1.116253	-2.965172
H	-2.652051	-4.827821	-0.529774
H	-1.866556	-5.224270	-2.857082
H	-0.826397	-3.331521	-4.133937
C	-2.936298	1.072241	1.916908
C	-3.657695	1.975280	2.699761
C	-3.635284	3.332082	2.368026
C	-2.895860	3.757895	1.259931
C	-2.166375	2.816813	0.532775
N	-2.161614	1.516004	0.881645
H	-4.279144	1.619203	3.511416
H	-4.219617	4.040678	2.943735
H	-2.901345	4.794150	0.946037
H	-1.596508	3.071140	-0.351099
H	-4.242250	-3.128225	3.613698

FS-1 E(I) = -2501.36362805 / E(II) = -2501.87524195

Mn	-1.725696	-0.197230	0.224420
Mn	0.846500	0.666601	-0.550405

O	-2.670803	-0.396202	1.743631
O	-0.591599	0.072206	-1.380275
O	1.921755	0.952059	-1.971927
O	-0.220447	0.418901	1.012023
H	4.484163	1.088010	-2.074240
C	5.581232	1.155177	-2.094550
H	5.881261	1.125203	-3.147911
H	5.863861	2.135611	-1.696268
C	6.232007	0.037332	-1.308671
C	6.745427	0.257786	-0.017575
C	7.355795	-0.776157	0.705629
C	7.465452	-2.055424	0.146400
C	6.960363	-2.289057	-1.140086
C	6.350280	-1.253819	-1.857005
H	6.694302	1.255688	0.410401
H	7.773854	-0.575171	1.687960
H	7.962905	-2.850827	0.692475
H	7.063984	-3.270207	-1.593738
H	5.979520	-1.439714	-2.861306
S	-4.300094	-0.957286	1.964877
O	-5.110569	0.028271	1.159227
O	-4.266689	-2.342755	1.367384
O	-4.442966	-0.878641	3.443320
N	2.265212	1.281875	0.747409
C	3.853896	2.004707	2.845372
C	3.029692	2.961988	2.239266
H	3.011613	3.980100	2.606371
C	2.224954	2.563627	1.166330
C	3.044125	0.337487	1.312041
C	3.874496	0.682654	2.385382
H	4.511892	-0.053169	2.857293
C	1.692681	-2.175648	-0.969718
N	1.876087	-1.060816	-0.238297
C	2.898718	-0.982590	0.671265
C	3.746601	-2.070710	0.878781
C	3.549719	-3.239522	0.134758
C	2.515442	-3.292865	-0.802799
H	0.882737	-2.142968	-1.685925
H	4.581260	-1.993318	1.562936
H	4.214000	-4.084221	0.271718
H	2.350782	-4.175466	-1.407950
C	1.303530	3.396281	0.369131
C	1.230493	4.789732	0.421915
C	0.390543	5.463457	-0.472419
C	-0.351476	4.731336	-1.403578
C	-0.254559	3.336995	-1.402001

N	0.539812	2.695039	-0.525519
H	1.836751	5.344088	1.127487
H	0.332917	6.545575	-0.451588
H	-0.991654	5.224938	-2.123781
H	-0.797778	2.708902	-2.095355
H	4.478801	2.290191	3.683449
N	-3.129624	-0.830609	-1.053575
C	-4.884266	-1.652788	-2.975481
C	-4.036076	-2.585805	-2.367968
H	-4.078271	-3.630052	-2.648445
C	-3.153632	-2.138014	-1.380340
C	-3.954709	0.084557	-1.599519
C	-4.857472	-0.306719	-2.592753
H	-5.533375	0.406037	-3.046704
C	-2.659652	2.594565	0.701358
N	-2.782055	1.511660	-0.089913
C	-3.814725	1.413463	-0.981046
C	-4.697962	2.478910	-1.160548
C	-4.554029	3.622229	-0.370148
C	-3.533999	3.675552	0.585259
H	-1.866880	2.554408	1.436513
H	-5.520539	2.394513	-1.859014
H	-5.253119	4.444066	-0.473605
H	-3.429765	4.525787	1.247471
C	-2.239818	-2.944970	-0.554611
C	-2.234405	-4.339021	-0.490621
C	-1.438651	-4.972594	0.467471
C	-0.667010	-4.200936	1.342472
C	-0.686769	-2.811751	1.215071
N	-1.430556	-2.210095	0.266929
H	-2.884603	-4.917720	-1.134067
H	-1.449658	-6.053108	0.552437
H	-0.078520	-4.661262	2.126087
H	-0.137753	-2.151442	1.873185
H	-5.580268	-1.978927	-3.739399

FS-TS1 E(I) = -2501.35265082 / E(II) = -2501.86483499

Mn	1.691145	-0.062090	-0.150016
Mn	-1.122664	0.220055	-0.146792
O	3.057488	-0.057096	-1.340212
O	0.152705	-0.052284	1.061708
O	-2.484330	0.199382	1.039530
O	0.377028	0.211832	-1.350680
H	-3.756307	0.429497	0.692665
C	-4.939830	0.687257	0.423156
H	-4.950526	1.780850	0.411391

H	-5.096462	0.270604	-0.575496
C	-5.770705	0.078531	1.475354
C	-6.321974	-1.213666	1.310675
C	-7.089124	-1.797454	2.318458
C	-7.316811	-1.106991	3.517997
C	-6.772229	0.172614	3.701067
C	-6.006683	0.758148	2.693472
H	-6.153085	-1.747470	0.379368
H	-7.515237	-2.784691	2.172490
H	-7.914508	-1.560714	4.301433
H	-6.949124	0.709212	4.627250
H	-5.584692	1.748312	2.838029
S	4.749849	-0.254953	-1.069246
O	5.086118	0.880429	-0.130981
O	4.840080	-1.616019	-0.419640
O	5.296334	-0.149473	-2.449865
N	-2.178574	0.540689	-1.853285
C	-3.050083	0.949562	-4.411435
C	-2.709173	2.047853	-3.611780
H	-2.776197	3.053712	-4.006270
C	-2.257684	1.807950	-2.308776
C	-2.483242	-0.536224	-2.606226
C	-2.939986	-0.356405	-3.917403
H	-3.184353	-1.202071	-4.547489
C	-1.498776	-2.741312	0.134978
N	-1.650601	-1.681036	-0.679605
C	-2.281431	-1.810018	-1.887785
C	-2.735349	-3.058329	-2.318971
C	-2.561219	-4.171184	-1.487538
C	-1.947299	-4.010734	-0.241968
H	-1.019836	-2.541045	1.084079
H	-3.237085	-3.160142	-3.273410
H	-2.915903	-5.145191	-1.804427
H	-1.818435	-4.848317	0.431869
C	-1.833337	2.802220	-1.303223
C	-2.031988	4.181345	-1.399055
C	-1.662153	4.999170	-0.324653
C	-1.110529	4.421422	0.822700
C	-0.920422	3.036989	0.861047
N	-1.261420	2.260004	-0.183784
H	-2.488500	4.609958	-2.282718
H	-1.818714	6.070305	-0.379961
H	-0.833185	5.026030	1.676998
H	-0.502936	2.520363	1.715130
H	-3.389978	1.111438	-5.427622
N	2.794252	-0.365630	1.493941

C	4.096335	-0.774334	3.856646
C	3.657059	-1.873246	3.109383
H	3.839138	-2.881507	3.457450
C	3.000915	-1.633859	1.898180
C	3.231447	0.710171	2.176594
C	3.893715	0.531329	3.394848
H	4.258670	1.376994	3.962776
C	2.097070	2.869750	-0.530775
N	2.234376	1.840040	0.326146
C	2.985959	1.973501	1.460586
C	3.539160	3.208953	1.801073
C	3.370250	4.291899	0.934814
C	2.655147	4.118146	-0.254756
H	1.556502	2.653967	-1.442693
H	4.142636	3.309256	2.694019
H	3.823108	5.248587	1.168569
H	2.551056	4.924896	-0.969399
C	2.534083	-2.625529	0.914706
C	2.833623	-3.988382	0.946488
C	2.479406	-4.788438	-0.142548
C	1.836183	-4.210288	-1.241864
C	1.534058	-2.848769	-1.208361
N	1.847375	-2.091147	-0.139965
H	3.387487	-4.406040	1.777382
H	2.735963	-5.841570	-0.147661
H	1.594560	-4.794125	-2.121161
H	1.065733	-2.328847	-2.033423
H	4.613036	-0.936595	4.795319

FS-2 E(I) = -2501.37776818 / E(II) = -2501.89743483

Mn	-1.699031	-0.155563	0.215759
Mn	0.948981	0.506171	-0.471203
O	-2.698086	-0.305457	1.714496
O	-0.520864	0.041742	-1.338819
O	2.039789	0.691399	-1.948522
O	-0.166341	0.319526	1.053269
H	3.007445	0.828545	-1.847207
C	5.310078	1.240580	-2.276966
H	4.904203	1.074097	-3.269434
H	5.307981	2.259013	-1.901534
C	5.948179	0.201002	-1.562302
C	6.559496	0.437084	-0.289463
C	7.205605	-0.585312	0.397044
C	7.269500	-1.880481	-0.148622
C	6.673997	-2.139868	-1.396574
C	6.023882	-1.126763	-2.092233

H	6.535695	1.441726	0.123564
H	7.685226	-0.377233	1.348723
H	7.795069	-2.669203	0.379622
H	6.737819	-3.133714	-1.828410
H	5.579592	-1.327945	-3.062459
S	-4.365786	-0.731595	1.885838
O	-5.075127	0.333082	1.083647
O	-4.435617	-2.103718	1.258494
O	-4.545651	-0.673362	3.361869
N	2.367728	1.011466	0.897312
C	3.830338	1.601032	3.128398
C	3.130633	2.620591	2.469736
H	3.154801	3.634341	2.848793
C	2.384027	2.288025	1.333504
C	3.019708	0.008084	1.518825
C	3.784004	0.282384	2.659239
H	4.314010	-0.503761	3.181154
C	1.654478	-2.377238	-0.888527
N	1.867146	-1.287729	-0.127498
C	2.816386	-1.297181	0.859883
C	3.547710	-2.455826	1.126754
C	3.314301	-3.601103	0.356814
C	2.365638	-3.560388	-0.668728
H	0.913957	-2.268793	-1.669857
H	4.310641	-2.457418	1.894541
H	3.881465	-4.505177	0.545532
H	2.179256	-4.423568	-1.295260
C	1.571061	3.187828	0.491030
C	1.598803	4.583199	0.542815
C	0.856627	5.315018	-0.391801
C	0.112982	4.637851	-1.362720
C	0.107780	3.239951	-1.360759
N	0.804961	2.544475	-0.443553
H	2.207413	5.092632	1.279739
H	0.875960	6.398553	-0.370582
H	-0.450949	5.176519	-2.113759
H	-0.437209	2.648935	-2.084728
H	4.404360	1.833710	4.017703
N	-3.122554	-0.648795	-1.099690
C	-4.901441	-1.292567	-3.066167
C	-4.144269	-2.301858	-2.460338
H	-4.266705	-3.334444	-2.759749
C	-3.246991	-1.944051	-1.449811
C	-3.858848	0.339848	-1.643697
C	-4.771419	0.040381	-2.659698
H	-5.377434	0.813865	-3.112823

C	-2.408462	2.699036	0.723147
N	-2.604583	1.640910	-0.086355
C	-3.621926	1.642774	-0.999940
C	-4.408804	2.781157	-1.180737
C	-4.186376	3.897341	-0.370316
C	-3.186009	3.851438	0.606069
H	-1.638225	2.582811	1.473845
H	-5.219938	2.775726	-1.897435
H	-4.811451	4.776623	-0.475362
H	-3.024471	4.680959	1.282904
C	-2.416383	-2.836298	-0.624018
C	-2.521309	-4.227569	-0.589409
C	-1.794596	-4.940799	0.367252
C	-0.980738	-4.249694	1.270897
C	-0.890347	-2.861019	1.173237
N	-1.567235	-2.184009	0.226072
H	-3.203174	-4.740151	-1.255678
H	-1.891588	-6.018620	0.428841
H	-0.444531	-4.770422	2.054258
H	-0.305009	-2.258705	1.855153
H	-5.607218	-1.548031	-3.847827

AFD2-1 E(I) = -2501.36666666 / E(II) = -2501.87827942

Mn	-1.728467	-0.197604	0.220189
Mn	0.848858	0.670871	-0.548555
O	-2.670534	-0.393467	1.743940
O	-0.594192	0.072862	-1.367732
O	1.914213	0.953516	-1.980363
O	-0.223517	0.420939	0.993078
H	4.471092	0.979446	-2.175923
C	5.558234	1.124364	-2.107013
H	5.940934	1.160019	-3.133547
H	5.738689	2.104432	-1.652607
C	6.225398	0.021370	-1.313679
C	6.738703	0.256767	-0.025585
C	7.363978	-0.764723	0.703135
C	7.488383	-2.045938	0.152188
C	6.983754	-2.294423	-1.131972
C	6.359055	-1.272013	-1.854089
H	6.674515	1.256607	0.396066
H	7.780762	-0.552193	1.683579
H	7.995798	-2.831872	0.702745
H	7.098120	-3.277536	-1.578841
H	5.987479	-1.469585	-2.855924
S	-4.297061	-0.956186	1.968925
O	-5.112026	0.024721	1.161832

O	-4.263854	-2.343855	1.376113
O	-4.437690	-0.873053	3.447640
N	2.266421	1.287411	0.748689
C	3.859517	2.012676	2.842733
C	3.033590	2.969160	2.237643
H	3.016087	3.987598	2.603858
C	2.227179	2.569733	1.166381
C	3.048656	0.344347	1.311137
C	3.880977	0.690683	2.382629
H	4.521013	-0.044063	2.852612
C	1.700964	-2.169974	-0.971340
N	1.883144	-1.054465	-0.240534
C	2.905599	-0.975404	0.669225
C	3.755031	-2.062375	0.876607
C	3.559746	-3.231445	0.132613
C	2.525204	-3.286137	-0.804518
H	0.890531	-2.139365	-1.687019
H	4.589135	-1.984272	1.561384
H	4.225125	-4.075279	0.269546
H	2.361220	-4.169099	-1.409335
C	1.306364	3.402197	0.368165
C	1.231213	4.795456	0.422265
C	0.391640	5.468785	-0.472770
C	-0.347376	4.736417	-1.406078
C	-0.247915	3.342197	-1.406035
N	0.545691	2.700520	-0.528700
H	1.835144	5.350053	1.129645
H	0.331983	6.550764	-0.450712
H	-0.987202	5.229696	-2.126816
H	-0.788692	2.714397	-2.101471
H	4.485788	2.298971	3.679519
N	-3.133188	-0.835368	-1.053815
C	-4.894179	-1.665166	-2.966563
C	-4.043330	-2.595648	-2.358897
H	-4.086206	-3.640895	-2.635480
C	-3.157925	-2.144092	-1.375620
C	-3.962055	0.077173	-1.598665
C	-4.867771	-0.318009	-2.587657
H	-5.546629	0.392437	-3.040793
C	-2.669978	2.593584	0.696781
N	-2.790814	1.508851	-0.092026
C	-3.823553	1.407444	-0.982699
C	-4.708517	2.471120	-1.164099
C	-4.566025	3.616416	-0.376330
C	-3.545775	3.673229	0.578532
H	-1.877444	2.556689	1.432237

H	-5.531142	2.384071	-1.862179
H	-5.266238	4.437080	-0.481466
H	-3.442301	4.525114	1.238745
C	-2.242644	-2.948322	-0.548795
C	-2.235767	-4.342257	-0.482629
C	-1.438793	-4.973604	0.475889
C	-0.667580	-4.199741	1.349208
C	-0.689120	-2.810731	1.219708
N	-1.433835	-2.211141	0.271138
H	-2.885599	-4.922641	-1.124922
H	-1.448425	-6.054008	0.562362
H	-0.077923	-4.658135	2.133082
H	-0.140343	-2.149514	1.876956
H	-5.592478	-1.994266	-3.727116

