

**Tables of Cartesian Coordinates (Å)
and Computed Energies (a.u.) for all
Stationary at the ωB97X-D/BS1(SMD)
level of theory.**

1_{C2}⁺

Energy = -4902.656669
Enthalpy 0K = -4902.314953
Enthalpy 298K = -4902.287725
Free Energy 298K = -4902.372191
Nimag = 0 (30.5366 cm⁻¹)

N -4.15460 -0.19417 -0.99394
C -5.03107 -0.44556 0.03727
C -4.42048 -0.04218 1.18474
N -3.18486 0.45032 0.82786
C -3.04860 0.34827 -0.49553
C -2.16979 0.90947 1.78043
C -1.12462 1.76362 1.11268
N 0.02263 1.21884 0.66610
C 0.93606 2.03041 0.09394
C 0.69884 3.39289 -0.09713
C -0.49795 3.94513 0.32980
C -1.41546 3.11820 0.95958
Mn 0.59292 -0.83620 0.53371
C 0.94871 -0.94839 2.29594
O 1.16965 -1.01725 3.41930
H -6.01003 -0.88433 -0.13528
C 2.24455 1.42383 -0.25354
N 2.43113 0.14725 0.14387
C 3.65873 -0.39717 0.04628
C 4.70728 0.30177 -0.56454
C 4.49255 1.57372 -1.06569
C 3.24453 2.15716 -0.88544
C 3.94232 -1.76161 0.59833
Br 0.09724 -0.63085 -1.98479
C -1.00239 -1.66122 0.70883
O -1.94868 -2.30762 0.79722
C 1.14362 -2.52257 0.16293
O 1.36656 -3.61840 -0.08776
H 5.29284 2.12154 -1.56627
H -0.70194 5.00775 0.18958
H 3.06582 3.17268 -1.23266
H 1.44910 4.02826 -0.56298
H -2.36245 3.50630 1.33705
H 5.68662 -0.17298 -0.63809
H -4.75267 -0.06241 2.21888
H -2.15752 0.60040 -1.07298
H -1.72852 0.04156 2.28329
H -2.69247 1.50368 2.53922
C -4.39766 -0.47075 -2.40263
H 3.35826 -1.96947 1.50306
H 5.00841 -1.84216 0.84806
H 3.72586 -2.53974 -0.14789
H -3.45619 -0.36087 -2.95203
H -4.76473 -1.49858 -2.50618

H -5.14225 0.23350 -2.79461

1_{C5}⁺

Energy = -4902.656267
Enthalpy 0K = -4902.314597
Enthalpy 298K = -4902.287321
Free Energy 298K = -4902.372717
Nimag = 0 (26.2408 cm⁻¹)

Br -0.41636 -0.50719 2.12386
Mn -0.73702 -0.89495 -0.39506
N 3.25122 0.31966 -0.58715
O -1.70795 -3.56942 0.39716
O 1.75450 -2.47295 -0.32291
N -2.54035 0.20883 -0.25440
N -0.04150 1.11472 -0.62000
C -2.32313 1.50438 0.05695
N 5.20297 -0.15457 0.21517
C -4.64664 1.85527 0.52393
H -5.46936 2.49400 0.85013
O -1.08579 -1.30689 -3.29296
C 0.82806 -1.79474 -0.36471
C -3.80332 -0.25893 -0.27241
C -0.94132 2.00404 -0.14828
C 0.66228 3.79200 -0.24145
H 0.93913 4.83443 -0.07663
C -3.34987 2.34995 0.46828
H -3.15498 3.38666 0.73434
C -0.61182 3.34182 0.07025
H -1.34377 4.03838 0.47312
C 1.56023 2.89269 -0.79290
H 2.56387 3.20236 -1.08929
C 1.17615 1.56354 -0.96797
C -4.87517 0.55060 0.12281
H -5.88451 0.13739 0.10562
C 4.53416 0.12916 -0.89668
H 4.96018 0.19956 -1.89493
C -1.40400 -2.51333 0.07098
C 3.09479 0.15462 0.77400
H 2.12670 0.24120 1.26990
C 2.19897 0.62761 -1.55920
H 1.74398 -0.29787 -1.92329
H 2.68346 1.11606 -2.41313
C 4.32386 -0.14374 1.27547
H 4.64748 -0.34808 2.29219
C 6.63247 -0.41842 0.30610
H 7.06044 -0.40000 -0.70185
H 6.78904 -1.40590 0.75705
H 7.10625 0.35326 0.92532
C -0.95373 -1.14505 -2.16453
C -4.09998 -1.65684 -0.72475
H -3.43723 -1.97577 -1.53826
H -5.13736 -1.71755 -1.07843
H -3.99987 -2.36700 0.10876

2_{C2}⁺
 Energy = -4941.942678
 Enthalpy 0K = -4941.573301
 Enthalpy 298K = -4941.544360
 Free Energy 298K = -4941.633469
 Nimag = 0 (16.4833 cm⁻¹)

Br	-0.41368	-1.53673	-1.68221
Mn	-1.33566	-0.81567	0.59392
N	0.03656	0.82711	0.60602
C	0.02041	3.21704	0.80466
H	-0.51711	4.15978	0.72782
N	-2.46166	0.72979	-0.35710
C	1.34479	3.20665	1.21660
H	1.84884	4.13570	1.48764
C	-2.65940	3.12472	-0.40882
H	-2.24899	4.10402	-0.17111
C	-1.96916	1.95878	-0.08784
C	-0.60103	2.00934	0.48725
C	-4.34927	1.76532	-1.39682
H	-5.28534	1.64221	-1.94297
C	2.02455	1.99798	1.24259
H	3.08045	1.96056	1.51249
C	1.34295	0.82600	0.91734
C	-3.88126	3.02389	-1.06173
H	-4.44529	3.92084	-1.32378
C	-3.62096	0.62508	-1.03483
O	0.22822	-2.91750	1.94696
O	-3.18287	-3.11482	0.52704
O	-2.42547	0.03435	3.19897
N	3.48504	-0.32110	0.49008
C	-2.52455	-2.17579	0.51208
C	-4.15202	-0.71890	-1.42443
H	-3.34271	-1.36616	-1.78723
H	-4.64596	-1.20515	-0.57055
H	-4.90262	-0.60890	-2.21758
C	-0.31958	-2.05800	1.41796
C	2.08928	-0.49020	0.86785
H	2.08215	-0.97784	1.85077
H	1.60891	-1.15651	0.13919
C	-1.99847	-0.28208	2.18267
C	4.56599	-0.46422	1.33528
N	5.25385	0.08606	-0.68047
C	5.67732	-0.20908	0.59771
C	3.91993	0.01241	-0.73571
C	3.08637	0.30247	-1.92360
H	2.07585	-0.11533	-1.81436
H	3.00417	1.39175	-2.06501
H	3.54667	-0.12735	-2.82351
C	6.11607	0.42425	-1.80352
H	7.14698	0.48603	-1.44009
H	6.04631	-0.35232	-2.57648
H	5.81765	1.39327	-2.22291
H	4.44318	-0.73619	2.37977
H	6.72999	-0.21443	0.86567

2_{C5}⁺
 Energy = -4941.942733
 Enthalpy 0K = -4941.573560
 Enthalpy 298K = -4941.544582
 Free Energy 298K = -4941.633129
 Nimag = 0 (25.5879 cm⁻¹)

C	-4.02639	-0.04573	-1.60206
N	-4.95934	-0.18333	-0.59665
C	-4.37843	0.06916	0.58114
N	-3.09225	0.36848	0.34129
C	-2.85180	0.29971	-1.01657
C	-2.11257	0.69293	1.37990
C	-1.03717	1.60461	0.84749
N	0.18749	1.13079	0.56263
C	1.13054	2.00189	0.14458
C	0.84384	3.34836	-0.08139
C	-0.43497	3.82515	0.16394
C	-1.38126	2.94304	0.65995
Mn	0.84971	-0.89081	0.37019
C	0.95642	-1.15788	2.14682
O	1.01925	-1.33553	3.27904
C	-6.35823	-0.53814	-0.79746
C	2.50914	1.47111	0.00722
N	2.68233	0.17297	0.33454
C	3.93194	-0.32236	0.41590
C	5.03919	0.46018	0.06652
C	4.85895	1.76657	-0.35346
C	3.57252	2.29060	-0.36093
C	4.17438	-1.72258	0.89279
Br	0.69570	-0.48986	-2.16312
C	-0.73366	-1.74998	0.24098
O	-1.67137	-2.40589	0.14037
C	1.50669	-2.52281	-0.06126
O	1.80708	-3.58490	-0.37110
H	5.71017	2.38423	-0.64538
H	-0.67956	4.87440	-0.00851
H	3.41248	3.32922	-0.64214
H	1.61266	4.03001	-0.43910
H	-2.39259	3.27305	0.90298
H	6.03697	0.02457	0.13384
C	-5.02014	0.03535	1.91476
H	-1.86557	0.46650	-1.44894
H	-1.69836	-0.22651	1.80638
H	-2.64415	1.21654	2.18358
H	-4.28026	-0.20943	-2.64533
H	-6.58693	-1.47495	-0.27384
H	-6.52382	-0.67382	-1.87129
H	-7.00692	0.26589	-0.42803
H	3.45828	-2.02287	1.66712
H	5.18781	-1.80004	1.30774
H	4.11058	-2.43694	0.05927
H	-6.05330	-0.32032	1.83854
H	-4.46429	-0.63372	2.58702
H	-5.02657	1.04256	2.35835

3_{C2}⁺
 Energy = -5020.511262
 Enthalpy 0K = -5020.086602
 Enthalpy 298K = -5020.054214
 Free Energy 298K = -5020.150855
 Nimag = 0 (20.3542 cm⁻¹)

Br -0.91038 -1.53661 -1.74423
 Mn -1.61264 -0.79319 0.60069
 N -0.32004 0.89779 0.39111
 C -0.38327 3.29603 0.34384
 H -0.95537 4.21654 0.25093
 N -2.91388 0.67017 -0.25369
 C 0.98877 3.35265 0.53111
 H 1.49930 4.31370 0.60980
 C -3.24057 3.05033 -0.29531
 H -2.85345 4.05284 -0.12621
 C -2.44681 1.92621 -0.08186
 C -1.00680 2.05075 0.25872
 C -4.98764 1.59324 -1.00462
 H -5.98727 1.41507 -1.40313
 C 1.70267 2.16473 0.58281
 H 2.78783 2.17746 0.68332
 C 1.01833 0.95302 0.50497
 C -4.54272 2.87811 -0.74721
 H -5.18832 3.74117 -0.91898
 C -4.15362 0.49710 -0.75070
 O 0.15481 -2.81419 1.81603
 O -3.35407 -3.16632 0.80158
 O -2.42934 0.11422 3.28518
 N 3.17980 -0.19927 0.14419
 C -2.74514 -2.20098 0.68786
 C -4.66414 -0.87669 -1.05531
 H -3.87574 -1.49507 -1.50386
 H -5.03288 -1.36774 -0.14300
 H -5.50740 -0.81381 -1.75521
 C -0.47154 -1.97991 1.33505
 C 1.78495 -0.35100 0.51763
 H 1.76237 -0.79151 1.52147
 H 1.30788 -1.05885 -0.17270
 C -2.11124 -0.22843 2.23791
 C 4.05300 -0.15533 2.51268
 H 3.34225 0.61476 2.84880
 H 3.67413 -1.13673 2.83760
 H 5.01141 0.02309 3.01542
 C 4.24173 -0.10607 1.03857
 N 4.96244 0.03265 -1.04583
 C 5.36973 0.03709 0.28236
 C 3.63685 -0.11124 -1.11450
 C 6.79873 0.17464 0.66692
 H 7.21495 1.13104 0.31510
 H 6.90075 0.13455 1.75832
 H 7.40454 -0.63632 0.23480
 C 2.82504 -0.13253 -2.35475
 H 1.77603 -0.37552 -2.14149
 H 2.86159 0.85154 -2.84577
 H 3.21795 -0.88301 -3.05486

C 5.86716 0.16890 -2.17484
 H 6.43786 1.10084 -2.07470
 H 6.55839 -0.68356 -2.20003
 H 5.29257 0.19779 -3.10571

3_{C5}⁺
 Energy = -5020.511767
 Enthalpy 0K = -5020.087292
 Enthalpy 298K = -5020.054820
 Free Energy 298K = -5020.151457
 Nimag = 0 (18.2502 cm⁻¹)

C -3.76959 0.57515 1.09590
 N -3.31033 -0.28621 0.17498
 C -4.36816 -0.76812 -0.58902
 C -5.49629 -0.17374 -0.09997
 N -5.09329 0.65195 0.94209
 C -1.91237 -0.63832 -0.00755
 C -1.12184 0.45694 -0.69198
 N 0.18277 0.58493 -0.40220
 C 0.86484 1.62806 -0.91670
 C 0.28129 2.51702 -1.81862
 C -1.04641 2.33948 -2.17743
 C -1.76531 1.31105 -1.58633
 C 2.24330 1.82242 -0.40311
 C 3.00908 2.92595 -0.76825
 C 4.24606 3.11435 -0.16443
 C 4.65182 2.21764 0.80878
 C 3.84450 1.11941 1.13003
 N 2.67586 0.91151 0.49508
 Mn 1.48985 -0.84382 0.47018
 C 0.49862 -2.32773 0.18533
 O -0.04396 -3.32440 0.01102
 C 4.31217 0.18111 2.20107
 C -6.00083 1.48096 1.71724
 C -2.95387 1.33921 2.07050
 C 2.75952 -2.03072 0.97970
 O 3.49498 -2.86523 1.25852
 C 0.89085 -0.59043 2.14471
 O 0.52355 -0.44591 3.22458
 Br 2.37099 -1.23756 -1.90718
 C -6.92191 -0.29448 -0.50197
 H 4.87030 3.96759 -0.43583
 H -1.52202 3.01143 -2.89361
 H 2.65050 3.64251 -1.50432
 H 0.84942 3.34448 -2.23833
 H -2.82221 1.17054 -1.81453
 H 5.59663 2.35237 1.33698
 C -4.17868 -1.73458 -1.70303
 H -1.88028 -1.55811 -0.60362
 H -1.48133 -0.87058 0.97143
 H 3.48031 -0.20172 2.80438
 H 5.01527 0.69916 2.86618
 H 4.84870 -0.67326 1.76337
 H -5.44302 2.01128 2.49521
 H -6.48477 2.21221 1.05682
 H -6.76499 0.84872 2.18698

H	-1.92156	0.97299	2.09372
H	-2.93783	2.40480	1.79639
H	-3.37542	1.24711	3.08093
H	-7.53558	-0.68611	0.32370
H	-7.33517	0.68221	-0.79626
H	-7.01546	-0.97903	-1.35379
H	-5.13919	-1.92209	-2.19851
H	-3.47559	-1.34326	-2.45390
H	-3.78995	-2.69778	-1.33831

1c2(red1-Br)

Energy	= -4902.752424
Enthalpy 0K	= -4902.414330
Enthalpy 298K	= -4902.386708
Free Energy 298K	= -4902.473562
Nimag	= 0 (22.3693 cm ⁻¹)

N	-4.05076	-0.21311	-0.98112
C	-4.95715	-0.42869	0.03252
C	-4.38755	0.03688	1.17844
N	-3.14883	0.53065	0.83721
C	-2.96933	0.37086	-0.47322
C	-2.15319	1.04251	1.78678
C	-1.09013	1.84987	1.08655
N	0.02303	1.23464	0.62673
C	0.98140	2.02051	-0.00135
C	0.71345	3.39642	-0.27276
C	-0.43974	3.98287	0.16728
C	-1.36073	3.19450	0.90120
Mn	0.56864	-0.80721	0.56468
C	0.96247	-0.84009	2.30819
O	1.21295	-0.84448	3.43063
H	-5.92384	-0.89031	-0.14921
C	2.23062	1.41305	-0.30194
N	2.40662	0.10488	0.10426
C	3.64423	-0.43619	0.04782
C	4.72224	0.23730	-0.51808
C	4.52591	1.52360	-1.06056
C	3.29500	2.11307	-0.94232
C	3.89239	-1.80909	0.60819
Br	-0.00058	-0.75836	-2.00694
C	-1.02770	-1.59534	0.82217
O	-1.97471	-2.23329	0.98018
C	1.07416	-2.51260	0.24971
O	1.26148	-3.62790	0.04577
H	5.34867	2.05181	-1.54854
H	-0.64084	5.03802	-0.02979
H	3.13625	3.11889	-1.32929
H	1.44520	3.99215	-0.81734
H	-2.28319	3.61941	1.29893
H	5.70198	-0.24156	-0.54254
H	-4.75138	0.05756	2.20183
H	-2.05716	0.59584	-1.02958
H	-1.72941	0.19655	2.34151
H	-2.69354	1.67708	2.49898
C	-4.23105	-0.55800	-2.38356
H	3.33925	-1.97846	1.54144

H	4.96316	-1.93999	0.81419
H	3.60234	-2.59051	-0.10859
H	-3.24455	-0.61101	-2.85926
H	-4.72058	-1.53652	-2.44864
H	-4.84830	0.20118	-2.88091

1c5(red1-Br)

Energy	= -4902.750647
Enthalpy 0K	= -4902.412224
Enthalpy 298K	= -4902.384686
Free Energy 298K	= -4902.471243
Nimag	= 0 (28.8855 cm ⁻¹)

Br	-0.34541	-0.66118	2.13836
Mn	-0.72346	-0.86896	-0.44219
N	3.21972	0.36546	-0.58669
O	-1.62962	-3.60042	0.20502
O	1.77387	-2.43050	-0.51755
N	-2.52860	0.18799	-0.20614
N	-0.03909	1.12725	-0.58923
C	-2.29899	1.51035	0.12222
N	5.14647	-0.14988	0.25217
C	-4.64407	1.82826	0.63178
H	-5.47102	2.44758	0.98787
O	-1.13118	-1.09183	-3.34331
C	0.84404	-1.75041	-0.49381
C	-3.80017	-0.26946	-0.22597
C	-0.98508	2.01029	-0.08394
C	0.60418	3.84467	-0.18215
H	0.87456	4.88669	0.00246
C	-3.36897	2.32700	0.59444
H	-3.17794	3.35140	0.91198
C	-0.62996	3.37108	0.16673
H	-1.35281	4.04296	0.62838
C	1.51645	2.96001	-0.80660
H	2.49978	3.29514	-1.14026
C	1.15192	1.63269	-0.96892
C	-4.87738	0.51399	0.17722
H	-5.88588	0.09975	0.14360
C	4.50767	0.17295	-0.86811
H	4.96199	0.27182	-1.85122
C	-1.35682	-2.51474	-0.05692
C	3.02549	0.16157	0.76284
H	2.04132	0.23137	1.23145
C	2.19273	0.72253	-1.57344
H	1.75012	-0.18919	-1.98612
H	2.70760	1.24296	-2.38916
C	4.23867	-0.16307	1.28811
H	4.53290	-0.40324	2.30592
C	6.56955	-0.43182	0.37224
H	7.03066	-0.35922	-0.61866
H	6.70624	-1.44503	0.76989
H	7.03017	0.29825	1.04929
C	-0.97412	-1.01150	-2.20617
C	-4.08880	-1.66950	-0.69177
H	-3.48310	-1.94564	-1.56510
H	-5.14858	-1.76251	-0.96425

H -3.89241 -2.40086 0.10519

2c2(red1-Br)

Energy = -4942.038330
Enthalpy 0K = -4941.672795
Enthalpy 298K = -4941.643401
Free Energy 298K = -4941.734134
Nimag = 0 (16.1172 cm⁻¹)

Br -0.32908 -1.71581 -1.59190
Mn -1.34504 -0.77855 0.62929
N 0.02146 0.82647 0.61686
C -0.00029 3.25815 0.78163
H -0.55245 4.19631 0.72469
N -2.43368 0.70031 -0.42296
C 1.31448 3.25902 1.15958
H 1.81784 4.19306 1.41934
C -2.70446 3.12111 -0.46647
H -2.34410 4.10975 -0.18280
C -1.94531 1.96172 -0.13176
C -0.64791 2.03034 0.44689
C -4.29372 1.70177 -1.56414
H -5.19324 1.56181 -2.16517
C 2.02505 2.03265 1.18130
H 3.08970 2.00788 1.41542
C 1.33536 0.86169 0.90735
C -3.87272 2.98882 -1.17118
H -4.45832 3.87078 -1.44238
C -3.55780 0.58959 -1.16181
O 0.17995 -2.77155 2.17451
O -3.20747 -3.06602 0.60259
O -2.53255 0.23601 3.12168
N 3.47380 -0.30885 0.49607
C -2.53590 -2.13362 0.56137
C -4.04218 -0.77274 -1.56694
H -3.19983 -1.41032 -1.86904
H -4.57453 -1.26425 -0.73913
H -4.74805 -0.68986 -2.40457
C -0.35644 -1.95917 1.55982
C 2.08079 -0.45908 0.89929
H 2.09014 -0.91799 1.89585
H 1.59082 -1.15044 0.20025
C -2.06514 -0.15302 2.14619
C 4.56858 -0.44744 1.32117
N 5.22170 0.09835 -0.70679
C 5.66798 -0.19289 0.56432
C 3.88567 0.02267 -0.73616
C 3.02644 0.31228 -1.90595
H 2.03852 -0.15902 -1.79855
H 2.88741 1.40053 -2.00557
H 3.49704 -0.06149 -2.82505
C 6.06285 0.43911 -1.84436
H 7.10122 0.49344 -1.50132
H 5.97509 -0.33164 -2.62133
H 5.76218 1.41245 -2.25220
H 6.72514 -0.19610 0.81392
H 4.46488 -0.71522 2.36877

2c5(red1-Br)

Energy = -4942.036877
Enthalpy 0K = -4941.670664
Enthalpy 298K = -4941.641435
Free Energy 298K = -4941.731894
Nimag = 0 (24.5537 cm⁻¹)

C -3.91496 0.02173 -1.60962
N -4.84148 -0.19231 -0.61105
C -4.28726 0.10278 0.57066
N -3.02977 0.50537 0.33980
C -2.77524 0.45892 -1.01441
C -2.08642 0.89969 1.39236
C -0.96583 1.74596 0.84249
N 0.21260 1.17194 0.52538
C 1.23528 1.99775 0.07690
C 0.97344 3.37467 -0.19734
C -0.24872 3.91961 0.08285
C -1.24238 3.09170 0.66067
Mn 0.78277 -0.85732 0.40641
C 0.91206 -1.02719 2.18034
O 0.99608 -1.12681 3.32399
C -6.20612 -0.65687 -0.81901
C 2.52839 1.42279 -0.04695
N 2.65973 0.09147 0.29784
C 3.89828 -0.43834 0.40057
C 5.04240 0.27863 0.06270
C 4.91455 1.60112 -0.40976
C 3.67070 2.17359 -0.45264
C 4.07411 -1.84878 0.89104
Br 0.59787 -0.62018 -2.19245
C -0.83602 -1.64099 0.34541
O -1.80194 -2.26779 0.30189
C 1.34526 -2.53389 0.04519
O 1.57741 -3.63039 -0.21104
H 5.79680 2.16912 -0.71513
H -0.44946 4.97398 -0.11955
H 3.55806 3.20594 -0.78188
H 1.75866 4.00012 -0.62155
H -2.22046 3.48508 0.94130
H 6.02097 -0.19312 0.16124
C -4.92275 0.00496 1.90416
H -1.79485 0.68117 -1.43349
H -1.71271 0.00268 1.89980
H -2.64867 1.48786 2.12795
H -4.14699 -0.16372 -2.65431
H -6.36697 -1.60302 -0.28694
H -6.35164 -0.81746 -1.89239
H -6.91997 0.09729 -0.46440
H 3.38553 -2.08738 1.71238
H 5.10203 -1.99478 1.24924
H 3.90594 -2.57433 0.08229
H -5.92438 -0.43194 1.82732
H -4.31134 -0.62367 2.56757
H -5.00760 1.00302 2.36009

3c2(red1-Br)

Energy = -5020.606762
 Enthalpy 0K = -5020.185622
 Enthalpy 298K = -5020.152874
 Free Energy 298K = -5020.250763
 Nimag = 0 (19.0955 cm⁻¹)

Br -0.85087 -1.61267 -1.74757
 Mn -1.63244 -0.78965 0.60606
 N -0.31644 0.85146 0.48276
 C -0.36272 3.28255 0.64725
 H -0.93318 4.21112 0.66467
 N -2.87424 0.68152 -0.27104
 C 0.99000 3.30971 0.84733
 H 1.50505 4.25409 1.03745
 C -3.19783 3.09599 -0.25400
 H -2.82930 4.09046 -0.00394
 C -2.38022 1.95029 -0.02437
 C -1.02418 2.04208 0.39497
 C -4.87665 1.65355 -1.17252
 H -5.83774 1.49967 -1.66502
 C 1.72076 2.09713 0.77877
 H 2.80679 2.09502 0.87107
 C 1.02299 0.91146 0.60669
 C -4.43820 2.94552 -0.81735
 H -5.06916 3.81736 -1.00730
 C -4.07578 0.55403 -0.87297
 O 0.08443 -2.81099 1.88873
 O -3.41788 -3.13435 0.72070
 O -2.54296 0.12559 3.24875
 N 3.16415 -0.23572 0.12417
 C -2.78600 -2.17771 0.63116
 C -4.57775 -0.81332 -1.23754
 H -3.76722 -1.42512 -1.65712
 H -4.98880 -1.33058 -0.35801
 H -5.38638 -0.73460 -1.97682
 C -0.52442 -1.98047 1.37299
 C 1.77859 -0.40031 0.53461
 H 1.78838 -0.89499 1.51253
 H 1.27679 -1.07140 -0.17562
 C -2.18513 -0.22648 2.21461
 C 4.14281 -0.49091 2.43532
 H 3.46968 0.24399 2.90256
 H 3.74991 -1.49742 2.64659
 H 5.12777 -0.40408 2.91033
 C 4.26403 -0.25129 0.97266
 N 4.89119 0.15250 -1.10751
 C 5.35794 -0.00804 0.19098
 C 3.56216 0.01340 -1.13079
 C 6.80306 0.08963 0.52532
 H 7.20989 1.07371 0.24647
 H 6.95136 -0.04980 1.60310
 H 7.38687 -0.67871 -0.00451
 C 2.68255 0.16494 -2.31465
 H 1.66688 -0.19640 -2.10305
 H 2.62291 1.22505 -2.60527
 H 3.08014 -0.40499 -3.16553

C 5.74381 0.44191 -2.24746
 H 6.27876 1.38495 -2.07574
 H 6.46897 -0.37095 -2.38298
 H 5.13286 0.53593 -3.15047

3c5(red1-Br)

Energy = -5020.605410
 Enthalpy 0K = -5020.184182
 Enthalpy 298K = -5020.151413
 Free Energy 298K = -5020.249732
 Nimag = 0 (15.4183 cm⁻¹)

Br 0.83806 -1.61960 1.76277
 Mn 1.62357 -0.80185 -0.59437
 N 0.32625 0.85867 -0.50033
 C 0.41458 3.28185 -0.74374
 H 1.00079 4.20015 -0.77981
 N 2.87561 0.66776 0.27184
 C -0.93314 3.32267 -0.97430
 H -1.42902 4.26796 -1.20635
 C 3.22937 3.07771 0.22022
 H 2.87440 4.07249 -0.04785
 C 2.40096 1.93851 -0.00180
 C 1.05175 2.04001 -0.44077
 C 4.87928 1.62946 1.18140
 H 5.83277 1.47167 1.68728
 C -1.68457 2.12442 -0.87884
 H -2.76921 2.13587 -0.98490
 C -1.01011 0.93612 -0.64655
 C 4.46062 2.92113 0.80178
 H 5.09922 3.78829 0.98762
 C 4.06878 0.53499 0.88905
 O -0.12067 -2.82041 -1.84449
 O 3.39567 -3.15759 -0.68856
 O 2.54278 0.07094 -3.24816
 N -3.16386 -0.16153 -0.10444
 C 2.76748 -2.19783 -0.60657
 C 4.55070 -0.83300 1.27752
 H 3.72789 -1.43041 1.69411
 H 4.96669 -1.36564 0.40951
 H 5.35123 -0.75385 2.02557
 C 0.50131 -1.99054 -1.34357
 C -1.78619 -0.35905 -0.52445
 H -1.80258 -0.89588 -1.47970
 H -1.29197 -1.00382 0.21583
 C 2.18151 -0.26301 -2.20904
 C -2.56698 0.40919 2.27755
 H -1.82256 -0.39958 2.34120
 H -2.01435 1.34631 2.10562
 H -3.08546 0.48664 3.24130
 C -3.54990 0.16835 1.18796
 N -5.31784 -0.04954 -0.12436
 C -4.91363 0.23887 1.17458
 C -4.24431 -0.28224 -0.88801
 C -5.88812 0.55205 2.25286
 H -6.58116 -0.28653 2.42116
 H -5.35697 0.75196 3.19159

H	-6.48811	1.44015	2.00187
C	-4.20736	-0.61197	-2.33463
H	-3.44004	-0.00639	-2.83613
H	-3.96291	-1.67494	-2.48155
H	-5.17039	-0.40728	-2.81418
C	-6.71233	-0.08321	-0.53322
H	-7.26048	-0.78997	0.10260
H	-7.15200	0.91763	-0.43255
H	-6.78893	-0.41062	-1.57384

1_{C2}⁺(red1)

Energy	= -2328.673243
Enthalpy 0K	= -2328.334223
Enthalpy 298K	= -2328.308659
Free Energy 298K	= -2328.390209
Nimag	= 0 (20.4469 cm ⁻¹)

C	-3.53918	1.35555	0.93886
C	-2.30507	0.95067	0.43217
N	-1.95317	-0.35060	0.34903
C	-2.78427	-1.29325	0.84511
C	-4.02683	-0.94005	1.37894
C	-4.41931	0.39010	1.40740
C	-1.26666	1.92649	0.02354
N	-0.06809	1.40862	-0.32506
C	0.96544	2.25416	-0.51804
C	0.80965	3.63561	-0.46158
C	-0.44731	4.17115	-0.20628
C	-1.49425	3.30460	0.06099
C	2.34686	1.71976	-0.80392
N	2.78398	0.67661	0.11877
C	3.67196	-0.32529	-0.20220
C	3.84810	-1.07249	0.92067
N	3.06358	-0.51241	1.90231
C	2.43260	0.54377	1.39776
C	2.90466	-1.03452	3.25130
Mn	-0.26333	-0.63850	-0.85746
C	0.59996	-1.92511	0.06878
O	1.15000	-2.81294	0.57306
C	-2.36756	-2.73172	0.84468
C	-1.18664	-1.69180	-1.97681
O	-1.74272	-2.40064	-2.70689
C	0.97716	-0.69374	-2.13890
O	1.74274	-0.82417	-3.00244
H	4.44963	-1.95840	1.10262
H	-5.39333	0.67700	1.80771
H	-0.60074	5.25113	-0.18321
H	-3.81316	2.40782	0.98152
H	-2.47680	3.70258	0.30729
H	1.67419	4.28149	-0.61874
H	-4.67873	-1.72327	1.76775
H	4.09429	-0.42048	-1.19840
H	1.73801	1.18093	1.94017
H	2.40229	1.30429	-1.81747
H	3.06507	2.54791	-0.75279
H	-2.21614	-3.11128	-0.17461
H	-3.13420	-3.34725	1.33172

H	-1.42156	-2.85990	1.38847
H	2.32012	-0.32090	3.84176
H	2.38057	-1.99751	3.20721
H	3.89364	-1.16838	3.70557

1_{C5}⁺(red1)

Energy	= -2328.674010
Enthalpy 0K	= -2328.335029
Enthalpy 298K	= -2328.309490
Free Energy 298K	= -2328.390416
Nimag	= 0 (29.4621 cm ⁻¹)

C	-2.25040	1.06644	-1.69370
N	-2.56807	1.09152	-0.35414
C	-3.45280	0.12597	-0.10663
N	-3.71026	-0.51698	-1.24014
C	-2.96704	0.05124	-2.24923
C	-2.06667	2.03528	0.63962
C	-0.61275	2.38900	0.44491
N	0.30524	1.41706	0.26752
C	1.57538	1.77757	-0.02049
C	1.99080	3.11127	0.00758
C	1.05939	4.10374	0.26511
C	-0.26983	3.73761	0.44306
C	2.48131	0.68096	-0.43685
C	3.75501	0.92858	-0.94639
C	4.50294	-0.13897	-1.42361
C	3.94368	-1.40822	-1.40093
C	2.66571	-1.60235	-0.86864
N	1.96332	-0.56400	-0.36568
Mn	0.22899	-0.62883	0.80624
C	-1.02412	-0.50833	2.07014
O	-1.81926	-0.53088	2.91722
C	2.06461	-2.97379	-0.88057
H	-3.01005	-0.31639	-3.27048
C	-0.78985	-1.77724	-0.14219
O	-1.45412	-2.58065	-0.65125
C	0.96711	-1.81662	1.92796
O	1.39903	-2.60601	2.65922
C	-4.59061	-1.66632	-1.38573
H	5.50402	0.02329	-1.82712
H	1.35820	5.15274	0.29249
H	4.15759	1.93876	-0.98931
H	3.03009	3.37649	-0.17796
H	-1.04538	4.49136	0.58252
H	4.48905	-2.26632	-1.79578
H	-3.88191	-0.10567	0.86569
H	-1.54547	1.76398	-2.13752
H	-2.23748	1.60286	1.63279
H	-2.66569	2.95229	0.57571
H	1.84766	-3.33220	0.13442
H	2.75113	-3.68374	-1.35849
H	1.11911	-2.97459	-1.44054
H	-5.35107	-1.44684	-2.14480
H	-3.99795	-2.53781	-1.68905
H	-5.07476	-1.86523	-0.42361

2_{C2}⁺(red1)

Energy = -2367.960104
 Enthalpy 0K = -2367.592890
 Enthalpy 298K = -2367.565912
 Free Energy 298K = -2367.649856
 Nimag = 0 (28.5534 cm⁻¹)

C	2.50922	0.46696	1.25589
N	2.72793	0.57894	-0.06395
C	3.53450	-0.46072	-0.47894
C	3.79297	-1.22369	0.61154
N	3.14180	-0.63762	1.67254
C	2.28041	1.63333	-0.96868
C	0.89230	2.17434	-0.72207
N	-0.13474	1.34844	-0.44693
C	-1.32525	1.89251	-0.10789
C	-1.56159	3.26577	-0.18790
C	-0.52468	4.10790	-0.55844
C	0.72965	3.55626	-0.78526
C	-2.33886	0.95101	0.42308
C	-3.52509	1.39711	1.00347
C	-4.38071	0.46572	1.57533
C	-4.01053	-0.87125	1.57035
C	-2.81291	-1.26550	0.96669
N	-2.00561	-0.35682	0.37738
Mn	-0.38383	-0.70700	-0.89910
C	0.77952	-0.77438	-2.25082
O	1.48952	-0.89452	-3.16191
C	-2.41605	-2.70908	0.99328
C	3.10925	-1.15827	3.03082
C	0.51425	-1.97277	0.02583
O	1.06916	-2.85598	0.53231
C	-1.35897	-1.79893	-1.93106
O	-1.95033	-2.53391	-2.60615
H	4.36736	-2.13821	0.72451
H	-5.31744	0.78433	2.03611
H	-0.68342	5.18483	-0.63310
H	-3.77493	2.45617	1.02730
H	-2.54341	3.67644	0.04117
H	1.58937	4.18963	-1.00693
H	-4.64416	-1.62802	2.03452
H	3.84472	-0.56523	-1.51427
C	1.70601	1.35343	2.13068
H	2.35146	1.22756	-1.98614
H	2.99311	2.46632	-0.90695
H	-2.32671	-3.12396	-0.01959
H	-3.16198	-3.29663	1.54299
H	-1.44271	-2.83276	1.48766
H	3.57050	-0.44077	3.72187
H	2.07163	-1.35101	3.33138
H	3.67381	-2.09604	3.05151
H	2.12181	1.34996	3.14609
H	1.70717	2.38433	1.75818
H	0.66643	0.99418	2.17872

2_{C5}⁺(red1)

Energy = -2367.961478
 Enthalpy 0K = -2367.594356
 Enthalpy 298K = -2367.567309
 Free Energy 298K = -2367.651065
 Nimag = 0 (30.5702 cm⁻¹)

N	2.08555	-0.54108	-0.40354
C	2.59865	0.70791	-0.44366
C	3.86451	0.97465	-0.96072
C	4.60339	-0.07584	-1.48941
C	4.04161	-1.34434	-1.51123
C	2.77424	-1.55892	-0.96135
C	1.68316	1.78366	0.00468
N	0.42814	1.38972	0.30697
C	-0.51865	2.33146	0.49192
C	-0.21431	3.68837	0.49653
C	1.10438	4.09152	0.30951
C	2.06179	3.12843	0.03430
C	-1.95723	1.91082	0.65744
N	-2.41588	1.06716	-0.44462
C	-1.98790	1.16210	-1.75242
C	-2.66112	0.21676	-2.45657
N	-3.49461	-0.42830	-1.57132
C	-3.33925	0.09865	-0.35123
C	-4.36995	-1.54422	-1.89588
Mn	0.41661	-0.64555	0.84583
C	1.18952	-1.89753	1.86776
O	1.64904	-2.71953	2.54445
C	2.16560	-2.92624	-1.00655
C	-0.68476	-0.48008	2.24254
O	-1.35914	-0.44834	3.18767
C	-0.71440	-1.73535	-0.04291
O	-1.44453	-2.50605	-0.51189
H	-2.62289	-0.05108	-3.50842
H	5.59856	0.10070	-1.90153
H	1.37353	5.14849	0.33989
H	4.26605	1.98635	-0.97061
H	3.09062	3.42325	-0.16604
H	-1.01012	4.41964	0.64254
H	4.57711	-2.18530	-1.95360
C	-4.03335	-0.36358	0.87216
H	-1.24522	1.88700	-2.07163
H	-2.09332	1.36006	1.59362
H	-2.59187	2.80498	0.70168
H	2.07033	-3.35836	-0.00079
H	2.78797	-3.59888	-1.61011
H	1.15940	-2.88734	-1.44587
H	-4.28081	-1.74973	-2.96764
H	-4.06536	-2.43170	-1.32720
H	-5.41046	-1.28656	-1.65990
H	-5.03403	-0.73567	0.61894
H	-3.46762	-1.18615	1.33639
H	-4.13818	0.44875	1.60083

3_{c2}⁺(red1)

Energy = -2446.528112
 Enthalpy 0K = -2446.105402
 Enthalpy 298K = -2446.074945
 Free Energy 298K = -2446.167122
 Nimag = 0 (22.9868 cm⁻¹)

C -4.11928 -0.44884 -0.60762
 N -2.91988 -0.29623 -0.02717
 C -3.07131 0.25555 1.23905
 C -4.41187 0.43751 1.41913
 N -5.03707 -0.00641 0.25824
 C -1.63690 -0.65905 -0.60549
 C -0.82298 0.56182 -0.97634
 N 0.48955 0.56644 -0.68163
 C 1.20020 1.69724 -0.88449
 C 0.64144 2.81882 -1.49691
 C -0.69562 2.78735 -1.86745
 C -1.44449 1.65441 -1.57523
 C 2.56999 1.69364 -0.32027
 N 2.94087 0.54773 0.29583
 C 4.08406 0.52587 1.01271
 C 4.92646 1.64159 1.04965
 C 4.59089 2.78947 0.34705
 C 3.38167 2.82510 -0.33625
 Mn 1.72664 -1.06481 -0.25141
 C 1.12271 -1.80550 1.28185
 O 0.76279 -2.36022 2.23384
 C 4.45195 -0.70151 1.78769
 C -1.91342 0.54821 2.12540
 C -5.17704 0.98497 2.56998
 C -6.48001 0.00971 0.07956
 C -4.33515 -1.01617 -1.96102
 C 0.87014 -2.15931 -1.37936
 O 0.34514 -2.90356 -2.09885
 C 3.06738 -2.23247 -0.46834
 O 3.87749 -3.04544 -0.63435
 H 5.24899 3.66028 0.35260
 H -1.15543 3.64764 -2.35639
 H 3.07070 3.72989 -0.85604
 H 1.23757 3.71261 -1.67389
 H -2.50915 1.61434 -1.80949
 H 5.84502 1.59278 1.63623
 H -1.81480 -1.29002 -1.48538
 H -1.08886 -1.26477 0.12431
 H 3.56391 -1.17208 2.22937
 H 5.15924 -0.44375 2.58671
 H 4.93993 -1.44470 1.14018
 H -4.49144 1.24335 3.38634
 H -5.73026 1.89308 2.28523
 H -5.90436 0.25122 2.94932
 H -1.29613 -0.34840 2.28611
 H -1.26700 1.32969 1.69672
 H -2.27006 0.89797 3.10175
 H -6.94634 -0.69732 0.77800
 H -6.85818 1.02091 0.27415
 H -6.73531 -0.27381 -0.94507

H -5.37528 -0.89694 -2.28044
 H -3.68788 -0.50979 -2.69051
 H -4.09156 -2.08916 -1.96641

3_{c5}⁺(red1)

Energy = -2446.528291
 Enthalpy 0K = -2446.105970
 Enthalpy 298K = -2446.075361
 Free Energy 298K = -2446.167958
 Nimag = 0 (24.5526 cm⁻¹)

N 2.92743 0.56701 0.29714
 C 2.54790 1.70231 -0.33280
 C 3.35147 2.83921 -0.36308
 C 4.56120 2.82030 0.32008
 C 4.90487 1.68387 1.03734
 C 4.07023 0.56193 1.01469
 C 1.17789 1.68785 -0.89651
 N 0.47738 0.55262 -0.68134
 C -0.83508 0.53331 -0.97461
 C -1.46776 1.61505 -1.58250
 C -0.72879 2.75080 -1.88827
 C 0.60900 2.79726 -1.52116
 C -1.63690 -0.69291 -0.59616
 N -2.92733 -0.34109 -0.02325
 C -3.09240 0.19897 1.19361
 N -4.39996 0.41056 1.36118
 C -5.09319 -0.01030 0.23267
 C -4.16125 -0.48326 -0.64732
 C -2.01078 0.53577 2.15065
 C -4.30805 -1.05334 -2.01285
 C -6.57331 0.08909 0.13530
 C -5.03279 0.98878 2.53528
 Mn 1.73459 -1.06289 -0.24398
 C 4.44511 -0.65311 1.80575
 C 0.88119 -2.18684 -1.34497
 O 0.36196 -2.95072 -2.04762
 C 3.10401 -2.18996 -0.49105
 O 3.93864 -2.97396 -0.67490
 C 1.17342 -1.81881 1.29972
 O 0.84981 -2.38650 2.25666
 H 5.21350 3.69546 0.31412
 H -1.19657 3.60178 -2.38586
 H 3.03400 3.73498 -0.89442
 H 1.19735 3.69386 -1.70992
 H -2.53291 1.56306 -1.81338
 H 5.82386 1.64909 1.62424
 H -1.81999 -1.32226 -1.47594
 H -1.08034 -1.30009 0.12562
 H 3.56002 -1.11968 2.25721
 H 5.15436 -0.38173 2.59850
 H 4.93225 -1.40498 1.16773
 H -4.26821 1.39208 3.20641
 H -5.69705 1.80411 2.22316
 H -5.61588 0.22125 3.06114
 H -1.09143 -0.01093 1.90928
 H -1.79204 1.61414 2.11433

H	-2.30523	0.27368	3.17514
H	-7.06234	-0.47085	0.94676
H	-6.90661	1.13637	0.19943
H	-6.91664	-0.32278	-0.82144
H	-5.36055	-1.01769	-2.31957
H	-3.71871	-0.48420	-2.74773
H	-3.97752	-2.10274	-2.04751

1c2(red2)

Energy	=	-2328.776748
Enthalpy 0K	=	-2328.439436
Enthalpy 298K	=	-2328.414192
Free Energy 298K	=	-2328.493569
Nimag	=	0 (28.9766 cm ⁻¹)

C	-3.49661	1.53811	0.89867
C	-2.26426	1.06921	0.36890
N	-2.00042	-0.27497	0.26864
C	-2.91291	-1.15730	0.77566
C	-4.11545	-0.73335	1.31611
C	-4.42337	0.64130	1.36086
C	-1.21947	1.93691	-0.06721
N	-0.06199	1.31052	-0.52326
C	1.01917	2.13745	-0.74291
C	0.95284	3.50872	-0.67621
C	-0.27526	4.14870	-0.36652
C	-1.33760	3.35012	-0.03893
C	2.36949	1.53896	-1.03681
N	2.83309	0.63086	0.01696
C	3.74734	-0.38258	-0.15573
C	3.87284	-1.01328	1.04371
N	3.03208	-0.37051	1.92350
C	2.41420	0.61610	1.28017
C	2.80349	-0.75474	3.30738
Mn	-0.26328	-0.70563	-0.78184
C	0.46078	-1.91676	0.31470
O	0.97048	-2.74856	0.95201
C	-2.60806	-2.62758	0.77324
C	-1.17118	-1.75911	-1.89500
O	-1.73661	-2.47353	-2.62084
C	1.06464	-0.99045	-1.92797
O	1.87165	-1.29933	-2.71139
H	4.47815	-1.86340	1.34516
H	-5.37525	0.98485	1.77182
H	-0.35481	5.23686	-0.35031
H	-3.70063	2.60711	0.94651
H	-2.28394	3.80413	0.25528
H	1.85568	4.09551	-0.85344
H	-4.81519	-1.47329	1.70736
H	4.22119	-0.57212	-1.11448
H	1.67939	1.28822	1.71590
H	2.37302	0.96993	-1.97303
H	3.10781	2.34424	-1.13705
H	-2.50997	-3.02613	-0.24523
H	-3.41173	-3.17848	1.27941
H	-1.66359	-2.83465	1.29486
H	2.15278	-0.01038	3.77894

H	2.31942	-1.73901	3.33473
H	3.76252	-0.79523	3.83789

1c5(red2)

Energy	=	-2328.776760
Enthalpy 0K	=	-2328.440115
Enthalpy 298K	=	-2328.414634
Free Energy 298K	=	-2328.494936
Nimag	=	0 (22.9393 cm ⁻¹)

C	3.70092	1.11570	-0.98199
C	2.42487	0.81476	-0.43445
N	1.99169	-0.48395	-0.31476
C	2.77683	-1.48128	-0.82142
C	4.01744	-1.22124	-1.37896
C	4.49939	0.10215	-1.44259
C	1.50315	1.81309	-0.00167
N	0.27246	1.34379	0.44823
C	-0.69919	2.29960	0.64594
C	-0.45403	3.65090	0.59133
C	0.85303	4.12626	0.30706
C	1.80535	3.19918	-0.02047
C	-2.13012	1.87636	0.86505
N	-2.62788	1.04478	-0.23470
C	-2.32235	1.20450	-1.56594
C	-2.96321	0.21111	-2.24129
N	-3.64702	-0.53296	-1.30754
C	-3.42559	-0.01247	-0.10439
C	-4.43491	-1.72246	-1.58960
Mn	0.23247	-0.67140	0.76625
C	-0.67168	-1.80650	-0.27575
O	-1.29941	-2.59300	-0.86354
C	2.28358	-2.89922	-0.79810
C	1.00855	-1.82918	1.87450
O	1.48522	-2.60592	2.59979
C	-1.07692	-0.71731	1.96253
O	-1.89946	-0.85488	2.77948
H	-2.98921	-0.03241	-3.29962
H	5.48201	0.31594	-1.86896
H	1.07417	5.19485	0.30193
H	4.03834	2.14949	-1.04728
H	2.80551	3.52763	-0.30383
H	-1.27716	4.35006	0.74809
H	4.61125	-2.04891	-1.76962
H	-1.67446	2.00282	-1.91720
H	-3.81231	-0.40347	0.83363
H	-2.27071	1.31112	1.79207
H	-2.76242	2.77090	0.92505
H	2.16511	-3.27693	0.22631
H	2.99359	-3.55289	-1.32175
H	1.30509	-2.98378	-1.29045
H	-4.84019	-2.11012	-0.64886
H	-5.25704	-1.46453	-2.26853
H	-3.78966	-2.47982	-2.05058

2c2(red2)

Energy = -2368.062360
 Enthalpy 0K = -2367.697426
 Enthalpy 298K = -2367.670578
 Free Energy 298K = -2367.753327
 Nimag = 0 (23.8714 cm⁻¹)

C	-3.54161	1.49157	0.93163
C	-2.32959	1.02415	0.35448
N	-2.04407	-0.31964	0.29287
C	-2.91241	-1.19685	0.87913
C	-4.09322	-0.77365	1.46592
C	-4.42469	0.59722	1.47614
C	-1.32599	1.89127	-0.16579
N	-0.16525	1.26965	-0.61925
C	0.89699	2.10138	-0.88058
C	0.79571	3.47290	-0.90723
C	-0.44670	4.09952	-0.62884
C	-1.48128	3.30080	-0.22344
C	2.27190	1.52833	-1.12220
N	2.75247	0.57549	-0.11454
C	3.60439	-0.46002	-0.43563
C	3.84190	-1.15394	0.70489
N	3.13325	-0.52906	1.70438
C	2.48246	0.52854	1.19888
C	3.05163	-0.97956	3.08461
Mn	-0.35878	-0.75268	-0.83405
C	0.44799	-1.93049	0.24146
O	0.99085	-2.75318	0.86265
C	-2.57847	-2.66038	0.91256
C	-1.29124	-1.87425	-1.85355
O	-1.87343	-2.63230	-2.52012
C	0.89167	-0.98520	-2.07477
O	1.64833	-1.23658	-2.92575
H	4.43962	-2.04092	0.89258
H	-5.35873	0.93978	1.92704
H	-0.55510	5.18390	-0.68686
H	-3.76031	2.55866	0.95488
H	-2.43416	3.74865	0.05924
H	1.68413	4.07149	-1.11449
H	-4.75724	-1.51016	1.92077
H	3.95388	-0.61630	-1.45152
H	2.31967	1.00110	-2.08248
H	2.99282	2.35449	-1.17275
H	-2.52607	-3.09254	-0.09558
H	-3.34246	-3.20823	1.47983
H	-1.60312	-2.83046	1.38880
H	3.47086	-0.22044	3.75809
H	2.00568	-1.17696	3.35132
H	3.62979	-1.90465	3.17765
C	1.60832	1.41869	1.99944
H	1.57499	2.42735	1.57464
H	0.58537	1.01218	2.02008
H	1.98242	1.48141	3.02898

2c5(red2)

Energy = -2368.063413
 Enthalpy 0K = -2367.698588
 Enthalpy 298K = -2367.671614
 Free Energy 298K = -2367.754628
 Nimag = 0 (27.3409 cm⁻¹)

C	-3.30223	0.07221	-0.36609
N	-2.43183	1.09101	-0.35455
C	-1.98775	1.31926	-1.63921
C	-2.60117	0.41069	-2.43990
N	-3.41416	-0.35054	-1.63206
C	-1.98270	1.84638	0.82146
C	-0.54641	2.28334	0.67454
N	0.42465	1.32935	0.47960
C	1.65880	1.79354	0.03965
C	1.97482	3.17722	0.06173
C	1.02632	4.10215	0.40722
C	-0.29179	3.63351	0.65660
C	2.55763	0.79183	-0.42895
C	3.83076	1.08114	-0.98835
C	4.59465	0.06478	-1.49958
C	4.07916	-1.24802	-1.47702
C	2.84480	-1.49782	-0.90098
N	2.09853	-0.50177	-0.33827
Mn	0.37991	-0.68393	0.80512
C	-0.81207	-0.65350	2.12236
O	-1.53778	-0.71612	3.03333
C	2.30912	-2.90029	-0.91853
C	-4.22738	-1.47502	-2.06495
C	-0.63881	-1.76920	-0.18191
O	-1.33586	-2.52982	-0.72553
C	1.16658	-1.90824	1.83120
O	1.65384	-2.72171	2.50771
H	-2.53248	0.23898	-3.51016
H	5.57410	0.26936	-1.93769
H	1.25754	5.16835	0.43553
H	4.18945	2.10940	-1.02617
H	2.98095	3.50366	-0.20354
H	-1.11318	4.33606	0.80749
H	4.64159	-2.07444	-1.91414
H	-1.27273	2.10292	-1.87098
C	-4.00318	-0.54576	0.78260
H	-2.13502	1.22231	1.70580
H	-2.62267	2.73190	0.92515
H	2.24285	-3.32696	0.09157
H	2.96355	-3.54697	-1.51793
H	1.29842	-2.92860	-1.34876
H	-3.87647	-2.39379	-1.57822
H	-5.28097	-1.29726	-1.81296
H	-4.12566	-1.57614	-3.15064
H	-5.05469	-0.73114	0.52312
H	-3.53594	-1.51157	1.02853
H	-3.97322	0.09774	1.66757

3c2(red2)

Energy = -2446.628428
 Enthalpy 0K = -2446.208566
 Enthalpy 298K = -2446.177877
 Free Energy 298K = -2446.271086
 Nimag = 0 (9.4427 cm⁻¹)

N	2.98959	0.49178	0.23660
C	2.57812	1.73480	-0.20346
C	3.43967	2.86278	-0.13010
C	4.66871	2.74355	0.46225
C	5.03115	1.49688	1.02054
C	4.18437	0.40947	0.89880
C	1.24094	1.79994	-0.68506
N	0.53575	0.60644	-0.63615
C	-0.81060	0.66927	-0.86699
C	-1.44962	1.81227	-1.29153
C	-0.70159	3.00256	-1.48009
C	0.62722	2.99320	-1.15111
C	-1.61775	-0.58364	-0.59447
N	-2.93824	-0.29460	-0.05633
C	-4.10247	-0.31754	-0.71736
N	-5.06456	-0.00945	0.15964
C	-4.50400	0.23077	1.40763
C	-3.15725	0.05081	1.27173
C	-4.30050	-0.60161	-2.15983
C	-2.04641	0.15822	2.25498
C	-5.32942	0.60114	2.58681
C	-6.48661	0.08003	-0.12512
Mn	1.70436	-1.03540	-0.27607
C	4.58365	-0.89002	1.53714
C	0.76075	-2.11147	-1.33491
O	0.19741	-2.85625	-2.03222
C	3.02325	-2.14602	-0.72688
O	3.83463	-2.91431	-1.05662
C	1.24103	-1.84713	1.24805
O	0.94650	-2.45957	2.19332
H	5.34284	3.60037	0.52929
H	-1.18508	3.91103	-1.84428
H	3.11383	3.82310	-0.52988
H	1.21625	3.90688	-1.23413
H	-2.52589	1.80559	-1.46991
H	5.97463	1.38028	1.55630
H	-1.73611	-1.19855	-1.49465
H	-1.08842	-1.20035	0.14073
H	3.73658	-1.34100	2.07320
H	5.40728	-0.72534	2.24482
H	4.92512	-1.62354	0.79350
H	-6.68744	-0.30275	-1.13060
H	-7.04213	-0.52526	0.60207
H	-6.81627	1.12548	-0.05935
H	-3.34273	-0.60369	-2.69121
H	-4.78359	-1.58029	-2.30015
H	-4.94112	0.16849	-2.61139
H	-5.90423	1.52025	2.39641
H	-6.04365	-0.19757	2.83988
H	-4.68454	0.77270	3.45736

H	-2.43718	0.47936	3.22830
H	-1.53648	-0.80795	2.39086
H	-1.29249	0.89002	1.92634

3c5(red2)

Energy = -2446.628612
 Enthalpy 0K = -2446.208935
 Enthalpy 298K = -2446.178215
 Free Energy 298K = -2446.271065
 Nimag = 0 (15.5535 cm⁻¹)

N	2.99890	0.52072	0.18805
C	2.56427	1.72044	-0.33980
C	3.41066	2.86196	-0.36463
C	4.64938	2.80354	0.21670
C	5.03787	1.60722	0.86073
C	4.20503	0.50252	0.83371
C	1.21926	1.73117	-0.80384
N	0.52986	0.53722	-0.64550
C	-0.82151	0.56814	-0.85053
C	-1.48229	1.66591	-1.35480
C	-0.75131	2.84296	-1.65909
C	0.58354	2.87448	-1.35668
C	-1.60896	-0.66377	-0.45242
N	-2.95175	-0.34271	0.00773
C	-3.22698	0.23124	1.18634
N	-4.54944	0.41369	1.24318
C	-5.13844	-0.05901	0.07709
C	-4.12607	-0.53430	-0.70841
C	-2.23596	0.62921	2.21543
C	-4.14585	-1.14293	-2.06520
C	-6.60742	-0.00020	-0.14352
C	-5.28559	1.01195	2.34356
Mn	1.72433	-1.05682	-0.18336
C	4.63258	-0.74102	1.55916
C	0.76414	-2.23332	-1.11254
O	0.19433	-3.04476	-1.72505
C	3.05308	-2.16724	-0.60294
O	3.87556	-2.93565	-0.90407
C	1.33116	-1.75645	1.41457
O	1.08141	-2.29629	2.41492
H	5.31183	3.67199	0.20980
H	-1.25188	3.71232	-2.08960
H	3.06553	3.78518	-0.83016
H	1.16040	3.78344	-1.52921
H	-2.56259	1.63420	-1.50498
H	5.99109	1.54369	1.38811
H	-1.70694	-1.36855	-1.28652
H	-1.07955	-1.19465	0.34814
H	3.80606	-1.15114	2.15653
H	5.47695	-0.51748	2.22495
H	4.95453	-1.53008	0.86547
H	-4.58425	1.42398	3.07572
H	-5.91730	1.82296	1.95999
H	-5.91594	0.25427	2.82761
H	-1.26831	0.14654	2.03149
H	-2.08623	1.71957	2.19754

H	-2.58222	0.34142	3.21720
H	-7.14932	-0.54455	0.64483
H	-6.96906	1.03967	-0.14480
H	-6.86166	-0.45333	-1.10945
H	-5.16724	-1.13139	-2.46515
H	-3.49992	-0.58412	-2.75938
H	-3.79913	-2.18747	-2.04224

1c2(I1)

Energy	= -2517.168112
Enthalpy 0K	= -2516.818696
Enthalpy 298K	= -2516.789014
Free Energy 298K	= -2516.880196
Nimag	= 0 (29.2092 cm ⁻¹)

N	1.75809	-0.96954	-0.40756
C	2.14349	0.06945	-1.21825
C	3.33682	-0.00191	-1.98615
C	4.10116	-1.13834	-1.95132
C	3.66707	-2.22152	-1.16101
C	2.50681	-2.11233	-0.41255
C	1.26243	1.19059	-1.24568
N	0.11299	1.07752	-0.46725
C	-0.83608	2.06003	-0.65631
C	-0.62299	3.18423	-1.41696
C	0.62416	3.37898	-2.06574
C	1.53767	2.36153	-1.99581
C	-2.19260	1.91692	-0.01965
N	-2.87777	0.67829	-0.40118
C	-3.85878	0.05813	0.33733
C	-4.19829	-1.07940	-0.32795
N	-3.41733	-1.12857	-1.46004
C	-2.62698	-0.05867	-1.48092
C	-3.40426	-2.21396	-2.42759
Mn	0.13463	-0.51827	0.80539
C	-0.82631	-2.00620	0.57625
O	-1.48839	-2.96393	0.51565
C	2.06126	-3.29721	0.39476
C	1.07731	-0.93314	2.25834
O	1.66737	-1.21992	3.22086
C	-1.06856	0.02845	1.99359
O	-1.80354	0.28488	2.86165
H	-2.13127	1.92466	1.07414
H	-2.82654	2.75992	-0.32151
H	3.63771	0.83992	-2.60859
H	-1.42406	3.91769	-1.52250
H	-1.89108	0.16486	-2.24880
H	2.48618	2.44917	-2.52589
H	0.82667	4.28752	-2.63524
H	4.23497	-3.15254	-1.13283
H	5.02078	-1.21012	-2.53626
H	-4.91903	-1.85736	-0.09327
H	-4.22136	0.47379	1.27277
H	-4.42790	-2.40775	-2.77007
H	-2.99078	-3.11456	-1.95626
H	-2.78003	-1.92353	-3.27943
H	2.74870	-4.13880	0.23765

H	2.03140	-3.07439	1.46945
H	1.05127	-3.61580	0.10225
C	1.35834	2.66881	1.92226
O	0.30128	3.03652	2.22607
O	2.43912	2.35041	1.64978

1c2(TS1)

Energy	= -2517.154875
Enthalpy 0K	= -2516.805718
Enthalpy 298K	= -2516.777167
Free Energy 298K	= -2516.864212
Nimag	= 0 (-626.5560 cm ⁻¹)

N	1.82425	-0.54511	-0.66166
C	2.07984	0.71362	-1.10214
C	3.20685	1.01490	-1.89245
C	4.06725	0.00413	-2.25399
C	3.77115	-1.30087	-1.84378
C	2.65241	-1.55370	-1.06242
C	1.09262	1.70923	-0.73974
N	0.02119	1.24283	-0.01694
C	-1.00177	2.14190	0.18786
C	-0.91007	3.47456	-0.16035
C	0.24847	3.97098	-0.77623
C	1.23274	3.06205	-1.09264
C	-2.30234	1.68086	0.78378
N	-2.95877	0.64497	-0.02145
C	-3.88441	-0.25753	0.44958
C	-4.23201	-1.05358	-0.59818
N	-3.51223	-0.61865	-1.68728
C	-2.75034	0.40555	-1.31465
C	-3.52873	-1.22751	-3.00793
Mn	0.23099	-0.65786	0.64582
C	-0.66650	-1.88219	-0.27297
O	-1.27340	-2.73752	-0.78026
C	2.35767	-2.97402	-0.67827
C	1.13111	-1.66245	1.80103
O	1.67003	-2.33083	2.58901
C	-1.01447	-0.73014	1.91330
O	-1.75898	-0.91419	2.78620
H	-2.17331	1.27680	1.79299
H	-2.98893	2.53347	0.85588
H	3.39505	2.03500	-2.22277
H	-1.75812	4.13189	0.03860
H	-2.06266	0.94468	-1.96134
H	2.12560	3.39480	-1.62004
H	0.34475	5.02667	-1.03334
H	4.41101	-2.13390	-2.13857
H	4.94954	0.21198	-2.86267
H	-4.92108	-1.89095	-0.66219
H	-4.20791	-0.25966	1.48618
H	-2.93088	-0.61291	-3.68962
H	-4.56232	-1.28202	-3.37045
H	-3.09994	-2.23559	-2.94732
H	3.02641	-3.65336	-1.22278
H	2.50579	-3.14628	0.39591
H	1.31976	-3.24427	-0.91189

C 1.46607 0.96522 2.29454
 O 0.72436 1.19283 3.20533
 O 2.53028 1.19917 1.80386

1c2(TS1)'

Energy = -2517.151635
 Enthalpy 0K = -2516.803310
 Enthalpy 298K = -2516.774425
 Free Energy 298K = -2516.862820
 Nimag = 1 (-510.9166 cm⁻¹)

C 4.22133 -0.40381 -1.28892
 N 3.12916 0.34544 -0.91493
 C 3.19834 0.57744 0.39298
 N 4.29467 -0.00234 0.87260
 C 4.95490 -0.62318 -0.16408
 C 2.04825 0.75342 -1.82210
 C 1.01164 1.61814 -1.15993
 N -0.13060 1.04779 -0.64059
 C -1.10579 1.93153 -0.22848
 C -0.87877 3.31835 -0.15085
 C 0.31543 3.85705 -0.57003
 C 1.25679 2.97482 -1.12938
 C -2.38068 1.34040 0.09630
 C -3.49673 2.10200 0.50496
 C -4.70453 1.47796 0.70482
 C -4.79396 0.10053 0.45518
 C -3.67142 -0.61405 0.06675
 N -2.45290 -0.00962 -0.06641
 Mn -0.62367 -0.89634 -0.38449
 C -1.02050 -1.70175 -1.91732
 O -1.22369 -2.30380 -2.89063
 C -3.82406 -2.07711 -0.23230
 C 4.70123 -0.02072 2.26927
 C 0.98254 -1.66774 -0.41153
 O 1.94470 -2.31756 -0.38529
 C 0.12080 -0.08048 2.09820
 C -0.96781 -2.20383 0.77242
 O -1.13736 -3.09039 1.50858
 H 1.59251 -0.15361 -2.23916
 H 2.52070 1.31049 -2.64080
 H -3.40672 3.17669 0.65550
 H 2.18961 3.35077 -1.55459
 H 2.47280 1.13256 0.97960
 H -1.66064 3.97237 0.23340
 H 0.50706 4.92952 -0.51432
 H -5.74688 -0.42138 0.55508
 H -5.58103 2.04512 1.02488
 H 5.88449 -1.16403 -0.00976
 H 4.37353 -0.72102 -2.31664
 H 5.73010 0.34951 2.35442
 H 4.64161 -1.04723 2.65227
 H 4.02781 0.62422 2.84328
 H -4.88927 -2.33393 -0.30224
 H -3.33504 -2.34289 -1.17855
 H -3.37981 -2.70472 0.55187
 O 1.16662 -0.59453 2.35187

O -0.75443 0.65417 2.42141

1c2(I2)

Energy = -2517.164641
 Enthalpy 0K = -2516.812806
 Enthalpy 298K = -2516.784558
 Free Energy 298K = -2516.871612
 Nimag = 0 (18.6514 cm⁻¹)

C -3.03467 0.15586 -0.58831
 N -3.23005 0.30077 0.72489
 C -4.53921 -0.00697 1.02787
 C -5.14354 -0.34242 -0.14457
 N -4.18588 -0.23456 -1.13033
 C -2.18888 0.64117 1.69483
 C -1.17821 1.58196 1.09018
 N -0.00496 1.11661 0.62613
 C 0.87198 2.00678 0.11590
 C 0.57324 3.36580 0.00117
 C -0.65315 3.83612 0.44450
 C -1.53294 2.92909 1.01443
 C 2.20519 1.47763 -0.25029
 N 2.42845 0.18557 0.06709
 C 3.67361 -0.30891 -0.06469
 C 4.70045 0.45989 -0.62628
 C 4.44807 1.75527 -1.04629
 C 3.18164 2.28367 -0.83182
 C 3.99675 -1.69415 0.40732
 Mn 0.64191 -0.90592 0.41130
 C 0.36270 -0.58118 -1.69335
 O -0.66515 0.05794 -2.06888
 C -4.37284 -0.51620 -2.54498
 C 1.22651 -2.51316 -0.09371
 O 1.48360 -3.58848 -0.43198
 C 0.90676 -1.16537 2.18652
 O 1.01784 -1.42906 3.30715
 C -0.90673 -1.76832 0.34666
 O -1.84724 -2.44630 0.27116
 O 1.26762 -0.96749 -2.45078
 H -1.71170 -0.27433 2.06178
 H -2.68750 1.13324 2.53825
 H 2.96560 3.31200 -1.11513
 H -2.50123 3.24785 1.40409
 H -2.05108 0.24218 -1.13748
 H 1.29789 4.06012 -0.42001
 H -0.90727 4.89424 0.36380
 H 5.69464 0.02182 -0.72757
 H 5.23097 2.35885 -1.50919
 H -6.16586 -0.63946 -0.36188
 H -4.92378 0.04512 2.04271
 H -5.05490 0.22135 -2.98717
 H -4.78870 -1.52429 -2.66475
 H -3.39467 -0.46129 -3.03666
 H 5.06674 -1.76542 0.64469
 H 3.41453 -1.95910 1.29878
 H 3.78200 -2.43579 -0.37494

1c5(I1)

Energy = -2517.168195
 Enthalpy 0K = -2516.818797
 Enthalpy 298K = -2516.789040
 Free Energy 298K = -2516.880902
 Nimag = 0 (17.4349 cm⁻¹)

C -2.55443 0.67872 -1.92485
 N -2.69327 1.05710 -0.61005
 C -3.58076 0.25472 -0.02739
 N -4.01939 -0.62310 -0.92462
 C -3.38858 -0.37895 -2.12282
 C -1.95730 2.13568 0.05654
 C -0.53257 2.22864 -0.42654
 N 0.28578 1.12361 -0.34866
 C 1.48801 1.21024 -1.04418
 C 1.95449 2.44508 -1.56200
 C 1.17377 3.56827 -1.49812
 C -0.13627 3.42679 -0.96944
 C 2.21952 -0.00710 -1.16740
 N 1.66593 -1.09718 -0.54131
 C 2.25963 -2.31595 -0.70867
 C 3.43074 -2.46390 -1.43307
 C 4.03848 -1.33984 -2.02850
 C 3.42938 -0.11885 -1.90358
 Mn 0.06662 -0.61788 0.69140
 C -1.07078 -0.04680 1.92776
 O -1.79011 0.22523 2.80560
 C 1.62320 -3.53854 -0.11359
 H -3.58496 -0.97828 -3.00732
 C -1.08147 -1.91290 0.25072
 O -1.86653 -2.75564 0.06936
 C 0.88341 -1.37565 2.08039
 O 1.39068 -1.88428 2.99714
 C 1.76734 2.16022 2.22214
 O 2.78432 1.67758 1.94467
 O 0.78075 2.68152 2.53730
 H -2.02622 1.96055 1.13514
 H -2.47180 3.08042 -0.15952
 H 3.86369 0.75977 -2.37945
 H -0.84176 4.25880 -1.00163
 H -1.87358 1.18599 -2.60277
 H 2.94449 2.49785 -2.01545
 H 1.52368 4.52657 -1.88558
 H 3.87086 -3.45649 -1.53964
 H 4.96738 -1.44459 -2.59353
 C -4.96524 -1.69956 -0.67440
 H -3.87807 0.29364 1.01792
 H 2.19368 -4.43412 -0.39285
 H 1.58045 -3.48717 0.98249
 H 0.59154 -3.65804 -0.47252
 H -5.82960 -1.58861 -1.34074
 H -4.47116 -2.66143 -0.85671
 H -5.29377 -1.64799 0.36911

1c5(TS1)

Energy = -2517.154633
 Enthalpy 0K = -2516.805419
 Enthalpy 298K = -2516.776851
 Free Energy 298K = -2516.863927
 Nimag = 1 (-647.2741 cm⁻¹)

C -2.65456 1.05327 -1.64673
 N -2.79602 1.00625 -0.27888
 C -3.63348 0.01853 0.02895
 N -4.03402 -0.56903 -1.09462
 C -3.43209 0.06039 -2.15936
 C -2.12773 1.88783 0.68487
 C -0.73908 2.25048 0.23282
 N 0.19104 1.26209 0.00562
 C 1.33567 1.65362 -0.64326
 C 1.64444 3.00431 -0.87727
 C 0.75647 3.99301 -0.51796
 C -0.48173 3.58709 0.00286
 C 2.21887 0.57924 -1.04721
 N 1.82064 -0.66700 -0.68398
 C 2.54989 -1.73471 -1.12168
 C 3.70761 -1.56033 -1.86709
 C 4.14543 -0.27441 -2.20388
 C 3.38671 0.80123 -1.80304
 Mn 0.18157 -0.68114 0.56902
 C -1.09720 -0.67786 1.79928
 O -1.89205 -0.81670 2.63763
 C 2.10134 -3.13380 -0.81690
 H -3.60383 -0.25471 -3.18466
 C -0.81410 -1.75136 -0.43665
 O -1.50159 -2.50812 -0.99541
 C 0.93625 -1.83042 1.69337
 O 1.37774 -2.58982 2.45951
 C 1.52892 0.72510 2.34506
 O 2.62344 0.87125 1.89000
 O 0.78585 0.97970 3.24648
 H -2.14243 1.38973 1.65882
 H -2.72595 2.80295 0.77419
 H 3.68336 1.81171 -2.07920
 H -1.26187 4.32102 0.21219
 H -2.01280 1.77996 -2.13720
 H 2.59394 3.27136 -1.33920
 H 0.98415 5.04773 -0.67822
 H 4.26538 -2.43951 -2.19312
 H 5.05636 -0.12955 -2.78812
 C -4.90792 -1.72846 -1.18357
 H -3.92483 -0.27335 1.03488
 H 2.70658 -3.85173 -1.38556
 H 2.20875 -3.37325 0.24938
 H 1.04561 -3.28133 -1.07892
 H -5.73110 -1.51049 -1.87452
 H -4.33177 -2.58865 -1.54652
 H -5.30981 -1.94645 -0.18820

1c5 (I2)

Energy = -2517.160459
 Enthalpy 0K = -2516.807781
 Enthalpy 298K = -2516.779579
 Free Energy 298K = -2516.866053
 Nimag = 0 (25.4905 cm⁻¹)

N	2.56296	0.21788	0.17485
C	2.32852	1.52474	-0.06276
C	3.34188	2.41420	-0.41742
C	4.64708	1.94809	-0.49681
C	4.89402	0.62295	-0.17629
C	3.83456	-0.22619	0.16438
C	0.93389	1.97375	0.14546
N	0.05817	1.02320	0.53965
C	-1.18047	1.41289	0.88419
C	-1.60907	2.73601	0.77307
C	-0.73449	3.69860	0.29494
C	0.56307	3.31031	-0.00524
C	-2.16963	0.41324	1.42853
N	-3.26309	0.18432	0.48375
C	-4.54763	0.06928	0.82140
N	-5.25720	-0.14441	-0.28101
C	-4.39777	-0.16441	-1.35954
C	-3.13764	0.04144	-0.88390
H	-4.94763	0.14611	1.82978
C	-6.70036	-0.31800	-0.34556
Mn	0.79818	-0.94995	0.26019
C	1.47180	-2.45098	-0.41850
O	1.79754	-3.45584	-0.89360
C	4.14852	-1.64499	0.53285
C	0.96176	-1.38866	2.00815
O	1.01942	-1.78382	3.09560
C	-0.71350	-1.85140	0.02588
O	-1.62745	-2.54276	-0.15898
C	0.61013	-0.43522	-1.83066
O	1.63165	-0.54749	-2.52985
O	-0.49730	0.02158	-2.21343
H	-4.75947	-0.32534	-2.37136
H	-1.67992	-0.53461	1.66987
H	-2.61799	0.81017	2.34780
H	3.12595	3.46047	-0.62515
H	-2.62899	2.99364	1.06491
H	1.28163	4.05138	-0.34927
H	-1.04613	4.73811	0.18111
H	5.91011	0.22543	-0.18297
H	5.46050	2.61859	-0.78022
H	5.19398	-1.72292	0.85987
H	3.49407	-2.00493	1.33644
H	4.02098	-2.31249	-0.33104
H	-2.14928	0.07318	-1.38677
H	-7.13216	0.45695	-0.99099
H	-6.93065	-1.31030	-0.75315
H	-7.11437	-0.22874	0.66471

2c2 (I1)

Energy = -2556.453689
 Enthalpy 0K = -2556.076653
 Enthalpy 298K = -2556.045368
 Free Energy 298K = -2556.139892
 Nimag = 0 (25.8999 cm⁻¹)

C	-2.76619	-0.00578	-1.27092
N	-2.79263	0.78591	-0.18789
C	-3.68056	0.26388	0.72847
C	-4.18895	-0.87357	0.19371
N	-3.60569	-1.02596	-1.04248
C	-2.03963	2.01863	0.07307
C	-0.67563	2.09962	-0.56411
N	0.22139	1.07004	-0.40896
C	1.34510	1.11669	-1.22979
C	1.67969	2.28784	-1.95683
C	0.83720	3.36690	-1.96407
C	-0.40820	3.23159	-1.29687
C	2.13565	-0.06768	-1.26282
N	1.72074	-1.08192	-0.43288
C	2.37591	-2.27892	-0.48983
C	3.47351	-2.47265	-1.31210
C	3.93987	-1.41969	-2.12603
C	3.26803	-0.22603	-2.10697
Mn	0.22612	-0.50577	0.88611
C	-0.81615	0.19512	2.14305
O	-1.44473	0.57230	3.04962
C	1.89221	-3.42926	0.34484
C	-3.82623	-2.14616	-1.94300
C	-0.86499	-1.91426	0.75262
O	-1.59177	-2.82546	0.76177
C	1.22527	-1.00255	2.27287
O	1.85571	-1.33876	3.19318
C	1.78017	2.59892	1.84421
O	2.80892	2.14783	1.55749
O	0.78102	3.09541	2.15991
H	-1.96880	2.10649	1.16397
H	-2.64498	2.86285	-0.28121
H	3.59038	0.59398	-2.74802
H	-1.16918	4.00940	-1.37857
C	-1.95960	0.13617	-2.50657
H	2.61785	2.32692	-2.51087
H	1.08732	4.27901	-2.50869
H	3.96676	-3.44567	-1.32407
H	4.80966	-1.56004	-2.77171
H	-4.90245	-1.59240	0.58537
H	-3.85927	0.74230	1.68635
H	-4.49474	-2.85846	-1.44781
H	-2.87197	-2.63957	-2.16648
H	-4.29273	-1.79930	-2.87452
H	2.48778	-4.32654	0.13108
H	1.96792	-3.21568	1.41947
H	0.83778	-3.65351	0.13323
H	-2.50614	-0.28584	-3.35937
H	-1.73798	1.18774	-2.71578
H	-1.00894	-0.40732	-2.39303

2c2(TS1)

Energy = -2556.440262
 Enthalpy 0K = -2556.063442
 Enthalpy 298K = -2556.033315
 Free Energy 298K = -2556.122987
 Nimag = 1 (-623.5763 cm⁻¹)

C	-2.86322	0.40146	-1.10706
N	-2.88067	0.59484	0.22134
C	-3.69736	-0.35215	0.80237
C	-4.16679	-1.14366	-0.19345
N	-3.63445	-0.66379	-1.36718
C	-2.19822	1.62623	1.01419
C	-0.88386	2.10819	0.45877
N	0.11195	1.21652	0.13660
C	1.14899	1.72181	-0.61030
C	1.31895	3.09937	-0.82578
C	0.39213	3.99672	-0.34447
C	-0.75718	3.46909	0.26379
C	2.07027	0.73733	-1.13435
N	1.82688	-0.54450	-0.75550
C	2.59599	-1.53657	-1.29258
C	3.64086	-1.25032	-2.15969
C	3.92011	0.07386	-2.51904
C	3.12012	1.07193	-2.01296
Mn	0.34462	-0.71495	0.66790
C	-0.78250	-0.80157	2.04076
O	-1.44546	-0.98272	2.97717
C	2.31349	-2.97360	-0.96596
C	-3.82977	-1.25755	-2.68078
C	-0.64468	-1.87166	-0.24450
O	-1.29763	-2.68943	-0.75577
C	1.30603	-1.80993	1.68331
O	1.88927	-2.53642	2.38364
C	1.76930	0.77731	2.30918
O	2.77951	1.03139	1.72393
O	1.13330	0.94787	3.30762
H	-2.08224	1.21098	2.02178
H	-2.87712	2.48447	1.09681
H	3.29140	2.10811	-2.30058
H	-1.57841	4.12514	0.55732
C	-2.12163	1.15603	-2.14568
H	2.19342	3.45962	-1.36606
H	0.51674	5.07172	-0.48183
H	4.23458	-2.07176	-2.56339
H	4.74099	0.30619	-3.20045
H	-4.82332	-2.00842	-0.17107
H	-3.86360	-0.38335	1.87445
H	-4.44178	-2.15791	-2.56222
H	-2.86006	-1.53295	-3.11393
H	-4.34729	-0.55189	-3.34386
H	2.93246	-3.62717	-1.59428
H	2.53665	-3.20515	0.08382
H	1.25808	-3.22277	-1.13729
H	-2.66395	1.10779	-3.09807
H	-2.00222	2.20743	-1.86483
H	-1.12390	0.71257	-2.28771

2c2(I2)

Energy = -2556.449107
 Enthalpy 0K = -2556.068997
 Enthalpy 298K = -2556.039210
 Free Energy 298K = -2556.128958
 Nimag = 0 (21.7307 cm⁻¹)