AFD2-TS1 E(I) = -2501.35132450 / E(II) = -2501.86311689

Mn	-1.079454	0.298996	-0.108338
Mn	1.713731	-0.077808	-0.167113
O	3.055251	-0.072469	-1.378664
O	0.173991	-0.051495	1.069585
O	-2.460627	0.305075	1.119028
O	0.391942	0.283125	-1.327363
H	-3.789830	0.563439	0.800158
C	-4.943309	0.864404	0.571523
H	-4.952012	1.944104	0.749117
H	-5.099035	0.637103	-0.487229
C	-5.815757	0.097215	1.483344
C	-6.407249	-1.119312	1.072413
C	-7.216469	-1.851101	1.941766
C	-7.446118	-1.387555	3.245396
C	-6.861201	-0.186137	3.672066
C	-6.054169	0.547054	2.802700
H	-6.237367	-1.475465	0.059842
H	-7.674473	-2.776351	1.607377
H	-8.076796	-1.955363	3.921288
H	-7.039454	0.175384	4.679353
H	-5.600316	1.475738	3.135387
S	4.748477	-0.338388	-1.134256
O	5.135139	0.748811	-0.161001
O	4.800880	-1.725061	-0.539810
O	5.270085	-0.196602	-2.521593
N	-2.185790	0.695415	-1.763341
C	-3.163515	1.198053	-4.266795
C	-2.752249	2.263944	-3.456533
H	-2.807824	3.281597	-3.821397
C	-2.248481	1.976188	-2.182547

C	-2.561025	-0.351059	-2.527614
C	-3.072175	-0.123161	-3.810980
H	-3.373340	-0.944144	-4.449108
C	-1.544459	-2.653853	0.118847
N	-1.687384	-1.568784	-0.664916
C	-2.372737	-1.647591	-1.847965
C	-2.890430	-2.868250	-2.286959
C	-2.724995	-4.005938	-1.488586
C	-2.056106	-3.896326	-0.265932
H	-1.021831	-2.494141	1.052219
H	-3.434717	-2.928489	-3.221412
H	-3.129088	-4.958556	-1.811230
H	-1.933401	-4.752815	0.384918
C	-1.755995	2.930438	-1.169907
C	-1.920332	4.316470	-1.223613
C	-1.491777	5.096302	-0.143291
C	-0.918593	4.473518	0.969397
C	-0.765028	3.084307	0.965596
N	-1.159853	2.342586	-0.086351
H	-2.395955	4.779411	-2.079441
H	-1.620812	6.172259	-0.166008
H	-0.597696	5.047315	1.829696
H	-0.336308	2.536137	1.793764
H	-3.545369	1.396951	-5.261291
N	2.819541	-0.487715	1.451430
C	4.119932	-1.037616	3.786397
C	3.637544	-2.089218	2.998726
H	3.785212	-3.116491	3.304998
C	2.982894	-1.778059	1.803144
C	3.298939	0.543597	2.173810
C	3.961452	0.292011	3.379008
H	4.359255	1.100364	3.978377
C	2.233035	2.850269	-0.438211
N	2.334993	1.782811	0.376138
C	3.096366	1.842836	1.510557
C	3.698024	3.041555	1.896105
C	3.566930	4.163840	1.074170
C	2.840098	4.064638	-0.116595
H	1.679288	2.693321	-1.354072
H	4.308774	3.083272	2.788777
H	4.057017	5.092601	1.342743
H	2.762788	4.902455	-0.798081
C	2.472617	-2.712199	0.785385
C	2.721408	-4.085209	0.760410
C	2.326466	-4.827962	-0.355211
C	1.694097	-4.183511	-1.423343

C	1.443782	-2.813905	-1.333409
N	1.796893	-2.111255	-0.240256
H	3.266520	-4.555934	1.568432
H	2.542785	-5.888959	-0.404200
H	1.420509	-4.723017	-2.321358
H	0.984757	-2.245869	-2.131504
H	4.635576	-1.255863	4.714235

AFD2-2 E(I) = -2501.38063521 / E(II) = -2501.90058814

Mn	0.974645	0.363570	-0.495229
Mn	-1.715688	-0.106892	0.209010
O	-2.698611	-0.220609	1.723418
O	-0.543759	0.042253	-1.341729
O	2.046440	0.502351	-1.990717
O	-0.138193	0.222939	1.023459
H	3.008917	0.683352	-1.914615
C	5.266443	1.095031	-2.538057
H	4.814246	0.715999	-3.448732
H	5.275024	2.170933	-2.396015
C	5.937999	0.234769	-1.639532
C	6.608606	0.742937	-0.481358
C	7.282562	-0.107285	0.388295
C	7.317221	-1.492828	0.146360
C	6.664719	-2.018261	-0.983846
C	5.986427	-1.178900	-1.860767
H	6.604801	1.814687	-0.303674
H	7.803701	0.302684	1.247949
H	7.863905	-2.149290	0.815377
H	6.707666	-3.084382	-1.184097
H	5.498172	-1.586209	-2.741154
S	-4.389961	-0.526360	1.911050
O	-5.031512	0.609894	1.150762
O	-4.572796	-1.871007	1.247698
O	-4.542478	-0.497258	3.391270
N	2.445681	0.702475	0.866323
C	3.982803	1.091039	3.091552
C	3.361558	2.187036	2.479236
H	3.475061	3.181543	2.891595
C	2.574721	1.957150	1.344784
C	3.020989	-0.372275	1.442991
C	3.820654	-0.201953	2.579138
H	4.291278	-1.046545	3.065345
C	1.433899	-2.552213	-1.021343
N	1.744797	-1.510684	-0.227525
C	2.700742	-1.632807	0.745187
C	3.332897	-2.857966	0.966323
C	2.994202	-3.953878	0.164483

C	2.044083	-3.797995	-0.848947
H	0.696849	-2.356592	-1.788623
H	4.097564	-2.949756	1.727249
H	3.480911	-4.909932	0.319354
H	1.778354	-4.621093	-1.500320
C	1.828223	2.949945	0.546348
C	1.967657	4.335736	0.649205
C	1.275883	5.159076	-0.247122
C	0.469483	4.580307	-1.231535
C	0.352553	3.188158	-1.280880
N	1.002872	2.404841	-0.400585
H	2.622871	4.766851	1.396100
H	1.381568	6.236103	-0.186063
H	-0.058856	5.190030	-1.953583
H	-0.247671	2.670680	-2.017154
H	4.586604	1.244225	3.978324
N	-3.192481	-0.448398	-1.095040
C	-5.051464	-0.894789	-3.042262
C	-4.364352	-1.976890	-2.480150
H	-4.572983	-2.987713	-2.805057
C	-3.424099	-1.719498	-1.478182
C	-3.860965	0.609510	-1.594768
C	-4.811937	0.411467	-2.600433
H	-5.365322	1.242106	-3.018351
C	-2.196888	2.778165	0.813000
N	-2.486665	1.762732	-0.022476
C	-3.514829	1.870214	-0.917418
C	-4.214302	3.070379	-1.051207
C	-3.894201	4.141452	-0.213110
C	-2.885064	3.989847	0.743286
H	-1.425461	2.581590	1.545384
H	-5.034302	3.148888	-1.753419
H	-4.451227	5.068754	-0.281832
H	-2.648937	4.783972	1.440374
C	-2.655122	-2.697712	-0.690983
C	-2.869675	-4.076781	-0.693327
C	-2.192858	-4.871934	0.234976
C	-1.317988	-4.273215	1.147320
C	-1.117426	-2.894035	1.085362
N	-1.747531	-2.139091	0.165412
H	-3.596711	-4.515029	-1.364856
H	-2.374919	-5.939940	0.268515
H	-0.817533	-4.856412	1.910046
H	-0.477650	-2.360321	1.775260
H	-5.788827	-1.072019	-3.816386

FO-1 E(I) = -2501.35656924 / E(II) = -2501.86657123

Mn	-1.776156	-0.083905	0.256782
Mn	0.885996	0.280907	-0.533644
O	-2.706883	-0.197447	1.785703
O	-0.622346	0.060422	-1.389768
O	1.878806	0.393483	-2.131601
O	-0.163085	0.148766	1.039525
H	4.224825	0.469773	-2.443343
C	5.310349	0.561984	-2.592434
H	5.550260	0.015354	-3.511987
H	5.532897	1.619499	-2.767135
C	6.094166	0.023649	-1.415703
C	6.794111	0.883402	-0.550371
C	7.531402	0.380881	0.529495
C	7.582849	-0.997894	0.766182
C	6.892112	-1.868325	-0.088226
C	6.155967	-1.361414	-1.165408
H	6.781368	1.953019	-0.741770
H	8.084491	1.062639	1.168758
H	8.175059	-1.391050	1.586596
H	6.954338	-2.942002	0.066192
H	5.645051	-2.044333	-1.839269
S	-4.423576	-0.434898	2.008710
O	-5.023592	0.754780	1.302654
O	-4.677338	-1.746560	1.309121
O	-4.519764	-0.444886	3.492572
N	2.504260	0.536006	0.642946
C	4.399086	0.843715	2.586942
C	3.739808	1.969650	2.078485
H	3.971818	2.957098	2.456365
C	2.775009	1.782688	1.082954
C	3.119236	-0.566499	1.120023
C	4.096973	-0.437928	2.112180
H	4.616572	-1.301478	2.503994
C	1.137643	-2.652069	-1.129814
N	1.583743	-1.632458	-0.371230
C	2.651561	-1.804711	0.469206
C	3.257109	-3.056366	0.597836
C	2.779290	-4.127281	-0.165335
C	1.717108	-3.920813	-1.050369
H	0.320366	-2.419656	-1.799100
H	4.109624	-3.185096	1.251979
H	3.245484	-5.102386	-0.083595
H	1.343431	-4.722261	-1.675109
C	1.985275	2.815367	0.385704
C	2.220236	4.190135	0.457140

C	1.474579	5.053250	-0.353599
C	0.518282	4.523051	-1.224450
C	0.310591	3.141540	-1.243757
N	1.014568	2.318593	-0.443267
H	2.990180	4.580701	1.110803
H	1.654314	6.121529	-0.318049
H	-0.054894	5.161949	-1.884350
H	-0.405273	2.662948	-1.898266
H	5.151707	0.965046	3.356546
N	-3.294987	-0.305843	-1.024531
C	-5.201352	-0.588177	-2.956420
C	-4.557354	-1.722511	-2.448523
H	-4.816842	-2.708773	-2.810256
C	-3.590979	-1.548976	-1.453425
C	-3.917878	0.801682	-1.474307
C	-4.893051	0.687475	-2.469498
H	-5.411692	1.558810	-2.847257
C	-2.084872	2.793847	0.964715
N	-2.450192	1.826869	0.101308
C	-3.494553	2.018285	-0.760704
C	-4.135459	3.255758	-0.830324
C	-3.739055	4.276555	0.038225
C	-2.713197	4.039645	0.958880
H	-1.301695	2.530996	1.663520
H	-4.968344	3.402537	-1.505895
H	-4.250226	5.232183	0.019760
H	-2.418123	4.794700	1.676548
C	-2.856619	-2.591670	-0.717240
C	-3.141417	-3.956922	-0.760183
C	-2.491241	-4.815443	0.130651
C	-1.572112	-4.292541	1.045990
C	-1.300372	-2.924157	1.024044
N	-1.906434	-2.108675	0.139785
H	-3.900787	-4.335636	-1.432179
H	-2.727497	-5.873285	0.133413
H	-1.089905	-4.925120	1.780530
H	-0.620104	-2.447227	1.717049
H	-5.957657	-0.700235	-3.724392

FO-TS1 E(I) = -2501.34864248 / E(II) = -2501.85952299

Mn	1.711942	-0.079857	-0.165556
Mn	-1.076828	0.301890	-0.100347
O	3.044562	-0.075125	-1.381236
O	0.170762	-0.051727	1.082576
O	-2.459913	0.309981	1.126801
O	0.391469	0.285562	-1.336332

H	-3.785600	0.563599	0.796435
C	-4.939364	0.861187	0.561314
H	-4.950653	1.941423	0.735425
H	-5.089968	0.629984	-0.497263
C	-5.813335	0.094862	1.472319
C	-6.400964	-1.123933	1.062666
C	-7.211744	-1.854925	1.931254
C	-7.446754	-1.388227	3.232783
C	-6.865692	-0.184501	3.658155
C	-6.057120	0.547921	2.789544
H	-6.226922	-1.482523	0.051656
H	-7.666787	-2.781988	1.597856
H	-8.078622	-1.955418	3.908081
H	-7.048087	0.179410	4.663833
H	-5.606192	1.478379	3.121239
S	4.741369	-0.344238	-1.143594
O	5.129366	0.742067	-0.169680
O	4.790008	-1.731350	-0.549596
O	5.261934	-0.202791	-2.530455
N	-2.184152	0.703343	-1.756147
C	-3.151869	1.210771	-4.262499
C	-2.740068	2.274801	-3.450066
H	-2.790999	3.292873	-3.814471
C	-2.241043	1.984438	-2.174799
C	-2.558316	-0.341432	-2.523066
C	-3.064793	-0.111149	-3.807844
H	-3.364997	-0.930830	-4.448111
C	-1.546555	-2.650040	0.120652
N	-1.687219	-1.563719	-0.661857
C	-2.372385	-1.639308	-1.845218
C	-2.892042	-2.858515	-2.286027
C	-2.729059	-3.997552	-1.489072
C	-2.060503	-3.890952	-0.265918
H	-1.023935	-2.492070	1.054399
H	-3.436179	-2.916448	-3.220714
H	-3.134947	-4.948937	-1.813120
H	-1.939901	-4.748539	0.383874
C	-1.746002	2.936168	-1.160976
C	-1.907178	4.322677	-1.212637
C	-1.476644	5.100009	-0.131307
C	-0.904486	4.474511	0.980440
C	-0.753794	3.085051	0.974596
N	-1.150588	2.345780	-0.078389
H	-2.382203	4.787822	-2.067603
H	-1.603530	6.176262	-0.152423
H	-0.582343	5.046449	1.841508

H	-0.326126	2.534317	1.801693
H	-3.530020	1.411571	-5.258023
N	2.820188	-0.492840	1.450291
C	4.122822	-1.046524	3.783076
C	3.636884	-2.096744	2.995723
H	3.782511	-3.124491	3.301398
C	2.980867	-1.783640	1.801426
C	3.301877	0.537178	2.172926
C	3.965885	0.283658	3.376873
H	4.365591	1.091009	3.976336
C	2.230270	2.846243	-0.434406
N	2.333440	1.778593	0.379671
C	3.098802	1.837137	1.511448
C	3.703325	3.034943	1.895321
C	3.571008	4.157530	1.073983
C	2.840177	4.059585	-0.114493
H	1.673332	2.689425	-1.348407
H	4.317182	3.075581	2.785911
H	4.063355	5.085532	1.341044
H	2.762139	4.897591	-0.795657
C	2.465397	-2.715858	0.784653
C	2.711481	-4.089291	0.756908
C	2.311783	-4.829494	-0.358729
C	1.677562	-4.182192	-1.424099
C	1.429911	-2.812328	-1.331395
N	1.787469	-2.112266	-0.237939
H	3.258267	-4.562235	1.562504
H	2.526074	-5.890792	-0.410077
H	1.400741	-4.719791	-2.322261
H	0.969977	-2.241441	-2.126999
H	4.639578	-1.266287	4.709934

FO-2 E(I) = -2501.37780350 / E(II) = -2501.89758179

Mn	-1.697705	-0.154124	0.215536
Mn	0.952192	0.503896	-0.466878
O	-2.699615	-0.301937	1.712503
O	-0.516194	0.041250	-1.337056
O	2.047912	0.688940	-1.941071
O	-0.166042	0.319011	1.055979
H	3.016110	0.819329	-1.837840
C	5.304761	1.242260	-2.295982
H	4.901115	1.074696	-3.289118
H	5.301898	2.261145	-1.921787
C	5.939038	0.203041	-1.577536
C	6.546483	0.440286	-0.302998
C	7.189440	-0.581816	0.386915