Mn	1.31594	-0.97036	-0.40568
N	0.01926	0.71691	-0.57390
C	0.07088	3.09244	-0.94056
H	0.62821	4.02697	-0.93615
N	2.53340	0.64578	0.32381
C	-1.25627	3.08161	-1.34067
H	-1.74685	3.99943	-1.66902
C	2.78812	3.03348	0.18457
H	2.38207	4.00319	-0.09634
C	2.05685	1.86098	-0.01284
C	0.67442	1.89685	-0.54593
C	4.51602	1.70460	1.14494
H	5.48918	1.59663	1.62610
C	-1.95185	1.88253	-1.28619
H	-3.00917	1.84337	-1.55107
C	-1.29126	0.72187	-0.88482
C	4.04623	2.95144	0.76326
H	4.64218	3.85124	0.92727
C	3.74007	0.56214	0.91875
O	-0.28257	-3.08333	-1.66033
O	2.66072	-3.43409	0.43194
O	2.75849	-0.68891	-2.97786
N	-3.45817	-0.35627	-0.41537
C	2.20293	-2.41254	0.12535
C	4.25169	-0.76842	1.36768
H	3.46457	-1.25179	1.96315
H	4.49667	-1.40681	0.50682
H	5.15968	-0.64510	1.97239
C	0.28140	-2.20786	-1.15030
C	-2.05656	-0.57551	-0.75277
H	-2.04125	-1.13640	-1.69548
H	-1.59005	-1.17918	0.04989
C	2.15842	-0.73221	-1.98960
C	-4.52626	-0.51325	-1.27240
N	-5.23886	0.14169	0.70315
C	-5.64569	-0.20254	-0.56833
C	-3.90583	0.04163	0.78588
C	-3.06704	0.35923	1.96246
H	-2.21067	-0.33750	2.02511
H	-2.67573	1.38560	1.87159
H	-3.66034	0.29648	2.88291
C	-6.12074	0.54998	1.78675
H	-7.14436	0.58882	1.39972
H	-6.07013	-0.17633	2.60830
H	-5.83180	1.54387	2.15099
C	0.53780	-1.24215	1.56888
O	-0.65592	-1.65139	1.65168
O	1.25607	-0.92375	2.53126
H	-6.69333	-0.19954	-0.85516
H	-4.39118	-0.83480	-2.30113

2c5(I1)

Energy = -2556.454623
 Enthalpy 0K = -2556.077535
 Enthalpy 298K = -2556.046235
 Free Energy 298K = -2556.140577
 Nimag = 0 (26.1289 cm⁻¹)

C -2.30577 0.62947 -2.06080
 N -2.54833 1.00322 -0.75627
 C -3.49230 0.20460 -0.24040
 N -3.84905 -0.66829 -1.19146
 C -3.11955 -0.42288 -2.33191
 C -1.84682 2.09267 -0.06685
 C -0.41216 2.19453 -0.52059
 N 0.40682 1.09780 -0.39087
 C 1.59859 1.13735 -1.10461
 C 2.07487 2.34852 -1.66937
 C 1.30268 3.47952 -1.64063
 C -0.01155 3.36785 -1.11139
 C 2.29649 -0.10104 -1.19694
 N 1.72246 -1.15243 -0.52190
 C 2.26282 -2.39681 -0.67429
 C 3.40984 -2.60765 -1.42148
 C 4.04841 -1.52112 -2.05495
 C 3.48681 -0.27520 -1.95166
 Mn 0.20184 -0.56997 0.76131
 C -0.76372 0.17899 2.05132
 O -1.34640 0.59537 2.97148
 C 1.58770 -3.57527 -0.03466
 H -3.24528 -1.01609 -3.23301
 C -1.05847 -1.79614 0.45852
 O -1.90639 -2.59424 0.38075
 C 1.03323 -1.34782 2.12984
 O 1.55504 -1.85929 3.03681
 C 2.12373 2.19272 2.03741
 O 3.07779 1.57564 1.80674
 O 1.20379 2.84681 2.30181
 H -1.92523 1.92167 1.01011
 H -2.36674 3.03246 -0.29325
 H 3.94019 0.57546 -2.46022
 H -0.71566 4.19824 -1.18697
 H -1.57412 1.13968 -2.68023
 H 3.06255 2.37457 -2.13089
 H 1.65955 4.42039 -2.06318
 H 3.80767 -3.61921 -1.51570
 H 4.96131 -1.67519 -2.63465
 C -4.81382 -1.74053 -1.01255
 C -4.05198 0.20940 1.13006
 H 2.08250 -4.50662 -0.34034
 H 1.61570 -3.51798 1.06191
 H 0.53005 -3.62701 -0.32869
 H -4.92367 -2.26878 -1.96548
 H -4.45099 -2.43845 -0.24723
 H -5.78477 -1.32636 -0.71144
 H -5.14963 0.17270 1.08403
 H -3.70232 -0.67912 1.67718
 H -3.75556 1.10544 1.68379

2c5(TS1)

Energy = -2556.440515
 Enthalpy 0K = -2556.063336
 Enthalpy 298K = -2556.033258
 Free Energy 298K = -2556.123600
 Nimag = 1 (-644.6951 cm⁻¹)

C -2.33766 1.10681 -1.75879
 N -2.63336 1.03952 -0.41324
 C -3.55347 0.08564 -0.21494
 N -3.83749 -0.45758 -1.40541
 C -3.09058 0.16314 -2.37936
 C -2.01183 1.88259 0.61757
 C -0.60421 2.25350 0.23125
 N 0.32213 1.26020 0.01298
 C 1.45774 1.63319 -0.65907
 C 1.78526 2.98066 -0.88660
 C 0.91769 3.97883 -0.50275
 C -0.32889 3.58783 0.01349
 C 2.30165 0.53998 -1.09224
 N 1.87708 -0.69707 -0.72454
 C 2.55299 -1.78267 -1.20167
 C 3.69175 -1.63734 -1.98144
 C 4.16353 -0.36173 -2.31459
 C 3.45281 0.73358 -1.88013
 Mn 0.31479 -0.66465 0.61907
 C -0.84226 -0.55887 1.96495
 O -1.53381 -0.61241 2.89685
 C 2.05516 -3.16753 -0.90937
 H -3.15919 -0.12201 -3.42513
 C -0.79190 -1.72678 -0.27184
 O -1.54965 -2.47778 -0.74113
 C 1.10752 -1.83416 1.69541
 O 1.58363 -2.60395 2.42956
 C 1.83652 0.70232 2.29732
 O 2.88763 0.83334 1.74410
 O 1.19242 0.96388 3.27049
 H -2.05869 1.35010 1.57024
 H -2.61165 2.79592 0.71936
 H 3.77246 1.73821 -2.15304
 H -1.10233 4.33041 0.21747
 H -1.61596 1.81322 -2.15774
 H 2.73157 3.23583 -1.36227
 H 1.16141 5.03160 -0.65238
 H 4.20703 -2.53020 -2.33883
 H 5.06110 -0.24043 -2.92436
 C -4.74776 -1.57161 -1.61252
 C -4.16084 -0.35072 1.06260
 H 2.62619 -3.90098 -1.49340
 H 2.15922 -3.42638 0.15252
 H 0.99206 -3.26814 -1.16603
 H -4.77902 -1.79764 -2.68357
 H -4.38769 -2.45146 -1.06416
 H -5.75497 -1.30428 -1.26711
 H -5.24853 -0.44971 0.94008
 H -3.75789 -1.33253 1.35304
 H -3.96442 0.36460 1.86741

2c5(I2)

Energy = -2556.446064
 Enthalpy 0K = -2556.066085
 Enthalpy 298K = -2556.036026
 Free Energy 298K = -2556.126995
 Nimag = 0 (20.6786 cm⁻¹)

N	2.71788	0.21530	0.19318
C	2.49195	1.52507	-0.04469
C	3.51186	2.40937	-0.39364
C	4.81614	1.93929	-0.46241
C	5.05515	0.61482	-0.13373
C	3.99032	-0.23011	0.19971
C	1.09754	1.98063	0.14676
N	0.20708	1.03123	0.50426
C	-1.04041	1.42099	0.81224
C	-1.45589	2.74958	0.72102
C	-0.55871	3.71694	0.29682
C	0.74203	3.32443	0.01941
C	-2.06647	0.41570	1.27079
N	-3.08148	0.20496	0.23986
C	-4.38521	-0.00176	0.47857
N	-4.98809	-0.15997	-0.70434
C	-4.04703	-0.05156	-1.70894
C	-2.84331	0.17506	-1.12095
C	-5.02727	-0.03925	1.81328
C	-6.40972	-0.39527	-0.91097
Mn	0.95106	-0.94764	0.26292
C	1.63205	-2.51622	-0.23634
O	1.94973	-3.57505	-0.57975
C	4.29822	-1.64429	0.58758
C	0.97739	-1.32175	2.03227
O	0.92565	-1.66574	3.13741
C	-0.55236	-1.80779	-0.11766
O	-1.46447	-2.47143	-0.39705
C	0.88395	-0.48676	-1.85015
H	-4.31962	-0.15502	-2.75529
H	-1.59945	-0.53748	1.53748
H	-2.57270	0.80868	2.16088
H	3.30094	3.45560	-0.60631
H	-2.48427	3.00642	0.98229
H	-1.82323	0.26895	-1.54030
H	1.47454	4.06770	-0.28816
H	-0.85806	4.76201	0.20228
H	6.07002	0.21418	-0.12769
H	5.63394	2.60597	-0.74204
H	5.34508	-1.72334	0.90968
H	3.64676	-1.98365	1.40335
H	4.16047	-2.32540	-0.26364
H	-6.99275	0.45945	-0.54475
H	-6.58230	-0.51729	-1.98549
H	-6.72058	-1.30957	-0.38983
H	-6.09569	-0.26374	1.72215
H	-4.55732	-0.80941	2.44169
H	-4.91570	0.93212	2.31814
O	1.85878	-0.85552	-2.52711
O	-0.08663	0.19668	-2.26251

3c2(I1)

Energy = -2635.019744
 Enthalpy 0K = -2634.586570
 Enthalpy 298K = -2634.551818
 Free Energy 298K = -2634.654908
 Nimag = 0 (11.1764 cm⁻¹)

C	3.68010	0.01936	-1.49924
N	3.10601	-0.27630	-0.26909
C	4.05382	-0.30845	0.67735
N	5.22288	-0.05698	0.08015
C	5.02091	0.15718	-1.27743
C	1.68592	-0.50498	-0.06035
C	0.88308	0.76145	0.12269
N	-0.48121	0.64186	0.00908
C	-1.20657	1.82910	0.01869
C	-0.58893	3.07056	0.31804
C	0.76181	3.14134	0.52447
C	1.52073	1.95044	0.38263
Mn	-1.63592	-1.03888	-0.14111
C	-1.74286	-1.99943	-1.64329
O	-1.78498	-2.70298	-2.57041
C	-2.59119	1.70890	-0.29497
N	-3.03170	0.43494	-0.56477
C	-4.32203	0.26880	-0.98432
C	-5.20421	1.33241	-1.07293
C	-4.77878	2.63320	-0.73198
C	-3.47547	2.82007	-0.35480
C	-4.80309	-1.09658	-1.38373
C	3.84882	-0.55060	2.12613
C	6.14268	0.46442	-2.20311
C	6.51903	0.00816	0.73356
C	2.87529	0.12899	-2.74457
C	-2.80531	-1.87327	0.90994
O	-3.55452	-2.44666	1.59376
C	-0.51477	-2.26001	0.50483
O	0.10179	-3.15184	0.93271
C	-0.72426	0.21059	3.08366
O	-1.75447	0.73622	3.14750
O	0.31544	-0.30421	3.08238
H	-1.19457	3.97507	0.37471
H	1.25033	4.08880	0.75891
H	-3.11534	3.81857	-0.10971
H	-6.22576	1.15204	-1.41096
H	2.60668	1.98565	0.46780
H	-5.47140	3.47625	-0.78370
H	-4.79015	-1.79909	-0.53991
H	-4.16543	-1.52442	-2.16956
H	-5.83129	-1.03734	-1.76442
H	1.29988	-1.06061	-0.92585
H	1.57825	-1.16393	0.80752
H	2.78699	-0.47957	2.38545
H	4.39502	0.19879	2.71496
H	4.21518	-1.54914	2.40852
H	7.23923	-0.60020	0.17283
H	6.44009	-0.38632	1.75143
H	6.86859	1.04868	0.76987

H	2.08187	0.88432	-2.63790
H	2.39727	-0.83021	-2.99689
H	3.51938	0.42101	-3.58313
H	6.86300	-0.36717	-2.24585
H	6.68638	1.36632	-1.88330
H	5.75763	0.63582	-3.21581

3c2(TS1)

Energy	= -2635.008310
Enthalpy 0K	= -2634.576062
Enthalpy 298K	= -2634.542188
Free Energy 298K	= -2634.641953
Nimag	= 1 (-645.7324 cm ⁻¹)

C	3.90737	-0.02285	-1.34928
N	3.14600	-0.24229	-0.20781
C	3.93478	-0.22396	0.87572
N	5.18457	-0.00876	0.45338
C	5.19918	0.12125	-0.92954
C	1.70769	-0.44074	-0.19913
C	0.91248	0.83399	-0.08735
N	-0.45699	0.70884	-0.12238
C	-1.17390	1.88021	-0.05037
C	-0.55716	3.13473	0.11243
C	0.81202	3.23087	0.17841
C	1.55489	2.04365	0.06180
Mn	-1.59409	-0.97637	-0.20843
C	-1.93892	-1.58999	-1.83805
O	-2.15960	-2.07412	-2.87317
C	-2.60975	1.74159	-0.14918
N	-3.06631	0.47201	-0.31240
C	-4.40667	0.28410	-0.49983
C	-5.29687	1.34778	-0.46869
C	-4.83429	2.65232	-0.25628
C	-3.48193	2.84978	-0.10814
C	-4.95288	-1.08943	-0.76031
C	3.50521	-0.37331	2.28792
C	6.45723	0.36313	-1.68327
C	6.36940	0.07300	1.28983
C	3.30563	0.02277	-2.70818
C	-2.54829	-2.03847	0.84746
O	-3.12411	-2.78985	1.52856
C	-0.40566	-2.29317	-0.06043
O	0.22983	-3.26281	0.02753
C	-1.03784	-0.29486	2.30650
O	-1.86586	0.49832	2.62101
O	-0.04911	-0.89839	2.59976
H	-1.16638	4.03437	0.18391
H	1.30882	4.19380	0.30509
H	-3.09131	3.85564	0.03475
H	-6.36009	1.15383	-0.61778
H	2.64389	2.08311	0.08527
H	-5.52938	3.49375	-0.22467
H	-4.86568	-1.73602	0.12261
H	-4.41872	-1.58595	-1.58066
H	-6.01584	-1.02289	-1.02632
H	1.43326	-0.97352	-1.11946

H	1.46169	-1.09849	0.64051
H	2.41538	-0.46465	2.36299
H	3.81820	0.50571	2.86962
H	3.96455	-1.26587	2.73744
H	7.06944	-0.72735	1.01703
H	6.08756	-0.03880	2.34132
H	6.85418	1.04740	1.14737
H	2.49917	0.77012	-2.75756
H	2.88208	-0.95316	-2.99178
H	4.06985	0.29140	-3.44772
H	7.17495	-0.45760	-1.53129
H	6.94086	1.29773	-1.36031
H	6.24536	0.43865	-2.75677

3c2(I2)

Energy	= -2635.016323
Enthalpy 0K	= -2634.581320
Enthalpy 298K	= -2634.547722
Free Energy 298K	= -2634.646834
Nimag	= 0 (17.2966 cm ⁻¹)

C	4.07482	-0.19048	-1.18283
N	3.13524	-0.24652	-0.16000
C	3.73916	-0.06611	1.02400
N	5.04380	0.09942	0.78112
C	5.28406	0.02345	-0.58499
C	1.70819	-0.44050	-0.34779
C	0.92661	0.84990	-0.40090
N	-0.42155	0.76159	-0.32998
C	-1.12609	1.91227	-0.24613
C	-0.51248	3.16882	-0.29622
C	0.86124	3.25235	-0.42609
C	1.59037	2.07028	-0.46757
Mn	-1.59974	-0.98322	-0.22381
C	-2.15980	-1.23648	-1.91478
O	-2.56243	-1.50528	-2.96884
C	-2.59108	1.78374	-0.09958
N	-3.08332	0.52985	-0.07901
C	-4.42060	0.35580	-0.00086
C	-5.28737	1.44687	0.10566
C	-4.78234	2.73870	0.11519
C	-3.41314	2.91058	-0.00124
C	-5.01511	-1.01999	-0.02891
C	3.08330	-0.00188	2.35254
C	6.65135	0.15980	-1.15228
C	6.07809	0.32965	1.77458
C	3.70236	-0.34334	-2.61455
C	-2.43137	-2.25345	0.68713
O	-2.87077	-3.14415	1.29398
C	-0.42673	-2.28963	-0.49383
O	0.20595	-3.24036	-0.70035
C	-1.01515	-0.67493	1.85900
O	-1.73660	0.06315	2.53445
O	0.09223	-1.17619	2.16730
H	-1.10261	4.08033	-0.23573
H	1.36051	4.22101	-0.47988
H	-2.99612	3.91506	-0.01456

H	-6.36082	1.26599	0.17648
H	2.67725	2.09950	-0.54391
H	-5.44626	3.60104	0.19968
H	-4.83301	-1.54365	0.91953
H	-4.58374	-1.62831	-0.83377
H	-6.10102	-0.95536	-0.17509
H	1.56686	-1.01415	-1.27112
H	1.31443	-1.02771	0.49534
H	2.02993	-0.32149	2.30536
H	3.12296	1.02978	2.73519
H	3.61013	-0.65058	3.06664
H	6.78919	-0.50693	1.77108
H	5.62543	0.41511	2.76713
H	6.60894	1.26162	1.54171
H	2.93145	0.38732	-2.90295
H	3.31109	-1.35118	-2.82273
H	4.58207	-0.18137	-3.24950
H	7.32430	-0.61548	-0.75509
H	7.08749	1.14085	-0.90912
H	6.61894	0.05877	-2.24398

3_{C5}(I1)

Energy	=	-2635.020085
Enthalpy 0K	=	-2634.587681
Enthalpy 298K	=	-2634.552665
Free Energy 298K	=	-2634.657149
Nimag	=	0 (14.2625 cm ⁻¹)

Mn	-1.63122	-1.00134	0.33487
N	-0.46020	0.59027	-0.17754
C	-0.55048	2.88551	-1.02654
H	-1.14768	3.76438	-1.27022
N	-2.98256	0.56136	0.51778
C	0.78929	2.87192	-1.30696
H	1.27649	3.72406	-1.78423
C	-3.39454	2.87211	-0.13380
H	-3.02633	3.79630	-0.57814
C	-2.53572	1.74567	-0.01978
C	-1.16822	1.76288	-0.41835
C	-5.11261	1.59714	0.93454
H	-6.11988	1.51238	1.34512
C	1.54028	1.73257	-0.91661
H	2.62232	1.71780	-1.05218
C	0.89926	0.65195	-0.35984
C	-4.68055	2.79693	0.33165
H	-5.35354	3.65379	0.25424
C	-4.25443	0.51340	1.01595
O	0.06435	-3.28444	-0.41065
O	-3.64261	-2.65589	-1.03999
O	-1.71657	-2.20067	3.02694
N	3.10898	-0.25580	0.30517
C	-2.85403	-1.98757	-0.50234
C	-4.74028	-0.73673	1.69115
H	-4.78154	-1.58798	0.99861
H	-4.07366	-1.02347	2.51607
H	-5.74780	-0.57773	2.09765
C	-0.54093	-2.33133	-0.12271

C	1.69821	-0.54538	0.09993
H	1.27359	-0.93586	1.03494
H	1.64100	-1.35654	-0.63393
C	-1.69839	-1.67385	1.98823
C	3.88093	-1.29374	-1.86091
H	3.49292	-2.30920	-1.68624
H	3.15004	-0.75269	-2.48041
H	4.81570	-1.37906	-2.42849
C	4.12972	-0.57965	-0.58045
N	4.93567	0.48820	1.17776
C	5.28664	-0.11102	-0.02497
C	3.61555	0.39383	1.36165
C	6.69541	-0.16306	-0.49635
H	7.33543	-0.69673	0.22284
H	6.75180	-0.68559	-1.45910
H	7.10832	0.84879	-0.62879
C	2.85374	0.94260	2.50943
H	2.92709	2.04014	2.52182
H	1.79479	0.66964	2.44229
H	3.25480	0.55748	3.45762
C	5.88381	1.11279	2.08363
H	5.34748	1.57534	2.91802
H	6.57860	0.35715	2.47308
H	6.44769	1.88648	1.54713
C	-0.87033	-0.41209	-3.11574
O	0.15786	-0.94588	-3.06028
O	-1.89234	0.12150	-3.23434

3_{C5}(TS1)

Energy	=	-2635.007844
Enthalpy 0K	=	-2634.575623
Enthalpy 298K	=	-2634.541740
Free Energy 298K	=	-2634.641306
Nimag	=	1 (-708.5915 cm ⁻¹)

Mn	-1.58309	-0.96793	0.23574
N	-0.44132	0.69876	-0.00150
C	-0.53792	3.09653	-0.42277
H	-1.14416	3.99432	-0.53264
N	-3.03029	0.50253	0.36418
C	0.82704	3.16929	-0.57507
H	1.32238	4.11140	-0.81433
C	-3.44899	2.85907	-0.00524
H	-3.06395	3.84558	-0.25755
C	-2.58145	1.75062	0.07163
C	-1.15189	1.86744	-0.12395
C	-5.24147	1.40842	0.59704
H	-6.29283	1.23720	0.83303
C	1.56748	1.99126	-0.38855
H	2.65419	2.01534	-0.47241
C	0.92481	0.80612	-0.09897
C	-4.79034	2.68592	0.24488
H	-5.48371	3.52735	0.18693
C	-4.35470	0.34271	0.65787
O	0.21036	-3.26634	-0.09995
O	-3.27061	-2.83463	-1.28371
O	-1.92702	-1.95874	2.97840

N	3.15317	-0.24810	0.18958
C	-2.62961	-2.06255	-0.68851
C	-4.88360	-0.99898	1.07312
H	-4.87174	-1.71689	0.24253
H	-4.28494	-1.43166	1.88509
H	-5.92087	-0.89951	1.41856
C	-0.41653	-2.29523	0.02358
C	1.71758	-0.45772	0.11143
H	1.37957	-0.96021	1.02725
H	1.53355	-1.14749	-0.71986
C	-1.79296	-1.51059	1.91192
C	3.55711	-0.72314	-2.25211
H	3.17775	-1.75638	-2.27906
H	2.74845	-0.05747	-2.58877
H	4.38605	-0.64585	-2.96619
C	4.02351	-0.35414	-0.88916
N	5.12024	0.21403	0.94263
C	5.26928	-0.06299	-0.41046
C	3.83464	0.10176	1.28932
C	6.59518	-0.01742	-1.08088
H	7.28994	-0.74679	-0.63683
H	6.48747	-0.25164	-2.14704
H	7.05126	0.98032	-0.99107
C	3.27228	0.35362	2.63800
H	3.45206	1.39767	2.93346
H	2.19213	0.17344	2.65058
H	3.74593	-0.30341	3.38151
C	6.21689	0.57155	1.82592
H	5.83568	0.74346	2.83729
H	6.95120	-0.24409	1.85054
H	6.69955	1.48764	1.46169
C	-1.21715	-0.42245	-2.33491
O	-0.26824	-1.05964	-2.68245
O	-2.04893	0.37947	-2.62542

3c5(I2)

Energy	= -2635.013039
Enthalpy 0K	= -2634.577850
Enthalpy 298K	= -2634.544187
Free Energy 298K	= -2634.643137
Nimag	= 0 (18.7926 cm ⁻¹)

Mn	-1.59403	-0.95862	0.27241
N	-0.42089	0.77735	0.11277
C	-0.52030	3.11915	-0.45166
H	-1.11883	4.00106	-0.66922
N	-3.08540	0.53856	0.13962
C	0.85856	3.19956	-0.49017
H	1.35880	4.13878	-0.73150
C	-3.43196	2.89326	-0.21466
H	-3.01769	3.88470	-0.38505
C	-2.60065	1.77580	-0.08343
C	-1.13224	1.89881	-0.14508
C	-5.29715	1.45578	0.13786
H	-6.36948	1.28477	0.24269
C	1.59246	2.04979	-0.21894
H	2.68118	2.07920	-0.25124

C	0.92917	0.86398	0.07250
C	-4.80259	2.72808	-0.11467
H	-5.47543	3.58155	-0.21725
C	-4.42148	0.37558	0.27099
O	0.22292	-3.22700	0.64666
O	-3.04288	-3.13784	-1.05142
O	-2.26164	-1.34554	3.12417
N	3.14182	-0.24117	0.22492
C	-2.52101	-2.24405	-0.51756
C	-5.00269	-0.97432	0.57043
H	-4.93983	-1.63494	-0.30474
H	-4.47403	-1.46777	1.39550
H	-6.06190	-0.87305	0.83989
C	-0.41550	-2.27272	0.47868
C	1.70239	-0.40999	0.30501
H	1.44606	-0.84117	1.28039
H	1.39646	-1.11654	-0.47857
C	-1.98529	-1.12521	2.01829
C	3.29025	-0.93595	-2.19852
H	3.08338	-2.01580	-2.13456
H	2.33473	-0.44331	-2.42959
H	3.98767	-0.77085	-3.02950
C	3.88883	-0.43671	-0.93122
N	5.18132	0.24926	0.72575
C	5.18048	-0.12666	-0.61156
C	3.94060	0.17854	1.21628
C	6.42531	-0.15593	-1.42343
H	7.14509	-0.88603	-1.02211
H	6.19242	-0.43830	-2.45757
H	6.91558	0.82938	-1.43591
C	3.52490	0.55105	2.58960
H	3.72679	1.61729	2.76918
H	2.45386	0.37316	2.73446
H	4.08094	-0.03671	3.33406
C	6.36386	0.67841	1.45232
H	6.11704	0.81617	2.50978
H	7.14600	-0.08606	1.36333
H	6.73004	1.62702	1.03788
C	-1.11440	-0.78199	-1.87754
O	-0.02600	-1.29667	-2.19673
O	-1.88181	-0.08678	-2.54684

1c2(I3)

Energy	= -2898.999311
Enthalpy 0K	= -2898.516479
Enthalpy 298K	= -2898.476658
Free Energy 298K	= -2898.587792
Nimag	= 0 (23.1233 cm ⁻¹)

N	3.10365	-0.55664	0.41213
C	2.62247	-0.58959	1.66970
C	3.45604	-0.60758	2.78682
C	4.83077	-0.61520	2.59791
C	5.31990	-0.64563	1.30211
C	4.43406	-0.62174	0.21857
C	1.15010	-0.68742	1.79992

N	0.45040	-0.73279	0.64568
C	-0.86998	-0.98204	0.70919
C	-1.54170	-1.12350	1.92108
C	-0.83659	-0.99733	3.10787
C	0.53189	-0.79457	3.04561
C	-1.62436	-1.09453	-0.59511
N	-2.87389	-1.83287	-0.48297
C	-2.99722	-3.20272	-0.57692
C	-4.31639	-3.49074	-0.41175
N	-4.96797	-2.29175	-0.21704
C	-4.08017	-1.30398	-0.26446
C	-6.39799	-2.13479	0.00525
Mn	1.59959	-0.14586	-1.04133
C	2.62511	0.82392	-2.12801
O	3.19381	1.52553	-2.85030
C	5.00638	-0.67241	-1.16689
C	1.82378	-1.79869	-1.76903
O	1.96141	-2.80896	-2.30847
C	0.36816	0.23798	-2.25621
O	-0.32452	0.50345	-3.14959
C	1.38847	1.73696	-0.11440
O	2.30209	2.16927	0.59221
O	0.25179	2.34748	-0.20062
O	-1.91362	2.29455	-1.44516
O	-3.54640	1.46693	0.55716
O	-2.92585	4.75873	-0.85415
O	-1.18757	2.27813	2.04978
O	-3.38392	3.91728	1.74476
H	-1.85155	-0.09165	-0.98017
H	-1.00718	-1.61595	-1.33501
H	3.04689	-0.61906	3.79477
H	-2.61255	-1.31991	1.94016
H	1.11172	-0.72940	3.96389
H	-1.34492	-1.07717	4.06995
H	6.39270	-0.68939	1.10865
H	5.50842	-0.62000	3.45375
H	-4.84878	-4.43767	-0.42206
H	-2.13967	-3.84405	-0.76165
H	-6.69197	-2.70571	0.89459
H	-6.94623	-2.50263	-0.87098
H	-6.61637	-1.07259	0.15916
H	6.01199	-1.11222	-1.13779
H	4.38115	-1.26307	-1.84646
H	5.10233	0.33914	-1.58667
H	-4.26550	-0.23819	-0.08470
H	-0.97807	2.24150	-1.01466
H	-3.04032	1.75364	-0.23294
H	-3.73096	2.31404	1.02024
H	-2.51068	3.92529	-1.16724
H	-3.79170	4.75592	-1.28001
H	-0.55596	2.41281	1.29983
H	-1.82701	1.65834	1.66310
H	-2.51309	3.53122	1.97840
H	-3.21622	4.34296	0.87806
H	-1.81545	1.97130	-2.34809

1c2(TS2)

Energy	=	-2898.997131
Enthalpy 0K	=	-2898.518849
Enthalpy 298K	=	-2898.479277
Free Energy 298K	=	-2898.590489
Nimag	=	1 (-685.1132 cm ⁻¹)

N	3.01875	-0.56201	0.54530
C	2.51170	-0.28602	1.76231
C	3.32115	0.00164	2.85877
C	4.70037	-0.04386	2.70325
C	5.21484	-0.41840	1.47346
C	4.35046	-0.67734	0.40244
C	1.03811	-0.38329	1.88711
N	0.35055	-0.60164	0.74639
C	-0.96827	-0.85055	0.83360
C	-1.64570	-0.84390	2.05143
C	-0.94961	-0.56025	3.21550
C	0.41475	-0.33863	3.13351
C	-1.71080	-1.11950	-0.45278
N	-3.01530	-1.73467	-0.26221
C	-3.25463	-3.09056	-0.19761
C	-4.59307	-3.24502	-0.01025
N	-5.14020	-1.98070	0.03999
C	-4.17155	-1.08352	-0.11533
C	-6.55321	-1.68337	0.22611
Mn	1.55644	-0.39415	-1.00795
C	2.66041	0.14451	-2.30383
O	3.27531	0.56370	-3.18562
C	4.94816	-1.09543	-0.90769
C	1.65870	-2.18901	-1.32220
O	1.73006	-3.30761	-1.58472
C	0.35480	-0.20581	-2.30602
O	-0.30072	-0.11755	-3.25744
C	1.57529	1.63837	-0.52770
O	2.59898	2.16051	-0.09286
O	0.47703	2.36707	-0.58989
O	-1.65654	1.95201	-1.57304
O	-3.34157	1.67179	0.44378
O	-2.46911	4.50579	-1.52908
O	-0.93378	2.54418	1.74486
O	-3.01292	4.30385	1.15795
H	-1.84636	-0.16828	-0.98914
H	-1.12643	-1.79728	-1.08474
H	2.89006	0.25733	3.82456
H	-2.71365	-1.05100	2.09121
H	0.98916	-0.15059	4.03818
H	-1.46202	-0.53102	4.17833
H	6.29096	-0.51308	1.32063
H	5.36077	0.18618	3.54143
H	-5.20371	-4.13853	0.08524
H	-2.45525	-3.81959	-0.29947
H	-6.90307	-2.15439	1.15283
H	-7.12373	-2.07233	-0.62662
H	-6.68218	-0.59763	0.29257
H	5.91971	-1.57744	-0.73487
H	4.29948	-1.79406	-1.44885

H	5.12678	-0.22180	-1.55095
H	-4.26061	0.00800	-0.05571
H	-0.53262	2.04409	-1.13355
H	-2.79351	1.76617	-0.37648
H	-3.48408	2.60027	0.72544
H	-2.11770	3.58179	-1.61545
H	-3.32934	4.46081	-1.96311
H	-0.32507	2.56722	0.97449
H	-1.63826	1.94613	1.44022
H	-2.18212	3.89733	1.47691
H	-2.80888	4.51253	0.22028
H	-1.64127	1.59575	-2.46685

1_{c2}(I4)

Energy	=	-2898.998787
Enthalpy 0K	=	-2898.516981
Enthalpy 298K	=	-2898.477265
Free Energy 298K	=	-2898.588748
Nimag	=	0 (16.8297 cm ⁻¹)

N	3.02194	-0.56164	0.54216
C	2.51399	-0.29296	1.76097
C	3.32273	0.00004	2.85612
C	4.70220	-0.03705	2.69923
C	5.21777	-0.40993	1.46965
C	4.35411	-0.67168	0.39869
C	1.04144	-0.40665	1.88903
N	0.35022	-0.60509	0.74701
C	-0.96539	-0.87167	0.83381
C	-1.63469	-0.90737	2.05584
C	-0.93541	-0.64628	3.22289
C	0.42520	-0.40252	3.13966
C	-1.71176	-1.10463	-0.45577
N	-3.02364	-1.70727	-0.27594
C	-3.28199	-3.06095	-0.24519
C	-4.62156	-3.20168	-0.05462
N	-5.15014	-1.93144	0.03165
C	-4.16972	-1.04374	-0.10570
C	-6.55734	-1.61806	0.23378
Mn	1.55854	-0.37194	-1.00844
C	2.66881	0.12605	-2.31869
O	3.28535	0.51969	-3.20946
C	4.95356	-1.08798	-0.91106
C	1.64167	-2.17138	-1.31872
O	1.70137	-3.29350	-1.56133
C	0.34938	-0.18105	-2.31212
O	-0.29238	-0.11377	-3.27084
C	1.61139	1.64282	-0.51887
O	2.61785	2.17703	-0.07858
O	0.51675	2.42463	-0.59199
O	-1.73512	1.87199	-1.52810
O	-3.37507	1.70032	0.45643
O	-2.37730	4.42585	-1.52118
O	-0.99380	2.47214	1.77054
O	-2.98967	4.34953	1.14112
H	-1.83125	-0.13155	-0.96479
H	-1.13817	-1.77692	-1.10341

H	2.89099	0.25384	3.82204
H	-2.69940	-1.13103	2.09618
H	1.00237	-0.23257	4.04619
H	-1.44196	-0.65167	4.18929
H	6.29413	-0.50035	1.31621
H	5.36190	0.19739	3.53671
H	-5.24438	-4.08870	0.02051
H	-2.49359	-3.79827	-0.37000
H	-6.90905	-2.10584	1.15115
H	-7.13899	-1.97764	-0.62434
H	-6.66948	-0.53239	0.32712
H	5.92257	-1.57433	-0.73628
H	4.30497	-1.78396	-1.45579
H	5.13891	-0.21304	-1.55066
H	-4.24307	0.04874	-0.01698
H	-0.32609	2.03898	-1.04325
H	-2.81821	1.76533	-0.37933
H	-3.51738	2.63476	0.71003
H	-2.07784	3.46955	-1.57796
H	-3.23576	4.41568	-1.96030
H	-0.37354	2.53140	1.01955
H	-1.72641	1.93833	1.40847
H	-2.19357	3.90764	1.49404
H	-2.75077	4.50456	0.19907
H	-1.84941	1.53714	-2.42302

1_{c2}⁺(I5)

Energy	=	-2517.670507
Enthalpy 0K	=	-2517.305019
Enthalpy 298K	=	-2517.276559
Free Energy 298K	=	-2517.363303
Nimag	=	0 (25.7834 cm ⁻¹)

N	-2.45876	0.17488	-0.07059
C	-2.24069	1.47541	0.22097
C	-3.24022	2.30073	0.72896
C	-4.51904	1.78416	0.89407
C	-4.75844	0.47768	0.50583
C	-3.71014	-0.31406	0.02031
C	-0.88982	1.99867	-0.09795
N	-0.00459	1.11410	-0.60320
C	1.18010	1.57699	-1.03751
C	1.54513	2.91829	-0.92017
C	0.66275	3.81669	-0.34244
C	-0.57953	3.35012	0.05904
C	2.18086	0.65103	-1.68041
N	3.26572	0.30040	-0.76203
C	4.54856	-0.01984	-1.14872
C	5.22987	-0.34791	-0.01765
N	4.34729	-0.22337	1.03240
C	3.16651	0.16935	0.56344
C	4.65624	-0.48788	2.43031
Mn	-0.65087	-0.91280	-0.34586
C	-1.25350	-2.54775	0.09242
O	-1.50795	-3.62996	0.38700
C	-4.01764	-1.71835	-0.40120
C	-0.96818	-1.12241	-2.14486

O -1.15138 -1.28259 -3.26504
 C 0.91394 -1.78113 -0.39694
 O 1.85487 -2.44826 -0.38452
 C -0.32631 -0.54999 1.64568
 O 0.61227 0.05216 2.15754
 O -1.28940 -0.99171 2.49020
 H 1.70803 -0.26089 -2.05942
 H 2.64473 1.16360 -2.53152
 H -3.03678 3.33770 0.98708
 H 2.52173 3.23890 -1.28662
 H -1.30398 4.04322 0.48152
 H 0.92588 4.86921 -0.22671
 H -5.75842 0.04725 0.57337
 H -5.32066 2.40661 1.29550
 H 6.26244 -0.65104 0.13217
 H 4.86239 0.01922 -2.18813
 H 5.00686 -1.52207 2.53387
 H 3.74860 -0.34547 3.02623
 H 5.43580 0.20505 2.77057
 H -5.08514 -1.80737 -0.64090
 H -3.43549 -2.01742 -1.28160
 H -3.80618 -2.42475 0.41432
 H 2.24964 0.30292 1.16065
 H -1.02522 -0.72263 3.38942

1c5(I3)

Energy = -2898.998190
 Enthalpy 0K = -2898.515610
 Enthalpy 298K = -2898.475545
 Free Energy 298K = -2898.588112
 Nimag = 0 (20.5696 cm⁻¹)

C -4.22294 -1.05341 -0.04240
 N -3.00398 -1.63332 -0.32749
 C -3.16616 -2.95392 -0.42426
 N -4.44464 -3.24100 -0.20853
 C -5.12729 -2.06811 0.03299
 C -1.73544 -0.93910 -0.50299
 C -0.95994 -0.76123 0.78138
 N 0.37523 -0.63056 0.68693
 C 1.09595 -0.56081 1.82709
 C 0.49041 -0.50043 3.08156
 C -0.89095 -0.56114 3.17037
 C -1.62376 -0.73045 2.00552
 C 2.56727 -0.61340 1.67171
 N 3.02911 -0.63800 0.40679
 C 4.34639 -0.81934 0.19427
 C 5.24223 -0.91832 1.26507
 C 4.77629 -0.84701 2.56821
 C 3.41145 -0.71072 2.77715
 Mn 1.52865 -0.18280 -1.03483
 C 1.40050 1.73530 -0.16033
 O 0.32189 2.42586 -0.32540
 C 4.89102 -0.91973 -1.19968
 H -6.19412 -2.06019 0.23828
 C 2.58679 0.71761 -2.14899

O 3.18287 1.37917 -2.88715
 C 1.66555 -1.86243 -1.71928
 O 1.74664 -2.89176 -2.23408
 C 0.30223 0.21430 -2.25102
 O -0.38728 0.47583 -3.14778
 O 2.30115 2.10996 0.59433
 O -1.88691 2.39096 -1.50898
 O -3.48884 1.81008 0.62402
 O -2.79546 4.93773 -1.13990
 O -1.07095 2.68122 1.94666
 O -3.20631 4.37363 1.54153
 H -1.94833 0.04058 -0.95146
 H -1.13739 -1.52071 -1.21252
 H 3.01592 -0.69182 3.79070
 H -2.70830 -0.82088 2.04738
 H 1.08910 -0.40534 3.98509
 H -1.38981 -0.49963 4.13873
 H 6.30414 -1.05646 1.05661
 H 5.46306 -0.91774 3.41382
 C -5.03863 -4.57004 -0.24226
 H -2.38153 -3.67241 -0.64993
 H 5.87299 -1.41030 -1.18233
 H 4.22398 -1.48679 -1.85955
 H 5.02890 0.07935 -1.63711
 H -4.30885 0.02426 0.11770
 H -0.94448 2.32684 -1.10175
 H -3.00636 1.99076 -0.20931
 H -3.63090 2.70935 0.99271
 H -2.41788 4.06009 -1.36915
 H -3.67239 4.92025 -1.54208
 H -0.44596 2.70524 1.17990
 H -1.74629 2.05639 1.63478
 H -2.34394 3.97457 1.78503
 H -3.05198 4.70443 0.63223
 H -1.82325 2.01108 -2.39287
 H -5.55968 -4.75583 0.70481
 H -5.74934 -4.63096 -1.07596
 H -4.24368 -5.31110 -0.37741

1c5(TS2)

Energy = -2898.996054
 Enthalpy 0K = -2898.516800
 Enthalpy 298K = -2898.477564
 Free Energy 298K = -2898.587463
 Nimag = 1 (-686.4041 cm⁻¹)

C -4.32833 -0.58674 0.03726
 N -3.20889 -1.36569 -0.17220
 C -3.56588 -2.65079 -0.14594
 N -4.87353 -2.72316 0.07517
 C -5.37372 -1.44430 0.19422
 C -1.85479 -0.88082 -0.39605
 C -1.08229 -0.60667 0.87126
 N 0.25407 -0.49674 0.76733
 C 0.96983 -0.29069 1.89299
 C 0.36398 -0.11212 3.13555

C	-1.01557	-0.18468	3.23215
C	-1.74646	-0.46100	2.08798
C	2.44446	-0.35967	1.75952
N	2.90918	-0.74258	0.55444
C	4.21966	-1.00691	0.41246
C	5.11538	-0.79832	1.46851
C	4.65388	-0.31865	2.68266
C	3.28912	-0.11618	2.84020
Mn	1.45989	-0.49096	-0.99905
C	1.69250	1.54673	-0.60657
O	0.67420	2.38198	-0.69214
C	4.75918	-1.54044	-0.88084
H	-6.42789	-1.25909	0.38092
C	2.60388	-0.12728	-2.32120
O	3.25347	0.18612	-3.22180
C	1.37314	-2.29809	-1.23948
O	1.32693	-3.42790	-1.45636
C	0.27200	-0.22717	-2.29741
O	-0.37980	-0.10482	-3.24736
O	2.76891	1.98008	-0.20295
O	-1.51666	2.12597	-1.60314
O	-3.14997	2.14897	0.48445
O	-2.08060	4.74196	-1.69456
O	-0.63921	2.83527	1.66489
O	-2.52755	4.78081	1.01773
H	-1.91611	0.05042	-0.97972
H	-1.33110	-1.63555	-0.99243
H	2.89683	0.22540	3.79606
H	-2.83006	-0.55229	2.13995
H	0.96151	0.06659	4.02691
H	-1.51473	-0.04613	4.19247
H	6.17382	-1.01513	1.31682
H	5.34179	-0.12715	3.50831
C	-5.65883	-3.94554	0.16426
H	-2.89689	-3.49629	-0.28973
H	5.67704	-2.11282	-0.69134
H	4.03692	-2.19012	-1.38872
H	5.02171	-0.71825	-1.56203
H	-4.24923	0.50188	0.09977
H	-0.37090	2.13190	-1.19188
H	-2.63182	2.12503	-0.35852
H	-3.18607	3.10447	0.69852
H	-1.82202	3.78362	-1.72644
H	-2.96358	4.74876	-2.08278
H	-0.05483	2.75177	0.88043
H	-1.41424	2.30392	1.40916
H	-1.73815	4.30090	1.33980
H	-2.33698	4.90238	0.06221
H	-1.55714	1.74169	-2.48440
H	-6.17019	-3.97659	1.13408
H	-6.39770	-3.96377	-0.64663
H	-4.98766	-4.80608	0.07309

1c5(I4)

Energy = -2898.997487
 Enthalpy 0K = -2898.515481

Enthalpy 298K = -2898.475833
 Free Energy 298K = -2898.587378
 Nimag = 0 (9.8963 cm⁻¹)

C	-4.32793	-0.53308	0.05921
N	-3.22204	-1.32857	-0.15955
C	-3.60039	-2.60765	-0.14503
N	-4.90892	-2.66073	0.07744
C	-5.38736	-1.37479	0.20961
C	-1.86030	-0.86417	-0.38074
C	-1.08353	-0.61081	0.88664
N	0.25178	-0.49172	0.77692
C	0.97290	-0.29260	1.90025
C	0.37425	-0.13765	3.14932
C	-1.00424	-0.22185	3.25307
C	-1.74063	-0.48472	2.10964
C	2.44772	-0.34735	1.75874
N	2.91009	-0.74466	0.55694
C	4.22107	-1.00632	0.41437
C	5.12001	-0.77443	1.46287
C	4.66145	-0.27292	2.66907
C	3.29595	-0.07660	2.82967
Mn	1.45834	-0.49168	-0.99558
C	1.72834	1.53067	-0.62408
O	0.71822	2.41448	-0.72609
C	4.75765	-1.56367	-0.86998
H	-6.43803	-1.17399	0.39989
C	2.60133	-0.19065	-2.33728
O	3.24784	0.08255	-3.25160
C	1.34940	-2.30414	-1.20697
O	1.29234	-3.43780	-1.39048
C	0.26061	-0.23832	-2.29930
O	-0.38315	-0.14664	-3.25454
O	2.79317	1.98189	-0.23009
O	-1.59841	2.04261	-1.58105
O	-3.14688	2.18801	0.49226
O	-1.96816	4.64450	-1.73841
O	-0.66964	2.80428	1.67407
O	-2.46589	4.83960	0.94362
H	-1.90052	0.08123	-0.95089
H	-1.35169	-1.62462	-0.98267
H	2.90537	0.28164	3.78017
H	-2.82352	-0.58232	2.16691
H	0.97661	0.02839	4.03997
H	-1.49805	-0.10248	4.21875
H	6.17868	-0.98973	1.31080
H	5.35203	-0.06035	3.48726
C	-5.71331	-3.87114	0.15804
H	-2.94619	-3.46305	-0.29797
H	5.67071	-2.14006	-0.66970
H	4.03195	-2.21701	-1.36823
H	5.02894	-0.75437	-1.56309
H	-4.23013	0.55422	0.13226
H	-0.17392	2.09239	-1.13539
H	-2.63671	2.12357	-0.36949
H	-3.18446	3.15030	0.66223
H	-1.77506	3.65909	-1.73000

H	-2.84485	4.69431	-2.13691
H	-0.07816	2.74004	0.90045
H	-1.46993	2.32965	1.37586
H	-1.71224	4.33633	1.30763
H	-2.25001	4.89180	-0.01487
H	-1.76604	1.67702	-2.45521
H	-6.21878	-3.90524	1.13088
H	-6.45780	-3.86848	-0.64789
H	-5.05672	-4.74121	0.05250

2c2(I3)

Energy	=	-2938.284420
Enthalpy 0K	=	-2937.774144
Enthalpy 298K	=	-2937.732480
Free Energy 298K	=	-2937.848400
Nimag	=	0 (17.5486 cm ⁻¹)

N	3.14233	-0.62684	0.46222
C	2.66551	-0.41550	1.70466
C	3.49393	-0.35861	2.82383
C	4.85978	-0.53990	2.65592
C	5.34043	-0.80490	1.38373
C	4.45935	-0.84962	0.29669
C	1.19263	-0.32887	1.82749
N	0.49478	-0.58769	0.70099
C	-0.83901	-0.70626	0.78810
C	-1.53152	-0.44865	1.97001
C	-0.82281	-0.07959	3.10238
C	0.56264	-0.05019	3.03823
C	-1.59901	-1.14200	-0.44317
N	-2.76997	-1.94224	-0.11527
C	-2.71313	-3.19548	0.45993
C	-3.99358	-3.61859	0.60543
N	-4.80806	-2.62031	0.11265
C	-4.05242	-1.60624	-0.32596
C	-6.26376	-2.67041	0.08213
Mn	1.66706	-0.34797	-1.05011
C	2.74484	0.34948	-2.28758
O	3.35611	0.87282	-3.11719
C	5.01822	-1.15081	-1.06185
C	1.76861	-2.09970	-1.53460
O	1.82906	-3.18220	-1.92900
C	0.42352	-0.02506	-2.27142
O	-0.29766	0.19860	-3.15286
C	1.59774	1.66415	-0.41856
O	2.59246	2.16808	0.11004
O	0.47314	2.29950	-0.48713
O	-1.82324	2.06736	-1.44468
O	-3.22860	2.04677	0.94068
O	-2.57425	4.69313	-1.52054
O	-0.66532	3.06710	1.81075
O	-2.77392	4.74393	1.23545
H	-1.92826	-0.25564	-0.99953
H	-0.95001	-1.74341	-1.08928
H	3.08446	-0.18793	3.81765
H	-2.61856	-0.51578	1.98978

H	1.14337	0.19685	3.92495
H	-1.34151	0.16234	4.03135
H	6.40272	-0.98517	1.21258
H	5.53517	-0.49596	3.51244
H	-4.40024	-4.54057	1.01074
H	-1.76773	-3.66832	0.71129
H	-6.57932	-3.62956	0.50561
H	-6.62167	-2.59563	-0.95241
H	-6.68130	-1.85282	0.68302
H	5.99424	-1.64377	-0.96370
H	4.35156	-1.79866	-1.64332
H	5.17233	-0.22413	-1.63306
H	-0.84577	2.06804	-1.11364
H	-2.80140	1.98921	0.06379
H	-3.30692	3.01532	1.07890
H	-2.26589	3.76064	-1.56723
H	-3.48355	4.64763	-1.84007
H	-0.12517	2.89403	0.99885
H	-1.38614	2.42256	1.71509
H	-1.91028	4.35196	1.48661
H	-2.68892	4.86671	0.26724
H	-1.81280	1.64073	-2.30907
C	-4.54071	-0.34002	-0.91681
H	-4.03909	-0.14834	-1.87589
H	-5.62071	-0.39226	-1.09305
H	-4.32843	0.50060	-0.23666

2c2(TS2)

Energy	=	-2938.282412
Enthalpy 0K	=	-2937.776292
Enthalpy 298K	=	-2937.735138
Free Energy 298K	=	-2937.849826
Nimag	=	1 (-659.9434 cm ⁻¹)

N	3.02516	-0.66720	0.60906
C	2.54222	-0.13095	1.74767
C	3.37171	0.26541	2.79362
C	4.74052	0.05868	2.67804
C	5.22105	-0.57310	1.54352
C	4.33965	-0.93109	0.51562
C	1.06534	-0.06390	1.85299
N	0.37307	-0.46115	0.76470
C	-0.95941	-0.59571	0.86765
C	-1.65114	-0.25638	2.02912
C	-0.94793	0.22187	3.12262
C	0.43323	0.30141	3.03979
C	-1.71594	-1.12455	-0.32770
N	-2.96760	-1.76881	0.03480
C	-3.05469	-2.99554	0.66053
C	-4.37480	-3.25345	0.83534
N	-5.06947	-2.18264	0.31129
C	-4.20251	-1.28607	-0.17517
C	-6.52111	-2.05746	0.29303
Mn	1.59350	-0.62629	-0.97667
C	2.73636	-0.44210	-2.33861
O	3.38443	-0.26152	-3.27523

C	4.89597	-1.62306	-0.69242
C	1.51092	-2.44870	-1.02796
O	1.46742	-3.59506	-1.12680
C	0.39198	-0.44837	-2.27694
O	-0.28462	-0.36073	-3.21288
C	1.83128	1.44183	-0.81404
O	2.93901	1.92303	-0.58735
O	0.79274	2.25656	-0.85625
O	-1.46646	1.85428	-1.51942
O	-2.83954	2.32280	0.73039
O	-2.04629	4.41133	-2.04003
O	-0.24393	3.22100	1.48753
O	-2.19637	5.01836	0.63153
H	-1.92855	-0.27883	-0.99565
H	-1.10858	-1.86029	-0.86557
H	2.96445	0.72701	3.69105
H	-2.73472	-0.35737	2.06850
H	1.00985	0.63490	3.89994
H	-1.46807	0.51352	4.03641
H	6.28329	-0.79610	1.43271
H	5.41683	0.36616	3.47783
H	-4.88487	-4.10286	1.28048
H	-2.16929	-3.56900	0.92081
H	-6.94641	-2.94963	0.76447
H	-6.87995	-1.98794	-0.74154
H	-6.82884	-1.16770	0.85656
H	5.81781	-2.15645	-0.42432
H	4.18339	-2.34060	-1.11604
H	5.15542	-0.89324	-1.47291
H	-0.27958	1.93265	-1.21356
H	-2.40892	2.09445	-0.12818
H	-2.86955	3.30123	0.70944
H	-1.79050	3.46130	-1.89323
H	-2.96993	4.35402	-2.31203
H	0.25504	2.95865	0.68363
H	-1.03914	2.66030	1.43169
H	-1.37979	4.59463	0.96491
H	-2.10555	4.93770	-0.34266
H	-1.56580	1.39235	-2.35737
C	-4.53561	0.00804	-0.81056
H	-4.08621	0.06570	-1.81244
H	-5.62108	0.11893	-0.90737
H	-4.14010	0.84100	-0.20634

3C₂(I4)

Energy	= -2938.283469
Enthalpy 0K	= -2937.774220
Enthalpy 298K	= -2937.732773
Free Energy 298K	= -2937.847935
Nimag	= 0 (15.4125 cm ⁻¹)

N	3.04069	-0.66910	0.57905
C	2.57243	-0.16118	1.73684
C	3.41565	0.20702	2.78214
C	4.78229	-0.00033	2.64546
C	5.24761	-0.60538	1.49033

C	4.35344	-0.93491	0.46406
C	1.09691	-0.09629	1.86488
N	0.38698	-0.45936	0.77547
C	-0.94349	-0.59983	0.89586
C	-1.61582	-0.30035	2.08001
C	-0.89541	0.14375	3.17599
C	0.48427	0.22902	3.07283
C	-1.71892	-1.07926	-0.30655
N	-2.97050	-1.73022	0.04583
C	-3.05493	-2.95788	0.67086
C	-4.37464	-3.23207	0.82093
N	-5.07223	-2.17111	0.28099
C	-4.20721	-1.26468	-0.19098
C	-6.52461	-2.06370	0.23593
Mn	1.58906	-0.58195	-0.98783
C	2.71622	-0.39802	-2.36482
O	3.35120	-0.21519	-3.30898
C	4.89465	-1.59829	-0.76660
C	1.49991	-2.40566	-1.06014
O	1.45417	-3.55059	-1.15832
C	0.36731	-0.40417	-2.28060
O	-0.30564	-0.34267	-3.21796
C	1.84569	1.46825	-0.78894
O	2.93363	1.96230	-0.53037
O	0.81095	2.32372	-0.85733
O	-1.54285	1.82807	-1.49866
O	-2.83567	2.25200	0.73820
O	-2.02813	4.36673	-1.97533
O	-0.30491	3.14701	1.56477
O	-2.24382	4.97621	0.67956
H	-1.92387	-0.19770	-0.93424
H	-1.12396	-1.79946	-0.87811
H	3.02018	0.64674	3.69567
H	-2.69844	-0.40404	2.13279
H	1.07481	0.53517	3.93366
H	-1.40040	0.40428	4.10754
H	6.30768	-0.82892	1.36174
H	5.46870	0.28542	3.44465
H	-4.88256	-4.08658	1.25872
H	-2.16797	-3.52026	0.94937
H	-6.94743	-2.96077	0.70031
H	-6.86557	-1.99938	-0.80501
H	-6.85365	-1.17739	0.79288
H	5.82066	-2.13574	-0.52243
H	4.17891	-2.30881	-1.19670
H	5.14359	-0.85065	-1.53348
H	-0.11035	1.95425	-1.16258
H	-2.41400	2.04724	-0.14366
H	-2.90516	3.22705	0.72814
H	-1.79899	3.39782	-1.83451
H	-2.94681	4.33571	-2.26670
H	0.21008	2.94282	0.76034
H	-1.10703	2.60117	1.44600
H	-1.44053	4.55103	1.03794
H	-2.12851	4.87909	-0.29244
H	-1.74311	1.38602	-2.32911
C	-4.54537	0.02038	-0.84120

H	-4.07921	0.07675	-1.83532
H	-5.63039	0.11767	-0.95586
H	-4.16510	0.85970	-0.23559

2_{C5}(I3)

Energy	=	-2938.286070
Enthalpy 0K	=	-2937.775129
Enthalpy 298K	=	-2937.733576
Free Energy 298K	=	-2937.848978
Nimag	=	0 (20.0099 cm ⁻¹)

C	3.44134	-0.67090	2.79789
C	2.59669	-0.55895	1.69428
N	3.04754	-0.64572	0.42809
C	4.35061	-0.91011	0.21441
C	5.24650	-1.02883	1.28316
C	4.79476	-0.89094	2.58601
C	1.13173	-0.42140	1.85424
N	0.40423	-0.48228	0.71796
C	-0.93500	-0.53275	0.81822
C	-1.59251	-0.43109	2.04207
C	-0.84793	-0.27424	3.20088
C	0.53479	-0.29469	3.10771
C	-1.73140	-0.70285	-0.45368
N	-2.98599	-1.40958	-0.25292
C	-4.21768	-0.82982	-0.02709
C	-5.10753	-1.84962	0.08921
N	-4.40426	-3.02691	-0.06898
C	-3.11360	-2.74522	-0.27361
C	-4.98278	-4.36313	-0.02998
Mn	1.56323	-0.15113	-1.01982
C	0.35492	0.28795	-2.23952
O	-0.32507	0.57139	-3.13680
C	4.87810	-1.08471	-1.17880
C	1.53188	1.79678	-0.20445
O	2.46123	2.15890	0.52090
C	2.66474	0.64970	-2.16861
O	3.29263	1.25320	-2.92976
C	1.58605	-1.86139	-1.64091
O	1.58699	-2.91545	-2.11017
O	0.47610	2.52213	-0.37075
O	-1.74766	2.57091	-1.53852
O	-3.41543	2.06388	0.57365
O	-2.59316	5.14780	-1.23724
O	-0.94696	2.90230	1.86366
O	-3.04508	4.63547	1.44744
H	-6.17779	-1.84611	0.27475
H	-1.95955	0.27894	-0.88912
H	-1.14157	-1.26528	-1.18391
H	3.05377	-0.59892	3.81218
H	-2.68081	-0.45340	2.08309
H	1.14099	-0.21008	4.00740
H	-1.33890	-0.15798	4.16827
H	6.29711	-1.23489	1.07357
H	5.48242	-0.97525	3.42965
C	-2.01952	-3.71341	-0.51853

H	5.82880	-1.63307	-1.15200
H	4.17299	-1.62998	-1.81728
H	5.07292	-0.10939	-1.64723
H	-4.31685	0.25266	0.07206
H	-0.80851	2.47168	-1.13500
H	-2.91612	2.22310	-0.25349
H	-3.52615	2.97069	0.93409
H	-2.23224	4.25663	-1.43934
H	-3.46191	5.14170	-1.65714
H	-0.30762	2.87612	1.10874
H	-1.63823	2.28868	1.56583
H	-2.19065	4.22051	1.69179
H	-2.88485	4.94914	0.53310
H	-1.70082	2.17363	-2.41590
H	-4.53284	-4.94318	0.78581
H	-6.05882	-4.26508	0.14649
H	-4.81538	-4.87291	-0.98711
H	-2.32354	-4.72302	-0.21958
H	-1.76014	-3.72784	-1.58850
H	-1.12089	-3.43411	0.04852

2_{C5}(TS2)

Energy	=	-2938.283681
Enthalpy 0K	=	-2937.777356
Enthalpy 298K	=	-2937.736209
Free Energy 298K	=	-2937.851149
Nimag	=	1 (-695.8701 cm ⁻¹)

C	3.34937	-0.22461	2.84355
C	2.48943	-0.40970	1.76358
N	2.92534	-0.82342	0.55788
C	4.21396	-1.17884	0.41525
C	5.12290	-1.03201	1.47050
C	4.69691	-0.52075	2.68484
C	1.02357	-0.23953	1.89781
N	0.29651	-0.39184	0.77094
C	-1.04369	-0.40523	0.87342
C	-1.69793	-0.21607	2.08973
C	-0.95100	0.00224	3.23587
C	0.43062	-0.02368	3.14057
C	-1.83897	-0.61445	-0.39144
N	-3.20325	-1.05729	-0.15912
C	-4.30311	-0.23655	-0.01158
C	-5.37327	-1.05469	0.16233
N	-4.90820	-2.35357	0.11621
C	-3.58512	-2.34099	-0.07479
C	-5.73555	-3.54552	0.24426
Mn	1.49419	-0.47129	-0.99536
C	0.32961	-0.11671	-2.29298
O	-0.31092	0.05879	-3.24228
C	4.71258	-1.75126	-0.87778
C	1.86667	1.54579	-0.60496
O	2.97718	1.90684	-0.22360
C	2.66077	-0.19447	-2.31946
O	3.33045	0.06960	-3.22098
C	1.27301	-2.26800	-1.23224

O	1.14068	-3.39174	-1.44590
O	0.90209	2.44534	-0.66629
O	-1.29743	2.34786	-1.58995
O	-2.97492	2.45743	0.46287
O	-1.69019	4.99058	-1.68872
O	-0.42873	2.97509	1.66927
O	-2.18057	5.04294	1.01593
H	-6.42509	-0.83212	0.31762
H	-1.87133	0.33424	-0.94887
H	-1.34529	-1.36192	-1.02027
H	2.98140	0.14419	3.79890
H	-2.78579	-0.22610	2.13586
H	1.03893	0.10844	4.03284
H	-1.43996	0.17305	4.19627
H	6.16364	-1.32195	1.31828
H	5.39741	-0.37681	3.50956
C	-2.69150	-3.51586	-0.19841
H	5.58198	-2.39461	-0.68743
H	3.94156	-2.34012	-1.38814
H	5.04057	-0.95115	-1.55691
H	-4.19115	0.84937	0.00793
H	-0.15489	2.27142	-1.17011
H	-2.44145	2.40919	-0.36907
H	-2.95165	3.41125	0.68494
H	-1.49236	4.01742	-1.71638
H	-2.56285	5.05310	-2.09482
H	0.16490	2.85043	0.89773
H	-1.23483	2.50109	1.39764
H	-1.42695	4.51169	1.34263
H	-1.97140	5.15705	0.06335
H	-1.35665	1.96488	-2.47082
H	-5.43822	-4.11627	1.13338
H	-6.77780	-3.22687	0.34942
H	-5.63531	-4.17049	-0.65185
H	-3.19341	-4.42352	0.15536
H	-2.39932	-3.66276	-1.24968
H	-1.77872	-3.36362	0.39398

2c5(14)

Energy	=	-2938.285044
Enthalpy 0K	=	-2937.775825
Enthalpy 298K	=	-2937.734299
Free Energy 298K	=	-2937.849751
Nimag	=	0 (12.6650 cm ⁻¹)

C	3.36788	-0.18829	2.83404
C	2.50259	-0.39239	1.76202
N	2.93510	-0.81319	0.55704
C	4.22533	-1.16166	0.41069
C	5.13909	-0.99777	1.45926
C	4.71677	-0.47569	2.67005
C	1.03567	-0.23568	1.90557
N	0.30217	-0.38515	0.78263
C	-1.03752	-0.41164	0.89323
C	-1.68458	-0.24092	2.11633
C	-0.93170	-0.02798	3.25923

C	0.44959	-0.03838	3.15448
C	-1.83684	-0.60442	-0.36989
N	-3.20551	-1.03477	-0.13998
C	-4.29601	-0.20370	0.01964
C	-5.37505	-1.01221	0.18498
N	-4.92461	-2.31565	0.12181
C	-3.60181	-2.31499	-0.07134
C	-5.76436	-3.50000	0.23722
Mn	1.49731	-0.46530	-0.99190
C	0.31587	-0.12856	-2.29078
O	-0.32446	0.01075	-3.24273
C	4.72105	-1.74501	-0.87838
C	1.90015	1.53551	-0.62153
O	2.99911	1.91604	-0.24705
C	2.65110	-0.24529	-2.34053
O	3.30816	-0.01991	-3.26026
C	1.26423	-2.26710	-1.19882
O	1.12829	-3.39481	-1.37824
O	0.94520	2.48126	-0.69840
O	-1.38702	2.27170	-1.56609
O	-2.98401	2.47817	0.46968
O	-1.64929	4.88372	-1.73703
O	-0.47677	2.95341	1.67156
O	-2.15551	5.08611	0.94453
H	-6.42411	-0.78014	0.34489
H	-1.85234	0.35656	-0.91468
H	-1.35359	-1.35307	-1.00509
H	3.00294	0.18867	3.78746
H	-2.77203	-0.26206	2.17001
H	1.06268	0.08870	4.04413
H	-1.41538	0.12680	4.22503
H	6.18079	-1.28253	1.30413
H	5.42120	-0.31690	3.48865
C	-2.72141	-3.49809	-0.21000
H	5.59459	-2.38162	-0.68451
H	3.95195	-2.34512	-1.37857
H	5.04306	-0.95056	-1.56700
H	-4.17053	0.88133	0.05286
H	0.03228	2.22438	-1.11088
H	-2.45679	2.39660	-0.37922
H	-2.96914	3.43890	0.65067
H	-1.49401	3.89144	-1.72228
H	-2.52155	4.96421	-2.14017
H	0.12737	2.84714	0.91270
H	-1.29749	2.52383	1.36155
H	-1.43117	4.53975	1.30593
H	-1.93382	5.13481	-0.01269
H	-1.55904	1.91061	-2.44137
H	-5.46777	-4.08769	1.11546
H	-6.80218	-3.17141	0.35469
H	-5.67765	-4.11240	-0.66895
H	-3.23958	-4.40721	0.11541
H	-2.41590	-3.62443	-1.26010
H	-1.81533	-3.37071	0.39840

2_{C5}⁺(I5)
 Energy = -2556.955424
 Enthalpy 0K = -2556.562510
 Enthalpy 298K = -2556.532227
 Free Energy 298K = -2556.622888
 Nimag = 0 (20.7891 cm⁻¹)

C	-4.39616	0.01329	0.50003
N	-3.10308	0.27089	0.24782
C	-2.88064	0.22825	-1.11485
C	-4.07659	-0.05792	-1.69012
N	-5.00137	-0.18767	-0.67517
C	-2.09226	0.52878	1.27325
C	-1.04191	1.49050	0.77738
N	0.19674	1.06455	0.48182
C	1.11966	1.98134	0.12093
C	0.79959	3.32968	-0.03939
C	-0.49505	3.75890	0.21253
C	-1.42100	2.82744	0.65226
C	2.51155	1.49157	-0.03413
N	2.71271	0.18135	0.22536
C	3.97340	-0.28892	0.27649
C	5.06263	0.53655	-0.02919
C	4.85379	1.85819	-0.38220
C	3.55558	2.35190	-0.36428
Mn	0.90446	-0.93900	0.21302
C	0.83832	-0.47757	-1.78396
O	1.90843	-0.88496	-2.51459
C	4.24664	-1.70896	0.66773
C	-6.41420	-0.48630	-0.86556
C	1.57917	-2.54540	-0.22154
O	1.88337	-3.61147	-0.52919
C	0.98165	-1.25103	2.02124
O	1.01589	-1.48443	3.14386
C	-0.64770	-1.80673	-0.00078
O	-1.57519	-2.46694	-0.18186
O	-0.02475	0.15085	-2.38301
H	-1.65467	-0.41446	1.61474
H	-2.59864	0.98662	2.13160
H	3.37139	3.39842	-0.59777
H	-2.44286	3.11807	0.90234
H	1.55337	4.04947	-0.35056
H	-0.76636	4.80865	0.09051
H	6.06990	0.12026	0.01456
H	5.69045	2.50847	-0.64356
H	-4.35206	-0.18562	-2.73296
H	-1.88661	0.36858	-1.55292
H	-7.02897	0.33706	-0.48060
H	-6.67405	-1.41985	-0.35075
H	-6.59532	-0.60297	-1.93914
H	5.27540	-1.79899	1.04011
H	3.56007	-2.05629	1.44949
H	4.15397	-2.37697	-0.20059
C	-5.02374	-0.03687	1.84055
H	1.76456	-0.57032	-3.42623
H	-6.08260	-0.30602	1.76203
H	-4.51521	-0.78065	2.47081

H -4.94659 0.94328 2.33464

3_{C2}(I3)
 Energy = -3016.854647
 Enthalpy 0K = -3016.288571
 Enthalpy 298K = -3016.243681
 Free Energy 298K = -3016.365739
 Nimag = 0 (19.7660 cm⁻¹)

C	-4.08211	-0.67977	-0.49741
N	-2.85647	-1.20680	-0.35793
C	-2.95193	-2.53561	0.03860
C	-4.28466	-2.80791	0.14667
N	-4.96152	-1.63984	-0.18944
C	-1.59676	-0.52494	-0.60199
C	-0.80585	-0.32052	0.66938
N	0.52699	-0.46229	0.62322
C	1.21699	-0.43795	1.78315
C	0.60754	-0.13352	2.99808
C	-0.75868	0.10767	3.02790
C	-1.48048	-0.02560	1.85271
C	2.64599	-0.81161	1.68618
N	3.12233	-1.00301	0.44023
C	4.37629	-1.46705	0.28467
C	5.20272	-1.69678	1.39110
C	4.72987	-1.46042	2.67191
C	3.42060	-1.02582	2.82474
Mn	1.78526	-0.32033	-1.07395
C	2.08884	1.61028	-0.27494
O	1.10723	2.45191	-0.29565
C	4.92188	-1.74831	-1.08330
C	-6.41226	-1.54330	-0.20289
C	-4.36139	0.71522	-0.91443
C	3.01715	0.24733	-2.23145
O	3.74203	0.70396	-3.00710
C	1.56370	-2.01254	-1.70520
O	1.43191	-3.04876	-2.19638
C	0.67054	0.33595	-2.28634
O	0.03575	0.76262	-3.15943
O	3.15090	1.86907	0.29786
O	-1.15921	2.73601	-1.31336
O	-1.40454	5.45308	-1.21381
O	-2.64909	2.78154	1.00939
O	0.01913	3.24643	2.01864
O	-1.72677	5.32148	1.52863
H	-1.80351	0.44639	-1.06728
H	-1.01661	-1.12937	-1.30720
H	3.00890	-0.87110	3.82054
H	-2.56026	0.11652	1.83994
H	1.19165	-0.07481	3.91459
H	-1.25579	0.37427	3.96190
H	6.21588	-2.06699	1.22786
H	5.36352	-1.63183	3.54413
C	-5.00100	-4.05150	0.53428
C	-1.75449	-3.38636	0.27429
H	-6.80577	-1.86782	0.76830

H	-6.81841	-2.18505	-0.99571
H	-6.71891	-0.50894	-0.38137
H	5.78640	-2.42096	-1.01051
H	4.17044	-2.20854	-1.73601
H	5.26444	-0.82044	-1.56331
H	-0.21286	2.52461	-0.96090
H	-2.20798	2.71380	0.13976
H	-2.55928	3.73520	1.22246
H	-1.27176	4.48463	-1.32142
H	-2.28812	5.60202	-1.57168
H	0.55770	3.03387	1.21556
H	-0.80262	2.75654	1.84743
H	-0.95888	4.76015	1.76903
H	-1.57892	5.50270	0.57728
H	-1.19799	2.37383	-2.20582
H	-3.88513	0.91971	-1.88450
H	-5.43710	0.88780	-1.01934
H	-3.95849	1.42472	-0.17419
H	-2.06198	-4.42569	0.44289
H	-1.07297	-3.36686	-0.58925
H	-1.18900	-3.04900	1.15668
H	-5.60066	-3.89759	1.44457
H	-5.67990	-4.38611	-0.26470
H	-4.28008	-4.85427	0.73171

3_{C2}(TS2)

Energy	=	-3016.852283
Enthalpy 0K	=	-3016.290208
Enthalpy 298K	=	-3016.245784
Free Energy 298K	=	-3016.367229
Nimag	=	1 (-668.8811 cm ⁻¹)

C	-4.13416	-0.39308	-0.46537
N	-2.97978	-1.05118	-0.28003
C	-3.23502	-2.33888	0.17752
C	-4.59153	-2.44848	0.27620
N	-5.12342	-1.22803	-0.12834
C	-1.65067	-0.52646	-0.53746
C	-0.85821	-0.28871	0.72556
N	0.47808	-0.40224	0.66997
C	1.18092	-0.29578	1.81761
C	0.57366	0.02604	3.02936
C	-0.79937	0.21541	3.06935
C	-1.52732	0.03092	1.90591
C	2.62236	-0.62950	1.73138
N	3.05898	-1.04540	0.52578
C	4.30938	-1.52639	0.41269
C	5.18428	-1.52387	1.50610
C	4.76464	-1.02331	2.72710
C	3.45252	-0.58495	2.84889
Mn	1.72202	-0.51728	-1.05464
C	2.26731	1.43725	-0.56231
O	1.37596	2.41183	-0.53382
C	4.80113	-2.08171	-0.89022
C	-6.55240	-0.96230	-0.16331
C	-4.24051	1.00442	-0.94798

C	2.93875	-0.30120	-2.34597
O	3.64848	-0.07532	-3.22652
C	1.36674	-2.27344	-1.39929
O	1.16749	-3.37020	-1.69002
C	0.61837	0.03379	-2.33762
O	0.00469	0.35269	-3.26644
O	3.41531	1.68968	-0.20496
O	-0.87628	2.49669	-1.32721
O	-1.00734	5.15717	-1.49704
O	-2.29450	2.87680	0.90611
O	0.35961	3.21218	1.88159
O	-1.21927	5.41435	1.22644
H	-1.73461	0.42906	-1.07233
H	-1.12596	-1.24107	-1.18007
H	3.08693	-0.22010	3.80669
H	-2.61057	0.14170	1.90285
H	1.16141	0.12377	3.93960
H	-1.29630	0.48549	4.00247
H	6.19401	-1.91684	1.37815
H	5.44061	-0.99461	3.58378
C	-5.45320	-3.57985	0.70910
C	-2.14801	-3.31229	0.46581
H	-6.97381	-1.10149	0.84042
H	-7.03769	-1.65387	-0.86395
H	-6.73578	0.06537	-0.48813
H	5.61983	-2.79018	-0.70752
H	4.00609	-2.59626	-1.44259
H	5.19848	-1.27917	-1.52827
H	0.29243	2.32573	-0.97300
H	-1.85336	2.70214	0.03972
H	-2.16779	3.83958	1.02910
H	-0.91541	4.16631	-1.48144
H	-1.91065	5.29227	-1.80699
H	0.86103	2.98186	1.06966
H	-0.51101	2.80829	1.71127
H	-0.50487	4.81619	1.52530
H	-1.08437	5.45077	0.25467
H	-1.01199	2.16159	-2.21866
H	-3.75693	1.10112	-1.93097
H	-5.28687	1.30955	-1.04889
H	-3.73780	1.68868	-0.24546
H	-2.57721	-4.29025	0.71591
H	-1.48740	-3.43962	-0.40481
H	-1.52775	-2.98314	1.31373
H	-6.05156	-3.30909	1.59249
H	-6.14783	-3.88044	-0.08996
H	-4.83222	-4.44604	0.96826

3_{C2}(I4)

Energy	=	-3016.853280
Enthalpy 0K	=	-3016.287767
Enthalpy 298K	=	-3016.243250
Free Energy 298K	=	-3016.364666
Nimag	=	0 (13.9278 cm ⁻¹)

C	-4.14249	-0.34885	-0.45404
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N	-2.99082	-1.01065	-0.26532
C	-3.25328	-2.30399	0.17330
C	-4.61071	-2.41195	0.25900
N	-5.13647	-1.18585	-0.13599
C	-1.65847	-0.48802	-0.51153
C	-0.85797	-0.29411	0.75248
N	0.47892	-0.39548	0.68262
C	1.19092	-0.31298	1.82697
C	0.59136	-0.03401	3.05279
C	-0.78332	0.13855	3.11040
C	-1.51907	-0.01678	1.94825
C	2.63479	-0.63247	1.72327
N	3.06130	-1.04774	0.51358
C	4.31230	-1.52438	0.38856
C	5.19942	-1.51283	1.47199
C	4.79166	-1.00700	2.69469
C	3.47822	-0.57644	2.83010
Mn	1.71591	-0.50032	-1.05447
C	2.30052	1.43090	-0.56803
O	1.43007	2.45461	-0.55674
C	4.79166	-2.08548	-0.91643
C	-6.56430	-0.91622	-0.18116
C	-4.24424	1.05197	-0.92606
C	2.91947	-0.32118	-2.36570
O	3.61913	-0.11717	-3.25842
C	1.34019	-2.25713	-1.38582
O	1.13346	-3.35699	-1.65350
C	0.59875	0.04800	-2.33824
O	-0.01218	0.33977	-3.27459
O	3.43874	1.68988	-0.20483
O	-0.93501	2.47199	-1.32697
O	-0.94129	5.09443	-1.47746
O	-2.25418	2.82775	0.90283
O	0.34242	3.14383	1.91810
O	-1.19886	5.38796	1.22788
H	-1.72536	0.49052	-1.01121
H	-1.14359	-1.18778	-1.17785
H	3.12209	-0.20741	3.78990
H	-2.60332	0.08269	1.95725
H	1.18605	0.03917	3.96077
H	-1.27483	0.37290	4.05600
H	6.20934	-1.90200	1.33442
H	5.47783	-0.96854	3.54281
C	-5.47871	-3.54633	0.67097
C	-2.17258	-3.28580	0.45718
H	-6.99448	-1.05765	0.81857
H	-7.04586	-1.60406	-0.88803
H	-6.74210	0.11296	-0.50467
H	5.60794	-2.79755	-0.73697
H	3.99083	-2.59889	-1.46150
H	5.18989	-1.28710	-1.55914
H	0.47589	2.29535	-0.93747
H	-1.82768	2.66733	0.01359
H	-2.15754	3.79293	1.02273
H	-0.89436	4.08980	-1.46306
H	-1.83338	5.26858	-1.79938
H	0.85838	2.95777	1.10998

H	-0.53437	2.77077	1.69917
H	-0.50333	4.78315	1.55196
H	-1.04760	5.39534	0.25596
H	-1.17060	2.16495	-2.20754
H	-3.77170	1.15162	-1.91407
H	-5.28992	1.36402	-1.01130
H	-3.72509	1.72659	-0.22580
H	-2.60768	-4.26809	0.67858
H	-1.49942	-3.39551	-0.40603
H	-1.56423	-2.97782	1.32148
H	-6.08575	-3.28376	1.55091
H	-6.16559	-3.83733	-0.13829
H	-4.86205	-4.41635	0.92768

3_{C2}⁺(15)

Energy	=	-2635.523370
Enthalpy 0K	=	-2635.074058
Enthalpy 298K	=	-2635.040662
Free Energy 298K	=	-2635.137993
Nimag	=	0 (19.3063 cm ⁻¹)

C	-3.61503	0.14487	1.18974
N	-3.14683	-0.28380	0.00743
C	-4.20145	-0.45436	-0.88394
C	-5.33745	-0.11941	-0.20389
N	-4.94152	0.24819	1.07615
C	-1.74619	-0.51502	-0.30160
C	-0.98545	0.75679	-0.60125
N	0.34725	0.74197	-0.44033
C	1.02664	1.89928	-0.56081
C	0.40946	3.07767	-0.98298
C	-0.95458	3.07199	-1.23148
C	-1.66779	1.90445	-1.00256
Mn	1.66093	-0.94928	-0.33496
C	1.15696	-1.14180	1.63588
O	1.81052	-2.11030	2.34073
C	2.45019	1.86947	-0.14045
N	2.94685	0.66572	0.22192
C	4.18501	0.60486	0.75183
C	4.97701	1.75395	0.86922
C	4.49155	2.97942	0.44816
C	3.19739	3.04161	-0.05105
C	4.74480	-0.69708	1.23422
C	-3.99747	-0.91513	-2.28295
C	-5.85777	0.67769	2.11848
C	-6.76528	-0.10775	-0.61708
C	-2.81032	0.47636	2.38942
C	2.83932	-2.30418	-0.27259
O	3.49754	-3.24707	-0.30867
C	0.52992	-2.27718	-0.72958
O	-0.09784	-3.21561	-0.96493
C	2.06236	-0.67178	-2.10643
O	2.30212	-0.55291	-3.22130
O	0.33643	-0.48289	2.25765
H	0.98116	3.99399	-1.11551
H	-1.46015	3.97591	-1.57494