C	7.253661	-1.877793	-0.156738
C	6.661674	-2.138402	-1.406150
C	6.014800	-1.125657	-2.105236
H	6.522547	1.445566	0.108478
H	7.666298	-0.372883	1.339792
H	7.776808	-2.666310	0.374214
H	6.725654	-3.132972	-1.836272
H	5.573116	-1.327776	-3.076445
S	-4.368130	-0.726210	1.880894
O	-5.074785	0.338521	1.076420
O	-4.438143	-2.098790	1.254580
O	-4.550830	-0.666525	3.356519
N	2.368900	1.006205	0.905025
C	3.825143	1.591920	3.141424
C	3.128591	2.612888	2.481569
H	3.152596	3.626213	2.861778
C	2.385189	2.282305	1.342679
C	3.017753	0.001496	1.527697
C	3.778760	0.273812	2.670819
H	4.305968	-0.513517	3.193811
C	1.654220	-2.380631	-0.883772
N	1.867071	-1.291651	-0.121991
C	2.814170	-1.303035	0.867453
C	3.542959	-2.463030	1.135534
C	3.309348	-3.607652	0.364717
C	2.362963	-3.565005	-0.662874
H	0.915403	-2.270773	-1.666521
H	4.303876	-2.466239	1.905321
H	3.874493	-4.512786	0.554434
H	2.176455	-4.427692	-1.290047
C	1.575675	3.183826	0.498780
C	1.605300	4.579133	0.551700
C	0.866703	5.312763	-0.384304
C	0.124637	4.637429	-1.357718
C	0.117358	3.239552	-1.356816
N	0.811105	2.542311	-0.438338
H	2.212715	5.087092	1.290625
H	0.887580	6.396253	-0.362208
H	-0.436511	5.177496	-2.109838
H	-0.426660	2.649956	-2.082661
H	4.396576	1.823078	4.032788
N	-3.119284	-0.646613	-1.102406
C	-4.895156	-1.289618	-3.071850
C	-4.140280	-2.299385	-2.463948
H	-4.263318	-3.332024	-2.762933
C	-3.244517	-1.941943	-1.451948

C	-3.853426	0.342519	-1.648424
C	-4.764396	0.043441	-2.665979
H	-5.368673	0.817314	-3.120759
C	-2.404950	2.701598	0.719722
N	-2.600720	1.643169	-0.089455
C	-3.616276	1.645587	-1.005025
C	-4.401542	2.784721	-1.188039
C	-4.179451	3.901166	-0.377879
C	-3.181008	3.854784	0.600441
H	-1.636247	2.585004	1.471932
H	-5.211293	2.779757	-1.906302
H	-4.803354	4.781067	-0.484681
H	-3.019831	4.684565	1.277044
C	-2.416472	-2.834590	-0.624012
C	-2.523030	-4.225721	-0.588711
C	-1.798932	-4.939141	0.369789
C	-0.985995	-4.248368	1.274518
C	-0.893846	-2.859862	1.176124
N	-1.568182	-2.182709	0.227244
H	-3.204220	-4.737972	-1.255924
H	-1.897264	-6.016813	0.431903
H	-0.451863	-4.769196	2.059228
H	-0.309106	-2.257748	1.858722
H	-5.599736	-1.544776	-3.854690

RMn1-1 E(I) = -3899.88284332 / E(II) = -3900.81660239

Mn	-5.093551	-0.873220	0.025354
Mn	-2.920220	0.892798	0.080981
O	-4.659164	1.080301	0.189193
O	-2.631872	2.749877	0.235032
O	-3.292678	-0.958412	-0.083000
N	-0.961454	0.470245	-0.031368
C	1.617900	-0.525060	-0.213843
C	0.891966	-0.171980	-1.374363
H	1.359512	-0.264977	-2.345589
C	-0.404859	0.322791	-1.253008
C	-0.309520	0.137958	1.103544
C	0.987829	-0.364810	1.041396
H	1.508259	-0.663397	1.941540
C	-3.217171	1.166581	3.057725
N	-2.409319	0.767292	2.056516
C	-1.115877	0.395205	2.311864
C	-0.633387	0.364713	3.622105
C	-1.476299	0.751547	4.669497
C	-2.778796	1.171474	4.383967
H	-4.207663	1.486566	2.764156

H	0.390237	0.072640	3.820584
H	-1.111939	0.743392	5.690302
H	-3.446024	1.503883	5.169189
C	-1.297431	0.780792	-2.335506
C	-0.920154	0.963259	-3.667571
C	-1.835710	1.520550	-4.566872
C	-3.104194	1.894138	-4.113633
C	-3.436781	1.674129	-2.774823
N	-2.559773	1.113706	-1.920290
H	0.078977	0.702366	-3.993400
H	-1.552371	1.678522	-5.601102
H	-3.824921	2.353553	-4.778216
H	-4.395190	1.946320	-2.354139
C	2.997919	-1.038004	-0.305389
C	3.407262	-1.832842	-1.395062
C	4.715104	-2.305315	-1.481555
C	5.641516	-1.980287	-0.483139
C	5.248834	-1.197813	0.609373
C	3.940013	-0.733185	0.697311
H	2.693864	-2.118009	-2.161065
H	5.016479	-2.917042	-2.321375
H	5.965168	-0.957330	1.380874
H	3.671202	-0.085868	1.524929
C	8.998522	-3.621798	0.446412
C	7.533150	-3.191878	0.516679
N	7.011257	-2.439248	-0.578495
C	7.743784	-2.105156	-1.753664
C	9.193674	-2.586566	-1.856564
C	9.377043	-3.868844	-1.025739
H	8.766241	-4.681991	-1.440584
O	7.206164	-1.431751	-2.646197
O	6.799952	-3.469762	1.475538
C	9.914621	-2.502012	1.044705
H	9.581672	-2.266054	2.059641
H	10.917985	-2.939257	1.120496
C	10.146341	-1.476416	-1.309328
H	11.168887	-1.819429	-1.510849
H	9.994225	-0.548860	-1.867077
C	10.021490	-1.204465	0.212170
C	8.964232	-0.172970	0.567925
O	8.886762	0.847891	-0.288484
O	8.275516	-0.234793	1.621570
H	8.229916	1.580664	-0.011368
C	9.523564	-2.838279	-3.342408
H	10.567942	-3.153603	-3.440129
H	8.887185	-3.627483	-3.757298

H	9.367614	-1.933425	-3.934112
C	9.173003	-4.904633	1.283906
H	10.219335	-5.227004	1.251433
H	8.884467	-4.734282	2.323698
H	8.549995	-5.715848	0.892952
H	7.237073	0.878914	2.186828
C	4.305240	3.756673	1.236327
C	4.293701	3.699964	-0.166993
C	3.089109	3.798142	-0.870800
C	1.862099	3.965524	-0.204925
C	1.879855	4.001005	1.201570
C	3.080432	3.894822	1.910430
H	5.227246	3.583081	-0.707219
H	3.104342	3.761471	-1.956660
H	0.946318	4.130594	1.743763
H	3.069739	3.939006	2.996379
C	5.613865	3.761448	2.034462
H	5.371895	3.579508	3.085568
C	0.563823	4.148056	-0.966172
H	-0.234677	3.562779	-0.487848
H	0.678400	3.762166	-1.990310
C	6.534377	2.638194	1.609461
O	6.576940	1.603419	2.463802
O	7.208899	2.671784	0.548902
C	6.346015	5.120765	1.903596
H	7.244654	5.145342	2.529535
H	6.643001	5.295666	0.866139
H	5.680271	5.928965	2.219582
C	1.054256	6.520070	-1.826439
C	0.069676	5.623342	-1.054912
H	2.051187	6.513066	-1.373712
H	1.152373	6.182808	-2.867634
H	0.699521	7.557057	-1.845973
C	-1.336582	5.670772	-1.683413
H	-0.005316	6.002482	-0.023885
H	-2.041649	5.047223	-1.121745
H	-1.721136	6.697165	-1.703644
H	-1.307247	5.308386	-2.720993
H	10.956193	-0.702053	0.512175
H	10.423190	-4.194282	-1.084953
S	-6.883203	-3.512899	-0.138932
O	-7.465092	-3.178688	1.212224
O	-6.410414	-4.910344	-0.328847
O	-7.637665	-2.897843	-1.291596
O	-5.374746	-2.640766	-0.143315
N	-7.000648	-0.297843	0.203958

C	-9.516242	0.724729	0.468032
C	-8.954997	0.587935	-0.807096
H	-9.515163	0.876226	-1.686870
C	-7.668052	0.052406	-0.913135
C	-7.525214	-0.204276	1.441837
C	-8.809338	0.323152	1.607533
H	-9.257257	0.406939	2.589022
C	-4.552934	-1.818883	2.797752
N	-5.398809	-1.117085	2.019182
C	-6.637780	-0.762087	2.476449
C	-7.009024	-1.033786	3.793722
C	-6.123385	-1.731674	4.619584
C	-4.887021	-2.144578	4.112774
H	-3.625655	-2.125038	2.331670
H	-7.993961	-0.761657	4.150960
H	-6.411406	-1.980594	5.634464
H	-4.200611	-2.727913	4.713423
C	-6.921157	-0.265148	-2.142096
C	-7.453363	-0.252386	-3.431817
C	-6.688715	-0.755522	-4.488094
C	-5.410764	-1.263227	-4.233938
C	-4.914330	-1.222368	-2.930431
N	-5.644218	-0.703910	-1.924385
H	-8.467472	0.086241	-3.601104
H	-7.101407	-0.783542	-5.489985
H	-4.814768	-1.704029	-5.023046
H	-3.945139	-1.617892	-2.656483
H	-10.514957	1.132066	0.572936

RMn1-TS1 E(I) = -3899.87417326 / E(II) = -3900.80840810

Mn	4.882947	-0.934234	-0.021881
Mn	2.714935	0.862615	0.002183
O	4.473769	0.991102	-0.103926
O	2.380096	2.691655	-0.051214
O	3.084804	-1.009487	0.112269
N	0.778543	0.319982	0.051358
C	-1.757262	-0.783332	0.110497
C	-1.060821	-0.504134	1.307731
H	-1.541254	-0.687346	2.259823
C	0.217021	0.049187	1.247171
C	0.164908	0.041589	-1.116561
C	-1.111546	-0.517330	-1.116996
H	-1.606470	-0.765503	-2.046459
C	3.065828	1.313592	-2.935053
N	2.249711	0.828808	-1.979571
C	0.980720	0.416451	-2.286885

C	0.530574	0.441456	-3.609090
C	1.380978	0.920962	-4.610975
C	2.658895	1.374774	-4.269800
H	4.036426	1.649647	-2.595927
H	-0.473763	0.116466	-3.850403
H	1.042044	0.954185	-5.640083
H	3.331378	1.772973	-5.019186
C	1.073229	0.461171	2.377815
C	0.684454	0.477686	3.719603
C	1.560065	0.999450	4.678474
C	2.800591	1.503419	4.275991
C	3.147486	1.446911	2.923467
N	2.309183	0.923007	2.009677
H	-0.291656	0.110280	4.010963
H	1.268181	1.025524	5.722106
H	3.490384	1.934011	4.990900
H	4.088022	1.818796	2.539940
C	-3.145149	-1.283948	0.141595
C	-3.602420	-2.129889	1.170349
C	-4.940941	-2.514447	1.237277
C	-5.849769	-2.045892	0.280124
C	-5.400000	-1.241497	-0.774828
C	-4.062831	-0.866232	-0.842202
H	-2.908844	-2.510599	1.912675
H	-5.279475	-3.154272	2.040157
H	-6.095749	-0.904517	-1.528408
H	-3.751658	-0.191987	-1.632513
C	-9.446384	-3.022989	-0.688871
C	-7.927248	-2.870346	-0.754355
N	-7.263565	-2.337246	0.392579
C	-7.905619	-2.049521	1.634589
C	-9.419119	-2.256833	1.724571
C	-9.854912	-3.368714	0.754767
H	-9.412037	-4.328701	1.052037
O	-7.243896	-1.619697	2.591014
O	-7.269657	-3.172860	-1.759592
C	-10.130653	-1.682209	-1.122522
H	-9.773051	-1.394570	-2.115443
H	-11.202001	-1.901396	-1.209311
C	-10.135483	-0.922671	1.338151
H	-11.205332	-1.081076	1.523571
H	-9.800808	-0.120171	2.000095
C	-9.962860	-0.497961	-0.140907
C	-8.717683	0.329610	-0.416160
O	-8.318754	1.097824	0.601984
O	-8.154839	0.350001	-1.543384

H	-7.522860	1.696668	0.387378
C	-9.784454	-2.617479	3.178656
H	-10.869775	-2.735350	3.267763
H	-9.311480	-3.558469	3.479494
H	-9.452616	-1.838244	3.868432
C	-9.873569	-4.136495	-1.665463
H	-10.962316	-4.253298	-1.638539
H	-9.565506	-3.900512	-2.686674
H	-9.417185	-5.093473	-1.392035
H	-6.937772	1.299215	-2.025768
C	-3.453309	3.696811	-0.974824
C	-3.299823	3.346117	0.377440
C	-2.040150	3.395489	0.982367
C	-0.896309	3.824892	0.275793
C	-1.053538	4.136701	-1.092982
C	-2.305648	4.066298	-1.703545
H	-4.169025	3.058737	0.958440
H	-1.947689	3.147163	2.036235
H	-0.190023	4.448224	-1.672568
H	-2.403532	4.328910	-2.753544
C	-4.816976	3.810575	-1.658714
H	-4.670081	3.701570	-2.737040
C	0.409114	4.013110	0.973274
H	1.267058	3.298130	0.457358
H	0.359834	3.663318	2.013760
C	-5.814227	2.743375	-1.260171
O	-6.178892	1.936693	-2.267781
O	-6.299766	2.650625	-0.103919
C	-5.448821	5.204971	-1.377360
H	-6.386887	5.327102	-1.929352
H	-5.652906	5.318628	-0.309186
H	-4.757166	5.992232	-1.690216
C	0.086833	6.474244	1.527858
C	1.040112	5.424216	0.909687
H	-0.876833	6.501928	1.009720
H	-0.100963	6.253063	2.586605
H	0.537048	7.471893	1.468970
C	2.412704	5.453361	1.607285
H	1.189429	5.680561	-0.149322
H	3.093829	4.727800	1.154028
H	2.859709	6.451166	1.533130
H	2.307057	5.216711	2.675514
H	-10.775907	0.215453	-0.358102
H	-10.944068	-3.490372	0.807242
S	6.635299	-3.605356	0.026184
O	7.202425	-3.239077	-1.325043

O	6.160780	-5.007620	0.181396
O	7.425201	-3.038230	1.182140
O	5.151238	-2.721208	0.085962
N	6.799859	-0.389194	-0.222753
C	9.330716	0.588281	-0.507259
C	8.790764	0.427678	0.774122
H	9.373496	0.679439	1.650469
C	7.495237	-0.085174	0.890035
C	7.303060	-0.273105	-1.467060
C	8.594630	0.232605	-1.643455
H	9.026165	0.333239	-2.630714
C	4.269510	-1.779652	-2.811957
N	5.146471	-1.123356	-2.028489
C	6.384032	-0.782546	-2.499086
C	6.723604	-1.021037	-3.831586
C	5.805934	-1.670660	-4.661181
C	4.569642	-2.070073	-4.143119
H	3.345462	-2.079727	-2.335668
H	7.708177	-0.761416	-4.199006
H	6.068370	-1.893988	-5.688921
H	3.858101	-2.617645	-4.748235
C	6.766930	-0.426004	2.123970
C	7.326515	-0.459218	3.401892
C	6.577518	-0.982338	4.459208
C	5.287419	-1.464510	4.217418
C	4.764458	-1.377291	2.926640
N	5.479147	-0.838579	1.920757
H	8.349175	-0.140922	3.558647
H	7.011026	-1.046274	5.450637
H	4.702237	-1.921661	5.005377
H	3.785240	-1.753442	2.661575
H	10.335762	0.977622	-0.620169

RMn1-2 E(I) = -3899.90511928 / E(II) = -3900.84674679

Mn	4.974875	-0.954914	-0.154178
Mn	2.794694	0.785350	0.207819
O	4.560843	0.929027	0.179895
O	2.426392	2.574133	0.532815
O	3.167887	-1.046047	-0.112182
N	0.854361	0.238216	0.160104
C	-1.680738	-0.860163	0.027367
C	-0.977593	-0.806514	1.252273
H	-1.453183	-1.164267	2.155935
C	0.299892	-0.250610	1.289084
C	0.234455	0.180721	-1.037049
C	-1.043286	-0.367066	-1.133557