H	2.77624	3.99979	-0.34778
H	5.97530	1.66461	1.29958
H	-2.74897	1.88111	-1.13962
H	5.10015	3.88204	0.52596
H	3.98657	-1.28527	1.76570
H	5.12357	-1.29162	0.38991
H	5.59029	-0.51130	1.90897
H	-1.70946	-1.19178	-1.16291
H	-1.27612	-1.02012	0.54904
H	-3.29570	-0.25815	-2.81896
H	-3.59744	-1.94044	-2.31344
H	-4.95239	-0.90672	-2.82243
H	-7.19635	0.90094	-0.52561
H	-6.86035	-0.42895	-1.66133
H	-7.36390	-0.78783	0.00797
H	-1.75280	0.21909	2.24492
H	-2.88427	1.55318	2.60409
H	-3.18690	-0.07419	3.26337
H	-6.41888	1.55596	1.77439
H	-6.55729	-0.13511	2.35301
H	-5.29471	0.94100	3.01916
H	1.47792	-2.06670	3.25644

3_{C5}(I3)

Energy	=	-3016.854393
Enthalpy 0K	=	-3016.287908
Enthalpy 298K	=	-3016.243113
Free Energy 298K	=	-3016.364555
Nimag	=	0 (22.7018 cm ⁻¹)

C	3.37763	-1.03284	2.83981
C	2.61378	-0.82526	1.69284
N	3.09930	-1.03198	0.45281
C	4.35102	-1.50600	0.31236
C	5.16677	-1.73053	1.42783
C	4.68522	-1.47774	2.70216
C	1.18652	-0.44107	1.77391
N	0.50805	-0.46567	0.60727
C	-0.82447	-0.31712	0.63958
C	-1.50930	-0.01337	1.81521
C	-0.79812	0.12033	2.99689
C	0.56697	-0.12817	2.98144
C	-1.60570	-0.52295	-0.63777
N	-2.88098	-1.18276	-0.40032
C	-4.13822	-0.60772	-0.54585
C	-5.04279	-1.57249	-0.20157
N	-4.31172	-2.70202	0.14497
C	-3.00701	-2.45337	0.01144
C	-4.33732	0.79609	-0.99347
C	-1.89464	-3.38997	0.30239
C	-4.90529	-3.95522	0.57997
C	-6.52867	-1.55336	-0.16155
Mn	1.78508	-0.34199	-1.07789
C	0.68688	0.33189	-2.29590
O	0.06173	0.77083	-3.16976
C	4.90604	-1.80447	-1.04812

C	2.11840	1.58524	-0.28311
O	3.19003	1.83265	0.27714
C	3.03236	0.19925	-2.23190
O	3.76814	0.63836	-3.00728
C	1.54816	-2.03276	-1.70803
O	1.41222	-3.06839	-2.19925
O	1.14635	2.43789	-0.29380
O	-1.12173	2.73922	-1.30176
O	0.08948	3.24438	2.03269
O	-1.31174	5.46047	-1.21211
O	-1.61096	5.35696	1.53369
O	-2.58690	2.82692	1.03816
H	-1.80698	0.44827	-1.10546
H	-1.02519	-1.12873	-1.34148
H	2.95929	-0.86451	3.83058
H	-2.58827	0.13600	1.79093
H	1.14224	-0.06883	3.90347
H	-1.30286	0.39416	3.92468
H	6.17860	-2.10936	1.27658
H	5.31061	-1.64420	3.58128
H	-6.90171	-1.72259	0.86038
H	-6.95403	-2.33451	-0.80983
H	-6.90155	-0.58073	-0.50487
H	5.76027	-2.48866	-0.96206
H	4.15473	-2.25854	-1.70518
H	5.26680	-0.88473	-1.53053
H	-0.17591	2.51922	-0.95295
H	-2.15879	2.73731	0.16439
H	-2.47650	3.78133	1.23572
H	-1.20133	4.48844	-1.31413
H	-2.19770	5.62523	-1.55695
H	0.61646	3.02356	1.22431
H	-0.74513	2.77473	1.86523
H	-0.85586	4.77924	1.77527
H	-1.46442	5.52662	0.58007
H	-1.16678	2.38146	-2.19563
H	-3.88490	0.96744	-1.98235
H	-5.41097	1.00812	-1.07204
H	-3.89670	1.51088	-0.28146
H	-2.13226	-4.39765	-0.06256
H	-0.96970	-3.05991	-0.18497
H	-1.71367	-3.44375	1.38704
H	-5.63073	-3.75432	1.37778
H	-5.41300	-4.44168	-0.26349
H	-4.12566	-4.61721	0.96938

3_{C5}(TS2)

Energy	=	-3016.851483
Enthalpy 0K	=	-3016.289779
Enthalpy 298K	=	-3016.245182
Free Energy 298K	=	-3016.366589
Nimag	=	1 (-628.0548 cm ⁻¹)

C	3.42273	-0.35434	2.85023
C	2.57499	-0.52769	1.75923
N	2.98711	-1.10029	0.61045

C	4.22451	-1.62027	0.54527
C	5.11617	-1.49455	1.61799
C	4.72563	-0.82902	2.76775
C	1.13968	-0.16383	1.81881
N	0.43220	-0.35093	0.68532
C	-0.90332	-0.21441	0.73440
C	-1.56462	0.19139	1.89206
C	-0.83026	0.45519	3.03664
C	0.54121	0.25831	3.00440
C	-1.70070	-0.51596	-0.51262
N	-3.05377	-0.96579	-0.23284
C	-4.20915	-0.20389	-0.35777
C	-5.24515	-1.02114	-0.00394
N	-4.69185	-2.25386	0.32402
C	-3.36497	-2.20420	0.17890
C	-4.19329	1.21637	-0.79666
C	-2.38718	-3.30130	0.37969
C	-5.48503	-3.40360	0.72500
C	-6.70978	-0.77474	0.05925
Mn	1.66950	-0.67686	-1.01870
C	0.59616	-0.15382	-2.33896
O	-0.00057	0.14943	-3.28346
C	4.68032	-2.35515	-0.67923
C	2.34123	1.27659	-0.72384
O	3.51843	1.49120	-0.44552
C	2.88387	-0.67607	-2.33046
O	3.59506	-0.59423	-3.23447
C	1.20961	-2.43467	-1.19883
O	0.94619	-3.53963	-1.38983
O	1.50830	2.30256	-0.73990
O	-0.78183	2.42625	-1.41527
O	-0.78420	5.06410	-1.79403
O	-1.99284	3.08846	0.88310
O	0.71621	3.33991	1.66852
O	-0.76102	5.58042	0.89916
H	-1.75443	0.40509	-1.10788
H	-1.19870	-1.28349	-1.10927
H	3.07866	0.14188	3.75583
H	-2.64784	0.30628	1.88931
H	1.13503	0.42002	3.90153
H	-1.32222	0.79500	3.94937
H	6.11610	-1.92202	1.52993
H	5.41659	-0.70008	3.60296
H	-7.25871	-1.46903	-0.59501
H	-6.93219	0.24945	-0.26416
H	-7.09194	-0.90242	1.08369
H	5.46877	-3.07115	-0.41145
H	3.85773	-2.89884	-1.15867
H	5.10739	-1.65784	-1.41430
H	0.40510	2.23086	-1.10669
H	-1.64639	2.80027	0.00497
H	-1.80687	4.04883	0.89387
H	-0.74499	4.07331	-1.69745
H	-1.70292	5.22739	-2.03813
H	1.14495	3.02124	0.84525
H	-0.18935	2.98778	1.57933
H	-0.06824	4.96364	1.21025

H	-0.69447	5.51631	-0.07831
H	-0.97229	2.04690	-2.27849
H	-3.78235	1.31292	-1.81358
H	-5.21733	1.61025	-0.80560
H	-3.58609	1.84212	-0.12427
H	-2.76783	-4.04563	1.08814
H	-2.17933	-3.80394	-0.57740
H	-1.44155	-2.90682	0.77308
H	-6.11351	-3.13190	1.58226
H	-6.12200	-3.72164	-0.11068
H	-4.82778	-4.23005	1.01005

3c5 (14)

Energy	=	-3016.852645
Enthalpy 0K	=	-3016.287332
Enthalpy 298K	=	-3016.242666
Free Energy 298K	=	-3016.364116
Nimag	=	0 (18.0275 cm ⁻¹)

C	3.42810	-0.60576	2.84540
C	2.59452	-0.65537	1.73090
N	3.02516	-1.08675	0.52827
C	4.26860	-1.58609	0.41876
C	5.14537	-1.58234	1.51070
C	4.73508	-1.06013	2.72565
C	1.15540	-0.31088	1.81792
N	0.45416	-0.38908	0.66673
C	-0.88181	-0.26865	0.72235
C	-1.55106	0.02508	1.90991
C	-0.82466	0.17813	3.07841
C	0.54785	-0.01441	3.03576
C	-1.67648	-0.45859	-0.54599
N	-3.01227	-0.97962	-0.30486
C	-4.20298	-0.28357	-0.47928
C	-5.20533	-1.14429	-0.12953
N	-4.59715	-2.33512	0.24818
C	-3.27241	-2.22267	0.12740
C	-4.25120	1.12250	-0.95964
C	-2.26662	-3.26375	0.44973
C	-5.31813	-3.51794	0.68805
C	-6.68206	-0.97301	-0.11176
Mn	1.70711	-0.52077	-1.05629
C	0.61288	0.05706	-2.34661
O	0.01433	0.37002	-3.28397
C	4.74920	-2.16538	-0.87766
C	2.32938	1.39949	-0.57126
O	3.47459	1.63529	-0.21340
C	2.92511	-0.37447	-2.35868
O	3.63577	-0.19209	-3.24729
C	1.29567	-2.26820	-1.39108
O	1.06300	-3.36248	-1.66166
O	1.47924	2.43884	-0.55713
O	-0.88602	2.49385	-1.31027
O	-2.17410	2.90756	0.93609
O	-0.84532	5.11162	-1.50021
O	-1.05873	5.45592	1.20205

O	0.43395	3.18591	1.91940
H	-1.75344	0.52349	-1.03546
H	-1.15734	-1.14344	-1.22332
H	3.06917	-0.22325	3.79888
H	-2.63377	0.14372	1.90683
H	1.13456	0.05663	3.94909
H	-1.32213	0.42723	4.01710
H	6.14951	-1.99026	1.38573
H	5.41382	-1.02731	3.57997
H	-7.08318	-1.07922	0.90803
H	-7.17711	-1.72140	-0.74913
H	-6.94903	0.02433	-0.48209
H	5.55155	-2.89005	-0.68621
H	3.94362	-2.66886	-1.42505
H	5.16604	-1.37896	-1.52327
H	0.51641	2.29705	-0.93054
H	-1.77017	2.71665	0.04370
H	-2.05572	3.87284	1.02926
H	-0.81819	4.10629	-1.46775
H	-1.73879	5.29768	-1.81146
H	0.93694	2.97608	1.10890
H	-0.45518	2.83485	1.71201
H	-0.37556	4.83867	1.52873
H	-0.91988	5.44232	0.22839
H	-1.13016	2.18587	-2.18811
H	-3.80650	1.21554	-1.96234
H	-5.29504	1.45534	-1.01841
H	-3.70661	1.79601	-0.27948
H	-2.59935	-4.24633	0.09043
H	-1.30433	-3.03445	-0.02258
H	-2.11229	-3.32316	1.53818
H	-6.06820	-3.22728	1.43339
H	-5.81632	-3.99397	-0.16715
H	-4.62058	-4.22553	1.14715

1_{c2}(I5-R)

Energy	= -2517.764879
Enthalpy 0K	= -2517.402715
Enthalpy 298K	= -2517.373983
Free Energy 298K	= -2517.461871
Nimag	= 0 (23.2779 cm ⁻¹)

N	-2.44376	0.12460	-0.06956
C	-2.22526	1.45765	0.22577
C	-3.29148	2.26191	0.72905
C	-4.55465	1.73866	0.82256
C	-4.78081	0.41368	0.39860
C	-3.70203	-0.35780	-0.03018
C	-0.93192	1.97762	-0.05098
N	0.00138	1.10554	-0.59594
C	1.15382	1.62225	-1.05872
C	1.50160	2.96159	-0.94352
C	0.61546	3.83646	-0.27133
C	-0.58593	3.34831	0.16305
C	2.16656	0.71784	-1.71792
N	3.23820	0.33627	-0.79275

C	4.51306	-0.02534	-1.16639
C	5.17337	-0.37584	-0.02892
N	4.28386	-0.22389	1.01139
C	3.12062	0.20818	0.52958
C	4.56373	-0.49607	2.41323
Mn	-0.61438	-0.91279	-0.32479
C	-1.19105	-2.54681	0.12873
O	-1.42966	-3.63243	0.43600
C	-3.97420	-1.77511	-0.45053
C	-0.94291	-1.11523	-2.11192
O	-1.13853	-1.25950	-3.23494
C	0.95777	-1.75463	-0.40588
O	1.90484	-2.41867	-0.42598
C	-0.28969	-0.52980	1.67040
O	0.66173	0.04810	2.19154
O	-1.25843	-0.95090	2.52379
H	1.70246	-0.18889	-2.12211
H	2.64780	1.24938	-2.54732
H	-3.10788	3.29471	1.02325
H	2.45334	3.31047	-1.34683
H	-1.28913	4.01263	0.66463
H	0.87903	4.88512	-0.11596
H	-5.78136	-0.02052	0.41189
H	-5.37896	2.34824	1.20114
H	6.19442	-0.71120	0.13091
H	4.83859	0.00372	-2.20250
H	4.96026	-1.51391	2.51193
H	3.63072	-0.40969	2.98079
H	5.29713	0.22697	2.79227
H	-5.03847	-1.89731	-0.69285
H	-3.38270	-2.06243	-1.32975
H	-3.74111	-2.47938	0.36096
H	2.19909	0.35439	1.11968
H	-0.97770	-0.67815	3.41642

1_{c2}(I6-R)

Energy	= -2899.578840
Enthalpy 0K	= -2899.087863
Enthalpy 298K	= -2899.046292
Free Energy 298K	= -2899.162582
Nimag	= 0 (22.1849 cm ⁻¹)

N	3.11870	-0.52859	0.44419
C	2.57227	-0.51722	1.71417
C	3.42372	-0.45540	2.85762
C	4.78345	-0.51480	2.69939
C	5.31624	-0.65730	1.40219
C	4.45479	-0.64864	0.30703
C	1.15925	-0.63636	1.81348
N	0.43733	-0.68158	0.62899
C	-0.86274	-1.03398	0.68786
C	-1.53408	-1.28666	1.87216
C	-0.83767	-1.12557	3.09423
C	0.48850	-0.80244	3.06379
C	-1.61559	-1.10431	-0.62551
N	-2.84998	-1.87207	-0.54914

C	-2.93953	-3.24401	-0.63758	N	3.22832	-0.42900	0.39198
C	-4.25324	-3.56305	-0.48434	C	2.70730	-0.53955	1.67057
N	-4.93508	-2.37909	-0.30139	C	3.58231	-0.56957	2.79687
C	-4.06891	-1.37086	-0.34414	C	4.93760	-0.59813	2.60762
C	-6.37073	-2.25515	-0.09607	C	5.44580	-0.61696	1.29057
Mn	1.64889	-0.10899	-1.02056	C	4.56743	-0.52106	0.21786
C	2.73749	0.51954	-2.30150	C	1.29761	-0.68118	1.78660
O	3.31941	0.98596	-3.17911	N	0.55601	-0.65967	0.61514
C	5.05961	-0.77564	-1.06315	C	-0.74514	-1.01162	0.67379
C	1.71298	-1.84613	-1.60088	C	-1.39375	-1.32627	1.85506
O	1.75334	-2.93134	-1.97133	C	-0.67651	-1.24093	3.07064
C	0.39543	0.36618	-2.18578	C	0.65172	-0.92538	3.03593
O	-0.32115	0.71886	-3.02694	C	-1.52658	-1.02279	-0.62419
C	1.70124	1.77987	-0.22646	N	-2.67662	-1.91569	-0.59579
O	2.66168	2.48325	-0.01200	C	-2.62633	-3.27454	-0.81931
O	0.46530	2.38582	0.11986	C	-3.89609	-3.74311	-0.68253
O	-1.85112	2.54253	-1.32332	N	-4.69186	-2.66043	-0.37488
O	-3.86075	1.52999	0.28778	C	-3.93578	-1.56737	-0.32609
O	-2.92802	5.00735	-0.64106	C	-6.12666	-2.70804	-0.13636
O	-1.61702	1.96382	2.03374	Mn	1.72005	0.07710	-0.99125
O	-3.65344	3.81567	1.74792	C	2.76666	0.76624	-2.29244
H	-1.87467	-0.09156	-0.96140	O	3.30762	1.24679	-3.18459
H	-0.99798	-1.57226	-1.39952	C	5.14489	-0.51506	-1.16891
H	2.99399	-0.36937	3.85508	C	1.80928	-1.62668	-1.68330
H	-2.58533	-1.57004	1.87159	O	1.87987	-2.69569	-2.07941
H	1.04410	-0.70052	3.99548	C	0.39942	0.61269	-2.10460
H	-1.35487	-1.26724	4.04569	O	-0.32476	0.97508	-2.91980
H	6.39019	-0.75866	1.24061	C	1.78614	1.82735	-0.06535
H	5.44410	-0.47085	3.56882	O	2.30784	2.69464	0.46551
H	-4.76254	-4.52257	-0.49477	O	-0.26856	2.59354	-0.14130
H	-2.06433	-3.86569	-0.80622	O	-2.41776	2.33760	-1.29185
H	-6.90095	-2.63891	-0.97662	O	-4.09085	1.23792	0.51802
H	-6.61612	-1.19790	0.05127	O	-3.62512	4.64063	-0.55751
H	-6.66167	-2.82909	0.79237	O	-1.63105	1.99034	2.03726
H	6.06398	-1.21399	-0.99021	O	-3.88329	3.54215	1.98225
H	4.45225	-1.40981	-1.72236	H	-1.88610	-0.00955	-0.85738
H	5.16800	0.20916	-1.53995	H	-0.89353	-1.36218	-1.45029
H	-4.28718	-0.30753	-0.18621	H	3.17215	-0.58095	3.80593
H	-0.99901	2.43644	-0.84417	H	-2.44629	-1.60465	1.85691
H	-3.23997	1.86620	-0.38627	H	1.22541	-0.88248	3.96086
H	-4.03208	2.32782	0.83749	H	-1.17743	-1.43782	4.02091
H	-2.49814	4.20894	-1.00470	H	6.51721	-0.69112	1.10096
H	-3.72817	5.10262	-1.17248	H	5.61574	-0.62464	3.46387
H	-0.80210	1.91172	1.50934	H	-4.30344	-4.74532	-0.78275
H	-2.24580	1.41773	1.53310	H	-1.69625	-3.78190	-1.06148
H	-2.81221	3.38043	1.98807	H	-6.62942	-3.12019	-1.01998
H	-3.41333	4.36097	0.97013	H	-6.48692	-1.69085	0.05167
H	-1.66911	2.25579	-2.22827	H	-6.33171	-3.34060	0.73633
H	0.68925	3.27851	0.44602	H	6.16791	-0.91319	-1.14956
				H	4.55275	-1.12565	-1.86388
				H	5.20271	0.50750	-1.56927
				H	-4.25957	-0.55326	-0.05367
				H	-1.44326	2.43776	-0.83569
				H	-3.54512	1.61440	-0.20773
				H	-4.23534	2.01049	1.10549
				H	-3.16416	3.85289	-0.92995
				H	-4.51753	4.57263	-0.91768

1_{c2}(TS3)			
Energy	=	-2899.558076	
Enthalpy 0K	=	-2899.071601	
Enthalpy 298K	=	-2899.030410	
Free Energy 298K	=	-2899.145966	
Nimag	=	1 (-210.5435 cm ⁻¹)	

H	-1.03675	2.22263	1.26739
H	-2.21102	1.31620	1.65351
H	-2.99340	3.14608	2.11570
H	-3.78248	4.05227	1.15226
H	-2.27188	2.10169	-2.21415
H	-0.10214	3.54327	-0.09540

1_{C2}(I7-R)

Energy	=	-2899.566929
Enthalpy 0K	=	-2899.078544
Enthalpy 298K	=	-2899.036763
Free Energy 298K	=	-2899.154097
Nimag	=	0 (18.5020 cm ⁻¹)

N	3.39004	-0.31118	0.37749
C	2.87349	-0.49070	1.65201
C	3.75554	-0.61544	2.76568
C	5.10812	-0.66286	2.56217
C	5.60779	-0.60134	1.24214
C	4.72628	-0.41347	0.18519
C	1.46130	-0.60793	1.76577
N	0.72808	-0.55958	0.59064
C	-0.57626	-0.90491	0.62699
C	-1.23985	-1.20829	1.80259
C	-0.53788	-1.12666	3.02581
C	0.79874	-0.84056	3.00797
C	-1.35270	-0.93651	-0.67435
N	-2.36351	-1.98779	-0.69230
C	-2.10505	-3.32559	-0.89864
C	-3.29745	-3.97520	-0.81796
N	-4.25652	-3.01987	-0.56046
C	-3.67191	-1.82639	-0.48816
C	-5.67910	-3.27733	-0.39344
Mn	1.87571	0.33608	-0.93145
C	2.91765	1.13048	-2.18879
O	3.46032	1.67364	-3.03971
C	5.29337	-0.31043	-1.20175
C	1.94903	-1.32414	-1.78193
O	2.00064	-2.35572	-2.26021
C	0.50871	0.96917	-1.95312
O	-0.24910	1.41756	-2.68524
C	1.91183	1.93030	0.09990
O	2.06184	2.88966	0.68764
O	-0.91172	2.35916	0.55784
O	-2.79499	1.97017	-1.10623
O	-4.70674	0.85900	0.20276
O	-3.91993	4.27680	-0.64745
O	-2.91075	1.57462	2.29217
O	-5.04998	3.21944	1.61571
H	-1.86372	0.02941	-0.84284
H	-0.68902	-1.13610	-1.52108
H	3.35175	-0.69159	3.77458
H	-2.29670	-1.46941	1.79116
H	1.36179	-0.80242	3.93984
H	-1.05588	-1.30373	3.97074
H	6.67630	-0.68313	1.04005

H	5.79165	-0.76611	3.40818
H	-3.54876	-5.02675	-0.92531
H	-1.09965	-3.69193	-1.08855
H	-6.07896	-3.72943	-1.30962
H	-6.19012	-2.32848	-0.19729
H	-5.82952	-3.95931	0.45269
H	6.31186	-0.71976	-1.22076
H	4.69187	-0.86040	-1.93804
H	5.36103	0.73903	-1.52335
H	-4.17522	-0.87678	-0.25566
H	-1.60385	2.20835	-0.17627
H	-4.01367	1.27809	-0.40064
H	-5.09720	1.63009	0.65966
H	-3.44615	3.41698	-0.87611
H	-4.64185	4.31170	-1.28548
H	-2.11494	1.85376	1.78852
H	-3.41045	1.07107	1.62320
H	-4.25795	2.81947	2.02810
H	-4.67151	3.70469	0.84836
H	-2.58760	1.84595	-2.03770
H	-0.79932	3.31589	0.58548

1_{C2}⁺(I8)

Energy	=	-2441.875625
Enthalpy 0K	=	-2441.528704
Enthalpy 298K	=	-2441.501042
Free Energy 298K	=	-2441.586411
Nimag	=	0 (27.1961 cm ⁻¹)

C	3.20058	0.47513	0.55446
N	3.18147	0.29209	-0.76571
C	4.31976	-0.38808	-1.13388
C	5.03145	-0.61389	0.00411
N	4.31266	-0.06752	1.04247
C	2.11675	0.68438	-1.69769
C	1.08972	1.58452	-1.05926
N	-0.04111	1.05809	-0.52981
C	-0.99537	1.93372	-0.02473
C	-0.69214	3.32420	0.09610
C	0.48071	3.82325	-0.39422
C	1.38162	2.93517	-1.03374
C	-2.27266	1.39503	0.29125
N	-2.45504	0.04001	0.07908
C	-3.70451	-0.47868	0.14967
C	-4.79625	0.29163	0.53036
C	-4.60687	1.64638	0.87082
C	-3.35985	2.19766	0.74382
Mn	-0.60028	-0.93405	-0.12035
C	-0.29480	-0.52146	1.69372
O	-0.11156	-0.28077	2.78837
C	-3.94266	-1.92428	-0.18022
C	4.71204	-0.07725	2.44277
C	-1.14982	-2.61094	0.33744
O	-1.35545	-3.69623	0.63585
C	-0.99362	-1.16336	-1.94275
O	-1.24764	-1.26602	-3.04518
C	1.01817	-1.74852	-0.25411

O	1.96720	-2.39024	-0.29708
H	1.67107	-0.22656	-2.11403
H	2.60273	1.21897	-2.52266
H	-3.20507	3.25177	0.96917
H	2.30672	3.29393	-1.48650
H	-1.40970	3.99379	0.56876
H	0.71232	4.88699	-0.31212
H	-5.78511	-0.16603	0.57109
H	-5.44841	2.25477	1.20989
H	5.98379	-1.11166	0.16518
H	4.51851	-0.65448	-2.16821
H	5.64569	0.48660	2.55989
H	4.85904	-1.11396	2.76912
H	3.92057	0.38902	3.03925
H	-5.00649	-2.08506	-0.39804
H	-3.36499	-2.25269	-1.05469
H	-3.68742	-2.57167	0.67127
H	2.43401	0.97721	1.14011

1_{C2}⁺(I5-P)

Energy	= -2899.483963
Enthalpy 0K	= -2898.989047
Enthalpy 298K	= -2898.947946
Free Energy 298K	= -2899.062628
Nimag	= 0 (20.1175 cm ⁻¹)

N	3.07740	-0.58440	0.51177
C	2.54942	-0.42628	1.74404
C	3.33347	-0.14682	2.85886
C	4.71456	-0.09406	2.70920
C	5.25606	-0.36993	1.46605
C	4.41454	-0.61500	0.37285
C	1.08734	-0.64440	1.85418
N	0.39531	-0.71477	0.69877
C	-0.90726	-1.05087	0.75307
C	-1.55476	-1.30985	1.95817
C	-0.85162	-1.20086	3.14761
C	0.49028	-0.86597	3.09515
C	-1.67291	-1.11830	-0.55057
N	-2.95864	-1.78641	-0.44042
C	-3.15514	-3.14963	-0.50359
C	-4.48930	-3.35990	-0.34427
N	-5.07631	-2.12251	-0.18592
C	-4.13623	-1.18585	-0.24801
C	-6.49926	-1.88677	0.01361
Mn	1.61315	-0.28769	-1.01407
C	2.71818	0.18070	-2.35534
O	3.31362	0.53665	-3.27088
C	5.03882	-0.92568	-0.95317
C	1.62401	-2.07012	-1.47986
O	1.63745	-3.16866	-1.80205
C	0.36827	0.15127	-2.21412
O	-0.33551	0.47813	-3.06951
C	1.74945	1.66345	-0.41070
O	2.75304	2.30460	-0.20491
O	0.54994	2.38153	-0.20486

O	-1.81734	2.58233	-1.57319
O	-3.71054	1.72930	0.24902
O	-2.52418	5.12509	-0.68298
O	-1.37942	1.92007	1.87593
O	-3.28553	3.97088	1.70519
H	-1.85427	-0.10032	-0.92029
H	-1.09303	-1.66068	-1.30522
H	2.88120	0.02879	3.83330
H	-2.60696	-1.58975	1.97149
H	1.07550	-0.81085	4.01077
H	-1.34208	-1.38953	4.10377
H	6.33635	-0.39344	1.31651
H	5.35585	0.13309	3.56268
H	-5.07284	-4.27625	-0.33608
H	-2.33205	-3.84150	-0.66056
H	-7.05504	-2.25982	-0.85554
H	-6.66794	-0.81047	0.12636
H	-6.82961	-2.41035	0.91913
H	6.03014	-1.37189	-0.79848
H	4.42824	-1.62555	-1.53677
H	5.18397	-0.00786	-1.54113
H	-4.27233	-0.10513	-0.11896
H	-0.93282	2.43391	-1.17664
H	-3.16147	2.02507	-0.50201
H	-3.80675	2.54544	0.79270
H	-2.25572	4.30501	-1.13948
H	-3.31920	5.40663	-1.15249
H	-0.64537	1.97834	1.24402
H	-2.10598	1.54174	1.34920
H	-2.48135	3.47626	1.95121
H	-3.00333	4.49847	0.92815
H	-1.73903	2.30906	-2.49659
H	0.81302	3.29031	0.04031

1_{C2}⁺(TS4)

Energy	= -2899.457959
Enthalpy 0K	= -2898.968405
Enthalpy 298K	= -2898.927656
Free Energy 298K	= -2899.041335
Nimag	= 1 (-254.8620 cm ⁻¹)

N	3.25632	-0.40564	0.44851
C	2.75038	-0.46868	1.70135
C	3.56551	-0.45003	2.82899
C	4.94413	-0.41676	2.66274
C	5.45689	-0.44558	1.37805
C	4.59313	-0.44170	0.27649
C	1.28018	-0.64005	1.80849
N	0.58360	-0.64264	0.65173
C	-0.72153	-0.96625	0.68637
C	-1.37863	-1.23946	1.88353
C	-0.68229	-1.16836	3.07785
C	0.67091	-0.87676	3.03962
C	-1.49380	-1.01729	-0.61382
N	-2.63458	-1.91807	-0.56306
C	-2.57277	-3.28282	-0.75163
C	-3.84133	-3.75471	-0.61895

N	-4.64760	-2.66952	-0.34959	C	2.94553	-0.68539	1.58582
C	-3.90105	-1.57093	-0.31947	C	3.78714	-1.04706	2.63318
C	-6.08568	-2.71971	-0.12843	C	5.15995	-1.04580	2.42459
Mn	1.75880	0.04998	-0.99074	C	5.63933	-0.71470	1.16936
C	2.82200	0.68711	-2.31866	C	4.75186	-0.34847	0.15121
O	3.37125	1.12682	-3.22178	C	1.47087	-0.77968	1.71361
C	5.19365	-0.48610	-1.09457	N	0.76051	-0.60105	0.57809
C	1.84929	-1.68484	-1.65501	C	-0.55364	-0.88078	0.58472
O	1.91924	-2.75111	-2.04881	C	-1.21640	-1.24094	1.75738
C	0.44050	0.56369	-2.13454	C	-0.51075	-1.31972	2.94529
O	-0.27867	0.91895	-2.95161	C	0.86030	-1.10976	2.92034
C	1.79644	1.82852	-0.16315	C	-1.34364	-0.81878	-0.70427
O	2.25001	2.76476	0.30231	N	-2.30980	-1.90518	-0.79668
O	-0.38368	2.40715	-0.08479	C	-1.99322	-3.22265	-1.05324
O	-2.46991	2.21253	-1.31844	C	-3.16415	-3.91423	-1.05662
O	-4.27350	1.27481	0.43370	N	-4.16793	-3.00453	-0.80190
O	-3.50139	4.62471	-0.64940	C	-3.63252	-1.79732	-0.64892
O	-1.89635	1.85749	2.03113	C	-5.58771	-3.31471	-0.71559
O	-4.03137	3.59578	1.86344	Mn	1.89621	0.46516	-0.87163
H	-1.86010	-0.01047	-0.86941	C	2.91604	1.41149	-2.05563
H	-0.85314	-1.37295	-1.42607	O	3.43162	2.04972	-2.85076
H	3.14041	-0.46932	3.82999	C	5.31310	-0.00778	-1.19384
H	-2.43749	-1.49376	1.88443	C	2.00726	-1.10066	-1.90645
H	1.24658	-0.85384	3.96202	O	2.08744	-2.06115	-2.50651
H	-1.18446	-1.35482	4.02817	C	0.51513	1.17078	-1.84436
H	6.53317	-0.46825	1.20363	O	-0.24394	1.67687	-2.53100
H	5.60568	-0.39521	3.53042	C	1.87494	1.97595	0.27644
H	-4.24151	-4.76160	-0.69913	O	1.96164	2.89389	0.93586
H	-1.63710	-3.79007	-0.97153	O	-0.99153	2.13528	0.82112
H	-6.57209	-3.16539	-1.00473	O	-2.81595	2.05969	-0.93668
H	-6.45496	-1.69924	0.01988	O	-4.88195	0.82851	-0.01629
H	-6.29703	-3.32455	0.76211	O	-3.92549	4.29377	-0.14103
H	6.21382	-0.88610	-1.03588	O	-3.15920	1.12057	2.23926
H	4.61493	-1.12168	-1.77656	O	-5.27176	2.90147	1.78859
H	5.26704	0.52414	-1.52272	H	-1.89392	0.13931	-0.78105
H	-4.24450	-0.55547	-0.07978	H	-0.68403	-0.91553	-1.57139
H	-1.48972	2.28735	-0.81518	H	3.38420	-1.34583	3.59852
H	-3.70027	1.61107	-0.29262	H	-2.28755	-1.43124	1.74265
H	-4.43134	2.07371	0.98189	H	1.44311	-1.20757	3.83374
H	-3.10464	3.78953	-0.99189	H	-1.01845	-1.56219	3.88003
H	-4.36082	4.66635	-1.08582	H	6.70800	-0.73675	0.95370
H	-1.24487	2.06066	1.30458	H	5.84219	-1.32344	3.22974
H	-2.56610	1.33056	1.56640	H	-3.37256	-4.96764	-1.22219
H	-3.17744	3.16034	2.07022	H	-0.96792	-3.54512	-1.21471
H	-3.83853	4.08665	1.03703	H	-5.93049	-3.72527	-1.67341
H	-2.31502	2.02276	-2.24989	H	-6.13615	-2.39375	-0.49023
H	-0.24518	3.36036	-0.02178	H	-5.75193	-4.04811	0.08347

1_{C2}⁺(I6-P)

Energy	=	-2899.465454
Enthalpy 0K	=	-2898.973703
Enthalpy 298K	=	-2898.932246
Free Energy 298K	=	-2899.049058
Nimag	=	0 (8.8172 cm ⁻¹)

N	3.42273	-0.30630	0.37792
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C	2.94553	-0.68539	1.58582
C	3.78714	-1.04706	2.63318
C	5.15995	-1.04580	2.42459
C	5.63933	-0.71470	1.16936
C	4.75186	-0.34847	0.15121
C	1.47087	-0.77968	1.71361
N	0.76051	-0.60105	0.57809
C	-0.55364	-0.88078	0.58472
C	-1.21640	-1.24094	1.75738
C	-0.51075	-1.31972	2.94529
C	0.86030	-1.10976	2.92034
C	-1.34364	-0.81878	-0.70427
N	-2.30980	-1.90518	-0.79668
C	-1.99322	-3.22265	-1.05324
C	-3.16415	-3.91423	-1.05662
N	-4.16793	-3.00453	-0.80190
C	-3.63252	-1.79732	-0.64892
C	-5.58771	-3.31471	-0.71559
Mn	1.89621	0.46516	-0.87163
C	2.91604	1.41149	-2.05563
O	3.43162	2.04972	-2.85076
C	5.31310	-0.00778	-1.19384
C	2.00726	-1.10066	-1.90645
O	2.08744	-2.06115	-2.50651
C	0.51513	1.17078	-1.84436
O	-0.24394	1.67687	-2.53100
C	1.87494	1.97595	0.27644
O	1.96164	2.89389	0.93586
O	-0.99153	2.13528	0.82112
O	-2.81595	2.05969	-0.93668
O	-4.88195	0.82851	-0.01629
O	-3.92549	4.29377	-0.14103
O	-3.15920	1.12057	2.23926
O	-5.27176	2.90147	1.78859
H	-1.89392	0.13931	-0.78105
H	-0.68403	-0.91553	-1.57139
H	3.38420	-1.34583	3.59852
H	-2.28755	-1.43124	1.74265
H	1.44311	-1.20757	3.83374
H	-1.01845	-1.56219	3.88003
H	6.70800	-0.73675	0.95370
H	5.84219	-1.32344	3.22974
H	-3.37256	-4.96764	-1.22219
H	-0.96792	-3.54512	-1.21471
H	-5.93049	-3.72527	-1.67341
H	-6.13615	-2.39375	-0.49023
H	-5.75193	-4.04811	0.08347
H	6.34406	-0.37475	-1.26964
H	4.73080	-0.45875	-2.00782
H	5.34440	1.08203	-1.33681
H	-4.18227	-0.87394	-0.41091
H	-1.66130	2.14463	0.04844
H	-4.13352	1.31923	-0.48142
H	-5.27998	1.51560	0.55467
H	-3.45985	3.47328	-0.48906
H	-4.57238	4.49627	-0.82670
H	-2.33181	1.47836	1.85204

H	-3.64331	0.80342	1.45417
H	-4.51675	2.42771	2.18718
H	-4.82758	3.50531	1.15088
H	-2.58141	2.10253	-1.86929
H	-0.87094	3.06487	1.04552

1_{C2}²⁺(I7-P)

Energy	=	-2441.767118
Enthalpy 0K	=	-2441.416870
Enthalpy 298K	=	-2441.389488
Free Energy 298K	=	-2441.474065
Nimag	=	0 (22.0941 cm ⁻¹)

C	3.16974	0.49965	0.64652
N	3.18261	0.28220	-0.67044
C	4.32661	-0.41441	-0.99241
C	5.00444	-0.61763	0.16965
N	4.26320	-0.04009	1.17520
C	2.16421	0.67707	-1.64792
C	1.11529	1.58210	-1.05814
N	-0.03565	1.09144	-0.55088
C	-0.95827	1.96563	-0.09527
C	-0.72151	3.34178	-0.06519
C	0.47616	3.84122	-0.54609
C	1.39646	2.94633	-1.06931
C	-2.27075	1.40900	0.31520
N	-2.44608	0.07778	0.14531
C	-3.66973	-0.45348	0.35021
C	-4.72751	0.33977	0.81069
C	-4.53174	1.68549	1.05996
C	-3.28505	2.23411	0.79082
Mn	-0.61303	-0.93839	-0.20529
C	-0.22150	-0.68625	1.62218
O	0.00615	-0.55369	2.72534
C	-3.94280	-1.90171	0.08850
C	4.62694	-0.01535	2.58563
C	-1.16414	-2.65200	0.14149
O	-1.35668	-3.75895	0.34084
C	-1.07588	-1.06584	-2.03305
O	-1.35734	-1.11576	-3.12980
C	0.98736	-1.78803	-0.44346
O	1.91322	-2.45056	-0.54690
H	1.73185	-0.22267	-2.09806
H	2.68241	1.21791	-2.44888
H	-3.11936	3.29763	0.94482
H	2.34107	3.28997	-1.49259
H	-1.47280	4.02759	0.31912
H	0.67866	4.91297	-0.53225
H	-5.70182	-0.12354	0.96914
H	-5.34229	2.31102	1.43732
H	5.94678	-1.12096	0.36832
H	4.55023	-0.70762	-2.01435
H	5.54347	0.57332	2.71526
H	4.79093	-1.04270	2.93228
H	3.80913	0.44014	3.15392
H	-5.02475	-2.06260	0.00679

H	-3.47811	-2.24567	-0.84455
H	-3.58710	-2.52259	0.92338
H	2.39607	1.02511	1.20222

1_{C5}(I6-R)

Energy	=	-2899.577552
Enthalpy 0K	=	-2899.086186
Enthalpy 298K	=	-2899.044708
Free Energy 298K	=	-2899.160519
Nimag	=	0 (20.2544 cm ⁻¹)

C	-4.25061	-1.01764	-0.07559
N	-3.03934	-1.62184	-0.33736
C	-3.21955	-2.94113	-0.40147
N	-4.50419	-3.20499	-0.18957
C	-5.17140	-2.01661	0.01706
C	-1.75636	-0.95089	-0.49501
C	-0.99289	-0.77185	0.80151
N	0.33037	-0.53501	0.69853
C	1.06805	-0.40778	1.86700
C	0.40165	-0.37374	3.13004
C	-0.94628	-0.57955	3.20134
C	-1.66929	-0.82332	2.00881
C	2.48460	-0.41578	1.74833
N	3.00993	-0.63158	0.48733
C	4.32892	-0.88110	0.36094
C	5.20284	-0.82392	1.44476
C	4.70303	-0.47220	2.71516
C	3.35535	-0.27950	2.87057
Mn	1.56197	-0.26397	-1.01186
C	1.78398	1.69341	-0.44754
O	2.80215	2.33673	-0.33430
C	4.89898	-1.23245	-0.98478
H	-6.23984	-1.98769	0.21175
C	2.68319	0.11474	-2.36143
O	3.29208	0.42273	-3.28914
C	1.47058	-2.05406	-1.39000
O	1.41316	-3.17355	-1.63590
C	0.33651	0.18866	-2.21614
O	-0.35972	0.51437	-3.08462
O	0.60902	2.43366	-0.15870
O	-1.76204	2.56120	-1.50873
O	-1.38486	2.43567	1.89109
O	-3.74959	1.99178	0.35045
O	-2.56074	5.19592	-1.14319
O	-3.23283	4.44483	1.43490
H	-1.95379	0.02805	-0.95164
H	-1.16769	-1.54220	-1.20350
H	2.94935	-0.02929	3.85025
H	-2.74074	-1.01464	2.04270
H	0.97540	-0.21220	4.04214
H	-1.46158	-0.56597	4.16420
H	6.26205	-1.03577	1.29317
H	5.37835	-0.37203	3.56853
C	-5.11568	-4.52619	-0.19483
H	-2.44257	-3.67622	-0.59828

H	5.86229	-1.74541	-0.86155
H	4.22796	-1.88836	-1.55519
H	5.08503	-0.32910	-1.58335
H	-4.32934	0.06529	0.04767
H	-0.89544	2.45520	-1.05620
H	-3.15434	2.15514	-0.40446
H	-3.81155	2.87901	0.76861
H	-2.23559	4.31108	-1.40007
H	-3.38700	5.29040	-1.63315
H	-0.61298	2.23423	1.33900
H	-2.09652	1.90415	1.49444
H	-2.42803	3.95470	1.69375
H	-2.99090	4.84242	0.57305
H	-1.63845	2.17261	-2.38502
H	0.90891	3.34023	0.04528
H	-5.82575	-4.59691	-1.02834
H	-4.33006	-5.28030	-0.31210
H	-5.64061	-4.68465	0.75509

1_{C5}(TS3)

Energy	=	-2899.556499
Enthalpy 0K	=	-2899.069705
Enthalpy 298K	=	-2899.028622
Free Energy 298K	=	-2899.144153
Nimag	=	1 (-212.7057 cm ⁻¹)

C	-4.12617	-1.29790	0.04459
N	-2.86918	-1.75363	-0.29267
C	-2.91589	-3.07800	-0.44154
N	-4.15836	-3.48822	-0.21216
C	-4.93525	-2.39213	0.09464
C	-1.66559	-0.94702	-0.45511
C	-0.87326	-0.76982	0.82374
N	0.44457	-0.50523	0.70388
C	1.20061	-0.38937	1.85995
C	0.55965	-0.39621	3.13514
C	-0.78389	-0.62245	3.22584
C	-1.52225	-0.85713	2.04319
C	2.61427	-0.35304	1.71486
N	3.12156	-0.47454	0.43123
C	4.44998	-0.67438	0.26572
C	5.33739	-0.65782	1.33502
C	4.85156	-0.40280	2.63620
C	3.50368	-0.26070	2.82656
Mn	1.62683	-0.09103	-1.00430
C	1.82454	1.77034	-0.35666
O	2.40385	2.67267	0.03766
C	5.00448	-0.91752	-1.10910
H	-5.99339	-2.48797	0.32180
C	2.68960	0.32610	-2.40363
O	3.24348	0.62806	-3.36365
C	1.60514	-1.87784	-1.44085
O	1.61115	-2.99416	-1.68366
C	0.31728	0.35310	-2.17410
O	-0.40081	0.62670	-3.02773
O	-0.17207	2.66262	-0.59810
O	-2.40783	2.28913	-1.51392

O	-1.30280	2.49847	1.78184
O	-3.89828	1.64405	0.65646
O	-3.41525	4.75977	-1.09516
O	-3.45955	4.17982	1.62395
H	-1.97161	0.03374	-0.84862
H	-1.05602	-1.44907	-1.21238
H	3.10972	-0.08847	3.82745
H	-2.58880	-1.06905	2.09340
H	1.14774	-0.24213	4.03899
H	-1.28177	-0.63680	4.19775
H	6.39931	-0.82709	1.15318
H	5.54010	-0.33773	3.48204
C	-4.63282	-4.86221	-0.28786
H	-2.07548	-3.71341	-0.71207
H	6.00619	-1.36093	-1.03557
H	4.37095	-1.59858	-1.69344
H	5.10661	0.02429	-1.66743
H	-4.30958	-0.23997	0.25190
H	-1.39256	2.43345	-1.15888
H	-3.43122	1.83813	-0.18495
H	-3.96146	2.52658	1.07833
H	-3.04015	3.88585	-1.35610
H	-4.34638	4.68797	-1.33733
H	-0.79728	2.57319	0.92308
H	-1.96003	1.81638	1.57480
H	-2.58659	3.74807	1.75788
H	-3.41134	4.51304	0.70437
H	-2.34782	1.91872	-2.40076
H	0.04309	3.59195	-0.74474
H	-5.37926	-4.94686	-1.08758
H	-3.78399	-5.52013	-0.50277
H	-5.08345	-5.14228	0.67213

1_{C5}(I7-R)

Energy	=	-2899.564716
Enthalpy 0K	=	-2899.076304
Enthalpy 298K	=	-2899.034492
Free Energy 298K	=	-2899.151784
Nimag	=	0 (17.4194 cm ⁻¹)

C	-3.76662	-1.88807	-0.17202
N	-2.42294	-2.02752	-0.44638
C	-2.14248	-3.32443	-0.57756
N	-3.25841	-4.02261	-0.39784
C	-4.28982	-3.14563	-0.14197
C	-1.43885	-0.95392	-0.55641
C	-0.67208	-0.73330	0.73199
N	0.63321	-0.39919	0.65591
C	1.36005	-0.28853	1.83088
C	0.68903	-0.34003	3.08930
C	-0.64972	-0.61299	3.13818
C	-1.34477	-0.86415	1.93427
C	2.77355	-0.19922	1.70850
N	3.29468	-0.18774	0.42321
C	4.63035	-0.32302	0.24949
C	5.50792	-0.38403	1.32455

C	5.00453	-0.27604	2.64026
C	3.65192	-0.19103	2.83189
Mn	1.78749	0.29409	-0.96256
C	1.82501	2.00634	-0.14182
O	1.97613	3.03372	0.31652
C	5.20086	-0.39584	-1.13799
H	-5.30387	-3.49223	0.03662
C	2.83361	0.92441	-2.30599
O	3.38013	1.35580	-3.21638
C	1.87258	-1.45740	-1.60258
O	1.94308	-2.53828	-1.95298
C	0.41870	0.80057	-2.05292
O	-0.34298	1.15803	-2.82926
O	-0.99520	2.48645	0.21903
O	-2.92584	1.82938	-1.30012
O	-2.89364	2.00649	2.16474
O	-4.75241	0.96344	0.30917
O	-3.99379	4.20084	-1.14881
O	-5.04013	3.54956	1.30019
H	-1.98033	-0.03340	-0.84344
H	-0.76447	-1.23331	-1.37047
H	3.24515	-0.13821	3.84107
H	-2.40279	-1.12163	1.95000
H	1.24621	-0.17068	4.01011
H	-1.17535	-0.64881	4.09465
H	6.57625	-0.49851	1.13796
H	5.68496	-0.27994	3.49503
C	-3.38014	-5.47136	-0.47031
H	-1.16195	-3.73999	-0.79928
H	6.21388	-0.81770	-1.10465
H	4.59303	-1.02164	-1.80520
H	5.28247	0.60668	-1.58293
H	-4.22822	-0.91115	-0.00109
H	-1.70942	2.21276	-0.45691
H	-4.10107	1.25640	-0.39985
H	-5.12545	1.80987	0.62339
H	-3.54991	3.30198	-1.26119
H	-4.74482	4.15771	-1.75168
H	-2.12688	2.19303	1.58008
H	-3.42473	1.39949	1.61441
H	-4.23811	3.20577	1.74315
H	-4.68626	3.89180	0.44881
H	-2.75682	1.57762	-2.21341
H	-0.89389	3.43524	0.08360
H	-4.06382	-5.73941	-1.28534
H	-2.39096	-5.90180	-0.66081
H	-3.77077	-5.85022	0.48207

1_{C5}⁺(I5-P)

Energy	= -2899.482822
Enthalpy 0K	= -2898.988467
Enthalpy 298K	= -2898.947038
Free Energy 298K	= -2899.063536
Nimag	= 0 (10.7610 cm ⁻¹)

C	-4.33672	-0.68846	0.00288
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N	-3.18624	-1.41383	-0.23137
C	-3.48937	-2.71356	-0.24309
N	-4.79169	-2.84593	-0.02397
C	-5.34494	-1.59321	0.13378
C	-1.85131	-0.87202	-0.42915
C	-1.07616	-0.67068	0.85473
N	0.25681	-0.50148	0.76405
C	0.96059	-0.33519	1.90218
C	0.35124	-0.29182	3.15611
C	-1.02104	-0.44674	3.24394
C	-1.74177	-0.65407	2.07800
C	2.43698	-0.30948	1.77447
N	2.93450	-0.72568	0.59036
C	4.25822	-0.93262	0.47484
C	5.12962	-0.61374	1.52474
C	4.63248	-0.07906	2.70011
C	3.25573	0.05447	2.83859
Mn	1.50561	-0.51200	-0.98172
C	1.90027	1.47979	-0.72023
O	2.98066	2.01640	-0.64528
C	4.83325	-1.52234	-0.77643
H	-6.40587	-1.45720	0.32465
C	2.64163	-0.42997	-2.37586
O	3.26190	-0.32016	-3.33644
C	1.27788	-2.33407	-1.13251
O	1.14233	-3.46527	-1.24763
C	0.31323	-0.10248	-2.24461
O	-0.35501	0.19235	-3.13888
O	0.80435	2.36623	-0.62526
O	-1.66051	2.54265	-1.80762
O	-0.90255	2.50579	1.69193
O	-3.36169	2.18835	0.35286
O	-2.11140	5.25326	-1.32155
O	-2.68423	4.63836	1.30847
H	-1.95794	0.08751	-0.95312
H	-1.31575	-1.56327	-1.08833
H	2.83234	0.43727	3.76528
H	-2.82058	-0.79704	2.12228
H	0.94479	-0.16663	4.05952
H	-1.52391	-0.42234	4.21177
H	6.19880	-0.78694	1.39476
H	5.30152	0.20657	3.51377
C	-5.52547	-4.10261	0.02693
H	-2.78513	-3.52541	-0.41085
H	5.76906	-2.04670	-0.54183
H	4.14237	-2.23388	-1.24486
H	5.07612	-0.73369	-1.50313
H	-4.30986	0.40033	0.08564
H	-0.75268	2.38906	-1.46906
H	-2.89870	2.30257	-0.49815
H	-3.37391	3.09976	0.72474
H	-1.93980	4.34519	-1.63581
H	-2.93686	5.50026	-1.75677
H	-0.24469	2.38516	0.98959
H	-1.70823	2.10318	1.31810
H	-1.89259	4.13192	1.57075
H	-2.45224	4.98397	0.42085

H	-1.68227	2.14770	-2.68918
H	1.18239	3.26550	-0.56249
H	-6.26617	-4.12346	-0.78214
H	-4.81998	-4.93151	-0.09463
H	-6.03111	-4.18593	0.99661

1_{C5}⁺(TS4)

Energy	=	-2899.45682004
Enthalpy 0K	=	-2898.967595
Enthalpy 298K	=	-2898.926658
Free Energy 298K	=	-2899.040988
Nimag	=	1 (-288.8837 cm ⁻¹)

C	-4.21479	-1.06759	0.15224
N	-2.98475	-1.60604	-0.16746
C	-3.10726	-2.93141	-0.26725
N	-4.36892	-3.26068	-0.02047
C	-5.08261	-2.11185	0.24552
C	-1.74360	-0.87713	-0.38489
C	-0.94228	-0.64648	0.87637
N	0.38445	-0.45130	0.76442
C	1.10700	-0.27219	1.89064
C	0.51423	-0.20727	3.14990
C	-0.85609	-0.37339	3.25935
C	-1.58855	-0.62247	2.11069
C	2.58278	-0.25304	1.74003
N	3.06087	-0.55955	0.51238
C	4.38277	-0.76828	0.35415
C	5.27127	-0.56604	1.41719
C	4.79682	-0.14731	2.64761
C	3.42505	-0.00924	2.82003
Mn	1.58932	-0.27514	-0.99680
C	1.89364	1.62727	-0.60140
O	2.48376	2.55665	-0.30824
C	4.93646	-1.22974	-0.95878
H	-6.14344	-2.13932	0.47846
C	2.68352	-0.09092	-2.43386
O	3.26169	0.06008	-3.41067
C	1.46466	-2.10887	-1.25800
O	1.41087	-3.23604	-1.41459
C	0.29835	0.11065	-2.23164
O	-0.40527	0.31267	-3.11029
O	-0.09251	2.58808	-1.05434
O	-2.40764	2.21829	-1.65215
O	-0.82105	2.57296	1.48752
O	-3.51818	1.80299	0.76496
O	-3.15790	4.77817	-1.24323
O	-2.92643	4.38417	1.48587
H	-1.99487	0.09005	-0.84882
H	-1.16034	-1.46445	-1.09902
H	3.02476	0.27994	3.78939
H	-2.66352	-0.78151	2.17281
H	1.11546	-0.05295	4.04327
H	-1.34567	-0.32916	4.23325
H	6.33607	-0.73726	1.25493
H	5.48044	0.04479	3.47628
C	-4.91894	-4.60880	-0.04755

H	-2.30583	-3.62277	-0.51795
H	5.89635	-1.73618	-0.79517
H	4.26083	-1.92938	-1.46630
H	5.13124	-0.37559	-1.62350
H	-4.33402	0.00426	0.32408
H	-1.32459	2.36551	-1.44145
H	-3.21386	1.92979	-0.16218
H	-3.54650	2.71922	1.11447
H	-2.89863	3.86203	-1.50232
H	-4.11060	4.79824	-1.39410
H	-0.47854	2.62639	0.55246
H	-1.60939	2.01551	1.38035
H	-2.05168	3.95074	1.56715
H	-2.96404	4.65067	0.54295
H	-2.49769	1.82197	-2.52503
H	0.15019	3.47814	-1.33645
H	-5.65134	-4.68707	-0.86072
H	-4.10326	-5.32097	-0.21239
H	-5.40533	-4.81884	0.91275

1_{C5}⁺(I6-P)

Energy	=	-2899.463952
Enthalpy 0K	=	-2898.971653
Enthalpy 298K	=	-2898.930321
Free Energy 298K	=	-2899.044768
Nimag	=	0 (19.5372 cm ⁻¹)

C	-4.21409	-0.96835	0.19880
N	-3.01586	-1.50201	-0.23109
C	-3.19519	-2.79585	-0.50428
N	-4.46237	-3.11006	-0.26378
C	-5.12086	-1.98319	0.17919
C	-1.75536	-0.79001	-0.39862
C	-0.91939	-0.73718	0.85864
N	0.41151	-0.56376	0.74716
C	1.15758	-0.54053	1.87303
C	0.58624	-0.61292	3.14125
C	-0.78637	-0.75733	3.25636
C	-1.54278	-0.84540	2.10110
C	2.63147	-0.52393	1.70280
N	3.09433	-0.62051	0.43505
C	4.41684	-0.78874	0.22736
C	5.31654	-0.77825	1.29922
C	4.85665	-0.59148	2.59048
C	3.48850	-0.48033	2.79862
Mn	1.58624	-0.16678	-0.99253
C	1.88407	1.62956	-0.42288
O	2.24980	2.64557	-0.08163
C	4.96234	-0.99281	-1.15169
H	-6.17448	-2.00365	0.44334
C	2.63700	0.16570	-2.44590
O	3.16875	0.41120	-3.42765
C	1.46335	-1.99028	-1.41867
O	1.40152	-3.09959	-1.65543
C	0.26073	0.29509	-2.17685
O	-0.44734	0.53896	-3.03772

O	-0.43634	3.00396	-1.30833
O	-2.82076	2.05534	-1.26415
O	-0.61896	2.39128	1.37816
O	-3.35163	1.74403	1.23184
O	-2.72702	4.62383	-0.88289
O	-2.60025	4.35668	1.83774
H	-2.00095	0.23634	-0.74527
H	-1.21296	-1.31474	-1.18932
H	3.10365	-0.36774	3.80956
H	-2.62022	-0.98192	2.16485
H	1.20219	-0.57915	4.03658
H	-1.25827	-0.81859	4.23807
H	6.37941	-0.91351	1.09623
H	5.54911	-0.55532	3.43319
C	-5.06662	-4.42214	-0.44661
H	-2.43067	-3.47558	-0.87424
H	5.96548	-1.43283	-1.08997
H	4.33139	-1.66394	-1.74788
H	5.06234	-0.03209	-1.67714
H	-4.28775	0.06942	0.52740
H	-1.31455	2.52804	-1.43932
H	-3.23639	1.86444	0.23672
H	-3.35892	2.66127	1.56721
H	-2.90822	3.65527	-1.10010
H	-3.39398	5.13555	-1.35297
H	-0.49720	2.61978	0.42971
H	-1.47942	1.92744	1.37685
H	-1.75317	3.87300	1.83927
H	-2.69550	4.59312	0.88971
H	-3.34204	1.71826	-1.99983
H	-0.73945	3.92286	-1.28279
H	-5.85760	-4.35572	-1.20399
H	-4.29535	-5.12573	-0.77767
H	-5.49174	-4.76018	0.50626

2c2(I6-R)

Energy	= -2938.862601
Enthalpy 0K	= -2938.343468
Enthalpy 298K	= -2938.300369
Free Energy 298K	= -2938.419603
Nimag	= 0 (22.8449 cm ⁻¹)

C	-4.07375	-1.62544	-0.33707
N	-2.79137	-1.93533	-0.09497
C	-2.72353	-3.18770	0.47935
C	-3.99831	-3.63703	0.59424
N	-4.82068	-2.65418	0.08360
C	-1.62570	-1.11795	-0.40099
C	-0.85960	-0.69644	0.83743
N	0.46505	-0.49108	0.70902
C	1.20053	-0.20183	1.84943
C	0.52974	0.03039	3.08822
C	-0.82544	-0.12069	3.17528
C	-1.54702	-0.52947	2.02885
C	2.61644	-0.24422	1.73247
N	3.13473	-0.61057	0.50282

C	4.45109	-0.88209	0.40042
C	5.33020	-0.71025	1.46781
C	4.83781	-0.21536	2.69313
C	3.49262	0.00728	2.83009
Mn	1.68383	-0.39970	-1.02099
C	1.92083	1.60563	-0.66326
O	2.94059	2.25718	-0.67284
C	5.01021	-1.38257	-0.90203
C	-6.27356	-2.73239	0.01712
C	2.79003	-0.16903	-2.41638
O	3.39173	0.03077	-3.37773
C	1.58781	-2.21693	-1.22660
O	1.53055	-3.35476	-1.36656
C	0.42973	-0.03824	-2.22620
O	-0.30585	0.23608	-3.07955
O	0.75942	2.36916	-0.38937
O	-1.73566	2.26790	-1.47260
O	-0.98487	2.82726	1.87454
O	-3.47020	2.18790	0.73119
O	-2.40615	4.96514	-1.54968
O	-2.80168	4.80909	1.18241
H	-1.96622	-0.23113	-0.94925
H	-0.98303	-1.70595	-1.06418
H	3.09252	0.36640	3.77784
H	-2.62322	-0.69156	2.07311
H	1.10219	0.31600	3.97024
H	-1.34554	0.06018	4.11841
H	6.38737	-0.94512	1.33738
H	5.51709	-0.02893	3.52869
H	-4.39597	-4.56708	0.98986
H	-1.77514	-3.64143	0.75314
H	-6.58236	-3.69029	0.44839
H	-6.60704	-2.68084	-1.02709
H	-6.72181	-1.91377	0.59394
H	5.97382	-1.88118	-0.73131
H	4.33267	-2.09521	-1.39100
H	5.19143	-0.55152	-1.59891
C	-4.57299	-0.37371	-0.94924
H	-0.82170	2.23045	-1.10979
H	-2.96028	2.14175	-0.09800
H	-3.49142	3.15273	0.91221
H	-2.14723	4.02708	-1.64002
H	-3.28259	5.00306	-1.95236
H	-0.29744	2.46537	1.29503
H	-1.76561	2.27999	1.67029
H	-1.99244	4.33471	1.45555
H	-2.64362	5.00532	0.23614
H	-1.69514	1.78942	-2.31123
H	1.05968	3.29505	-0.31170
H	-5.64464	-0.45383	-1.16273
H	-4.40649	0.47757	-0.27015
H	-4.04351	-0.17389	-1.89177

2c2(TS3)

Energy	= -2938.841499
Enthalpy 0K	= -2938.327444
Enthalpy 298K	= -2938.284610

Free Energy 298K = -2938.403659
Nimag = 1 (-209.3725 cm⁻¹)

C	-3.93002	-1.80225	-0.31071
N	-2.61723	-1.99274	-0.11133
C	-2.41184	-3.25307	0.41107
C	-3.63258	-3.82980	0.53939
N	-4.56093	-2.91474	0.08849
C	-1.53857	-1.05943	-0.41158
C	-0.75394	-0.66813	0.82436
N	0.56987	-0.45049	0.69534
C	1.31092	-0.19418	1.83786
C	0.64945	-0.00310	3.08741
C	-0.70486	-0.16315	3.17778
C	-1.42965	-0.54440	2.02620
C	2.72638	-0.21884	1.70752
N	3.23833	-0.49878	0.44978
C	4.56115	-0.75082	0.31871
C	5.44196	-0.64238	1.38818
C	4.95477	-0.23486	2.65004
C	3.61046	-0.03318	2.81129
Mn	1.76460	-0.22126	-1.02997
C	2.01076	1.68932	-0.56215
O	2.62218	2.61501	-0.28809
C	5.11541	-1.15131	-1.01901
C	-6.00073	-3.13307	0.05778
C	2.84019	0.03990	-2.45729
O	3.41020	0.23781	-3.43489
C	1.70240	-2.03863	-1.30447
O	1.68443	-3.17264	-1.44365
C	0.44812	0.16196	-2.21510
O	-0.29306	0.39526	-3.06054
O	0.01501	2.58231	-0.77504
O	-2.27795	2.07152	-1.45124
O	-0.91200	2.87181	1.68514
O	-3.56772	1.85448	0.97877
O	-3.29539	4.57316	-1.35088
O	-3.07370	4.53726	1.41507
H	-1.96855	-0.15974	-0.87326
H	-0.88888	-1.55325	-1.14063
H	3.21441	0.25448	3.78458
H	-2.50635	-0.70086	2.06716
H	1.22692	0.26106	3.97263
H	-1.22009	-0.01248	4.12890
H	6.50004	-0.85851	1.23577
H	5.63947	-0.10068	3.49087
H	-3.92619	-4.80843	0.90806
H	-1.41632	-3.62119	0.64300
H	-6.20435	-4.12286	0.47982
H	-6.36623	-3.09756	-0.97644
H	-6.50966	-2.37049	0.66048
H	6.09918	-1.62202	-0.89183
H	4.45967	-1.86169	-1.54035
H	5.25636	-0.27379	-1.66681
C	-4.57071	-0.58374	-0.85463
H	-1.24041	2.27013	-1.19910
H	-3.15414	1.86825	0.09216

H	-3.61793	2.80615	1.20543
H	-2.92401	3.66730	-1.47455
H	-4.24385	4.44731	-1.47504
H	-0.48444	2.77816	0.78752
H	-1.58190	2.17016	1.66966
H	-2.19615	4.11373	1.54562
H	-3.11276	4.68857	0.44861
H	-2.27914	1.65429	-2.31923
H	0.22442	3.46723	-1.09830
H	-5.62761	-0.77316	-1.07269
H	-4.49398	0.24170	-0.12868
H	-4.07305	-0.27196	-1.78329

2c2(I7-R)

Energy = -2938.849793
Enthalpy 0K = -2938.333746
Enthalpy 298K = -2938.290233
Free Energy 298K = -2938.410343
Nimag = 0 (22.1177 cm⁻¹)

C	-3.44880	-2.36192	-0.33086
N	-2.14344	-2.15955	-0.10122
C	-1.59773	-3.29290	0.46538
C	-2.60317	-4.19491	0.58977
N	-3.74313	-3.59938	0.09145
C	-1.37136	-0.96466	-0.43590
C	-0.60301	-0.45963	0.76628
N	0.72369	-0.24763	0.66300
C	1.43993	0.05239	1.80998
C	0.74757	0.31386	3.03013
C	-0.61357	0.18353	3.08570
C	-1.30968	-0.25772	1.93885
C	2.85679	0.01459	1.70174
N	3.38099	-0.25344	0.44499
C	4.70293	-0.51312	0.32106
C	5.57105	-0.43306	1.40281
C	5.07285	-0.04473	2.66723
C	3.72930	0.17092	2.81822
Mn	1.91921	0.08811	-1.02974
C	2.07307	1.90804	-0.50665
O	2.28515	2.98856	-0.23095
C	5.26539	-0.88541	-1.02099
C	-5.05871	-4.22210	0.04259
C	3.00706	0.41148	-2.44664
O	3.59015	0.64311	-3.40596
C	1.87398	-1.74378	-1.38290
O	1.86295	-2.86799	-1.56267
C	0.56595	0.51596	-2.17701
O	-0.20154	0.80481	-2.97518
O	-0.71803	2.65685	-0.39347
O	-2.88705	1.70151	-1.32016
O	-2.16664	2.93545	1.93106
O	-4.17078	1.23029	0.91948
O	-4.23198	3.90960	-1.56251
O	-4.62671	3.97297	1.14484
H	-2.05447	-0.17267	-0.78511

H	-0.70103	-1.24222	-1.25379
H	3.32238	0.43887	3.79295
H	-2.39214	-0.38852	1.94382
H	1.30493	0.62150	3.91456
H	-1.15425	0.40498	4.00814
H	6.62885	-0.65590	1.25862
H	5.74932	0.06228	3.51848
H	-2.61166	-5.20639	0.98546
H	-0.54539	-3.35222	0.72868
H	-4.97473	-5.23106	0.45947
H	-5.40664	-4.28830	-0.99614
H	-5.77365	-3.64172	0.63934
H	6.24322	-1.36914	-0.89768
H	4.60860	-1.57567	-1.56755
H	5.42147	0.00754	-1.64397
C	-4.39967	-1.39528	-0.92380
H	-1.54696	2.24478	-0.82899
H	-3.71383	1.33289	0.03519
H	-4.60367	2.10017	1.02763
H	-3.68166	3.06246	-1.51805
H	-5.07929	3.60434	-1.90647
H	-1.54892	2.91020	1.16702
H	-2.70812	2.14008	1.76667
H	-3.71048	3.83503	1.46016
H	-4.51137	4.06067	0.17200
H	-2.85525	1.24867	-2.16876
H	-0.57938	3.47976	-0.87505
H	-5.34513	-1.89248	-1.16755
H	-4.59164	-0.57062	-0.21763
H	-3.98123	-0.96082	-1.84140

2_{C2}⁺(I5-P)

Energy	= -2938.768350
Enthalpy 0K	= -2938.246170
Enthalpy 298K	= -2938.203240
Free Energy 298K	= -2938.322204
Nimag	= 0 (18.6061 cm ⁻¹)

C	-4.17591	-1.43181	-0.24902
N	-2.90749	-1.80695	-0.01701
C	-2.89819	-3.05652	0.57056
C	-4.19366	-3.43477	0.70447
N	-4.96891	-2.41553	0.19069
C	-1.70715	-1.06032	-0.35572
C	-0.93271	-0.61293	0.86553
N	0.39898	-0.45414	0.76083
C	1.09881	-0.13957	1.87108
C	0.47911	0.08830	3.09862
C	-0.89910	-0.01673	3.18965
C	-1.61224	-0.38965	2.06147
C	2.57591	-0.15051	1.74451
N	3.06736	-0.66133	0.59480
C	4.38829	-0.89267	0.49368
C	5.26480	-0.51237	1.51844
C	4.77554	0.10940	2.65373
C	3.40124	0.27462	2.78049

Mn	1.63421	-0.58320	-0.97980
C	1.99605	1.42993	-0.86856
O	3.06795	1.98844	-0.85559
C	4.95434	-1.57389	-0.71471
C	-6.42515	-2.42023	0.13690
C	2.75642	-0.57313	-2.38822
O	3.37031	-0.51668	-3.35741
C	1.45353	-2.41608	-1.00784
O	1.35883	-3.55672	-1.04940
C	0.40822	-0.26967	-2.23906
O	-0.29794	-0.02978	-3.12030
O	0.88608	2.30199	-0.82270
O	-1.69395	2.26793	-1.71614
O	-0.55970	2.82838	1.64074
O	-3.13581	2.31036	0.69048
O	-2.12733	5.02677	-1.63957
O	-2.37409	4.89960	1.10680
H	-1.99615	-0.18581	-0.95306
H	-1.08750	-1.71221	-0.97889
H	2.98406	0.72710	3.67803
H	-2.69430	-0.50796	2.10346
H	1.06572	0.33310	3.98190
H	-1.41014	0.17156	4.13499
H	6.33145	-0.70867	1.40125
H	5.44876	0.44007	3.44662
H	-4.63633	-4.33806	1.11423
H	-1.97143	-3.55786	0.83622
H	-6.77762	-3.36584	0.56114
H	-6.76318	-2.34151	-0.90392
H	-6.82590	-1.58551	0.72553
H	5.89561	-2.07392	-0.45086
H	4.26396	-2.32329	-1.12098
H	5.18455	-0.84250	-1.50273
C	-4.61087	-0.16207	-0.87207
H	-0.74695	2.17952	-1.47475
H	-2.75337	2.25399	-0.20415
H	-3.12710	3.27653	0.87145
H	-1.98097	4.07416	-1.79536
H	-3.00477	5.19229	-2.00629
H	0.00463	2.56381	0.89858
H	-1.40395	2.37320	1.45729
H	-1.56111	4.41868	1.35169
H	-2.25367	5.08058	0.15129
H	-1.79786	1.79886	-2.55434
H	1.24579	3.21022	-0.85659
H	-5.69634	-0.15869	-1.01816
H	-4.33306	0.69012	-0.23191
H	-4.12605	-0.03460	-1.85111

2_{C2}⁺(TS4)

Energy	= -2938.742611
Enthalpy 0K	= -2938.226020
Enthalpy 298K	= -2938.184314
Free Energy 298K	= -2938.299083
Nimag	= 1 (-265.6261 cm ⁻¹)

C	-4.02642	-1.64578	-0.20522
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N	-2.71064	-1.89610	-0.10482
C	-2.52271	-3.18796	0.34541
C	-3.75532	-3.72287	0.52690
N	-4.67277	-2.75259	0.18037
C	-1.61752	-0.98979	-0.42501
C	-0.83487	-0.58845	0.80663
N	0.49537	-0.41537	0.72050
C	1.18605	-0.15046	1.85022
C	0.55332	0.03873	3.07639
C	-0.82515	-0.07878	3.15161
C	-1.52378	-0.42237	2.00693
C	2.66561	-0.17669	1.74223
N	3.17096	-0.54800	0.54327
C	4.49342	-0.78312	0.43026
C	5.35571	-0.55749	1.50972
C	4.85511	-0.08616	2.71053
C	3.48288	0.08915	2.83666
Mn	1.73771	-0.34698	-1.01411
C	2.05918	1.57043	-0.73737
O	2.65844	2.51824	-0.53543
C	5.07423	-1.29652	-0.85091
C	-6.12004	-2.91690	0.23037
C	2.84722	-0.26998	-2.44908
O	3.43409	-0.19956	-3.43010
C	1.60556	-2.19366	-1.16265
O	1.55604	-3.32945	-1.23852
C	0.45618	0.00417	-2.27143
O	-0.24771	0.19521	-3.15199
O	0.03432	2.48670	-1.11305
O	-2.30991	2.06572	-1.55970
O	-0.51168	2.78296	1.45541
O	-3.26510	2.04076	1.00942
O	-2.97043	4.68498	-1.37923
O	-2.53346	4.67602	1.35120
H	-2.02111	-0.08704	-0.90883
H	-0.97611	-1.51395	-1.13887
H	3.06312	0.42165	3.78360
H	-2.60515	-0.54696	2.03219
H	1.12737	0.26342	3.97261
H	-1.34546	0.07720	4.09774
H	6.42117	-0.75331	1.38408
H	5.51857	0.12047	3.55200
H	-4.06454	-4.70735	0.86617
H	-1.52967	-3.60408	0.49164
H	-6.33550	-3.93284	0.57703
H	-6.54894	-2.77665	-0.76981
H	-6.55650	-2.19337	0.93022
H	6.04605	-1.76686	-0.65438
H	4.42319	-2.04094	-1.32623
H	5.25016	-0.47293	-1.55790
C	-4.64757	-0.37487	-0.63925
H	-1.22203	2.22674	-1.41302
H	-3.01307	2.00987	0.06317
H	-3.24133	2.99930	1.21328
H	-2.75094	3.73525	-1.53186
H	-3.93237	4.71158	-1.44855
H	-0.23710	2.71007	0.49928

H	-1.31734	2.23983	1.47555
H	-1.67872	4.20330	1.43343
H	-2.62923	4.81093	0.38519
H	-2.43949	1.68180	-2.43330
H	0.25591	3.34078	-1.50328
H	-5.73058	-0.49652	-0.74987
H	-4.44663	0.41811	0.09835
H	-4.23034	-0.05510	-1.60403

2_{C2}⁺(16-P)

Energy	=	-2938.749364
Enthalpy 0K	=	-2938.228614
Enthalpy 298K	=	-2938.185890
Free Energy 298K	=	-2938.302947
Nimag	=	0 (15.8031 cm ⁻¹)

C	-4.05040	-1.59776	-0.26394
N	-2.72596	-1.80716	-0.33908
C	-2.47038	-3.16035	-0.23791
C	-3.66890	-3.77785	-0.09710
N	-4.63486	-2.79343	-0.11595
C	-1.67563	-0.81047	-0.50933
C	-0.85921	-0.65075	0.75420
N	0.47768	-0.52353	0.68812
C	1.18083	-0.48216	1.84142
C	0.55702	-0.45565	3.08582
C	-0.82608	-0.52283	3.15152
C	-1.53745	-0.65364	1.97286
C	2.65749	-0.56215	1.72183
N	3.15819	-0.67590	0.46952
C	4.47637	-0.91366	0.30562
C	5.33565	-0.97279	1.40844
C	4.84000	-0.78602	2.68658
C	3.47473	-0.59354	2.84790
Mn	1.71954	-0.16122	-1.00643
C	2.08961	1.61766	-0.42229
O	2.50034	2.61304	-0.07122
C	5.05932	-1.11861	-1.05777
C	-6.06722	-3.03123	0.00563
C	2.81497	0.11936	-2.43733
O	3.37886	0.32351	-3.41065
C	1.53307	-1.97334	-1.45170
O	1.44006	-3.07727	-1.70383
C	0.43281	0.38274	-2.20098
O	-0.26107	0.68215	-3.05546
O	-0.19897	3.05103	-1.22384
O	-2.61321	2.18605	-1.22698
O	-0.37269	2.50184	1.45999
O	-3.11965	1.93888	1.31523
O	-2.43710	4.75197	-0.86675
O	-2.28183	4.54734	1.85457
H	-2.11465	0.16537	-0.79989
H	-1.05305	-1.17098	-1.33103
H	3.05871	-0.48180	3.84620
H	-2.62288	-0.73632	1.98526
H	1.13815	-0.39654	4.00330

H	-1.33856	-0.49416	4.11416
H	6.39605	-1.16409	1.24079
H	5.50176	-0.81012	3.55401
H	-3.92413	-4.82831	0.00929
H	-1.45894	-3.55452	-0.27991
H	-6.22480	-4.10896	0.11961
H	-6.58499	-2.68207	-0.89659
H	-6.46140	-2.51201	0.88818
H	6.05044	-1.58065	-0.97036
H	4.43245	-1.77152	-1.67846
H	5.19454	-0.15558	-1.57118
C	-4.73575	-0.28835	-0.31133
H	-1.09644	2.60120	-1.34458
H	-3.02961	2.00435	0.32011
H	-3.09562	2.87098	1.60496
H	-2.64544	3.78266	-1.06288
H	-3.10516	5.26988	-1.32833
H	-0.24596	2.71151	0.50735
H	-1.24618	2.06201	1.46415
H	-1.45675	4.02651	1.86869
H	-2.37311	4.75936	0.90022
H	-3.07382	1.91576	-2.02759
H	-0.46678	3.98084	-1.23741
H	-5.82127	-0.42072	-0.25123
H	-4.39871	0.35191	0.51896
H	-4.49089	0.23684	-1.24457

2_{C5}(I5-R)

Energy	=	-2557.048705
Enthalpy 0K	=	-2556.659467
Enthalpy 298K	=	-2556.628753
Free Energy 298K	=	-2556.721329
Nimag	=	0 (21.9072 cm ⁻¹)

C	-4.38496	0.01572	0.51340
N	-3.09220	0.27588	0.27049
C	-2.85982	0.23387	-1.08912
C	-4.05124	-0.05542	-1.67378
N	-4.98379	-0.18686	-0.66587
C	-2.08705	0.54771	1.30147
C	-1.03140	1.50531	0.80186
N	0.18617	1.04360	0.47317
C	1.15263	1.96411	0.08960
C	0.79275	3.33359	-0.10856
C	-0.47136	3.76724	0.18419
C	-1.40745	2.83887	0.69648
C	2.48502	1.48865	-0.04370
N	2.70491	0.15065	0.22790
C	3.97164	-0.29909	0.32214
C	5.07180	0.51357	0.05269
C	4.85974	1.84823	-0.34845
C	3.58004	2.33725	-0.38715
Mn	0.89122	-0.94363	0.19389
C	0.82603	-0.47158	-1.80656
O	1.92655	-0.81559	-2.53149
C	4.22996	-1.72451	0.72343

C	-6.39467	-0.48568	-0.86477
C	1.56503	-2.54077	-0.25124
O	1.87194	-3.60618	-0.57066
C	0.97475	-1.24180	1.99400
O	1.01516	-1.45548	3.12313
C	-0.66293	-1.80242	-0.00057
O	-1.59606	-2.46599	-0.15893
O	-0.06715	0.09209	-2.42853
H	-1.65285	-0.39601	1.64805
H	-2.60668	1.00783	2.15030
H	3.40203	3.37486	-0.66790
H	-2.41467	3.14209	0.98684
H	1.53296	4.04029	-0.48296
H	-0.74688	4.81460	0.04072
H	6.07875	0.10403	0.14301
H	5.70535	2.49091	-0.60615
H	-4.31871	-0.18644	-2.71830
H	-1.86054	0.36525	-1.52083
H	-7.01303	0.33901	-0.48812
H	-6.65964	-1.41696	-0.34819
H	-6.56896	-0.60734	-1.93903
H	5.26293	-1.83370	1.08049
H	3.55002	-2.05385	1.52031
H	4.10490	-2.40500	-0.13094
C	-5.02369	-0.02936	1.84931
H	1.76170	-0.50782	-3.44136
H	-6.07127	-0.33902	1.76695
H	-4.49542	-0.73993	2.50090
H	-4.98833	0.96335	2.32299