H	-1.545514	-0.436443	-2.089364
C	3.107236	1.821502	-2.586792
N	2.305116	1.145401	-1.743049
C	1.041580	0.776438	-2.120667
C	0.584919	1.045076	-3.412859
C	1.422164	1.724219	-4.305139
C	2.692380	2.130140	-3.884937
H	4.071977	2.108614	-2.190299
H	-0.414357	0.754037	-3.711668
H	1.077266	1.947586	-5.308189
H	3.352880	2.678895	-4.544380
C	1.163113	-0.056708	2.471893
C	0.775076	-0.265912	3.797246
C	1.657581	0.074128	4.828930
C	2.903958	0.624723	4.515857
C	3.250297	0.797144	3.173051
N	2.405012	0.445306	2.186200
H	-0.206908	-0.662000	4.024240
H	1.365482	-0.073310	5.862324
H	3.597844	0.920483	5.292580
H	4.193353	1.221617	2.855424
C	-3.063261	-1.372034	-0.026474
C	-3.492561	-2.413803	0.818753
C	-4.821260	-2.833780	0.814479
C	-5.749412	-2.205155	-0.025131
C	-5.330236	-1.191563	-0.896433
C	-4.000199	-0.783604	-0.898557
H	-2.783371	-2.919907	1.465399
H	-5.138486	-3.630264	1.473331
H	-6.042628	-0.722362	-1.559066
H	-3.708249	0.039024	-1.542395
C	-9.299284	-3.178727	-1.160943
C	-7.794110	-2.914131	-1.199277
N	-7.150391	-2.565406	0.027183
C	-7.794542	-2.539659	1.300499
C	-9.291534	-2.851532	1.351406
C	-9.665872	-3.801001	0.199374
H	-9.157740	-4.766963	0.322054
O	-7.146978	-2.249267	2.317202
O	-7.131078	-2.979996	-2.243449
C	-10.077123	-1.833061	-1.348568
H	-9.757479	-1.354020	-2.278415
H	-11.133661	-2.104870	-1.463245
C	-10.093157	-1.517755	1.205557
H	-11.149146	-1.772306	1.361141
H	-9.800643	-0.823835	1.997501

C	-9.964163	-0.831834	-0.175940
C	-8.771092	0.100825	-0.306519
O	-8.409332	0.709529	0.826210
O	-8.220814	0.341311	-1.414283
H	-7.665554	1.399384	0.712336
C	-9.619199	-3.485549	2.718311
H	-10.694219	-3.684794	2.783926
H	-9.086268	-4.433645	2.848397
H	-9.329107	-2.821334	3.535465
C	-9.662376	-4.128662	-2.319475
H	-10.740623	-4.321213	-2.314808
H	-9.382087	-3.694887	-3.282111
H	-9.140584	-5.086091	-2.219577
H	-7.124332	1.487678	-1.743114
C	-4.002499	4.213456	-0.368410
C	-3.712293	3.701685	0.914136
C	-2.456511	3.883674	1.483030
C	-1.422218	4.614846	0.817067
C	-1.721225	5.081683	-0.500607
C	-2.973393	4.878477	-1.067825
H	-4.487147	3.183393	1.468693
H	-2.264562	3.508729	2.485102
H	-0.966237	5.622589	-1.060703
H	-3.175148	5.266639	-2.062968
C	-5.403734	4.203077	-0.977356
H	-5.306318	4.311998	-2.061341
C	-0.195317	4.902187	1.481130
H	1.502989	2.885987	0.642559
H	-0.081119	4.517220	2.495434
C	-6.185220	2.927030	-0.753492
O	-6.476164	2.261524	-1.881857
O	-6.580273	2.548065	0.379234
C	-6.244337	5.393952	-0.429507
H	-7.223594	5.440415	-0.918459
H	-6.394420	5.286404	0.648205
H	-5.716063	6.332396	-0.619693
C	0.314871	7.358266	1.240610
C	0.836431	5.907302	1.024113
H	-0.630738	7.528956	0.716133
H	0.149959	7.549349	2.307545
H	1.051153	8.083704	0.874858
C	2.184551	5.714219	1.750004
H	1.014043	5.783002	-0.056367
H	2.615607	4.729873	1.541311
H	2.903327	6.476522	1.428969
H	2.052884	5.819006	2.835495

H	-10.818527	-0.139021	-0.261440
H	-10.744014	-4.002170	0.230208
S	6.745637	-3.567019	-0.660494
O	7.379624	-2.878305	-1.846165
O	6.278838	-4.962407	-0.883781
O	7.466609	-3.305710	0.640950
O	5.254039	-2.717810	-0.462692
N	6.892588	-0.386099	-0.124215
C	9.423403	0.629322	-0.041523
C	8.828380	0.157457	1.134226
H	9.368041	0.184120	2.071739
C	7.533709	-0.365385	1.060386
C	7.450470	0.032205	-1.276946
C	8.742662	0.565718	-1.262940
H	9.216694	0.907467	-2.173685
C	4.508431	-1.115866	-3.094075
N	5.334265	-0.660804	-2.132674
C	6.587170	-0.211020	-2.444883
C	6.993809	-0.119084	-3.776756
C	6.128387	-0.554866	-4.783478
C	4.876893	-1.075753	-4.439147
H	3.568720	-1.528988	-2.752208
H	7.990081	0.226900	-4.020561
H	6.443095	-0.522223	-5.820221
H	4.205351	-1.467234	-5.192870
C	6.750363	-0.990689	2.139232
C	7.248166	-1.337653	3.395955
C	6.448577	-2.090344	4.259832
C	5.170373	-2.483151	3.849953
C	4.710680	-2.082688	2.595063
N	5.474098	-1.327350	1.782591
H	8.262403	-1.079006	3.671807
H	6.833737	-2.396573	5.225665
H	4.547384	-3.108173	4.477297
H	3.744677	-2.370801	2.202047
H	10.428195	1.033952	-0.008576

RMn2-1 E(I) = -3899.87901045 / E(II) = -3900.81237327

Mn	-3.357920	-1.611978	0.012913
Mn	-4.826364	0.769229	0.193359
O	-3.126597	0.400294	0.071544
O	-4.494662	2.622773	0.257331
O	-5.094500	-1.099494	0.127480
N	-6.833822	0.982792	0.324622
C	-9.554796	0.780462	0.483536
C	-8.790749	0.783153	1.657281
H	-9.271454	0.694786	2.623040

C	-7.399225	0.884000	1.545883
C	-7.544515	0.979265	-0.822259
C	-8.939850	0.880539	-0.770644
H	-9.535048	0.867637	-1.674565
C	-4.455898	1.259615	-2.749250
N	-5.348802	1.034885	-1.767255
C	-6.693244	1.108180	-2.020171
C	-7.159870	1.363716	-3.310865
C	-6.236337	1.574289	-4.341324
C	-4.869228	1.534709	-4.055840
H	-3.415438	1.224238	-2.457272
H	-8.223093	1.425164	-3.507098
H	-6.583288	1.785126	-5.346248
H	-4.129849	1.719979	-4.824622
C	-6.407007	0.919777	2.637232
C	-6.710695	1.076829	3.991082
C	-5.667013	1.211446	4.913628
C	-4.344898	1.195103	4.460971
C	-4.096363	1.019052	3.097157
N	-5.104238	0.867326	2.217503
H	-7.741555	1.121979	4.319771
H	-5.887113	1.345850	5.966326
H	-3.515979	1.321516	5.145895
H	-3.099249	1.003481	2.678663
S	-2.582368	-4.706291	-0.148843
O	-1.849773	-4.432734	-1.437581
O	-3.521928	-5.859824	-0.152822
O	-1.733806	-4.534333	1.084476
O	-3.704767	-3.368224	-0.042822
N	-1.372722	-1.685346	-0.085422
C	1.386365	-1.568652	-0.210431
C	0.720763	-1.639858	1.032973
H	1.298495	-1.691213	1.946128
C	-0.669179	-1.710104	1.065643
C	-0.780044	-1.635048	-1.295938
C	0.607951	-1.567947	-1.388172
H	1.095492	-1.506885	-2.352074
C	-4.050008	-1.980481	-2.865122
N	-3.057979	-1.703363	-1.996824
C	-1.750993	-1.726207	-2.399367
C	-1.429624	-1.934302	-3.741414
C	-2.455730	-2.185036	-4.656108
C	-3.781478	-2.226502	-4.211619
H	-5.046571	-2.022623	-2.446070
H	-0.394427	-1.958190	-4.056653
H	-2.218934	-2.381506	-5.695472

H	-4.592602	-2.468111	-4.886891
C	-1.530353	-1.906296	2.244002
C	-1.081891	-2.228403	3.525783
C	-2.015851	-2.572837	4.506456
C	-3.377630	-2.591151	4.186711
C	-3.773992	-2.230055	2.899081
N	-2.869570	-1.865023	1.969418
H	-0.021310	-2.270050	3.737977
H	-1.680587	-2.859420	5.496623
H	-4.119798	-2.902801	4.910856
H	-4.805711	-2.247183	2.573626
H	-10.633206	0.694073	0.546325
C	2.862092	-1.526606	-0.272348
C	3.556548	-2.223445	-1.280927
C	4.949325	-2.216658	-1.318901
C	5.670314	-1.497979	-0.358437
C	4.995851	-0.788713	0.641635
C	3.603522	-0.809852	0.686944
H	3.010376	-2.815314	-2.007576
H	5.474248	-2.769081	-2.087632
H	5.559426	-0.236338	1.379971
H	3.093478	-0.233712	1.451638
C	9.330726	-1.999430	0.729525
C	7.801379	-1.991195	0.762666
N	7.119329	-1.504193	-0.390970
C	7.759005	-1.028579	-1.567570
C	9.287798	-1.106919	-1.638596
C	9.796450	-2.231171	-0.720105
H	9.440981	-3.206659	-1.078508
O	7.079643	-0.560847	-2.495186
O	7.153449	-2.392316	1.739075
C	9.890453	-0.634980	1.251750
H	9.470339	-0.428170	2.240509
H	10.971039	-0.779140	1.376527
C	9.900827	0.250820	-1.173583
H	10.981438	0.180075	-1.350122
H	9.518320	1.065345	-1.794126
C	9.678847	0.583787	0.326367
C	8.385127	1.332755	0.594617
O	8.135659	2.305362	-0.284775
O	7.653844	1.111707	1.596795
H	7.311474	2.870289	-0.065001
C	9.695826	-1.362257	-3.104574
H	10.788039	-1.382999	-3.185780
H	9.307925	-2.323988	-3.457888
H	9.303749	-0.579724	-3.758088

C	9.831307	-3.126050	1.656291
H	10.926421	-3.151283	1.648720
H	9.484867	-2.970599	2.680598
H	9.461149	-4.101219	1.323170
H	6.364702	1.974939	2.074250
C	2.975410	4.194163	0.967427
C	3.037044	4.087282	-0.431360
C	1.870623	3.902464	-1.180356
C	0.609242	3.829624	-0.564372
C	0.557911	3.921985	0.837829
C	1.721329	4.097611	1.592010
H	3.996829	4.148264	-0.933608
H	1.940989	3.822678	-2.261559
H	-0.404027	3.860264	1.340592
H	1.655821	4.171150	2.674387
C	4.220546	4.485736	1.812093
H	3.977572	4.277464	2.858118
C	-0.665772	3.697959	-1.373785
H	-1.356517	3.015735	-0.858712
H	-0.438967	3.248979	-2.352379
C	5.363903	3.564582	1.448503
O	5.566946	2.560812	2.314821
O	6.069194	3.729102	0.420037
C	4.665041	5.962708	1.670213
H	5.512822	6.183729	2.327944
H	4.963779	6.173509	0.639955
H	3.835719	6.623819	1.937760
C	-0.583080	6.016331	-2.480728
C	-1.408092	5.047046	-1.615148
H	0.395126	6.224481	-2.035389
H	-0.416023	5.596892	-3.482629
H	-1.108217	6.970913	-2.603302
C	-2.793439	4.789407	-2.238958
H	-1.563494	5.513554	-0.630106
H	-3.408335	4.157202	-1.587366
H	-3.328528	5.732489	-2.403469
H	-2.690175	4.294905	-3.216250
H	10.445883	1.330670	0.588760
H	10.892914	-2.259471	-0.753592

RMn2-TS1 E(I) = -3899.86859243 / E(II) = -3900.80169855

Mn	-3.117266	-1.810686	0.079066
Mn	-4.245124	0.764497	0.074212
O	-2.616628	0.099256	-0.064190
O	-3.865493	2.601242	0.047571
O	-4.763120	-1.066077	0.170534

N	-6.219654	1.191216	0.256019
C	-8.928284	1.416706	0.512519
C	-8.122626	1.402328	1.658642
H	-8.569905	1.471208	2.641968
C	-6.737376	1.286162	1.496180
C	-6.966941	1.203629	-0.863787
C	-8.359267	1.322357	-0.763035
H	-8.988448	1.330820	-1.643693
C	-3.966976	0.844788	-2.923468
N	-4.821167	0.887398	-1.883378
C	-6.159047	1.099932	-2.093629
C	-6.657595	1.249636	-3.389540
C	-5.775112	1.199346	-4.473789
C	-4.412103	1.001562	-4.238745
H	-2.928391	0.679981	-2.671357
H	-7.714454	1.419883	-3.552548
H	-6.148322	1.322122	-5.483926
H	-3.701056	0.966998	-5.054577
C	-5.701052	1.282778	2.548275
C	-5.926243	1.563753	3.897296
C	-4.834882	1.638144	4.770418
C	-3.543071	1.441533	4.274473
C	-3.375039	1.147717	2.918535
N	-4.431676	1.052059	2.090702
H	-6.930326	1.747193	4.259105
H	-4.993587	1.864515	5.818495
H	-2.677051	1.516156	4.919997
H	-2.406176	0.990581	2.463902
S	-2.710592	-4.971515	0.176529
O	-1.942025	-4.885270	-1.119936
O	-3.759586	-6.025656	0.248561
O	-1.848119	-4.802680	1.403233
O	-3.670642	-3.526866	0.167981
N	-1.152046	-2.131959	0.020397
C	1.603898	-2.057224	-0.076306
C	0.925065	-2.060298	1.161395
H	1.489424	-2.045154	2.084278
C	-0.466070	-2.098363	1.179509
C	-0.547428	-2.189101	-1.181984
C	0.843248	-2.149800	-1.261727
H	1.342232	-2.147136	-2.221991
C	-3.821890	-2.403912	-2.764680
N	-2.817176	-2.128409	-1.911576
C	-1.514464	-2.308291	-2.287120
C	-1.200677	-2.680406	-3.594859
C	-2.237409	-2.930955	-4.497885

C	-3.565091	-2.807966	-4.075258
H	-4.822336	-2.317027	-2.361643
H	-0.168997	-2.834388	-3.884500
H	-2.010535	-3.255319	-5.507029
H	-4.388930	-3.044966	-4.736684
C	-1.351854	-2.138221	2.354895
C	-0.950055	-2.427594	3.659671
C	-1.923886	-2.599974	4.646713
C	-3.276670	-2.480942	4.310074
C	-3.621063	-2.162029	2.996543
N	-2.674724	-1.964564	2.058582
H	0.097510	-2.580217	3.886191
H	-1.630878	-2.861422	5.657087
H	-4.054354	-2.657776	5.042417
H	-4.645392	-2.083091	2.657105
H	-10.003987	1.499024	0.614795
C	3.073463	-1.907935	-0.124958
C	3.848178	-2.556415	-1.105177
C	5.227589	-2.360854	-1.166795
C	5.851183	-1.498099	-0.257825
C	5.097149	-0.859544	0.733659
C	3.723038	-1.068303	0.800617
H	3.379265	-3.241825	-1.803254
H	5.812576	-2.864657	-1.924568
H	5.584821	-0.207606	1.444180
H	3.147585	-0.536100	1.550329
C	9.545078	-1.116324	0.764942
C	8.059494	-1.472393	0.825368
N	7.275428	-1.242646	-0.343956
C	7.792636	-0.772691	-1.584917
C	9.292576	-0.475474	-1.671640
C	10.059392	-1.353218	-0.667086
H	9.957934	-2.413990	-0.932811
O	7.031202	-0.597547	-2.548343
O	7.527392	-1.933464	1.844584
C	9.744570	0.386217	1.155620
H	9.294214	0.569819	2.135571
H	10.826792	0.534158	1.258056
C	9.535688	1.029284	-1.330661
H	10.601474	1.219326	-1.509161
H	8.967465	1.660829	-2.018021
C	9.216839	1.420076	0.133946
C	7.768460	1.813982	0.372902
O	7.188036	2.437046	-0.656998
O	7.190094	1.646418	1.479754
H	6.246458	2.774741	-0.463035