2_{C5}(I6-R)

Energy	=	-2938.865499
Enthalpy 0K	=	-2938.346485
Enthalpy 298K	=	-2938.303286
Free Energy 298K	=	-2938.422685
Nimag	=	0 (21.0076 cm ⁻¹)

C	3.41853	-0.34247	2.87369
C	2.53587	-0.43277	1.75609
N	3.04223	-0.67288	0.49177
C	4.34664	-0.98710	0.35761
C	5.22831	-0.97588	1.43662
C	4.75394	-0.60233	2.71051
C	1.12256	-0.35103	1.88296
N	0.37255	-0.44166	0.71903
C	-0.96075	-0.60347	0.83043
C	-1.63254	-0.61574	2.04159
C	-0.89077	-0.40897	3.22931
C	0.46611	-0.27718	3.14965
C	-1.74763	-0.73712	-0.45737
N	-3.05157	-1.35716	-0.28490
C	-4.24139	-0.69012	-0.08105
C	-5.20198	-1.64316	0.03937
N	-4.58172	-2.86893	-0.09246
C	-3.27178	-2.68012	-0.28500
C	-5.25489	-4.15927	-0.03886

Mn	1.60346	-0.23739	-0.99901
C	0.39558	0.26832	-2.20008
O	-0.28741	0.62147	-3.06850
C	4.89245	-1.36180	-0.99193
C	1.91913	1.70799	-0.43783
O	2.96690	2.30099	-0.32009
C	2.73559	0.08975	-2.35264
O	3.35532	0.37161	-3.28150
C	1.43106	-2.02210	-1.37825
O	1.33472	-3.13716	-1.63248
O	0.78012	2.50502	-0.15582
O	-1.57617	2.75340	-1.51798
O	-1.24185	2.61850	1.86735
O	-2.26191	5.42295	-1.18629
O	-3.62170	2.30366	0.31190
O	-2.97536	4.72635	1.39651
H	-6.27160	-1.56084	0.20960
H	-1.91281	0.25571	-0.89660
H	-1.18941	-1.33426	-1.18534
H	3.03126	-0.07419	3.85612
H	-2.71339	-0.74398	2.07913
H	1.05306	-0.14445	4.05797
H	-1.39870	-0.36421	4.19516
H	6.27490	-1.23940	1.27845
H	5.43807	-0.53787	3.56030
C	-2.23993	-3.72383	-0.48207
H	5.82857	-1.92415	-0.87478
H	4.18653	-1.97940	-1.56276
H	5.12266	-0.46653	-1.58732
H	-4.27602	0.39859	-0.00552
H	-0.71958	2.60470	-1.05867
H	-3.00683	2.43379	-0.43367
H	-3.63812	3.19250	0.73063
H	-1.96994	4.52363	-1.43245
H	-3.08323	5.54257	-1.67911
H	-0.47523	2.37165	1.32651
H	-1.97781	2.12664	1.46416
H	-2.19959	4.19382	1.65969
H	-2.71063	5.10501	0.53286
H	-1.46996	2.34341	-2.38675
H	1.12357	3.39550	0.05028
H	-5.09718	-4.70494	-0.97762
H	-4.87263	-4.74847	0.80448
H	-6.32633	-3.98072	0.10099
H	-2.64256	-4.71462	-0.24333
H	-1.89646	-3.72599	-1.52768
H	-1.37350	-3.52834	0.16500

2_{C5}(TS3)

Energy	=	-2938.844435
Enthalpy 0K	=	-2938.330007
Enthalpy 298K	=	-2938.287276
Free Energy 298K	=	-2938.405651
Nimag	=	1 (-201.0375 cm ⁻¹)

C	3.53755	-0.25821	2.84164
C	2.64369	-0.31818	1.73129

N	3.14344	-0.46812	0.44756
C	4.46259	-0.72251	0.28168
C	5.35133	-0.73676	1.34992
C	4.87814	-0.45652	2.65057
C	1.23013	-0.29074	1.87832
N	0.46856	-0.38965	0.72415
C	-0.85983	-0.58691	0.84926
C	-1.51190	-0.62313	2.07002
C	-0.76253	-0.40656	3.24856
C	0.59073	-0.24826	3.15374
C	-1.67121	-0.74947	-0.41921
N	-2.86877	-1.55701	-0.23762
C	-4.13815	-1.08388	0.02261
C	-4.94381	-2.17385	0.11837
N	-4.15341	-3.28681	-0.08328
C	-2.89215	-2.89697	-0.29514
C	-4.62649	-4.66394	-0.07496
Mn	1.66170	-0.03807	-0.98920
C	0.36660	0.44195	-2.16152
O	-0.34412	0.73152	-3.01600
C	5.00690	-0.99309	-1.09228
C	1.91994	1.81921	-0.34978
O	2.52636	2.70221	0.04724
C	2.74051	0.34309	-2.38682
O	3.30806	0.62968	-3.34349
C	1.59325	-1.82404	-1.42840
O	1.58923	-2.93729	-1.68627
O	-0.04266	2.78252	-0.61844
O	-2.28899	2.48574	-1.54605
O	-1.20315	2.68922	1.74987
O	-3.27121	4.96906	-1.15377
O	-3.80846	1.86427	0.61379
O	-3.33503	4.40126	1.56795
H	-6.00828	-2.25940	0.31697
H	-1.98304	0.23500	-0.79806
H	-1.07115	-1.23522	-1.19407
H	3.15229	-0.06670	3.84234
H	-2.58865	-0.77756	2.11843
H	1.18645	-0.10800	4.05484
H	-1.25927	-0.38003	4.22081
H	6.40533	-0.94944	1.16757
H	5.56971	-0.41673	3.49550
C	-1.72432	-3.76636	-0.56657
H	5.98619	-1.48371	-1.01642
H	4.34367	-1.64345	-1.67827
H	5.15554	-0.05738	-1.65051
H	-4.32480	-0.01681	0.16306
H	-1.27426	2.59614	-1.18583
H	-3.33042	2.05086	-0.22293
H	-3.86223	2.74933	1.03141
H	-2.90021	4.09092	-1.40625
H	-4.20156	4.90051	-1.39987
H	-0.68703	2.73828	0.89533
H	-1.87033	2.01524	1.54852
H	-2.46894	3.95745	1.70661
H	-3.27950	4.72898	0.64687
H	-2.23337	2.09565	-2.42470

H	0.21105	3.70052	-0.77437
H	-4.43723	-5.13363	-1.04845
H	-4.12158	-5.23043	0.71779
H	-5.70395	-4.65243	0.11918
H	-1.97067	-4.81747	-0.37998
H	-1.40971	-3.66084	-1.61593
H	-0.88127	-3.48153	0.07843

2_{C5}(I7-R)

Energy	=	-2938.852710
Enthalpy 0K	=	-2938.336382
Enthalpy 298K	=	-2938.292913
Free Energy 298K	=	-2938.414128
Nimag	=	0 (15.3536 cm ⁻¹)

C	3.68755	-0.20031	2.84285
C	2.80792	-0.17521	1.72059
N	3.32750	-0.14259	0.43492
C	4.66317	-0.27779	0.25758
C	5.54118	-0.36633	1.33007
C	5.03931	-0.28889	2.64860
C	1.39359	-0.24701	1.84517
N	0.66180	-0.33428	0.67155
C	-0.65112	-0.63692	0.74983
C	-1.32328	-0.76267	1.95277
C	-0.61900	-0.53921	3.15658
C	0.72558	-0.29705	3.10533
C	-1.42949	-0.83749	-0.53558
N	-2.45982	-1.86140	-0.40606
C	-3.80464	-1.63725	-0.19691
C	-4.39306	-2.85998	-0.12170
N	-3.40044	-3.80356	-0.28472
C	-2.22857	-3.18192	-0.45313
C	-3.60405	-5.24522	-0.28212
Mn	1.81915	0.35780	-0.94417
C	0.45594	0.87266	-2.03593
O	-0.29794	1.23574	-2.81753
C	5.23468	-0.31726	-1.13081
C	1.86949	2.06386	-0.10965
O	2.03509	3.08526	0.35680
C	2.86460	0.99836	-2.28343
O	3.40771	1.43819	-3.19179
C	1.91616	-1.38387	-1.60850
O	2.01966	-2.45182	-1.98921
O	-0.93443	2.55727	0.31098
O	-2.82346	2.01867	-1.30124
O	-2.94104	2.06484	2.14844
O	-3.73164	4.45204	-1.11134
O	-4.79389	1.24188	0.17556
O	-4.92927	3.80324	1.26859
H	-5.42991	-3.14355	0.03428
H	-1.93406	0.10171	-0.82830
H	-0.76646	-1.14602	-1.35043
H	3.28190	-0.17059	3.85335
H	-2.38773	-0.99165	1.96810
H	1.28890	-0.14742	4.02574

H	-1.14202	-0.57183	4.11463
H	6.60901	-0.47934	1.13985
H	5.72018	-0.31808	3.50251
C	-0.90985	-3.81797	-0.67375
H	6.25161	-0.73000	-1.10555
H	4.63388	-0.93500	-1.81171
H	5.30687	0.69512	-1.55456
H	-4.22180	-0.63296	-0.09014
H	-1.62953	2.32753	-0.40048
H	-4.08579	1.50875	-0.48798
H	-5.11266	2.10181	0.51096
H	-3.34957	3.52751	-1.24176
H	-4.45738	4.48817	-1.74482
H	-2.14004	2.23565	1.60660
H	-3.48896	1.53031	1.54226
H	-4.17756	3.38103	1.73105
H	-4.51208	4.14492	0.44615
H	-2.62633	1.77586	-2.21116
H	-0.81748	3.51004	0.22502
H	-3.28742	-5.67215	-1.24207
H	-3.03486	-5.70422	0.53624
H	-4.67142	-5.43975	-0.13342
H	-0.95612	-4.89124	-0.45748
H	-0.59647	-3.68496	-1.72031
H	-0.15176	-3.35962	-0.02336

2_{C5}⁺(I8)

Energy	=	-2481.163028
Enthalpy 0K	=	-2480.788955
Enthalpy 298K	=	-2480.759371
Free Energy 298K	=	-2480.849322
Nimag	=	0 (26.1107 cm ⁻¹)

C	3.82385	1.93214	-0.58423
C	2.63181	1.24311	-0.21522
N	2.66466	-0.12124	0.01442
C	3.86093	-0.75659	0.04910
C	5.04877	-0.09828	-0.24380
C	5.01833	1.26352	-0.60720
C	1.39254	1.90652	-0.00212
N	0.31251	1.12981	0.40013
C	-0.80542	1.76572	0.82666
C	-0.95428	3.13912	0.80095
C	0.09108	3.93603	0.27143
C	1.24646	3.32250	-0.12025
C	-1.98555	0.97140	1.32106
N	-2.92461	0.65600	0.23699
C	-2.74474	0.88785	-1.11029
C	-3.83379	0.37907	-1.74334
N	-4.65667	-0.15088	-0.77445
C	-4.09267	0.02557	0.42594
C	-4.61379	-0.43518	1.73112
C	-5.93060	-0.81168	-1.02373
Mn	0.71428	-0.91367	0.05426
C	-0.97374	-1.57858	0.03818
O	-1.97468	-2.13696	-0.00520
C	3.93384	-2.21364	0.40538

C	0.61679	-0.51385	-1.78502
O	0.56128	-0.28353	-2.89560
C	1.14197	-2.64564	-0.32323
O	1.26483	-3.75378	-0.58061
C	0.90395	-1.12051	1.91163
O	1.03214	-1.19613	3.03773
H	-4.09743	0.35223	-2.79667
H	-1.68192	0.03633	1.80918
H	-2.52946	1.56641	2.06570
H	3.78842	2.99182	-0.83203
H	-1.88078	3.58565	1.16317
H	-1.86802	1.39308	-1.50353
H	2.07082	3.92014	-0.50724
H	-0.02013	5.01924	0.19275
H	5.98925	-0.64839	-0.20077
H	5.93826	1.78414	-0.88285
H	4.95729	-2.47119	0.70750
H	3.26160	-2.47374	1.23404
H	3.68605	-2.84583	-0.45951
H	-6.73682	-0.28481	-0.49813
H	-6.12285	-0.78456	-2.10130
H	-5.88295	-1.85500	-0.68728
H	-5.66280	-0.73962	1.64578
H	-4.02463	-1.29447	2.08745
H	-4.53503	0.36615	2.47878

2_{C5}⁺(I5-P)

Energy	= -2938.770832
Enthalpy 0K	= -2938.248227
Enthalpy 298K	= -2938.205393
Free Energy 298K	= -2938.323608
Nimag	= 0 (17.8131 cm ⁻¹)

C	3.33703	-0.09274	2.84808
C	2.49476	-0.37312	1.77693
N	2.96234	-0.78831	0.58049
C	4.26984	-1.07651	0.45472
C	5.16190	-0.84294	1.50972
C	4.70201	-0.31056	2.70128
C	1.02001	-0.30505	1.90801
N	0.30592	-0.40917	0.76859
C	-1.03449	-0.49090	0.85974
C	-1.69760	-0.44360	2.08381
C	-0.96460	-0.30041	3.25135
C	0.41535	-0.23825	3.16308
C	-1.83129	-0.62186	-0.41998
N	-3.16845	-1.15090	-0.21887
C	-4.32000	-0.40689	-0.05593
C	-5.33446	-1.29733	0.09228
N	-4.78552	-2.56150	0.01718
C	-3.46635	-2.45924	-0.16839
C	-5.53395	-3.80763	0.11676
Mn	1.54385	-0.44920	-0.97921
C	0.37209	0.04750	-2.22981
O	-0.28221	0.38762	-3.11821
C	4.80406	-1.66847	-0.81360

C	2.03715	1.51223	-0.66095
O	3.14264	1.98697	-0.54588
C	2.68547	-0.37590	-2.36907
O	3.31457	-0.26120	-3.32331
C	1.23337	-2.25277	-1.19388
O	1.06221	-3.37238	-1.36391
O	0.98882	2.45576	-0.57532
O	-1.45688	2.79213	-1.77849
O	-0.77158	2.65544	1.69909
O	-3.22855	2.43997	0.32470
O	-1.86745	5.50224	-1.26516
O	-2.48530	4.84789	1.34574
H	-6.39916	-1.14702	0.24665
H	-1.92983	0.36274	-0.89699
H	-1.31597	-1.28346	-1.12326
H	2.94028	0.29041	3.78638
H	-2.78417	-0.51031	2.12386
H	1.01741	-0.16729	4.06687
H	-1.46379	-0.25307	4.22023
H	6.21766	-1.08010	1.37144
H	5.38941	-0.09127	3.52019
C	-2.49447	-3.56730	-0.30961
H	5.70585	-2.25563	-0.59530
H	4.06990	-2.32386	-1.29808
H	5.09455	-0.87826	-1.52084
H	-4.28506	0.68297	-0.02119
H	-0.56301	2.58875	-1.42974
H	-2.74072	2.56393	-0.51084
H	-3.21878	3.34068	0.72124
H	-1.69557	4.59646	-1.58597
H	-2.68667	5.75594	-1.70828
H	-0.10279	2.51019	1.01199
H	-1.58430	2.28607	1.30696
H	-1.71037	4.31316	1.60137
H	-2.23686	5.20655	0.46785
H	-1.48453	2.40694	-2.66414
H	1.41447	3.33090	-0.48363
H	-5.39130	-4.40420	-0.79284
H	-5.20079	-4.37651	0.99414
H	-6.59501	-3.56018	0.22569
H	-2.95119	-4.52087	-0.02223
H	-2.15266	-3.64119	-1.35333
H	-1.61841	-3.38845	0.32922

2_{C5}⁺(TS4)

Energy	= -2938.744779
Enthalpy 0K	= -2938.227826
Enthalpy 298K	= -2938.185314
Free Energy 298K	= -2938.302688
Nimag	= 1 (-272.1155 cm ⁻¹)

C	3.46647	-0.17182	2.85273
C	2.62334	-0.30769	1.75391
N	3.09736	-0.56278	0.51295
C	4.41222	-0.81224	0.34956
C	5.29910	-0.71532	1.42821
C	4.83192	-0.35970	2.68103

C	1.14725	-0.25803	1.89643
N	0.42360	-0.37543	0.76226
C	-0.91161	-0.50421	0.86440
C	-1.56491	-0.46618	2.09492
C	-0.82893	-0.27700	3.25201
C	0.54936	-0.18567	3.15284
C	-1.72708	-0.68150	-0.39616
N	-2.97084	-1.40187	-0.17824
C	-4.20703	-0.84000	0.07191
C	-5.08084	-1.87175	0.19639
N	-4.36573	-3.03906	0.01948
C	-3.08311	-2.74023	-0.20469
C	-4.92926	-4.38191	0.06680
Mn	1.63848	-0.18581	-0.98936
C	0.36066	0.26926	-2.21544
O	-0.33280	0.51268	-3.09172
C	4.96110	-1.20427	-0.98745
C	1.98675	1.69250	-0.52599
O	2.59178	2.59669	-0.18830
C	2.73618	0.01888	-2.42104
O	3.31306	0.18459	-3.39632
C	1.48870	-2.00774	-1.31685
O	1.44707	-3.12758	-1.52325
O	0.02885	2.72065	-0.98230
O	-2.28857	2.44956	-1.63076
O	-0.75852	2.69446	1.54047
O	-3.46799	2.02776	0.75350
O	-2.97449	5.02254	-1.19600
O	-2.79978	4.57720	1.53088
H	-6.14772	-1.88247	0.40015
H	-1.97298	0.30279	-0.82493
H	-1.15665	-1.24373	-1.13966
H	3.07241	0.07112	3.83709
H	-2.64806	-0.56501	2.14327
H	1.15085	-0.07865	4.05261
H	-1.32157	-0.22063	4.22372
H	6.35744	-0.91885	1.26115
H	5.51549	-0.25352	3.52508
C	-1.97405	-3.68876	-0.45644
H	5.92210	-1.71715	-0.85458
H	4.28451	-1.87817	-1.52780
H	5.15147	-0.31588	-1.60698
H	-4.32333	0.23763	0.19281
H	-1.20785	2.55218	-1.39630
H	-3.13765	2.16179	-0.16330
H	-3.47266	2.93784	1.11898
H	-2.73483	4.10425	-1.46589
H	-3.92432	5.06860	-1.35887
H	-0.39054	2.74835	0.61492
H	-1.56384	2.16821	1.40543
H	-1.94256	4.11114	1.61875
H	-2.81277	4.85942	0.59202
H	-2.37261	2.06248	-2.50837
H	0.30757	3.60663	-1.24314
H	-4.77623	-4.88748	-0.89485
H	-4.45716	-4.95850	0.87225
H	-6.00245	-4.29462	0.26474

H	-2.29753	-4.72066	-0.28205
H	-1.63038	-3.59946	-1.49825
H	-1.12730	-3.46642	0.20881

2_{C5}⁺(16-P)

Energy	=	-2938.751822
Enthalpy 0K	=	-2938.231381
Enthalpy 298K	=	-2938.188590
Free Energy 298K	=	-2938.305407
Nimag	=	0 (20.5365 cm ⁻¹)

C	3.51943	-0.52213	2.82476
C	2.66355	-0.51928	1.72715
N	3.12141	-0.64672	0.46030
C	4.43471	-0.88174	0.25592
C	5.33168	-0.91570	1.32952
C	4.87984	-0.70655	2.62017
C	1.19157	-0.44706	1.89810
N	0.44418	-0.45881	0.77288
C	-0.89356	-0.55499	0.88920
C	-1.52186	-0.58627	2.13386
C	-0.76079	-0.50428	3.28624
C	0.61823	-0.44666	3.16746
C	-1.73886	-0.60653	-0.36135
N	-3.01531	-1.27711	-0.16551
C	-4.21001	-0.67014	0.16751
C	-5.14341	-1.65499	0.21604
N	-4.50559	-2.84020	-0.08918
C	-3.21116	-2.59710	-0.31500
C	-5.15022	-4.14514	-0.16109
Mn	1.63268	-0.14680	-0.97491
C	0.32777	0.35850	-2.16541
O	-0.36768	0.62306	-3.03038
C	4.97403	-1.11290	-1.12137
C	2.01054	1.64306	-0.43226
O	2.41595	2.64727	-0.10128
C	2.69350	0.10913	-2.43651
O	3.23160	0.30410	-3.42611
C	1.43677	-1.96715	-1.38322
O	1.35215	-3.07424	-1.62386
O	-0.25001	3.10616	-1.34331
O	-2.67290	2.26117	-1.30618
O	-0.47474	2.56691	1.35179
O	-3.23259	2.03393	1.19504
O	-2.47580	4.83223	-0.99404
O	-2.37024	4.63144	1.73459
H	-6.20441	-1.62102	0.44609
H	-1.95696	0.42032	-0.72473
H	-1.21329	-1.15261	-1.14893
H	3.13799	-0.39059	3.83441
H	-2.60618	-0.65185	2.19718
H	1.23592	-0.41984	4.06198
H	-1.23407	-0.50310	4.26919
H	6.38675	-1.10439	1.12877
H	5.57142	-0.70769	3.46438
C	-2.16909	-3.58340	-0.68042

H	5.96407	-1.58096	-1.05602
H	4.32478	-1.77189	-1.71164
H	5.10116	-0.15976	-1.65465
H	-4.26088	0.39260	0.40055
H	-1.14779	2.66628	-1.47138
H	-3.10405	2.12365	0.19941
H	-3.20234	2.95952	1.50440
H	-2.69549	3.86633	-1.18665
H	-3.12504	5.35773	-1.47361
H	-0.33671	2.76740	0.39915
H	-1.35464	2.14098	1.35450
H	-1.54697	4.10869	1.75677
H	-2.44972	4.84340	0.77934
H	-3.19331	1.92483	-2.04276
H	-0.51006	4.03839	-1.34991
H	-5.04309	-4.56170	-1.17046
H	-4.70303	-4.82592	0.57427
H	-6.21329	-4.01397	0.06601
H	-2.55484	-4.60491	-0.59174
H	-1.84002	-3.42189	-1.71815
H	-1.29798	-3.47652	-0.01829

2_{C5}²⁺(I7-P)

Energy	=	-2481.054865
Enthalpy 0K	=	-2480.676807
Enthalpy 298K	=	-2480.647958
Free Energy 298K	=	-2480.734663
Nimag	=	0 (23.8823 cm ⁻¹)

C	3.78808	1.98774	-0.57689
C	2.65645	1.26830	-0.20630
N	2.69221	-0.06873	0.00403
C	3.87845	-0.70990	-0.04226
C	5.04890	-0.02472	-0.38994
C	5.00300	1.32418	-0.68900
C	1.35817	1.94366	0.04102
N	0.31885	1.15916	0.40032
C	-0.83549	1.75217	0.76998
C	-1.00228	3.13436	0.72582
C	0.04104	3.93799	0.29383
C	1.24122	3.33272	-0.03734
C	-2.01175	0.94797	1.25812
N	-2.94606	0.62211	0.17853
C	-2.75122	0.79360	-1.17637
C	-3.85450	0.29859	-1.79454
N	-4.69970	-0.16367	-0.81034
C	-4.13731	0.03909	0.38575
C	-4.68636	-0.33166	1.70808
C	-6.00006	-0.77957	-1.04230
Mn	0.74776	-0.91356	0.10487
C	-0.94154	-1.60531	0.11407
O	-1.93460	-2.17107	0.07949
C	3.98787	-2.16868	0.27553
C	0.62787	-0.62019	-1.75658
O	0.57337	-0.46558	-2.87859
C	1.18092	-2.66968	-0.20218

O	1.29758	-3.78771	-0.39801
C	0.96124	-1.09120	1.97618
O	1.10086	-1.17428	3.09794
H	-4.11441	0.23998	-2.84755
H	-1.70024	0.02457	1.76114
H	-2.55559	1.54609	2.00045
H	3.73980	3.05608	-0.77375
H	-1.95643	3.56389	1.03284
H	-1.85973	1.25784	-1.58623
H	2.08401	3.94758	-0.34331
H	-0.07007	5.02160	0.23613
H	5.98981	-0.57469	-0.42386
H	5.90361	1.86526	-0.98377
H	5.03001	-2.41440	0.51480
H	3.36782	-2.45472	1.13443
H	3.70579	-2.77862	-0.59477
H	-6.78479	-0.19660	-0.54446
H	-6.18413	-0.78888	-2.12146
H	-5.99883	-1.80897	-0.66284
H	-5.70341	-0.72627	1.61074
H	-4.05160	-1.09776	2.17825
H	-4.70661	0.54715	2.36891

3_{C2}(I5-R)

Energy	=	-2635.616851
Enthalpy 0K	=	-2635.171397
Enthalpy 298K	=	-2635.137441
Free Energy 298K	=	-2635.237241
Nimag	=	0 (16.9206 cm ⁻¹)

C	-3.65254	0.04380	1.18981
N	-3.15687	-0.29107	-0.00889
C	-4.18649	-0.37497	-0.93802
C	-5.33964	-0.08859	-0.26362
N	-4.97655	0.16724	1.05261
C	-1.74592	-0.48390	-0.30196
C	-0.98795	0.81308	-0.49155
N	0.35005	0.75022	-0.38984
C	1.07365	1.93162	-0.44035
C	0.41240	3.15581	-0.76969
C	-0.94520	3.18090	-0.93253
C	-1.68335	1.98631	-0.75206
Mn	1.65371	-0.93076	-0.37074
C	1.12515	-1.27244	1.58020
O	1.81665	-2.26208	2.22784
C	2.44938	1.86741	-0.08425
N	2.95388	0.62920	0.27942
C	4.19268	0.55938	0.80972
C	5.01682	1.67727	0.92888
C	4.56000	2.92505	0.45797
C	3.28691	3.02267	-0.03894
C	4.72619	-0.76317	1.28243
C	-3.94422	-0.70991	-2.36654
C	-5.91585	0.52131	2.10218
C	-6.75518	-0.02917	-0.71385
C	-2.87347	0.27995	2.42859

C	2.83947	-2.27490	-0.38355
O	3.51153	-3.20713	-0.48295
C	0.52844	-2.22239	-0.86638
O	-0.09873	-3.14444	-1.17342
C	2.07018	-0.51797	-2.10667
O	2.31522	-0.31290	-3.21006
O	0.26625	-0.71209	2.24760
H	0.98677	4.07563	-0.87562
H	-1.45734	4.11340	-1.18093
H	2.91103	3.98463	-0.38561
H	6.00912	1.56823	1.36862
H	-2.77027	1.98658	-0.82905
H	5.20567	3.80575	0.50231
H	3.94961	-1.35539	1.78258
H	5.11399	-1.35201	0.43777
H	5.56078	-0.60475	1.97902
H	-1.68642	-1.09892	-1.20673
H	-1.29122	-1.04604	0.52066
H	-3.22857	-0.00759	-2.82046
H	-3.54121	-1.72832	-2.47824
H	-4.88392	-0.65239	-2.92950
H	-7.18387	0.97083	-0.54649
H	-6.82146	-0.25654	-1.78479
H	-7.37605	-0.75717	-0.16935
H	-1.81524	0.02240	2.28720
H	-2.94176	1.34014	2.71590
H	-3.27490	-0.32548	3.25393
H	-6.44017	1.44687	1.83093
H	-6.64636	-0.28755	2.23327
H	-5.37709	0.67651	3.04203
H	1.46639	-2.29276	3.13705

3_{C2}(I6-R)

Energy	=	-3017.432212
Enthalpy 0K	=	-3016.857550
Enthalpy 298K	=	-3016.811034
Free Energy 298K	=	-3016.937344
Nimag	=	0 (20.7222 cm ⁻¹)

N	3.13149	-0.97264	0.50934
C	2.62736	-0.59841	1.74292
C	3.47894	-0.58394	2.88780
C	4.76761	-1.03767	2.78487
C	5.22438	-1.53041	1.54462
C	4.38279	-1.46921	0.43588
C	1.23897	-0.30199	1.81097
N	0.51830	-0.38422	0.62848
C	-0.82571	-0.34044	0.69466
C	-1.52574	-0.10591	1.86693
C	-0.79736	0.09196	3.06306
C	0.56450	-0.01849	3.03710
C	-1.60418	-0.57291	-0.58658
N	-2.88501	-1.22179	-0.35722
C	-3.01850	-2.53578	0.07459
C	-4.35828	-2.77069	0.18590
N	-5.00255	-1.59441	-0.18287

C	-4.09559	-0.66992	-0.52009
C	-1.84668	-3.41888	0.31518
C	-4.34953	0.71218	-0.99204
C	-6.44913	-1.44953	-0.21900
C	-5.10407	-3.98859	0.59996
Mn	1.81262	-0.40772	-1.04595
C	3.00856	-0.27831	-2.37951
O	3.68279	-0.12055	-3.29940
C	4.91061	-1.97126	-0.87893
C	1.43161	-2.15994	-1.40813
O	1.21883	-3.25846	-1.66804
C	0.69395	0.24667	-2.26281
O	0.05278	0.69864	-3.11636
C	2.38457	1.49628	-0.53810
O	3.50282	1.95597	-0.48291
O	1.36841	2.43255	-0.23067
O	-1.07668	2.81895	-1.34593
O	-0.31641	3.09416	2.03413
O	-1.24518	5.59598	-1.31502
O	-2.84180	2.95959	0.83105
O	-1.72735	5.40089	1.39983
H	-1.78737	0.38309	-1.09113
H	-1.03057	-1.21166	-1.26626
H	3.10196	-0.22195	3.84388
H	-2.61420	-0.06605	1.85993
H	1.13695	0.10097	3.95642
H	-1.31904	0.31694	3.99578
H	6.22832	-1.94274	1.43568
H	5.42663	-1.03396	3.65668
H	-6.85524	-1.93986	-1.11406
H	-6.72128	-0.39003	-0.22476
H	-6.87765	-1.91250	0.67735
H	5.76888	-2.63551	-0.71066
H	4.14884	-2.52672	-1.44185
H	5.26021	-1.13938	-1.50722
H	-0.19166	2.60356	-0.97294
H	-2.33604	2.85106	0.00530
H	-2.69594	3.90630	1.04628
H	-1.15990	4.62983	-1.43583
H	-2.09039	5.80757	-1.73041
H	0.30488	2.63322	1.45070
H	-1.18075	2.71284	1.79084
H	-1.02279	4.77774	1.66384
H	-1.51425	5.60559	0.46627
H	-1.09358	2.40339	-2.21813
H	-3.78641	0.90200	-1.91696
H	-5.41252	0.86416	-1.20538
H	-4.02963	1.44637	-0.23622
H	-1.20548	-3.02799	1.11965
H	-2.18624	-4.42137	0.60295
H	-1.22984	-3.51334	-0.59081
H	-4.40218	-4.80714	0.80100
H	-5.68832	-3.80717	1.51541
H	-5.80028	-4.31716	-0.18647
H	1.82378	3.28356	-0.08312

3C2(TS3)

Energy = -3017.410701
 Enthalpy 0K = -3016.841109
 Enthalpy 298K = -3016.794791
 Free Energy 298K = -3016.921206
 Nimag = 1 (-210.3288 cm⁻¹)

N 3.25437 -0.81315 0.46540
 C 2.72802 -0.56408 1.72390
 C 3.57367 -0.60987 2.87166
 C 4.87963 -0.99849 2.74264
 C 5.36480 -1.36333 1.46665
 C 4.53214 -1.24643 0.36040
 C 1.32843 -0.32795 1.80524
 N 0.61088 -0.38197 0.62140
 C -0.73568 -0.38835 0.68696
 C -1.43760 -0.23141 1.86922
 C -0.71656 -0.05429 3.07103
 C 0.64828 -0.11911 3.04170
 C -1.51961 -0.59123 -0.59610
 N -2.73755 -1.36017 -0.38380
 C -2.74522 -2.70377 -0.02567
 C -4.05452 -3.05576 0.12648
 N -4.80772 -1.91973 -0.14710
 C -3.99628 -0.90419 -0.46536
 C -1.49915 -3.50606 0.09617
 C -4.39400 0.47649 -0.82701
 C -6.26027 -1.89619 -0.09660
 C -4.68379 -4.35089 0.49650
 Mn 1.90688 -0.20657 -1.03521
 C 3.07136 0.02148 -2.39671
 O 3.70601 0.22013 -3.33352
 C 5.09082 -1.60356 -0.98769
 C 1.63685 -1.96566 -1.49059
 O 1.52269 -3.06898 -1.76754
 C 0.70676 0.44999 -2.22545
 O 0.04009 0.84778 -3.07090
 C 2.40456 1.60360 -0.39762
 O 3.12691 2.40415 -0.02024
 O 0.57894 2.80881 -0.64335
 O -1.74974 2.69934 -1.36773
 O -0.25673 3.11140 1.84816
 O -2.24969 5.34548 -1.14555
 O -3.02821 2.63207 1.09141
 O -2.06162 5.16632 1.61660
 H -1.78642 0.38814 -1.01558
 H -0.91865 -1.13504 -1.33192
 H 3.17525 -0.35007 3.85178
 H -2.52618 -0.21801 1.86242
 H 1.21848 -0.01695 3.96427
 H -1.24491 0.11494 4.01180
 H 6.38671 -1.72031 1.33355
 H 5.53318 -1.04242 3.61714
 H -6.67401 -2.47519 -0.93297
 H -6.62168 -0.86556 -0.15152
 H -6.59404 -2.33409 0.85190
 H 5.99896 -2.20914 -0.86933

H 4.37528 -2.17561 -1.59346
 H 5.37307 -0.70092 -1.54889
 H -0.69647 2.71605 -1.09251
 H -2.64018 2.59254 0.19471
 H -2.90768 3.57217 1.33876
 H -2.07234 4.38847 -1.30983
 H -3.20282 5.42416 -1.27255
 H 0.13637 2.99916 0.93718
 H -1.05429 2.56047 1.79445
 H -1.28090 4.58275 1.74385
 H -2.05618 5.35300 0.65544
 H -1.79733 2.35166 -2.26462
 H -3.80612 0.82687 -1.68550
 H -5.45326 0.51777 -1.10166
 H -4.21017 1.16786 0.01041
 H -0.81309 -3.08247 0.84481
 H -1.74345 -4.53237 0.39641
 H -0.96622 -3.55005 -0.86516
 H -3.91068 -5.11396 0.64853
 H -5.26320 -4.26005 1.42816
 H -5.36575 -4.70340 -0.29216
 H 0.93163 3.66135 -0.92635

3C2(I7-R)

Energy = -3017.418810
 Enthalpy 0K = -3016.846922
 Enthalpy 298K = -3016.800106
 Free Energy 298K = -3016.927828
 Nimag = 0 (20.8591 cm⁻¹)

N 3.44970 -0.48616 0.42562
 C 2.90598 -0.33124 1.69347
 C 3.74555 -0.41436 2.84253
 C 5.06728 -0.74025 2.69888
 C 5.57673 -0.99900 1.40593
 C 4.74743 -0.85003 0.30166
 C 1.49721 -0.15467 1.77232
 N 0.79303 -0.25260 0.58416
 C -0.55209 -0.32685 0.63513
 C -1.27207 -0.15516 1.80369
 C -0.57156 0.08397 3.00626
 C 0.79648 0.05304 2.99811
 C -1.32005 -0.64060 -0.63246
 N -2.36790 -1.63193 -0.39893
 C -2.12586 -2.91676 0.08392
 C -3.33517 -3.54717 0.13920
 N -4.27810 -2.63609 -0.31329
 C -3.67877 -1.48637 -0.64515
 C -0.76928 -3.41224 0.44187
 C -4.38380 -0.30801 -1.20116
 C -5.69725 -2.91812 -0.44217
 C -3.70630 -4.91982 0.57327
 Mn 2.07723 0.16542 -1.02816
 C 3.23467 0.59078 -2.36069
 O 3.86602 0.90659 -3.26382
 C 5.32971 -1.08343 -1.06321

C	1.93996	-1.58133	-1.65647
O	1.90484	-2.65394	-2.04004
C	0.79773	0.83494	-2.14173
O	0.07820	1.27251	-2.91675
C	2.38881	1.88457	-0.26435
O	2.73020	2.88274	0.15381
O	-0.21712	2.94401	-0.12357
O	-2.41976	2.30512	-1.24030
O	-1.61111	3.13372	2.23045
O	-3.40152	4.71394	-1.21009
O	-3.83441	1.89156	1.02214
O	-3.82461	4.63931	1.48659
H	-1.78354	0.28965	-0.99820
H	-0.65849	-1.04507	-1.40582
H	3.32780	-0.24366	3.83427
H	-2.36145	-0.16332	1.77269
H	1.35273	0.20076	3.92339
H	-1.11590	0.27391	3.93346
H	6.61501	-1.29873	1.25951
H	5.71627	-0.81771	3.57435
H	-5.87654	-3.56293	-1.31342
H	-6.24941	-1.98074	-0.56290
H	-6.05140	-3.42232	0.46496
H	6.26349	-1.65480	-0.98066
H	4.64683	-1.64086	-1.71810
H	5.57573	-0.13024	-1.55375
H	-1.07073	2.66207	-0.61131
H	-3.36523	1.95178	0.15509
H	-4.09009	2.82061	1.18847
H	-3.00638	3.78562	-1.26192
H	-4.28560	4.60144	-1.57769
H	-0.99832	3.10287	1.46234
H	-2.26778	2.45640	1.97899
H	-2.95725	4.32301	1.81191
H	-3.66488	4.78045	0.52626
H	-2.28574	2.06106	-2.16176
H	-3.69595	0.52154	-1.40410
H	-4.90317	-0.58992	-2.12895
H	-5.12473	0.06051	-0.47804
H	-0.39457	-2.94285	1.36363
H	-0.80136	-4.49742	0.60011
H	-0.04689	-3.20740	-0.35978
H	-2.80624	-5.49092	0.83184
H	-4.36057	-4.89376	1.45853
H	-4.23944	-5.45860	-0.22467
H	-0.00180	3.80555	-0.49797

3_{C2}⁺ (I8)

Energy	= -2559.732212
Enthalpy 0K	= -2559.302494
Enthalpy 298K	= -2559.269480
Free Energy 298K	= -2559.367265
Nimag	= 0 (14.4553 cm ⁻¹)

C	-3.62182	0.25608	1.21354
N	-3.13836	-0.30699	0.09674
C	-4.17805	-0.55318	-0.79375

C	-5.32094	-0.12779	-0.17859
N	-4.94419	0.36493	1.06430
C	-1.73564	-0.58589	-0.16001
C	-0.94099	0.64218	-0.55670
N	0.40229	0.59152	-0.41039
C	1.14048	1.74082	-0.66390
C	0.50269	2.88135	-1.23821
C	-0.84842	2.88409	-1.43848
C	-1.60502	1.75004	-1.04947
Mn	1.69388	-1.04215	-0.08913
C	1.23511	-1.01015	1.72874
C	2.50484	1.73543	-0.26407
N	2.99472	0.56859	0.29689
C	4.21995	0.57582	0.87502
C	5.03749	1.69868	0.84514
C	4.59716	2.86307	0.18275
C	3.34056	2.88580	-0.36031
C	4.73711	-0.65465	1.56326
C	-3.95737	-1.15880	-2.13364
C	-5.87144	0.92202	2.03421
C	-6.73832	-0.12994	-0.62618
C	-2.83844	0.71261	2.38676
C	2.88551	-2.40645	0.11817
O	3.53262	-3.34734	0.19344
C	0.54545	-2.38904	-0.50254
O	-0.07926	-3.31324	-0.76391
C	2.17931	-0.86513	-1.90305
O	2.47083	-0.76732	-2.99601
O	0.97350	-0.94334	2.83286
H	1.09392	3.75498	-1.51009
H	-1.34409	3.75250	-1.87711
H	2.97135	3.78904	-0.84386
H	6.01531	1.66129	1.32621
H	-2.68971	1.74728	-1.15033
H	5.24181	3.74291	0.12258
H	3.96908	-1.14446	2.17708
H	5.11793	-1.38376	0.83336
H	5.57548	-0.38930	2.22015
H	-1.70299	-1.33002	-0.96417
H	-1.31034	-1.05459	0.73541
H	-3.24314	-0.56454	-2.72385
H	-3.56510	-2.18428	-2.05196
H	-4.90472	-1.20115	-2.68469
H	-7.15709	0.88784	-0.61864
H	-6.81194	-0.52414	-1.64699
H	-7.36161	-0.75607	0.03058
H	-1.77254	0.49807	2.25639
H	-2.95844	1.79757	2.52081
H	-3.18642	0.20998	3.30068
H	-6.33516	1.82864	1.62408
H	-6.65046	0.18355	2.26191
H	-5.33601	1.17430	2.95479