C	9.765447	-0.744009	-3.114895
H	10.829741	-0.501090	-3.207008
H	9.630097	-1.797691	-3.381848
H	9.198706	-0.140659	-3.827594
C	10.303583	-1.997571	1.777121
H	11.369803	-1.747262	1.759070
H	9.918998	-1.848983	2.788722
H	10.194143	-3.058918	1.531111
H	5.761264	2.251386	1.953625
C	1.850517	3.940208	0.816859
C	1.789356	3.316886	-0.440088
C	0.563899	3.165998	-1.096994
C	-0.634176	3.666836	-0.548371
C	-0.569711	4.260965	0.732039
C	0.645662	4.383406	1.400942
H	2.699730	2.975831	-0.918111
H	0.540702	2.691674	-2.073927
H	-1.480220	4.626481	1.196499
H	0.669974	4.848627	2.382959
C	3.151131	4.240244	1.564596
H	2.985817	4.063089	2.631898
C	-1.907253	3.633425	-1.322745
H	-2.742857	3.042339	-0.670557
H	-1.796137	3.048899	-2.246062
C	4.338910	3.389507	1.173624
O	4.881181	2.708032	2.192796
O	4.823332	3.377466	0.013087
C	3.556466	5.732938	1.366830
H	4.442481	5.978697	1.961987
H	3.774003	5.925203	0.312642
H	2.736135	6.383801	1.681798
C	-1.623136	5.897011	-2.453568
C	-2.570506	4.999669	-1.623404
H	-0.676949	6.075309	-1.933558
H	-1.396875	5.432568	-3.422335
H	-2.095250	6.866940	-2.649096
C	-3.920539	4.820918	-2.341840
H	-2.760367	5.500166	-0.662890
H	-4.597198	4.208842	-1.738365
H	-4.392268	5.793476	-2.523467
H	-3.778896	4.334498	-3.317199
H	9.753006	2.364899	0.326601
H	11.128994	-1.112894	-0.717156

RMn2-2 E(I) = -3899.90356978 / E(II) = -3900.84567917
Mn 3.294077 -1.906517 -0.216576

Mn	4.458180	0.621082	0.165027
O	2.811980	-0.012671	0.114654
O	4.011756	2.396456	0.470139
O	4.955366	-1.182025	-0.146198
N	6.440364	1.040157	0.165843
C	9.162746	1.235923	0.105753
C	8.431550	1.383456	-1.079454
H	8.941073	1.565507	-2.016871
C	7.036754	1.276703	-1.018267
C	7.115665	0.898740	1.322510
C	8.512483	0.995663	1.322539
H	9.084280	0.879105	2.234143
C	3.977383	0.400515	3.127496
N	4.907830	0.499600	2.160022
C	6.227583	0.675845	2.480091
C	6.634197	0.707289	3.815741
C	5.673961	0.586088	4.826209
C	4.327879	0.442308	4.479531
H	2.955289	0.293225	2.790083
H	7.677819	0.850014	4.066767
H	5.974048	0.620109	5.867132
H	3.558011	0.366788	5.237059
C	6.072299	1.420289	-2.126162
C	6.391354	1.872347	-3.408378
C	5.365859	2.066987	-4.340139
C	4.043448	1.811613	-3.967693
C	3.781374	1.344394	-2.677066
N	4.774115	1.141496	-1.791096
H	7.418266	2.094330	-3.670583
H	5.598041	2.427896	-5.335415
H	3.224676	1.971460	-4.657816
H	2.782145	1.127876	-2.324262
S	2.864408	-5.026011	-0.720366
O	2.078868	-5.097746	0.566160
O	3.909187	-6.068368	-0.913022
O	2.023373	-4.690728	-1.927044
O	3.835328	-3.599063	-0.509098
N	1.326892	-2.210720	-0.211495
C	-1.431889	-2.177665	-0.126382
C	-0.745278	-1.998114	-1.346969
H	-1.305329	-1.863012	-2.262865
C	0.647082	-2.025795	-1.360587
C	0.714460	-2.430018	0.968585
C	-0.676266	-2.417050	1.041736
H	-1.181434	-2.552354	1.988993
C	3.978028	-2.824090	2.538178

N	2.976952	-2.453752	1.716556
C	1.672992	-2.685102	2.056888
C	1.352046	-3.217296	3.306274
C	2.383922	-3.571232	4.179443
C	3.713971	-3.388117	3.786456
H	4.980083	-2.678166	2.156920
H	0.319314	-3.409976	3.567378
H	2.152035	-4.018485	5.139232
H	4.534260	-3.698696	4.421297
C	1.541415	-1.918559	-2.525699
C	1.145484	-2.027949	-3.859243
C	2.123728	-2.084205	-4.855629
C	3.475552	-2.031994	-4.499721
C	3.815127	-1.893994	-3.153710
N	2.865506	-1.806138	-2.202591
H	0.097515	-2.132358	-4.109788
H	1.833753	-2.205368	-5.893041
H	4.255663	-2.123354	-5.244999
H	4.838391	-1.874650	-2.802407
H	10.243879	1.305807	0.080615
C	-2.905633	-2.088076	-0.064731
C	-3.646893	-2.918819	0.797320
C	-5.032875	-2.801622	0.878386
C	-5.698316	-1.836246	0.113825
C	-4.977968	-1.007609	-0.754012
C	-3.594462	-1.141254	-0.847371
H	-3.145158	-3.684505	1.379484
H	-5.593674	-3.449216	1.539566
H	-5.498311	-0.267943	-1.346696
H	-3.043817	-0.472527	-1.500645
C	-9.421911	-1.632354	-0.854854
C	-7.907234	-1.812755	-0.968822
N	-7.135771	-1.691494	0.224504
C	-7.677314	-1.438783	1.515344
C	-9.198565	-1.324813	1.647705
C	-9.883125	-2.127639	0.527951
H	-9.663081	-3.198023	0.637556
O	-6.920908	-1.303689	2.489859
O	-7.344711	-2.055011	-2.045424
C	-9.795817	-0.122574	-1.023191
H	-9.382351	0.249840	-1.965035
H	-10.889313	-0.088447	-1.107256
C	-9.611566	0.175514	1.534025
H	-10.685940	0.219483	1.752880
H	-9.095793	0.762549	2.298370
C	-9.378996	0.808627	0.137198

C	-7.999520	1.419847	-0.045002
O	-7.547692	2.071226	1.031009
O	-7.376838	1.396631	-1.139432
H	-6.688300	2.597364	0.869960
C	-9.610761	-1.852600	3.037593
H	-10.692832	-1.742632	3.168229
H	-9.358820	-2.913340	3.144404
H	-9.097459	-1.302574	3.829511
C	-10.096173	-2.438188	-1.983479
H	-11.183241	-2.315837	-1.926018
H	-9.750141	-2.100850	-2.963227
H	-9.863781	-3.504661	-1.896415
H	-6.140596	2.374127	-1.583026
C	-2.811924	4.970243	-0.476422
C	-2.546973	4.538499	0.840394
C	-1.271843	4.652967	1.380627
C	-0.187711	5.230706	0.647617
C	-0.469469	5.630800	-0.695294
C	-1.743583	5.495956	-1.232452
H	-3.352458	4.127925	1.439312
H	-1.093006	4.328634	2.402294
H	0.319472	6.059156	-1.304035
H	-1.928026	5.823000	-2.252670
C	-4.215328	5.010142	-1.078240
H	-4.120894	5.015365	-2.167906
C	1.077916	5.420939	1.265287
H	3.045181	2.553475	0.514683
H	1.178635	5.095975	2.301176
C	-5.082590	3.818807	-0.737380
O	-5.450538	3.088133	-1.800904
O	-5.477992	3.564724	0.429680
C	-4.964474	6.301344	-0.635027
H	-5.943816	6.374413	-1.120965
H	-5.108706	6.300061	0.448866
H	-4.373375	7.179391	-0.910190
C	1.981920	7.735408	0.844829
C	2.231191	6.207121	0.691818
H	1.045941	8.035815	0.362774
H	1.919255	8.009017	1.904814
H	2.803902	8.304578	0.393782
C	3.570281	5.814330	1.351162
H	2.313626	5.997958	-0.386808
H	3.819344	4.762553	1.172452
H	4.387549	6.428353	0.954632
H	3.526292	5.981237	2.435899
H	-10.033449	1.695256	0.092289

H -10.971392 -2.014980 0.612897

NRA-1 E(I) = -3899.86014834 / E(II) = -3900.78899618

Mn	4.552628	-1.184180	-0.366838
Mn	2.743823	0.698166	0.644317
O	4.492005	0.605053	0.530503
O	2.840165	2.374238	1.498340
O	2.766612	-1.000845	-0.205632
N	0.739424	0.602918	0.675989
C	-1.959163	0.010539	0.469838
C	-1.208033	-0.402213	1.594921
H	-1.694875	-0.943995	2.395159
C	0.147192	-0.090147	1.672163
C	0.060335	1.017805	-0.415642
C	-1.301698	0.746902	-0.542262
H	-1.848383	1.081631	-1.413666
C	3.144054	2.418638	-1.780003
N	2.256417	1.703868	-1.061833
C	0.921365	1.739489	-1.370620
C	0.461577	2.472143	-2.467233
C	1.386548	3.188283	-3.234983
C	2.739462	3.173796	-2.882755
H	4.170497	2.372854	-1.442415
H	-0.599079	2.518367	-2.685037
H	1.048106	3.768894	-4.085703
H	3.472531	3.740751	-3.443007
C	1.080859	-0.400431	2.771765
C	0.712122	-0.872281	4.033730
C	1.688933	-1.000922	5.026817
C	3.010916	-0.645999	4.741465
C	3.329454	-0.197274	3.457771
N	2.388894	-0.099665	2.498619
H	-0.323279	-1.105921	4.248319
H	1.414989	-1.353397	6.014587
H	3.784056	-0.707640	5.496920
H	4.328316	0.102156	3.170387
C	-3.394118	-0.323960	0.357709
C	-3.899865	-1.522929	0.899641
C	-5.251096	-1.845251	0.793702
C	-6.126152	-0.957117	0.156077
C	-5.642591	0.238694	-0.387155
C	-4.286587	0.547230	-0.298685
H	-3.229280	-2.233967	1.370568
H	-5.629499	-2.779060	1.187876
H	-6.323137	0.918560	-0.883662
H	-3.924365	1.477592	-0.720573

C	-9.716307	-1.915656	1.171691
C	-8.242290	-1.518253	1.274880
N	-7.535970	-1.279428	0.057838
C	-8.111754	-1.357536	-1.237819
C	-9.609954	-1.662860	-1.344745
C	-10.329324	-1.220567	-0.058812
H	-10.269711	-0.129897	0.056447
O	-7.401812	-1.191215	-2.243410
O	-7.658530	-1.390226	2.359427
C	-9.855640	-3.467790	1.024122
H	-9.327738	-3.955872	1.849107
H	-10.924034	-3.688034	1.141858
C	-9.811148	-3.198393	-1.540554
H	-10.883338	-3.351926	-1.716110
H	-9.281196	-3.532351	-2.436313
C	-9.393205	-4.066803	-0.322489
C	-7.922115	-4.441820	-0.317990
O	-7.510099	-4.897026	-1.546967
O	-7.161288	-4.416962	0.656773
H	-6.567035	-5.169223	-1.525833
C	-10.173838	-0.924257	-2.576424
H	-11.236074	-1.163089	-2.696562
H	-10.078481	0.161006	-2.460177
H	-9.638087	-1.215776	-3.482614
C	-10.430733	-1.477106	2.465972
H	-11.489590	-1.753000	2.415478
H	-9.979768	-1.952504	3.340087
H	-10.362731	-0.392911	2.603532
H	-4.526163	3.261095	-4.245314
C	-2.323933	5.019209	-0.782932
C	-2.774896	4.345599	0.363802
C	-1.929017	4.153993	1.460333
C	-0.603948	4.625355	1.453636
C	-0.159148	5.305525	0.305009
C	-1.005602	5.501396	-0.790519
H	-3.793029	3.970050	0.410438
H	-2.302843	3.635232	2.338646
H	0.857600	5.686348	0.270825
H	-0.637020	6.037811	-1.661425
C	-3.234775	5.241452	-1.982774
H	-2.714802	5.912530	-2.685036
C	0.318952	4.413162	2.637540
H	1.246094	3.930361	2.294308
H	-0.154053	3.720203	3.348698
C	-3.448643	3.957586	-2.772256
O	-4.423298	4.088547	-3.724980

O	-2.818106	2.894386	-2.645999
C	-4.576736	5.926108	-1.618610
H	-5.163052	6.130994	-2.516376
H	-5.177488	5.298313	-0.953098
H	-4.372459	6.867931	-1.102309
C	-0.524005	6.387446	4.041803
C	0.703935	5.710514	3.405357
H	-1.282562	6.636493	3.291729
H	-0.988161	5.725762	4.785769
H	-0.237482	7.313763	4.553016
C	1.777400	5.397478	4.464928
H	1.140877	6.410235	2.675738
H	2.664315	4.940939	4.009847
H	2.090998	6.308847	4.987092
H	1.386258	4.700422	5.218607
H	-9.901897	-5.035579	-0.447721
H	-11.394075	-1.475545	-0.132065
S	5.822068	-3.788001	-1.713094
O	6.517392	-2.901869	-2.717620
O	5.095724	-4.964684	-2.262666
O	6.626177	-4.024388	-0.457979
O	4.503942	-2.800702	-1.159664
N	6.538989	-0.948706	-0.348485
C	9.209593	-0.409928	-0.215812
C	8.588304	-1.092329	0.836662
H	9.161680	-1.414611	1.695851
C	7.220121	-1.362399	0.737948
C	7.114724	-0.315655	-1.389389
C	8.480194	-0.019074	-1.344822
H	8.970182	0.485512	-2.167155
C	3.942341	-0.423353	-3.180251
N	4.876608	-0.398440	-2.210692
C	6.174944	-0.079719	-2.498669
C	6.534377	0.323581	-3.785054
C	5.563356	0.333872	-4.790286
C	4.255415	-0.059802	-4.490541
H	2.958662	-0.759489	-2.879913
H	7.564239	0.566133	-4.013734
H	5.834553	0.612063	-5.802218
H	3.493407	-0.106835	-5.258179
C	6.382436	-2.133449	1.672421
C	6.860843	-2.889060	2.743604
C	5.976862	-3.718554	3.439058
C	4.635341	-3.778310	3.048609
C	4.203214	-2.977865	1.990523
N	5.054056	-2.155106	1.348329

H	7.914152	-2.877652	2.992847
H	6.340144	-4.336649	4.252017
H	3.937988	-4.447192	3.536997
H	3.187180	-2.990292	1.618785
H	10.270437	-0.195003	-0.162624

NRA-TS1 E(I) = -3899.85367408 / E(II) = -3900.79085630

Mn	4.255283	-1.319832	-0.360617
Mn	2.711729	0.825920	0.609975
O	4.428843	0.498063	0.390258
O	3.004857	2.518477	1.326047
O	2.514041	-0.941363	-0.108007
N	0.695382	0.813246	0.671789
C	-2.001738	0.206926	0.484228
C	-1.259350	-0.131461	1.639390
H	-1.751552	-0.624298	2.467726
C	0.097684	0.180132	1.702686
C	0.027131	1.147490	-0.451789
C	-1.333564	0.866456	-0.571420
H	-1.871593	1.134332	-1.469952
C	3.141642	2.350217	-1.931292
N	2.235303	1.727223	-1.153957
C	0.900240	1.783197	-1.455749
C	0.455888	2.449080	-2.600553
C	1.397312	3.071684	-3.427304
C	2.753190	3.032123	-3.086620
H	4.169277	2.287992	-1.599205
H	-0.604514	2.518733	-2.810092
H	1.071286	3.598506	-4.317082
H	3.500706	3.523804	-3.696721
C	1.033388	-0.090574	2.811978
C	0.667798	-0.495730	4.098153
C	1.654674	-0.614867	5.082769
C	2.983957	-0.318251	4.765268
C	3.297923	0.068365	3.460060
N	2.345981	0.160555	2.512077
H	-0.370980	-0.690090	4.335122
H	1.384064	-0.918517	6.087604
H	3.766244	-0.379731	5.511299
H	4.302079	0.317584	3.144020
C	-3.438255	-0.127610	0.381750
C	-3.953418	-1.289432	0.990908
C	-5.304621	-1.614277	0.890343
C	-6.170174	-0.764801	0.190381
C	-5.677367	0.394847	-0.418794
C	-4.321205	0.705154	-0.335012

H	-3.289748	-1.972410	1.510729
H	-5.689639	-2.522188	1.335227
H	-6.350215	1.044378	-0.963949
H	-3.953049	1.607052	-0.812126
C	-9.773151	-1.669632	1.211593
C	-8.301236	-1.263584	1.311907
N	-7.579315	-1.091124	0.093290
C	-8.138716	-1.242651	-1.203124
C	-9.635490	-1.553192	-1.312561
C	-10.371622	-1.043421	-0.061901
H	-10.314839	0.052018	-0.005198
O	-7.416229	-1.133893	-2.207544
O	-7.732753	-1.073342	2.395580
C	-9.909563	-3.227894	1.146909
H	-9.390052	-3.669532	2.002793
H	-10.978978	-3.443076	1.264979
C	-9.834164	-3.097041	-1.428453
H	-10.904046	-3.260560	-1.609223
H	-9.292762	-3.478058	-2.298254
C	-9.431578	-3.898883	-0.160141
C	-7.960241	-4.271415	-0.117105
O	-7.533730	-4.795991	-1.312742
O	-7.211264	-4.189030	0.863668
H	-6.590532	-5.064590	-1.265837
C	-10.183272	-0.882185	-2.589368
H	-11.244770	-1.124917	-2.708064
H	-10.086097	0.207625	-2.532091
H	-9.638171	-1.224343	-3.471940
C	-10.504596	-1.163578	2.471371
H	-11.562654	-1.442817	2.421771
H	-10.064956	-1.591500	3.375322
H	-10.438649	-0.073559	2.552235
H	-4.381769	4.045903	-4.000153
C	-1.732922	5.225474	-0.596994
C	-2.063350	4.413204	0.501541
C	-1.100074	4.069726	1.449998
C	0.231531	4.526577	1.345267
C	0.555315	5.347124	0.243696
C	-0.410949	5.689275	-0.704587
H	-3.077778	4.045439	0.619474
H	-1.380563	3.448387	2.295813
H	1.569109	5.716231	0.129573
H	-0.134956	6.327410	-1.539838
C	-2.774412	5.618798	-1.632606
H	-2.317793	6.336622	-2.329919
C	1.250100	4.127688	2.358636

H	2.010420	3.330084	1.830853
H	0.792114	3.550687	3.173725
C	-3.191318	4.439789	-2.498926
O	-4.123454	4.806011	-3.433587
O	-2.763150	3.276283	-2.437333
C	-4.014947	6.320454	-1.013958
H	-4.704122	6.641969	-1.797612
H	-4.551369	5.652907	-0.332181
H	-3.688613	7.195273	-0.445171
C	1.370128	6.311983	3.652307
C	2.185052	5.216101	2.926148
H	0.646073	6.788440	2.983393
H	0.821056	5.887180	4.502585
H	2.040404	7.087726	4.040310
C	3.237897	4.598908	3.865802
H	2.717582	5.685204	2.086044
H	3.829924	3.843152	3.341215
H	3.914094	5.371970	4.247770
H	2.752945	4.124611	4.730401
H	-9.938922	-4.873118	-0.239009
H	-11.434952	-1.304240	-0.134513
S	5.155140	-4.135123	-1.571729
O	5.857309	-3.408926	-2.694721
O	4.287917	-5.277956	-1.970117
O	6.029737	-4.354700	-0.359844
O	3.989757	-2.984400	-1.020437
N	6.254979	-1.299182	-0.487970
C	8.969594	-1.044481	-0.568601
C	8.357904	-1.574039	0.573599
H	8.954678	-1.890670	1.418898
C	6.965651	-1.702001	0.582964
C	6.817115	-0.812701	-1.611264
C	8.205731	-0.663541	-1.677925
H	8.685079	-0.278881	-2.568545
C	3.530572	-0.693722	-3.181580
N	4.529342	-0.708937	-2.278903
C	5.829497	-0.556589	-2.673443
C	6.135944	-0.285271	-4.007558
C	5.101604	-0.233409	-4.945706
C	3.784018	-0.455420	-4.532708
H	2.541743	-0.897896	-2.793101
H	7.166717	-0.176083	-4.319498
H	5.326900	-0.056553	-5.991158
H	2.967327	-0.467080	-5.243408
C	6.122598	-2.308593	1.627405
C	6.599469	-3.029370	2.723149

C	5.690320	-3.707233	3.539345
C	4.324838	-3.653559	3.242283
C	3.899875	-2.893018	2.152422
N	4.779128	-2.214172	1.391511
H	7.664009	-3.110816	2.901449
H	6.047935	-4.298514	4.374493
H	3.601213	-4.207530	3.826920
H	2.863667	-2.828502	1.848107
H	10.048072	-0.942567	-0.600211

NRA-2 E(I) = -3899.88636371 / E(II) = -3900.83154791

Mn	4.304557	-1.370035	-0.385569
Mn	2.709843	0.657682	0.740719
O	4.445445	0.346001	0.533500
O	2.878764	2.274803	1.628995
O	2.549306	-1.009866	-0.155312
N	0.690590	0.622406	0.783236
C	-2.012100	0.067439	0.555864
C	-1.269100	-0.384321	1.671190
H	-1.764259	-0.942694	2.454870
C	0.091611	-0.094469	1.756688
C	0.022220	1.071493	-0.299642
C	-1.342569	0.818406	-0.437471
H	-1.881852	1.176326	-1.303645
C	3.143131	2.422113	-1.639766
N	2.233713	1.724533	-0.932395
C	0.899060	1.802897	-1.235410
C	0.458625	2.579904	-2.309064
C	1.403139	3.286870	-3.062176
C	2.757664	3.215807	-2.722633
H	4.168866	2.330451	-1.308105
H	-0.600639	2.666617	-2.518338
H	1.079042	3.902236	-3.893799
H	3.505998	3.768981	-3.276427
C	1.025639	-0.462368	2.839577
C	0.656164	-0.969671	4.087615
C	1.639459	-1.161657	5.064606
C	2.968404	-0.834299	4.778564
C	3.287391	-0.346780	3.508525
N	2.338958	-0.187269	2.566895
H	-0.382950	-1.184321	4.304626
H	1.365488	-1.543933	6.041285
H	3.746964	-0.948388	5.522301
H	4.291520	-0.067845	3.217892
C	-3.452532	-0.243195	0.432801
C	-3.975984	-1.448114	0.943121

C	-5.331792	-1.747906	0.829181
C	-6.194004	-0.831430	0.214766
C	-5.692884	0.370516	-0.297852
C	-4.332379	0.656942	-0.201167
H	-3.315931	-2.180947	1.394945
H	-5.723316	-2.685998	1.199733
H	-6.363132	1.072649	-0.777071
H	-3.957713	1.591287	-0.604151
C	-9.796018	-1.766268	1.209255
C	-8.317456	-1.388756	1.320641
N	-7.608320	-1.131410	0.109057
C	-8.185943	-1.168833	-1.187723
C	-9.687310	-1.456412	-1.300823
C	-10.401498	-1.036254	-0.004602
H	-10.330059	0.050771	0.135859
O	-7.475147	-0.982585	-2.189153
O	-7.732063	-1.292116	2.407598
C	-9.953170	-3.312908	1.025849
H	-9.431293	-3.826243	1.839249
H	-11.024095	-3.523262	1.138339
C	-9.904724	-2.984884	-1.531910
H	-10.978412	-3.122721	-1.711243
H	-9.377783	-3.303755	-2.434892
C	-9.497060	-3.885703	-0.334272
C	-8.030501	-4.277986	-0.337934
O	-7.621321	-4.703992	-1.578103
O	-7.271791	-4.288755	0.638745
H	-6.681722	-4.988401	-1.563108
C	-10.243953	-0.683781	-2.514752
H	-11.308394	-0.909612	-2.640591
H	-10.138221	0.397474	-2.372892
H	-9.710737	-0.958910	-3.427538
C	-10.505017	-1.349243	2.513566
H	-11.566706	-1.612969	2.457835
H	-10.058489	-1.848518	3.376557
H	-10.425699	-0.269096	2.674972
H	-4.463487	3.687150	-3.860648
C	-1.925608	5.384054	-0.581367
C	-2.060145	4.509621	0.519473
C	-1.067050	4.413666	1.483171
C	0.131234	5.194944	1.409927
C	0.257436	6.064396	0.282705
C	-0.747729	6.150237	-0.675629
H	-2.958152	3.908563	0.623617
H	-1.202896	3.749746	2.332859
H	1.141903	6.682750	0.180212

H	-0.627182	6.837366	-1.509466
C	-3.039154	5.560232	-1.598855
H	-2.717847	6.304315	-2.341893
C	1.108936	5.103611	2.438201
H	2.137484	2.916268	1.651299
H	0.879210	4.454207	3.284323
C	-3.317429	4.297736	-2.397579
O	-4.290037	4.502119	-3.339674
O	-2.761761	3.193585	-2.277053
C	-4.351395	6.100931	-0.959931
H	-5.110114	6.275879	-1.725972
H	-4.751327	5.396047	-0.223921
H	-4.139619	7.042414	-0.446125
C	2.008893	7.325722	3.208922
C	2.349629	5.950995	2.564300
H	1.257571	7.867745	2.624801
H	1.615386	7.187369	4.222890
H	2.910225	7.946208	3.275908
C	3.444063	5.227489	3.378510
H	2.754797	6.150999	1.560473
H	3.721298	4.275234	2.914437
H	4.340614	5.852705	3.455000
H	3.092080	5.023813	4.398707
H	-10.016815	-4.845447	-0.481910
H	-11.469013	-1.277843	-0.083286
S	5.248101	-4.053930	-1.846931
O	5.998125	-3.221789	-2.861011
O	4.400660	-5.148377	-2.395575
O	6.072994	-4.400384	-0.628839
O	4.069171	-2.959302	-1.230501
N	6.306006	-1.353687	-0.429257
C	9.023166	-1.120155	-0.375667
C	8.362854	-1.761083	0.678988
H	8.923250	-2.172022	1.508410
C	6.970680	-1.875155	0.619996
C	6.915939	-0.758673	-1.472450
C	8.306973	-0.617191	-1.467875
H	8.824115	-0.146449	-2.293642
C	3.699534	-0.456239	-3.158316
N	4.658480	-0.568810	-2.219878
C	5.974530	-0.386177	-2.541920
C	6.338411	0.017382	-3.827316
C	5.345622	0.170876	-4.798348
C	4.011210	-0.084133	-4.466397
H	2.694148	-0.693329	-2.836593
H	7.381868	0.150390	-4.082625

H	5.615893	0.451363	-5.809922
H	3.225858	-0.019705	-5.208915
C	6.082354	-2.580153	1.559498
C	6.507952	-3.418018	2.591379
C	5.560470	-4.167197	3.293466
C	4.208734	-4.066353	2.948952
C	3.835049	-3.190364	1.929487
N	4.750637	-2.446040	1.280998
H	7.563521	-3.530337	2.803102
H	5.878550	-4.847563	4.075066
H	3.457557	-4.670274	3.442231
H	2.813195	-3.080280	1.591668
H	10.102620	-1.026436	-0.353772

NRB-1 E(I) = -3899.87535788 / E(II) = -3900.80872769

Mn	-5.039702	-0.558760	-0.594328
Mn	-3.009991	0.425333	1.057250
O	-4.753314	0.674982	0.923069
O	-2.804934	1.582120	2.593805
O	-3.241147	-0.756267	-0.364271
N	-1.044986	0.054990	0.981498
C	1.600334	-0.645696	0.624415
C	1.059703	0.484349	-0.027658
H	1.703744	1.109437	-0.631671
C	-0.279579	0.813212	0.171394
C	-0.563182	-1.011064	1.648590
C	0.764607	-1.396192	1.478215
H	1.160100	-2.266566	1.985153
C	-3.788947	-1.366717	3.325592
N	-2.812418	-1.038131	2.456918
C	-1.566996	-1.603810	2.551731
C	-1.312434	-2.583323	3.512949
C	-2.330058	-2.952213	4.399503
C	-3.578497	-2.327880	4.316220
H	-4.723231	-0.834504	3.208717
H	-0.328164	-3.026998	3.591782
H	-2.140377	-3.701160	5.159758
H	-4.374766	-2.570218	5.008534
C	-1.008159	1.982766	-0.353753
C	-0.423630	3.060682	-1.021183
C	-1.215178	4.162421	-1.362054
C	-2.571371	4.170743	-1.022801
C	-3.110423	3.065679	-0.362033
N	-2.347838	1.996935	-0.052215
H	0.639623	3.065406	-1.224756
H	-0.769953	5.012515	-1.865925

H	-3.202438	5.020347	-1.251127
H	-4.147223	3.008196	-0.058393
C	3.024712	-0.994538	0.443465
C	3.649438	-0.829985	-0.808024
C	5.010868	-1.081261	-0.966100
C	5.769145	-1.485724	0.138231
C	5.161858	-1.680599	1.383143
C	3.795570	-1.446028	1.532481
H	3.065506	-0.520209	-1.668368
H	5.492208	-0.956349	-1.927973
H	5.756913	-1.999244	2.230267
H	3.341813	-1.556739	2.511601
C	9.482674	-0.699907	-0.470738
C	7.973503	-0.513018	-0.304119
N	7.201993	-1.665203	0.002408
C	7.725408	-2.974051	0.171620
C	9.246026	-3.153383	0.115963
C	9.941526	-1.828202	0.474532
H	9.728954	-1.554956	1.516849
O	6.950121	-3.926496	0.351434
O	7.417001	0.592185	-0.407940
C	9.834841	-1.074952	-1.949912
H	9.406721	-0.324857	-2.622016
H	10.926592	-0.998550	-2.026650
C	9.666885	-3.574778	-1.325818
H	10.742923	-3.785509	-1.287601
H	9.161349	-4.502583	-1.606103
C	9.425822	-2.490926	-2.413682
C	8.027881	-2.531050	-3.002858
O	7.677237	-3.802088	-3.385668
O	7.279953	-1.562963	-3.186923
H	6.783666	-3.818579	-3.791915
C	9.642604	-4.273317	1.100662
H	10.722501	-4.448425	1.046584
H	9.392057	-3.996903	2.130723
H	9.118272	-5.201693	0.863013
C	10.182904	0.628957	-0.120579
H	11.267643	0.510334	-0.215594
H	9.854753	1.431162	-0.785742
H	9.957911	0.933044	0.906854
H	-1.532597	2.609856	2.774002
C	2.465916	3.563012	2.192538
C	3.429269	2.556745	2.011708
C	4.247934	2.539947	0.876652
C	4.125764	3.521743	-0.123621
C	3.149836	4.520808	0.054207

C	2.337118	4.543479	1.193264
H	3.546633	1.781363	2.760762
H	5.001431	1.765975	0.763998
H	3.043953	5.302430	-0.694602
H	1.603978	5.336058	1.317109
C	1.565042	3.609027	3.432454
H	1.119241	4.606352	3.484554
C	5.036873	3.521506	-1.335031
H	4.443269	3.718578	-2.239905
H	5.488302	2.528142	-1.454097
C	0.410031	2.627624	3.258300
O	-0.740928	3.239077	2.883403
O	0.508140	1.395158	3.410785
C	2.314237	3.319114	4.749533
H	1.657610	3.490053	5.609262
H	2.651063	2.279676	4.789821
H	3.183431	3.976744	4.842074
C	7.147800	4.305211	-0.106322
C	6.187458	4.570916	-1.280511
H	6.630595	4.362602	0.857627
H	7.591201	3.305302	-0.192213
H	7.959115	5.042929	-0.096687
C	6.947091	4.582631	-2.621028
H	5.728598	5.562044	-1.135832
H	6.276763	4.801634	-3.461582
H	7.739336	5.340140	-2.615785
H	7.415425	3.607486	-2.807519
H	10.070220	-2.762315	-3.264059
H	11.028266	-1.954969	0.393246
S	-6.579589	-2.188862	-2.874877
O	-7.491927	-2.758407	-1.816705
O	-5.997309	-3.159336	-3.839525
O	-7.063504	-0.879882	-3.449064
O	-5.174217	-1.718150	-1.963685
N	-6.961859	-0.037770	-0.490286
C	-9.534099	0.815673	-0.173092
C	-8.682898	1.495445	-1.052057
H	-9.040543	2.349353	-1.612233
C	-7.372826	1.031383	-1.201411
C	-7.766670	-0.729763	0.340691
C	-9.086495	-0.309269	0.529112
H	-9.755319	-0.846216	1.188784
C	-5.098022	-3.151843	0.877281
N	-5.782010	-2.025812	0.598262
C	-7.111183	-1.922255	0.902429
C	-7.759538	-2.945572	1.594601

C	-7.047995	-4.103758	1.919552
C	-5.705748	-4.216771	1.543468
H	-4.072546	-3.181724	0.533377
H	-8.814168	-2.866204	1.824911
H	-7.546056	-4.920594	2.428976
H	-5.142209	-5.120208	1.739495
C	-6.336748	1.533957	-2.118652
C	-6.545787	2.463071	-3.138457
C	-5.513152	2.722660	-4.043589
C	-4.294781	2.048505	-3.912550
C	-4.129284	1.149941	-2.858204
N	-5.118833	0.929869	-1.971122
H	-7.514128	2.931043	-3.260804
H	-5.670929	3.416953	-4.860839
H	-3.492978	2.194992	-4.625167
H	-3.224720	0.574560	-2.711571
H	-10.555307	1.155243	-0.046041

NRB-TS1 E(I) = -3899.86601294 / E(II) = -3900.80189074

Mn	-4.878249	-0.823897	-0.451432
Mn	-2.919473	0.711928	0.830566
O	-4.671425	0.809698	0.648969
O	-2.882943	2.279339	1.940934
O	-3.074056	-0.833169	-0.211049
N	-0.947152	0.370064	0.853806
C	1.704671	-0.389117	0.680257
C	1.142005	0.500005	-0.262225
H	1.767287	0.926354	-1.034288
C	-0.198286	0.861695	-0.151630
C	-0.449473	-0.458083	1.791492
C	0.882404	-0.866807	1.723739
H	1.284581	-1.560832	2.450320
C	-3.671209	-0.390456	3.506409
N	-2.701549	-0.310155	2.576068
C	-1.442613	-0.785491	2.831264
C	-1.165391	-1.428180	4.039225
C	-2.176089	-1.543939	4.999634
C	-3.439689	-1.005825	4.738511
H	-4.618947	0.057428	3.240212
H	-0.169834	-1.802158	4.242344
H	-1.970054	-2.027759	5.947483
H	-4.232409	-1.051101	5.474478
C	-0.946784	1.806831	-1.000766
C	-0.381537	2.643129	-1.964845
C	-1.194290	3.570293	-2.625771
C	-2.551823	3.650250	-2.304009

C	-3.069160	2.788345	-1.335507
N	-2.286387	1.882951	-0.715586
H	0.681960	2.606671	-2.163343
H	-0.764340	4.236417	-3.364775
H	-3.199972	4.376428	-2.777922
H	-4.105271	2.807968	-1.025166
C	3.129727	-0.771355	0.582991
C	3.753180	-0.895831	-0.674590
C	5.110385	-1.194827	-0.776333
C	5.867302	-1.365040	0.387828
C	5.264509	-1.265187	1.645747
C	3.903775	-0.976953	1.742456
H	3.170481	-0.783793	-1.582621
H	5.588725	-1.293913	-1.742717
H	5.859032	-1.400885	2.541031
H	3.457120	-0.862618	2.724403
C	9.606099	-0.869997	-0.362466
C	8.106995	-0.591514	-0.242471
N	7.291356	-1.623220	0.293426
C	7.759806	-2.897972	0.707720
C	9.271167	-3.149562	0.690415
C	10.023425	-1.810492	0.785624
H	9.828390	-1.330732	1.754231
O	6.945641	-3.764881	1.063232
O	7.593744	0.488540	-0.575344
C	9.932748	-1.540449	-1.739624
H	9.528024	-0.919662	-2.544964
H	11.025955	-1.522314	-1.830856
C	9.666518	-3.862440	-0.639372
H	10.732617	-4.107815	-0.556435
H	9.120423	-4.804751	-0.734550
C	9.467769	-3.003110	-1.919577
C	8.068870	-3.105875	-2.498033
O	7.681220	-4.414302	-2.650101
O	7.347827	-2.164966	-2.852170
H	6.786362	-4.477400	-3.048856
C	9.625873	-4.071537	1.876219
H	10.697994	-4.295394	1.862574
H	9.388804	-3.590514	2.831498
H	9.065231	-5.007472	1.821081
C	10.363003	0.470982	-0.276111
H	11.441108	0.290260	-0.345015
H	10.064158	1.142763	-1.084188
H	10.158565	0.977574	0.672867
H	-2.503995	3.342340	1.613839
C	1.690408	4.471023	1.203543

C	2.523686	3.407094	1.589197
C	3.598733	3.011499	0.786526
C	3.880012	3.656195	-0.432551
C	3.035771	4.713814	-0.819697
C	1.963204	5.115422	-0.015891
H	2.328484	2.882364	2.518355
H	4.236866	2.194557	1.109988
H	3.232137	5.238899	-1.751143
H	1.336962	5.945930	-0.330909
C	0.526507	4.941465	2.074264
H	0.129642	5.865454	1.643710
C	5.064013	3.249091	-1.287140
H	4.756899	3.223226	-2.342836
H	5.390473	2.234655	-1.023798
C	-0.637648	3.944479	2.022997
O	-1.731819	4.328119	1.424080
O	-0.526507	2.783087	2.549474
C	0.929861	5.207201	3.543046
H	0.081553	5.606507	4.109013
H	1.261619	4.288461	4.034261
H	1.743885	5.937471	3.578458
C	6.900434	4.178299	0.244092
C	6.297584	4.195226	-1.172760
H	6.166961	4.476600	1.001365
H	7.261704	3.171630	0.489985
H	7.750475	4.867885	0.310135
C	7.356391	3.801265	-2.220977
H	5.953837	5.218922	-1.390940
H	6.950025	3.850558	-3.239021
H	8.221570	4.473024	-2.171992
H	7.707097	2.777781	-2.040724
H	10.100330	-3.460590	-2.695632
H	11.103650	-1.995097	0.733309
S	-6.309033	-3.124374	-2.150600
O	-7.174412	-3.435970	-0.954827
O	-5.660806	-4.284145	-2.819108
O	-6.886946	-2.064902	-3.056002
O	-4.935238	-2.324294	-1.440098
N	-6.831706	-0.413857	-0.449607
C	-9.450415	0.340924	-0.312394
C	-8.651368	0.802189	-1.365067
H	-9.067082	1.447241	-2.127921
C	-7.315654	0.393079	-1.415036
C	-7.583609	-0.896125	0.559968
C	-8.926111	-0.519261	0.659369
H	-9.553792	-0.892833	1.457646

C	-4.758585	-2.909820	1.672898
N	-5.516529	-1.946512	1.115629
C	-6.847888	-1.845970	1.410972
C	-7.423191	-2.679284	2.370727
C	-6.635035	-3.659089	2.980954
C	-5.290905	-3.788447	2.617259
H	-3.735780	-2.967687	1.324922
H	-8.479316	-2.605354	2.596121
H	-7.075382	-4.334914	3.704954
H	-4.668354	-4.568192	3.037476
C	-6.321961	0.682627	-2.462021
C	-6.599381	1.279142	-3.692489
C	-5.595439	1.333751	-4.663319
C	-4.337450	0.789132	-4.386261
C	-4.104934	0.229948	-3.129232
N	-5.067631	0.212341	-2.187758
H	-7.595555	1.641514	-3.911541
H	-5.804925	1.764859	-5.635471
H	-3.554948	0.774937	-5.134354
H	-3.165911	-0.231891	-2.854416
H	-10.490080	0.641530	-0.257254

NRB-2 E(I) = -3899.87091421 / E(II) = -3900.80670140

Mn	-4.909966	-0.778600	-0.504892
Mn	-2.881201	0.527732	0.920221
O	-4.639819	0.680534	0.790635
O	-2.680483	1.884499	2.269691
O	-3.096909	-0.845706	-0.325241
N	-0.916410	0.141457	0.858702
C	1.746694	-0.543843	0.616655
C	1.173190	0.436195	-0.222627
H	1.797178	0.961756	-0.931973
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H	1.343885	-1.922348	2.234124
C	-3.620046	-0.932327	3.431175
N	-2.659610	-0.734391	2.508969
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C	-1.117839	-2.047720	3.793778
C	-2.120360	-2.285889	4.740182
C	-3.381508	-1.708586	4.567686
H	-4.567591	-0.447799	3.238753
H	-0.123950	-2.453778	3.933642
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H	-4.167448	-1.847075	5.299281

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C	-2.526483	3.813323	-1.841288
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N	-2.257904	1.875561	-0.466575
H	0.689777	2.712238	-1.896236
H	-0.752368	4.488278	-2.870132
H	-3.172027	4.598130	-2.214264
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C	3.183305	-0.875088	0.500941
C	3.820794	-0.882753	-0.755520
C	5.186644	-1.138456	-0.864196
C	5.938048	-1.376295	0.292178
C	5.321265	-1.388361	1.547494
C	3.952003	-1.147540	1.649947
H	3.242856	-0.714724	-1.658157
H	5.675022	-1.153884	-1.830304
H	5.910308	-1.575835	2.436800
H	3.491830	-1.122946	2.632115
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N	7.369067	-1.588202	0.194187
C	7.877401	-2.857331	0.579138
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C	10.108943	-1.705953	0.684554
H	9.902649	-1.259877	1.666806
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H	10.878844	-3.944320	-0.725244
H	9.285937	-4.680568	-0.918746
C	9.578391	-2.836513	-2.051786
C	8.179935	-2.956893	-2.628711
O	7.817074	-4.269655	-2.803311
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H	6.923325	-4.342215	-3.202996
C	9.780715	-4.007005	1.711513
H	10.858433	-4.201136	1.687429
H	9.535415	-3.558617	2.680529
H	9.245402	-4.955966	1.633058
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H	11.462066	0.465916	-0.385980

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H	10.161048	1.086755	0.651090
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C	1.904275	5.185152	0.201451
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H	3.221738	5.434313	-1.483527
H	1.295650	6.046408	-0.061859
C	0.410615	4.866418	2.228744
H	0.022309	5.817494	1.849852
C	5.021534	3.393946	-1.134359
H	4.747668	3.467182	-2.196734
H	5.326380	2.354872	-0.953841
C	-0.795076	3.909382	2.109241
O	-1.922969	4.338448	1.728467
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H	-0.077974	5.395973	4.294493
H	1.132227	4.107859	4.159676
H	1.585322	5.789490	3.811059
C	6.822399	4.153493	0.527860
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H	6.071538	4.397244	1.287664
H	7.160596	3.122600	0.693076
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C	7.348106	3.993445	-1.947065
H	5.938497	5.351110	-1.033201
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H	10.218908	-3.254343	-2.843648
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C	-7.582182	-0.962133	0.577671
C	-8.914280	-0.587062	0.775164
H	-9.521852	-1.061433	1.534561
C	-4.758454	-3.149485	1.293577
N	-5.516130	-2.104816	0.907948
C	-6.835654	-2.032164	1.259228
C	-7.395029	-2.988191	2.107778
C	-6.605639	-4.056380	2.542279
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H	-3.748186	-3.170678	0.906848
H	-8.442285	-2.934382	2.376094
H	-7.034740	-4.825010	3.174673
H	-4.654985	-4.990026	2.398481
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C	-6.704000	1.769745	-3.364533
C	-5.733674	1.944028	-4.355105
C	-4.477070	1.349782	-4.201699
C	-4.210524	0.621616	-3.041701
N	-5.140046	0.487292	-2.076442
H	-7.700662	2.171214	-3.495328
H	-5.968933	2.507280	-5.250768
H	-3.721455	1.427630	-4.973162
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H	-10.487947	0.708463	0.083373

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N	1.056394	0.460827	0.335519
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C	-0.755721	-0.648624	1.402644
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C	0.517967	-0.084311	1.447892
C	0.405410	0.479163	-0.847634
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H	-1.394391	-0.082552	-1.897786
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N	2.482874	1.424291	-1.556931
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C	0.704642	1.489332	-3.169515
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C	2.828182	2.537944	-3.644278

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H	-0.313700	1.250027	-3.449343
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H	3.483313	3.111068	-4.288142
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C	1.930585	0.091234	4.974191
C	3.186363	0.618845	4.660046
C	3.519360	0.823303	3.318833
N	2.654263	0.523987	2.331182
H	0.036105	-0.566858	4.171867
H	1.647166	-0.077703	6.006643
H	3.897040	0.875674	5.435396
H	4.468542	1.235991	3.004758
C	-2.828629	-1.236818	0.103656
C	-3.154587	-2.401877	0.826309
C	-4.425597	-2.965172	0.733898
C	-5.402689	-2.359184	-0.066557
C	-5.096288	-1.196132	-0.785038
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H	-2.401307	-2.898419	1.429075
H	-4.658861	-3.866073	1.284777
H	-5.851290	-0.729431	-1.400531
H	-3.612299	0.272302	-1.244018
C	-8.664999	-3.763261	-1.558608
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N	-6.730532	-2.928303	-0.154939
C	-7.433631	-3.177227	1.060522
C	-8.835809	-3.785267	0.967895
C	-8.956571	-4.625165	-0.315885
H	-8.267954	-5.480159	-0.278789
O	-6.909138	-2.891034	2.147350
O	-6.531539	-3.016610	-2.453953
C	-9.691096	-2.582991	-1.631959
H	-9.425791	-1.923167	-2.463004
H	-10.660846	-3.038267	-1.868747
C	-9.895010	-2.637751	0.935084
H	-10.878055	-3.122879	0.983606
H	-9.790636	-2.012234	1.824987
C	-9.854231	-1.755518	-0.337400
C	-8.882437	-0.589961	-0.246822
O	-8.796126	-0.040141	0.963901
O	-8.268901	-0.136993	-1.251171
H	-8.180444	0.781775	1.013368
C	-9.078587	-4.652414	2.220471
H	-10.091086	-5.069158	2.189466

H	-8.367206	-5.484235	2.266889
H	-8.964694	-4.060142	3.131194
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H	-9.793038	-5.000269	-2.940563
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H	-8.074769	-5.438072	-2.836932
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C	-5.781035	3.717874	0.105366
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C	-4.800757	5.446369	1.500345
C	-4.171776	6.035837	0.387060
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C	-5.160400	4.292142	-1.019065
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H	-4.680086	5.879070	2.484962
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O	-6.717677	1.997382	-1.247246
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H	-9.971315	-5.036434	-0.386212
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O	7.640209	-2.488453	-1.938028
O	6.603716	-4.638520	-1.049884
O	7.782206	-3.022381	0.525947
O	5.526746	-2.445826	-0.513458
N	7.107794	-0.086005	-0.092280
C	9.606243	1.005971	0.000444
C	9.044355	0.463913	1.162352
H	9.597183	0.467127	2.092514
C	7.765982	-0.096562	1.083558
C	7.633848	0.402349	-1.232807
C	8.908966	0.975095	-1.213026
H	9.357863	1.372285	-2.113957
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N	5.525909	-0.316717	-2.086898
C	6.758947	0.186659	-2.397741
C	7.138050	0.354369	-3.730074
C	6.267352	-0.059467	-4.742023
C	5.037941	-0.633328	-4.402499
H	3.773329	-1.203880	-2.717292
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H	6.561892	0.032471	-5.781099
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C	7.019284	-0.794068	2.144266
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C	6.782676	-1.994773	4.217892
C	5.512522	-2.411725	3.807286
C	5.022096	-1.972463	2.577110
N	5.749719	-1.158009	1.789152
H	8.554030	-0.897820	3.653140
H	7.190854	-2.329343	5.164653
H	4.918762	-3.083138	4.414651
H	4.059927	-2.273595	2.184349
H	10.598208	1.440707	0.037447
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H	-3.986259	8.144125	-1.423692
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H	-3.300619	9.334708	-0.304992
C	-3.189014	7.813247	1.953584
H	-2.730794	7.067874	2.613992
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H	-4.168619	8.084305	2.362975
C	-1.865358	6.986042	-0.014941
H	-1.399478	6.196148	0.585934
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H	-1.237752	7.882237	0.053569

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O	0.703617	-2.207197	0.032560
N	2.641045	-0.305153	-0.131117
C	5.362447	-0.820241	-0.204986
C	4.602091	-0.759998	-1.395246
H	5.093355	-0.900062	-2.349160
C	3.234272	-0.502457	-1.327847
C	3.325639	-0.358394	1.031571
C	4.697112	-0.608493	1.024298
H	5.250844	-0.686623	1.950777
C	0.226915	0.254160	2.864975
N	1.121931	-0.074817	1.914067
C	2.459800	-0.125539	2.203986
C	2.911703	0.106928	3.504688
C	1.984248	0.423552	4.503291
C	0.627521	0.511978	4.178221
H	-0.803528	0.311077	2.541177
H	3.970093	0.068250	3.730394

H	2.321286	0.615771	5.515394
H	-0.111692	0.779547	4.922677
C	2.286195	-0.380149	-2.452290
C	2.642823	-0.288974	-3.799302
C	1.647003	-0.061326	-4.755334
C	0.318871	0.081239	-4.343672
C	0.014271	-0.033857	-2.985000
N	0.974269	-0.277378	-2.072518
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H	1.910429	0.022009	-5.803458
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C	6.810546	-1.102643	-0.246717
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C	8.708799	-2.261590	-1.241444
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H	9.727335	-0.246054	1.305964
H	7.320308	0.234773	1.383677
C	13.157017	-2.543048	0.740779
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N	10.998590	-1.877390	-0.403283
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C	13.539150	-3.028292	-0.669821
H	13.044004	-3.984422	-0.887200
O	11.008620	-1.310797	-2.642620
O	10.981299	-2.482857	1.824728
C	13.917723	-1.213233	1.061725
H	13.582506	-0.826931	2.028574
H	14.975866	-1.484872	1.162897
C	13.946949	-0.657578	-1.452521
H	15.005288	-0.887317	-1.628898
H	13.649669	0.107671	-2.173757
C	13.806929	-0.106974	-0.011642
C	12.600647	0.795925	0.189336
O	12.281206	1.537591	-0.871049
O	12.001250	0.886136	1.294935
H	11.493798	2.179342	-0.717015
C	13.497317	-2.475231	-3.147539
H	14.574748	-2.655934	-3.227060
H	12.975440	-3.412233	-3.370519
H	13.203001	-1.738686	-3.898550

C	13.526980	-3.595213	1.805530
H	14.607328	-3.774838	1.786454
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H	13.016190	-4.544574	1.613327
H	10.802394	1.909604	1.659348
C	8.497397	4.108567	0.876763
C	8.029948	4.839286	-0.226292
C	6.936749	5.696283	-0.091882
C	6.280189	5.856179	1.143353
C	6.767420	5.115977	2.242999
C	7.854801	4.255351	2.119559
H	8.533611	4.728935	-1.179902
H	6.601901	6.247335	-0.961086
H	6.295291	5.222684	3.213743
H	8.223642	3.702469	2.975160
C	5.077337	6.802479	1.331033
C	9.650751	3.213566	0.710705
O	9.991545	2.506254	1.805607
O	10.276043	3.106920	-0.380615
H	14.654611	0.581339	0.143003
H	14.619894	-3.212687	-0.713113
S	-2.178881	-5.522671	0.299812
O	-2.879688	-5.161430	1.585483
O	-1.377041	-6.776382	0.314280
O	-3.005205	-5.269550	-0.935492
O	-0.918465	-4.322331	0.186165
N	-3.057821	-2.397758	0.192026
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C	-5.112336	-2.081261	-0.952663
H	-5.680701	-2.051724	-1.872802
C	-3.743893	-2.338734	-0.967472
C	-3.651773	-2.265611	1.395005
C	-5.019871	-2.014883	1.470416
H	-5.506473	-1.880798	2.427465
C	-0.454642	-2.951155	3.003869
N	-1.402896	-2.578523	2.122587
C	-2.709404	-2.461290	2.509746
C	-3.066334	-2.627220	3.848408
C	-2.082467	-2.979086	4.776106
C	-0.763098	-3.159857	4.348279
H	0.537490	-3.095818	2.597007
H	-4.102073	-2.541882	4.151227
H	-2.350558	-3.144435	5.813317
H	0.010878	-3.479439	5.034648
C	-2.897590	-2.643783	-2.133791
C	-3.366051	-2.926513	-3.417606

C	-2.465610	-3.379675	-4.385413
C	-1.117474	-3.544549	-4.050839
C	-0.697042	-3.219316	-2.761052
N	-1.565024	-2.749499	-1.844440
H	-4.422903	-2.854605	-3.640324
H	-2.820353	-3.636202	-5.377064
H	-0.406476	-3.940885	-4.764781
H	0.322983	-3.347548	-2.423581
C	5.440292	7.889550	2.381651
H	5.690669	7.449135	3.352474
H	6.298520	8.483370	2.048278
H	4.591100	8.567313	2.527944
C	4.676672	7.511838	0.017496
H	4.387023	6.794856	-0.759518
H	3.817717	8.165587	0.203196
H	5.489053	8.135705	-0.371616
C	3.853206	5.988430	1.836414
H	3.569680	5.217318	1.110192
H	4.059333	5.497647	2.793568
H	2.994610	6.654940	1.979366
C	-7.223508	-1.620778	0.328655
C	-8.039998	-2.185463	1.327551
C	-9.405368	-1.909157	1.371394
C	-9.974152	-1.043800	0.428813
C	-9.175796	-0.475276	-0.571199
C	-7.815216	-0.769197	-0.624113
H	-7.616744	-2.876947	2.048480
H	-10.022895	-2.356621	2.138529
H	-9.616207	0.186417	-1.302866
H	-7.205585	-0.296550	-1.387096
C	-13.648317	-0.589396	-0.647255
C	-12.164544	-0.959848	-0.690197
N	-11.389004	-0.732209	0.485862
C	-11.912580	-0.232980	1.713441
C	-13.410167	0.083239	1.781417
C	-14.175824	-0.803084	0.783496
H	-14.084565	-1.860820	1.064980
O	-11.159498	-0.056707	2.682969
O	-11.629797	-1.440524	-1.699059
C	-13.838934	0.908440	-1.059515
H	-13.382673	1.076829	-2.039322
H	-14.920132	1.060058	-1.168210
C	-13.639282	1.584486	1.417781
H	-14.704574	1.785492	1.587968
H	-13.068825	2.221090	2.098590
C	-13.307629	1.951477	-0.049640

C	-11.849072	2.311924	-0.282170
O	-11.259241	2.926886	0.743040
O	-11.271921	2.112355	-1.385139
H	-10.286638	3.205771	0.565630
C	-13.897315	-0.161417	3.224408
H	-14.960119	0.092351	3.303945
H	-13.773586	-1.212474	3.507190
H	-13.331052	0.446858	3.933272
C	-14.404162	-1.480679	-1.652939
H	-15.468842	-1.223184	-1.646921
H	-14.010495	-1.348322	-2.663287
H	-14.303556	-2.539219	-1.391251
H	-9.780125	2.580351	-1.790811
C	-6.818792	3.824522	-1.121609
C	-6.093828	4.381691	-0.057342
C	-4.771188	4.787346	-0.241029
C	-4.132792	4.657304	-1.489241
C	-4.878463	4.094728	-2.548288
C	-6.196759	3.682002	-2.375066
H	-6.579720	4.494390	0.905158
H	-4.240040	5.214471	0.599785
H	-4.424304	3.986880	-3.527565
H	-6.758323	3.260820	-3.200234
C	-2.682587	5.120678	-1.735944
C	-8.214120	3.414793	-0.906897
O	-8.810310	2.834229	-1.965326
O	-8.812217	3.592122	0.190520
H	-13.828760	2.900448	-0.260106
H	-15.243880	-0.553755	0.821303
C	-2.686205	6.243503	-2.811360
H	-3.105124	5.894559	-3.761109
H	-3.278326	7.102445	-2.476370
H	-1.661613	6.586231	-2.999259
C	-2.017062	5.675964	-0.456344
H	-1.967351	4.918701	0.334256
H	-0.991096	5.984469	-0.684721
H	-2.549353	6.552153	-0.069278
C	-1.828817	3.924424	-2.242755
H	-1.768935	3.133750	-1.486590
H	-2.240986	3.496128	-3.163410
H	-0.807197	4.261652	-2.455002

HP2-1

Mn	0.946342	-2.546939	0.045291
Mn	-0.814723	-0.369500	0.022935
O	0.926728	-0.532295	-0.040530

O	-0.698534	1.514736	-0.032335
O	-0.840727	-2.256896	0.100072
N	-2.823390	-0.381092	0.079057
C	-5.555029	-0.828637	0.163500
C	-4.804348	-0.697841	1.353747
H	-5.308417	-0.747117	2.309934
C	-3.431010	-0.473819	1.281364
C	-3.497771	-0.512188	-1.083238
C	-4.873488	-0.733694	-1.070706
H	-5.421701	-0.865950	-1.994034
C	-0.384313	-0.040334	-2.933133
N	-1.286097	-0.294115	-1.965341
C	-2.621306	-0.375683	-2.262301
C	-3.061981	-0.255360	-3.581831
C	-2.126871	-0.019671	-4.595479
C	-0.773959	0.103027	-4.267001
H	0.642653	0.053500	-2.607538
H	-4.117947	-0.318506	-3.813060
H	-2.455649	0.085045	-5.623022
H	-0.029160	0.312384	-5.024319
C	-2.494386	-0.262812	2.402253
C	-2.864047	-0.077824	3.736165
C	-1.880688	0.236905	4.680354
C	-0.551505	0.371680	4.269436
C	-0.233066	0.158816	2.925888
N	-1.180464	-0.169439	2.026979
H	-3.903603	-0.149933	4.030686
H	-2.154812	0.393554	5.717283
H	0.228468	0.640193	4.970666
H	0.772249	0.251288	2.537930
C	-7.013192	-1.050876	0.205352
C	-7.598178	-1.835194	1.219413
C	-8.976205	-2.036897	1.258529
C	-9.796429	-1.442880	0.291349
C	-9.230116	-0.663211	-0.724548
C	-7.851667	-0.473661	-0.768675
H	-6.973539	-2.324121	1.959707
H	-9.412490	-2.645692	2.039100
H	-9.865389	-0.212016	-1.472470
H	-7.437020	0.170388	-1.536678
C	-13.396677	-2.276544	-0.793349
C	-11.874279	-2.141502	-0.824211
N	-11.232137	-1.624211	0.341271
C	-11.905420	-1.272534	1.546222
C	-13.422327	-1.473100	1.607690
C	-13.840223	-2.598771	0.645884

H	-13.407998	-3.555716	0.968019
O	-11.263307	-0.806318	2.499958
O	-11.195436	-2.461416	-1.809635
C	-14.063492	-0.940474	-1.263939
H	-13.668774	-0.666431	-2.246601
H	-15.131005	-1.161467	-1.387422
C	-14.134515	-0.147815	1.189155
H	-15.207200	-0.305912	1.357487
H	-13.815110	0.667862	1.842762
C	-13.933322	0.255793	-0.294501
C	-12.689773	1.094507	-0.537974
O	-12.438607	1.989235	0.419967
O	-11.999701	1.006244	-1.588856
H	-11.644464	2.603282	0.224018
C	-13.814527	-1.812780	3.060511
H	-14.901676	-1.925580	3.131923
H	-13.350667	-2.751409	3.382666
H	-13.491946	-1.024868	3.744840
C	-13.808002	-3.403103	-1.762591
H	-14.897787	-3.513318	-1.758654
H	-13.475361	-3.183694	-2.779774
H	-13.363561	-4.358448	-1.464677
H	-10.757860	1.951189	-2.031195
C	-7.348232	4.086059	-0.811280
C	-7.356543	3.867547	0.576073
C	-6.161433	3.636020	1.264702
C	-4.922836	3.624346	0.599503
C	-4.924822	3.826333	-0.792844
C	-6.117518	4.049161	-1.487434
H	-8.297315	3.882240	1.116518
H	-6.190177	3.477259	2.339286
H	-3.981617	3.823919	-1.333722
H	-6.091829	4.213624	-2.561416
C	-8.625053	4.444300	-1.579849
H	-8.416631	4.344964	-2.649056
C	-3.618351	3.443171	1.350650
H	-2.959569	2.762352	0.792910
H	-3.815322	2.973867	2.326232
C	-9.749011	3.478261	-1.274295
O	-9.968771	2.563517	-2.231419
O	-10.424519	3.529668	-0.214799
C	-9.076123	5.894466	-1.275729
H	-9.949205	6.169205	-1.877543
H	-9.338841	5.998958	-0.219742
H	-8.262897	6.588624	-1.506154
C	-3.602299	5.750250	2.483155

C	-2.825338	4.761690	1.595616
H	-4.577895	6.000303	2.053602
H	-3.771186	5.325456	3.482428
H	-3.039679	6.682472	2.609732
C	-1.442393	4.441063	2.195238
H	-2.668267	5.232726	0.612841
H	-0.883217	3.752182	1.551366
H	-0.850467	5.354987	2.323096
H	-1.549618	3.975255	3.185443
H	-14.747685	0.959312	-0.534826
H	-14.930760	-2.715641	0.675336
S	2.112495	-5.518469	0.126997
O	2.819299	-5.258590	-1.179588
O	1.334344	-6.783827	0.217261
O	2.921218	-5.141064	1.342190
O	0.829360	-4.336927	0.123637
N	2.926979	-2.376576	-0.035755
C	5.644122	-1.888516	-0.156235
C	4.976869	-1.962671	1.086057
H	5.541841	-1.865705	2.003444
C	3.608858	-2.219579	1.117236
C	3.524915	-2.338041	-1.243559
C	4.891842	-2.086252	-1.334292
H	5.380210	-2.028176	-2.297999
C	0.348267	-3.219676	-2.796411
N	1.284806	-2.752527	-1.948311
C	2.590201	-2.640209	-2.341101
C	2.955160	-2.909349	-3.660861
C	1.982339	-3.358784	-4.557608
C	0.665935	-3.533302	-4.118069
H	-0.641401	-3.353483	-2.379940
H	3.989808	-2.827007	-3.968129
H	2.257402	-3.603871	-5.577072
H	-0.098221	-3.926971	-4.776382
C	2.761661	-2.436865	2.302430
C	3.227667	-2.603135	3.607301
C	2.329565	-2.988785	4.606008
C	0.985914	-3.202961	4.281256
C	0.566920	-2.992573	2.967553
N	1.432242	-2.586901	2.018229
H	4.281857	-2.494915	3.827707
H	2.683271	-3.155706	5.616966
H	0.277675	-3.550213	5.022940
H	-0.449452	-3.163514	2.638041
C	7.098665	-1.632508	-0.214834
C	7.902929	-2.273510	-1.177612

C	9.278479	-2.054569	-1.213708
C	9.870629	-1.178033	-0.297142
C	9.084843	-0.523795	0.657797
C	7.711566	-0.755549	0.700963
H	7.461914	-2.983044	-1.869619
H	9.890154	-2.563086	-1.947952
H	9.547469	0.151975	1.362786
H	7.111253	-0.220171	1.428795
C	13.559502	-1.061729	0.807363
C	12.045089	-1.275951	0.846340
N	11.303845	-0.962691	-0.330664
C	11.869549	-0.451583	-1.529474
C	13.393470	-0.304103	-1.601452
C	14.059028	-1.294700	-0.630565
H	13.850326	-2.328115	-0.938518
O	11.131928	-0.133932	-2.476078
O	11.459569	-1.711496	1.847041
C	13.912223	0.393715	1.258954
H	13.463852	0.585508	2.238286
H	15.001891	0.415452	1.386485
C	13.796284	1.150941	-1.207501
H	14.875043	1.234260	-1.388988
H	13.295834	1.867385	-1.864202
C	13.527298	1.521235	0.275954
C	12.138596	2.087407	0.515850
O	11.758888	2.981383	-0.399717
O	11.440747	1.801154	1.525105
H	10.864209	3.435946	-0.199701
C	13.840193	-0.568111	-3.054847
H	14.924147	-0.433581	-3.138963
H	13.597658	-1.592013	-3.359875
H	13.340714	0.116317	-3.744282
C	14.215893	-2.055496	1.787455
H	15.302479	-1.916741	1.781669
H	13.842094	-1.904696	2.802822
H	13.998347	-3.089908	1.501666
H	10.041718	2.487822	1.970881
C	6.379145	4.148820	0.746787
C	6.479673	4.043848	-0.650030
C	5.369179	3.673849	-1.414758
C	4.125024	3.407160	-0.817385
C	4.037352	3.496822	0.583168
C	5.146447	3.858108	1.353328
H	7.426652	4.249442	-1.137858
H	5.468956	3.597740	-2.493866
H	3.089752	3.284986	1.072045

H	5.052979	3.924896	2.434134
C	7.549853	4.639739	1.605344
H	7.319362	4.420468	2.651889
C	2.900934	3.072541	-1.646322
H	2.315004	2.295087	-1.136596
H	3.213027	2.657997	-2.616488
C	8.823938	3.890535	1.283332
O	9.161500	2.955077	2.183189
O	9.512441	4.128824	0.257830
C	7.774042	6.162975	1.435496
H	8.565292	6.521509	2.103097
H	8.060629	6.393701	0.406071
H	6.850330	6.699061	1.671793
C	2.644935	5.375342	-2.761589
C	1.961293	4.287160	-1.914232
H	3.556351	5.748411	-2.283405
H	2.918523	4.982978	-3.750877
H	1.971654	6.226831	-2.915939
C	0.653231	3.810771	-2.575037
H	1.707008	4.723227	-0.935759
H	0.128662	3.090931	-1.935645
H	-0.019430	4.656555	-2.763172
H	0.862794	3.334552	-3.544180
H	14.177340	2.383728	0.496016
H	15.148011	-1.164638	-0.667337