3_{C2}⁺ (I5-P)

Energy	= -3017.338237
Enthalpy 0K	= -3016.759928

Enthalpy 298K = -3016.713819
 Free Energy 298K = -3016.838593
 Nimag = 0 (19.9425 cm⁻¹)

N	3.06724	-1.03824	0.57492
C	2.60060	-0.59995	1.76451
C	3.41384	-0.50175	2.88955
C	4.73689	-0.91671	2.80057
C	5.18351	-1.45017	1.60454
C	4.32744	-1.50309	0.49709
C	1.14907	-0.30125	1.82589
N	0.47054	-0.38404	0.66149
C	-0.87078	-0.29416	0.69265
C	-1.56673	-0.02910	1.87062
C	-0.86528	0.12195	3.05534
C	0.51057	-0.04122	3.03703
C	-1.65128	-0.52219	-0.58562
N	-2.95257	-1.11814	-0.34030
C	-3.13416	-2.42547	0.09854
C	-4.48071	-2.60364	0.22287
N	-5.08094	-1.40522	-0.15027
C	-4.14295	-0.51595	-0.49267
C	-1.99838	-3.35923	0.32015
C	-4.33168	0.88154	-0.94888
C	-6.52232	-1.21177	-0.14327
C	-5.27562	-3.78457	0.65032
Mn	1.76402	-0.52931	-1.03112
C	2.95447	-0.52219	-2.38260
O	3.62482	-0.44362	-3.31188
C	4.84753	-2.09715	-0.77595
C	1.32347	-2.29242	-1.32231
O	1.09567	-3.39192	-1.55145
C	0.67076	0.11966	-2.28559
O	0.05581	0.56336	-3.15618
C	2.43957	1.36670	-0.64796
O	3.58673	1.73038	-0.53297
O	1.48679	2.39922	-0.51664
O	-0.99908	2.89205	-1.51768
O	0.00111	3.00868	1.91830
O	-0.94089	5.67420	-1.27608
O	-2.55587	3.00773	0.80875
O	-1.39069	5.39780	1.43238
H	-1.79421	0.43249	-1.10768
H	-1.10103	-1.19527	-1.25030
H	3.02788	-0.11266	3.82934
H	-2.65242	0.05733	1.85364
H	1.07648	0.02703	3.96355
H	-1.38616	0.34459	3.98768
H	6.20122	-1.82993	1.50514
H	5.39923	-0.84500	3.66508
H	-6.99184	-1.93875	-0.81799
H	-6.76863	-0.20047	-0.47763
H	-6.90416	-1.35654	0.87533
H	5.68300	-2.77377	-0.55432
H	4.07421	-2.66309	-1.30950
H	5.23250	-1.31170	-1.44206
H	-0.09831	2.62116	-1.23706

H	-2.14127	2.93630	-0.07038
H	-2.39528	3.94682	1.05025
H	-0.95644	4.71996	-1.48273
H	-1.74741	6.01506	-1.68236
H	0.55928	2.67189	1.20169
H	-0.89724	2.72757	1.65650
H	-0.68643	4.76877	1.67812
H	-1.18188	5.62385	0.50199
H	-1.11963	2.52821	-2.40441
H	-3.81657	1.03578	-1.90817
H	-5.39227	1.11239	-1.08997
H	-3.91199	1.58503	-0.21309
H	-1.28174	-2.96349	1.05571
H	-2.37303	-4.32033	0.69259
H	-1.45359	-3.54522	-0.61745
H	-4.60610	-4.61588	0.90263
H	-5.88628	-3.55246	1.53616
H	-5.95379	-4.11921	-0.14934
H	1.99119	3.23143	-0.42514

3_{C2}⁺(TS4)

Energy = -3017.312243
 Enthalpy 0K = -3016.739171
 Enthalpy 298K = -3016.693605
 Free Energy 298K = -3016.815999
 Nimag = 1 (-284.1803 cm⁻¹)

N	3.19804	-0.88817	0.51579
C	2.70091	-0.61083	1.74322
C	3.49625	-0.64023	2.88512
C	4.82898	-1.01255	2.76967
C	5.31001	-1.37378	1.52361
C	4.47612	-1.30328	0.40179
C	1.24265	-0.34718	1.82203
N	0.56011	-0.37353	0.65705
C	-0.78323	-0.32147	0.69895
C	-1.47686	-0.15185	1.89589
C	-0.77342	-0.04964	3.08348
C	0.60596	-0.17235	3.04848
C	-1.58282	-0.48506	-0.57754
N	-2.82388	-1.21043	-0.35461
C	-2.87764	-2.56117	-0.02245
C	-4.19738	-2.86656	0.13544
N	-4.91096	-1.69872	-0.11140
C	-4.06763	-0.70664	-0.41537
C	-1.66209	-3.41285	0.06554
C	-4.40939	0.69764	-0.74004
C	-6.36203	-1.63035	-0.04574
C	-4.87166	-4.14353	0.48835
Mn	1.86548	-0.30110	-1.03313
C	3.02352	-0.20421	-2.42807
O	3.64503	-0.09413	-3.38379
C	5.04138	-1.69764	-0.92734
C	1.51461	-2.08158	-1.42159
O	1.36402	-3.18429	-1.66795
C	0.68271	0.35437	-2.26712
O	0.03717	0.72188	-3.13609

C	2.45531	1.50191	-0.52327
O	3.17942	2.31309	-0.18399
O	0.64137	2.78179	-0.94160
O	-1.72655	2.76274	-1.42547
O	0.13479	2.87185	1.65091
O	-1.93253	5.42296	-0.99245
O	-2.68619	2.66718	1.13892
O	-1.52300	5.09853	1.72285
H	-1.81160	0.51021	-0.98806
H	-1.01019	-1.04652	-1.32143
H	3.08762	-0.38563	3.86036
H	-2.56357	-0.08834	1.88777
H	1.17531	-0.14085	3.97443
H	-1.29407	0.10342	4.02990
H	6.33926	-1.71080	1.39559
H	5.47418	-1.03944	3.64943
H	-6.79891	-2.22350	-0.85969
H	-6.69492	-0.59267	-0.13238
H	-6.69778	-2.02906	0.91931
H	5.94253	-2.30608	-0.78030
H	4.32753	-2.28150	-1.52143
H	5.34007	-0.80827	-1.50100
H	-0.62178	2.74379	-1.26386
H	-2.43652	2.67520	0.19122
H	-2.50435	3.58654	1.42540
H	-1.87999	4.46804	-1.23740
H	-2.87529	5.62098	-1.04458
H	0.39140	2.87039	0.68743
H	-0.75486	2.48091	1.62147
H	-0.76616	4.47764	1.76553
H	-1.58018	5.32873	0.77179
H	-1.90218	2.48463	-2.33043
H	-3.86947	1.01954	-1.64055
H	-5.48198	0.80936	-0.92730
H	-4.11598	1.36419	0.08592
H	-0.93726	-3.02138	0.79515
H	-1.93970	-4.42836	0.37296
H	-1.16137	-3.47909	-0.91167
H	-4.12638	-4.93551	0.63061
H	-5.44824	-4.04294	1.42059
H	-5.56504	-4.46069	-0.30523
H	1.00578	3.62075	-1.24795

$3\text{C}_2^+(16\text{-P})$

Energy	=	-3017.319276
Enthalpy 0K	=	-3016.742582
Enthalpy 298K	=	-3016.696738
Free Energy 298K	=	-3016.818877
Nimag	=	0 (27.6502 cm^{-1})

N	3.20564	-0.94199	0.46468
C	2.66718	-0.93410	1.70565
C	3.40399	-1.29078	2.83184
C	4.72722	-1.67986	2.67825
C	5.26157	-1.72116	1.40245
C	4.48290	-1.34814	0.30194

C	1.22559	-0.59967	1.80774
N	0.55255	-0.46815	0.64382
C	-0.78840	-0.36945	0.68350
C	-1.48075	-0.28798	1.89124
C	-0.78152	-0.31673	3.08431
C	0.59171	-0.50100	3.04314
C	-1.59398	-0.37712	-0.59974
N	-2.82335	-1.14561	-0.44664
C	-2.83559	-2.53234	-0.30933
C	-4.13946	-2.89578	-0.14045
N	-4.88483	-1.72548	-0.18107
C	-4.07971	-0.67555	-0.37556
C	-1.60101	-3.35629	-0.39747
C	-4.52946	0.73208	-0.46901
C	-6.33026	-1.67599	-0.03916
C	-4.77046	-4.22881	0.04488
Mn	1.88934	-0.13187	-0.98845
C	3.04654	0.17966	-2.36111
O	3.65197	0.43196	-3.29779
C	5.10479	-1.40269	-1.05818
C	1.58738	-1.87404	-1.60656
O	1.46635	-2.94169	-1.97671
C	0.69306	0.61754	-2.16630
O	0.05423	1.03651	-3.01328
C	2.44500	1.53536	-0.23800
O	2.98213	2.42771	0.20672
O	0.45232	3.32748	-1.06524
O	-2.05322	2.74410	-1.17173
O	0.16661	2.65437	1.57977
O	-1.58706	5.25829	-0.67002
O	-2.63067	2.51714	1.41399
O	-1.41434	4.95214	2.03894
H	-1.83084	0.66449	-0.89223
H	-1.02699	-0.85058	-1.40661
H	2.95368	-1.28591	3.82177
H	-2.56243	-0.16987	1.88660
H	1.15835	-0.56651	3.96919
H	-1.30039	-0.21732	4.03883
H	6.28962	-2.04394	1.23559
H	5.32508	-1.96280	3.54627
H	-6.80931	-2.11110	-0.92644
H	-6.65408	-0.63748	0.07901
H	-6.62604	-2.24309	0.85203
H	6.04928	-1.95835	-1.01379
H	4.45250	-1.89936	-1.78807
H	5.33692	-0.38926	-1.41641
H	-0.49108	2.99571	-1.21103
H	-2.53470	2.58251	0.43051
H	-2.45268	3.42721	1.71975
H	-1.90525	4.33158	-0.91024
H	-2.19932	5.87098	-1.09124
H	0.32599	2.90227	0.64163
H	-0.76195	2.34812	1.56477
H	-0.67404	4.31679	2.03809
H	-1.47918	5.19908	1.09084
H	-2.41902	2.61495	-2.05293
H	-3.72240	1.39054	-0.81257

H	-5.37411	0.80819	-1.16795
H	-4.85431	1.09358	0.51753
H	-0.84813	-3.05038	0.34452
H	-1.84349	-4.41113	-0.22006
H	-1.14949	-3.27542	-1.39746
H	-4.00553	-5.01455	0.02420
H	-5.29829	-4.28787	1.00908
H	-5.50028	-4.43612	-0.75244
H	0.30375	4.28328	-1.04664

3C2+(I7-P)

Energy	=	-2559.624776
Enthalpy 0K	=	-2559.191193
Enthalpy 298K	=	-2559.158715
Free Energy 298K	=	-2559.254035
Nimag	=	0 (15.2090 cm ⁻¹)

C	-3.64054	0.21123	1.21212
N	-3.14535	-0.29575	0.07101
C	-4.17892	-0.50925	-0.83747
C	-5.32682	-0.11589	-0.21156
N	-4.96084	0.32198	1.05528
C	-1.74442	-0.57864	-0.18221
C	-0.94233	0.65174	-0.55241
N	0.39210	0.64066	-0.36848
C	1.08724	1.77723	-0.59415
C	0.48471	2.91693	-1.12484
C	-0.87701	2.90476	-1.38018
C	-1.60337	1.76882	-1.05929
Mn	1.69800	-1.02900	-0.06831
C	1.33685	-0.98179	1.78495
C	2.51614	1.77493	-0.19549
N	3.03523	0.59649	0.22018
C	4.30136	0.56703	0.68928
C	5.08537	1.72634	0.71102
C	4.56925	2.92596	0.25617
C	3.25711	2.95301	-0.19514
C	4.91174	-0.70203	1.19610
C	-3.94660	-1.06629	-2.19634
C	-5.89791	0.83980	2.03830
C	-6.74167	-0.10726	-0.66654
C	-2.87390	0.60752	2.41806
C	2.86726	-2.42882	0.12011
O	3.47408	-3.39269	0.19461
C	0.51822	-2.38997	-0.38190
O	-0.10779	-3.32561	-0.57700
C	2.10129	-0.93640	-1.91040
O	2.35017	-0.88926	-3.01551
O	1.13996	-0.93688	2.90089
H	1.06757	3.80948	-1.34135
H	-1.36990	3.77979	-1.80611
H	2.81795	3.89146	-0.52468
H	6.10389	1.66517	1.09528
H	-2.68256	1.74598	-1.20743
H	5.17110	3.83608	0.26564
H	4.25154	-1.22296	1.90186

H	5.15404	-1.37529	0.36161
H	5.85092	-0.47937	1.71667
H	-1.70518	-1.30645	-1.00192
H	-1.32870	-1.05783	0.71001
H	-3.21833	-0.46020	-2.75650
H	-3.56717	-2.09871	-2.14600
H	-4.88689	-1.07826	-2.76057
H	-7.16923	0.90503	-0.60721
H	-6.80750	-0.44833	-1.70667
H	-7.36132	-0.77227	-0.04559
H	-1.80763	0.38448	2.30282
H	-2.98455	1.68703	2.59714
H	-3.24754	0.07010	3.30143
H	-6.32856	1.78274	1.67678
H	-6.69975	0.10826	2.19766
H	-5.37986	1.01701	2.98584

3C5(I6-R)

Energy	=	-3017.432181
Enthalpy 0K	=	-3016.857147
Enthalpy 298K	=	-3016.810742
Free Energy 298K	=	-3016.936938
Nimag	=	0 (18.8312 cm ⁻¹)

C	-3.05775	-2.45706	0.04995
N	-2.90580	-1.19813	-0.38514
C	-4.15276	-0.61302	-0.57195
C	-5.07735	-1.55915	-0.22833
N	-4.36826	-2.68914	0.15746
C	-1.61496	-0.55999	-0.60454
C	-0.83722	-0.34890	0.68024
N	0.50598	-0.40653	0.61810
C	1.22329	-0.34340	1.80414
C	0.54786	-0.05867	3.02954
C	-0.81271	0.06800	3.05165
C	-1.53969	-0.11566	1.85197
C	2.60778	-0.65770	1.73739
C	3.45474	-0.67359	2.88544
C	4.73797	-1.14236	2.77936
C	5.19329	-1.61976	1.53287
C	4.35665	-1.52942	0.42221
N	3.11164	-1.01841	0.49988
Mn	1.80638	-0.41254	-1.05123
C	1.41159	-2.15240	-1.45568
O	1.18676	-3.24146	-1.74430
C	4.88310	-2.01459	-0.89951
C	-4.33052	0.78186	-1.05488
C	-6.56353	-1.52206	-0.22134
C	-4.98375	-3.92895	0.59914
C	-1.97037	-3.40828	0.38328
C	0.69847	0.27366	-2.26024
O	0.06275	0.74580	-3.10685
C	2.38670	1.47740	-0.50251
O	1.37280	2.41031	-0.18228
C	3.01373	-0.26565	-2.37292
O	3.69790	-0.09488	-3.28294

O	3.50706	1.92997	-0.43059	C	0.70634	-0.07335	3.02663
O	-1.05402	2.85235	-1.32071	C	-0.65792	0.00895	3.06372
O	-1.06764	5.63471	-1.28566	C	-1.39043	-0.17813	1.86976
O	-2.82203	3.10049	0.84323	C	2.77259	-0.54681	1.68979
O	-0.31730	3.08848	2.07985	C	3.62948	-0.61904	2.82716
O	-1.57743	5.47746	1.42769	C	4.93073	-1.01685	2.67635
H	-1.80156	0.40482	-1.09076	C	5.39886	-1.36399	1.38937
H	-1.04377	-1.18232	-1.30115	C	4.55500	-1.22231	0.29434
H	3.07848	-0.32405	3.84642	N	3.28268	-0.78001	0.42171
H	-2.62801	-0.06026	1.83979	Mn	1.92360	-0.13195	-1.05105
H	1.11860	0.05065	3.95122	C	1.64719	-1.87150	-1.57427
H	-1.33463	0.29588	3.98349	O	1.50934	-2.95935	-1.89783
H	6.19241	-2.04274	1.42052	C	5.09402	-1.56215	-1.06631
H	5.39339	-1.16230	3.65366	C	-4.37404	0.29402	-1.13085
H	-6.98439	-2.30922	-0.86537	C	-6.23742	-2.32392	-0.33233
H	-6.91815	-0.55128	-0.58852	C	-4.32956	-4.43058	0.60540
H	-6.96018	-1.66983	0.79500	C	-1.43190	-3.44451	0.48205
H	5.72227	-2.70496	-0.74007	C	0.70731	0.55682	-2.20418
H	4.11167	-2.53480	-1.48235	O	0.02366	0.98103	-3.02300
H	5.25970	-1.17720	-1.50473	C	2.40232	1.66416	-0.35917
H	-0.17985	2.60919	-0.93966	O	0.51808	2.82821	-0.45030
H	-2.32421	2.96694	0.01662	C	3.08549	0.15171	-2.40573
H	-2.62733	4.03760	1.05971	O	3.72337	0.38908	-3.33083
H	-1.04012	4.66573	-1.41050	O	3.11615	2.47366	0.01429
H	-1.89649	5.89854	-1.70414	O	-1.78386	2.71786	-1.26295
H	0.29095	2.59944	1.50599	O	-2.49324	5.31495	-1.10513
H	-1.19725	2.76505	1.80805	O	-3.21085	2.51613	1.08505
H	-0.91513	4.81372	1.70158	O	-0.52165	3.19800	1.96433
H	-1.34387	5.66388	0.49524	O	-2.45676	5.12030	1.65934
H	-1.07751	2.43691	-2.19274	H	-1.82452	0.37353	-0.98463
H	-3.83465	0.93556	-2.02562	H	-0.87811	-1.09038	-1.34262
H	-5.39933	0.99226	-1.18604	H	3.24292	-0.37605	3.81637
H	-3.92617	1.51273	-0.33855	H	-2.47919	-0.14636	1.86447
H	-1.88199	-3.52034	1.47460	H	1.28455	0.03624	3.94356
H	-2.17512	-4.39498	-0.05400	H	-1.17708	0.20068	4.00524
H	-1.00952	-3.05320	-0.00415	H	6.41612	-1.72738	1.23913
H	-4.21624	-4.59993	0.99747	H	5.59318	-1.08296	3.54270
H	-5.71117	-3.71136	1.39090	H	-6.49706	-3.19616	-0.95129
H	-5.49345	-4.41466	-0.24359	H	-6.72530	-1.44039	-0.76185
H	1.83015	3.25572	-0.01097	H	-6.65257	-2.48853	0.67411

3_{C5}(TS3)

Energy	=	-3017.410346
Enthalpy 0K	=	-3016.840924
Enthalpy 298K	=	-3016.794629
Free Energy 298K	=	-3016.920793
Nimag	=	1 (-204.4705 cm ⁻¹)

C	-2.64135	-2.67865	0.09409	H	5.38495	-0.65372	-1.61351
N	-2.67425	-1.41775	-0.36172	H	-0.74112	2.73561	-0.94942
C	-3.99040	-1.04516	-0.61128	H	-2.75233	2.51470	0.22006
C	-4.76525	-2.12153	-0.28083	H	-3.18065	3.46172	1.33716
N	-3.90158	-3.11545	0.15955	H	-2.22147	4.37511	-1.24112
C	-1.49117	-0.59266	-0.58413	H	-3.43907	5.30529	-1.29508
C	-0.69736	-0.35960	0.68580	H	-0.04822	3.06116	1.09638
N	0.64777	-0.35991	0.60974	H	-1.28405	2.60330	1.87534
C	1.37571	-0.30050	1.78710	H	-1.64015	4.59467	1.81005
				H	-2.42355	5.32173	0.70174
				H	-1.80611	2.34687	-2.15123
				H	-3.85467	0.52323	-2.07349
				H	-5.45350	0.31535	-1.32582
				H	-4.14161	1.08560	-0.40299
				H	-1.36548	-3.52485	1.57775

H	-1.46669	-4.45760	0.05906
H	-0.52397	-2.95106	0.12059
H	-3.49360	-4.94887	1.08535
H	-5.14148	-4.31927	1.33445
H	-4.68399	-5.01996	-0.25088
H	0.86161	3.68847	-0.72127

3C₅(I7-R)

Energy	=	-3017.417431
Enthalpy 0K	=	-3016.845230
Enthalpy 298K	=	-3016.798566
Free Energy 298K	=	-3016.925628
Nimag	=	0 (16.7013 cm ⁻¹)

C	-2.05009	-2.87097	0.14484
N	-2.33232	-1.66867	-0.38061
C	-3.67714	-1.62005	-0.73287
C	-4.21358	-2.82711	-0.38243
N	-3.18346	-3.57800	0.16633
C	-1.35561	-0.60027	-0.60238
C	-0.57220	-0.27022	0.65153
N	0.77315	-0.20106	0.58803
C	1.48802	-0.10082	1.76942
C	0.79878	0.11977	2.99974
C	-0.56890	0.15397	3.02032
C	-1.28110	-0.09206	1.82515
C	2.89413	-0.29261	1.67868
C	3.74432	-0.37568	2.81971
C	5.06035	-0.71995	2.66512
C	5.55271	-0.99764	1.36975
C	4.71371	-0.84813	0.27272
N	3.42255	-0.46580	0.40695
Mn	2.04510	0.19514	-1.03869
C	1.87235	-1.55376	-1.65626
O	1.80775	-2.62883	-2.02868
C	5.27712	-1.10339	-1.09614
C	-4.31609	-0.43913	-1.37128
C	-5.59687	-3.35797	-0.50715
C	-3.34231	-4.93214	0.66967
C	-0.72766	-3.33759	0.62902
C	0.75819	0.87956	-2.13753
O	0.02974	1.32396	-2.89957
C	2.38099	1.91456	-0.28772
O	-0.22644	2.95766	-0.09629
C	3.19506	0.59728	-2.38487
O	3.82383	0.89819	-3.29493
O	2.73242	2.91382	0.11967
O	-2.45829	2.39459	-1.15794
O	-3.44280	4.79260	-1.19903
O	-3.87522	1.89207	0.99418
O	-1.69547	3.17371	2.22597
O	-3.94170	4.64601	1.48709
H	-1.90002	0.30448	-0.91606
H	-0.69759	-0.92044	-1.41642
H	3.33939	-0.19057	3.81418
H	-2.37118	-0.09748	1.80181

H	1.36401	0.27223	3.91887
H	-1.10443	0.35207	3.95090
H	6.58532	-1.31265	1.21544
H	5.71752	-0.79761	3.53445
H	-5.61592	-4.28610	-1.09850
H	-6.24004	-2.62095	-1.00317
H	-6.02999	-3.57819	0.48089
H	6.20437	-1.68597	-1.01843
H	4.57917	-1.65857	-1.73696
H	5.52926	-0.15874	-1.59987
H	-1.08508	2.69316	-0.59015
H	-3.36426	2.01072	0.14218
H	-4.18516	2.80156	1.17053
H	-3.03217	3.86801	-1.23120
H	-4.31242	4.66156	-1.59395
H	-1.06598	3.13838	1.47198
H	-2.34318	2.48999	1.96723
H	-3.07185	4.33626	1.81130
H	-3.77188	4.80903	0.53211
H	-2.47964	2.01256	-2.04058
H	-3.78123	-0.14059	-2.28503
H	-5.34808	-0.68917	-1.64824
H	-4.33810	0.41960	-0.68494
H	-0.65395	-3.22441	1.72150
H	-0.57630	-4.39398	0.37278
H	0.07914	-2.75566	0.17318
H	-2.45461	-5.22285	1.23958
H	-4.21416	-4.97072	1.33419
H	-3.48752	-5.62947	-0.16633
H	0.00408	3.81682	-0.46688

3C₅⁺(I5-P)

Energy	=	-3017.337855
Enthalpy 0K	=	-3016.759301
Enthalpy 298K	=	-3016.713252
Free Energy 298K	=	-3016.837668
Nimag	=	0 (20.8741 cm ⁻¹)

C	-3.12814	-2.37372	0.08192
N	-2.94945	-1.11962	-0.36343
C	-4.18462	-0.50820	-0.55361
C	-5.12767	-1.43099	-0.19919
N	-4.44237	-2.57325	0.19508
C	-1.64898	-0.51259	-0.60126
C	-0.86820	-0.29767	0.67782
N	0.47192	-0.39790	0.64849
C	1.14800	-0.33487	1.81573
C	0.50908	-0.07648	3.02682
C	-0.86499	0.10402	3.04261
C	-1.56526	-0.03297	1.85542
C	2.59544	-0.65261	1.75365
C	3.40246	-0.60300	2.88620
C	4.71961	-1.03538	2.79192
C	5.16654	-1.53523	1.58159
C	4.31740	-1.53848	0.46747
N	3.06301	-1.05979	0.55332

Mn	1.77129	-0.49629	-1.04266
C	1.33456	-2.24526	-1.40983
O	1.10398	-3.33135	-1.69510
C	4.83895	-2.09277	-0.82282
C	-4.33010	0.88438	-1.05219
C	-6.61245	-1.36092	-0.18965
C	-5.08651	-3.79317	0.65319
C	-2.06196	-3.34649	0.42236
C	0.68240	0.18530	-2.28364
O	0.06788	0.64717	-3.14507
C	2.43720	1.38830	-0.59078
O	1.48051	2.41358	-0.44014
C	2.97671	-0.43603	-2.37984
O	3.66022	-0.32074	-3.29541
O	3.58214	1.74986	-0.44911
O	-0.99479	2.92932	-1.46372
O	-0.94773	5.70873	-1.21316
O	-2.58318	3.02049	0.84231
O	-0.04292	3.01245	1.98310
O	-1.41969	5.41002	1.48963
H	-1.81198	0.45012	-1.10166
H	-1.09164	-1.15905	-1.28596
H	3.01565	-0.23926	3.83585
H	-2.65008	0.06850	1.83256
H	1.07371	-0.02155	3.95498
H	-1.38515	0.32946	3.97466
H	6.17925	-1.92655	1.47580
H	5.37682	-1.00285	3.66272
H	-7.05117	-2.14233	-0.82860
H	-6.94580	-0.38454	-0.56172
H	-7.00962	-1.49479	0.82832
H	5.65725	-2.79586	-0.62038
H	4.05961	-2.61793	-1.38832
H	5.24785	-1.28898	-1.45206
H	-0.09852	2.65375	-1.17393
H	-2.15779	2.95115	-0.03168
H	-2.42517	3.95891	1.08648
H	-0.95626	4.75466	-1.42150
H	-1.75608	6.04419	-1.62034
H	0.52405	2.66783	1.27748
H	-0.93949	2.73816	1.70703
H	-0.71965	4.77695	1.73660
H	-1.20262	5.64296	0.56291
H	-1.10670	2.56834	-2.35274
H	-3.85319	1.00774	-2.03675
H	-5.39449	1.12683	-1.16081
H	-3.88318	1.60909	-0.35499
H	-1.96281	-3.43834	1.51477
H	-2.29990	-4.33584	0.00918
H	-1.09625	-3.03026	0.01401
H	-4.33368	-4.48136	1.05000
H	-5.80024	-3.54842	1.44942
H	-5.61683	-4.27056	-0.18132
H	1.98183	3.24365	-0.31754

3_{C5}⁺(TS4)

Energy = -3017.311513

Enthalpy 0K = -3016.738640
 Enthalpy 298K = -3016.693094
 Free Energy 298K = -3016.815553
 Nimag = 1 (-310.4638 cm⁻¹)

C	-2.90130	-2.47531	0.05311
N	-2.82980	-1.19082	-0.33336
C	-4.11505	-0.68259	-0.50238
C	-4.97428	-1.69959	-0.19548
N	-4.19279	-2.79386	0.14968
C	-1.58342	-0.46873	-0.55907
C	-0.77091	-0.31505	0.70857
N	0.57142	-0.37359	0.65324
C	1.26455	-0.36100	1.81221
C	0.63955	-0.19117	3.04536
C	-0.73880	-0.05815	3.09374
C	-1.45379	-0.14763	1.91199
C	2.72008	-0.63406	1.71679
C	3.52679	-0.67621	2.85025
C	4.85612	-1.05543	2.71840
C	5.32230	-1.41001	1.46483
C	4.47756	-1.32612	0.35199
N	3.20291	-0.90545	0.48214
Mn	1.86058	-0.29202	-1.04927
C	1.48223	-2.06243	-1.46224
O	1.30388	-3.15704	-1.72627
C	5.02776	-1.71106	-0.98621
C	-4.39206	0.71174	-0.93542
C	-6.45949	-1.76019	-0.18791
C	-4.72433	-4.09023	0.53549
C	-1.76366	-3.37918	0.34868
C	0.66965	0.39033	-2.26177
O	0.01567	0.77255	-3.11775
C	2.47328	1.49791	-0.52374
O	0.66149	2.80679	-0.91622
C	3.00627	-0.19040	-2.45497
O	3.61946	-0.07624	-3.41542
O	3.20370	2.30185	-0.18204
O	-1.70864	2.80368	-1.35992
O	-1.97956	5.44358	-0.89773
O	-2.67219	2.63624	1.18122
O	0.14973	2.87045	1.67986
O	-1.53656	5.07907	1.80735
H	-1.82689	0.53056	-0.95057
H	-1.01925	-1.01108	-1.32300
H	3.12969	-0.42520	3.83123
H	-2.54022	-0.07280	1.90868
H	1.21718	-0.17124	3.96651
H	-1.24935	0.09349	4.04589
H	6.34845	-1.75115	1.32366
H	5.51029	-1.09203	3.59116
H	-6.82787	-2.55699	-0.85172
H	-6.87793	-0.80608	-0.53034
H	-6.84337	-1.95975	0.82451
H	5.92589	-2.32735	-0.85391
H	4.30425	-2.28329	-1.57994
H	5.32791	-0.81774	-1.55300

H	-0.59303	2.77985	-1.21937
H	-2.40838	2.66680	0.23646
H	-2.50815	3.55267	1.48462
H	-1.89877	4.49324	-1.15650
H	-2.92955	5.60837	-0.93085
H	0.40979	2.88023	0.71796
H	-0.73816	2.47552	1.64494
H	-0.77345	4.46523	1.82862
H	-1.60908	5.32454	0.86113
H	-1.91491	2.50518	-2.25154
H	-3.92710	0.92905	-1.90854
H	-5.47497	0.85390	-1.03798
H	-4.01616	1.43803	-0.20042
H	-1.72714	-3.60631	1.42482
H	-1.87167	-4.32302	-0.20358
H	-0.81258	-2.91996	0.06346
H	-3.91962	-4.71482	0.93579
H	-5.48792	-3.95295	1.31082
H	-5.17258	-4.58415	-0.33689
H	1.02794	3.64561	-1.22023

3_{C5}⁺(I6-P)

Energy	=	-3017.317066
Enthalpy 0K	=	-3016.741357
Enthalpy 298K	=	-3016.695191
Free Energy 298K	=	-3016.819315
Nimag	=	0 (12.8035 cm ⁻¹)

C	-2.83881	-2.45706	-0.19957
N	-2.82469	-1.13693	-0.45140
C	-4.13141	-0.66871	-0.55174
C	-4.94420	-1.74656	-0.34131
N	-4.11493	-2.83796	-0.12093
C	-1.60479	-0.34547	-0.59065
C	-0.78911	-0.36698	0.68361
N	0.54780	-0.48567	0.62763
C	1.22936	-0.66579	1.78030
C	0.60778	-0.59431	3.02355
C	-0.76176	-0.38242	3.08310
C	-1.47141	-0.30539	1.89834
C	2.66116	-1.02996	1.64593
C	3.41180	-1.42846	2.74815
C	4.71669	-1.86092	2.55480
C	5.21491	-1.90820	1.26464
C	4.42443	-1.48709	0.18968
N	3.17195	-1.02753	0.39276
Mn	1.87539	-0.08325	-0.99492
C	1.51350	-1.74856	-1.76855
O	1.33320	-2.75880	-2.25828
C	5.00435	-1.55826	-1.18861
C	-4.47563	0.74681	-0.84171
C	-6.42572	-1.86844	-0.32457
C	-4.59888	-4.17912	0.16177
C	-1.65293	-3.32454	0.00101
C	0.69037	0.76894	-2.11524
O	0.05304	1.24310	-2.93311

C	2.45520	1.51887	-0.12437
O	0.55447	3.43102	-0.93217
C	3.05595	0.30781	-2.32835
O	3.69008	0.62066	-3.22665
O	2.99674	2.36952	0.39019
O	-1.94027	2.89214	-1.05213
O	-1.46907	5.36796	-0.44997
O	-2.66051	2.47281	1.40254
O	0.13596	2.62048	1.66665
O	-1.47889	4.87502	2.23839
H	-1.87292	0.69969	-0.83528
H	-1.03489	-0.76565	-1.42562
H	2.98557	-1.42220	3.74884
H	-2.55179	-0.17090	1.89924
H	1.17987	-0.70451	3.94219
H	-1.26942	-0.30203	4.04542
H	6.22348	-2.27215	1.06641
H	5.32643	-2.17641	3.40312
H	-6.77580	-2.57547	-1.09211
H	-6.88689	-0.89253	-0.51926
H	-6.78351	-2.22711	0.65280
H	5.89752	-2.19509	-1.18243
H	4.29449	-1.97757	-1.91328
H	5.31822	-0.56126	-1.53002
H	-0.39067	3.11871	-1.11614
H	-2.47233	2.61850	0.42714
H	-2.52448	3.35937	1.78629
H	-1.78473	4.45274	-0.74379
H	-2.05228	6.00335	-0.87856
H	0.33645	2.91767	0.75113
H	-0.79159	2.31845	1.59817
H	-0.74184	4.23635	2.21950
H	-1.49611	5.19173	1.30912
H	-2.43225	2.73692	-1.86403
H	-4.06406	1.06503	-1.81072
H	-5.56653	0.85400	-0.88500
H	-4.08744	1.41909	-0.06319
H	-1.46262	-3.47273	1.07523
H	-1.80848	-4.30514	-0.46645
H	-0.76209	-2.87292	-0.44623
H	-3.75550	-4.83688	0.39251
H	-5.27299	-4.14633	1.02718
H	-5.14004	-4.56972	-0.70985
H	0.41054	4.38428	-0.85067

1_{C2}(I9)

Energy	=	-2710.594123
Enthalpy 0K	=	-2710.128150
Enthalpy 298K	=	-2710.089915
Free Energy 298K	=	-2710.197440
Nimag	=	0 (21.6925 cm ⁻¹)

C	1.38173	3.47729	0.94444
C	1.29788	2.06379	0.84120
N	1.83021	1.39803	-0.23619
C	2.34464	2.13497	-1.27038
C	2.41518	3.51522	-1.21219

C	1.94845	4.20035	-0.07176
C	0.61925	1.24637	1.79227
N	0.61373	-0.12046	1.52642
C	-0.17979	-0.89122	2.35108
C	-0.86845	-0.38712	3.42875
C	-0.78434	0.99214	3.75129
C	-0.04824	1.79205	2.91796
C	-0.34996	-2.36299	2.07772
N	-0.97168	-2.64082	0.77927
C	-1.82105	-1.84236	0.13746
N	-2.18838	-2.43471	-0.99695
C	-1.55358	-3.65109	-1.08445
C	-0.79011	-3.78257	0.03522
C	-3.07936	-1.86398	-1.99725
Mn	1.80735	-0.65963	-0.03993
C	2.09093	-2.36299	0.38157
O	2.40069	-3.47082	0.56753
C	2.79570	1.44077	-2.52183
C	1.12832	-1.18652	-1.60427
O	0.75653	-1.63130	-2.61492
C	3.54378	-0.72074	-0.42781
O	4.67542	-0.79596	-0.68630
H	0.60395	-2.89937	2.10134
H	-0.99045	-2.80119	2.85320
H	0.98830	3.98730	1.82268
H	-1.48833	-1.05696	4.02615
H	0.01026	2.86299	3.10979
H	-1.30699	1.40085	4.61723
H	2.83007	4.06376	-2.05889
H	2.01941	5.28830	-0.00970
H	-1.69760	-4.31407	-1.93274
H	-0.13183	-4.58277	0.36012
H	-3.88933	-1.32293	-1.49408
H	-3.50095	-2.68110	-2.59258
H	-2.52172	-1.18214	-2.65144
H	3.05799	2.18207	-3.28779
H	3.67330	0.80372	-2.35066
H	1.99818	0.79629	-2.91749
H	-2.14706	-0.85799	0.47448
H	-2.24286	1.38928	1.75466
O	-2.67835	1.33319	0.89225
H	-0.23320	0.75987	-1.07806
O	-4.42364	3.21651	-0.49420
H	-3.79818	2.88946	0.17173
H	-4.02857	2.88352	-1.32373
O	-5.01533	0.49930	-0.38952
H	-4.26085	0.50376	0.22573
H	-5.22740	1.45158	-0.40159
O	-0.95672	1.40273	-1.20928
H	-1.96215	1.40640	0.22426
H	-0.50230	2.25353	-1.30529
O	-3.44215	1.52691	-2.50758
H	-2.52913	1.38243	-2.20646
H	-3.97102	0.95728	-1.91848

1c2(TS5)

Energy = -2710.565951

Enthalpy 0K = -2710.103600
 Enthalpy 298K = -2710.067038
 Free Energy 298K = -2710.171027
 Nimag = 1 (-1164.7140 cm⁻¹)

C	3.02627	2.45122	1.03611
C	2.32131	1.25640	0.86615
N	2.65813	0.35015	-0.07482
C	3.75152	0.57101	-0.84234
C	4.49575	1.74428	-0.70427
C	4.12431	2.70246	0.23030
C	1.17756	0.89171	1.72125
N	0.58050	-0.29412	1.44969
C	-0.44323	-0.67086	2.25483
C	-0.90657	0.11647	3.30307
C	-0.30043	1.33942	3.56936
C	0.75970	1.72287	2.76712
C	-1.12424	-1.99130	2.03382
N	-2.22364	-1.91201	1.06740
C	-2.42351	-0.96612	0.14830
N	-3.47181	-1.31470	-0.59343
C	-3.95862	-2.51860	-0.13834
C	-3.17102	-2.89638	0.90492
C	-4.03779	-0.52905	-1.68102
Mn	1.26112	-1.19663	-0.30360
C	0.11468	-2.51136	-0.62638
O	-0.53844	-3.41568	-0.96258
C	4.18613	-0.44999	-1.85047
C	1.05550	-0.81834	-1.99899
O	0.93063	-0.63908	-3.15871
C	2.46995	-2.47119	0.00244
O	3.24137	-3.34292	0.07239
H	-0.40499	-2.74394	1.68855
H	-1.56287	-2.33825	2.97664
H	2.72578	3.17794	1.78792
H	-1.73957	-0.24243	3.90925
H	1.26326	2.66888	2.95650
H	-0.64377	1.97423	4.38747
H	5.36787	1.89632	-1.34146
H	4.69133	3.62892	0.33772
H	-4.81837	-2.99979	-0.59596
H	-3.19414	-3.77914	1.53760
H	-4.77284	0.18328	-1.28538
H	-4.51359	-1.21228	-2.39299
H	-3.23804	0.02671	-2.18292
H	5.13050	-0.13927	-2.31563
H	4.33285	-1.43050	-1.37897
H	3.43291	-0.57883	-2.63909
H	-1.83230	-0.05994	0.01590
H	-1.51147	2.42967	1.60105
O	-1.87346	2.52130	0.71278
H	0.26131	0.15358	-1.06549
O	-2.43984	4.61358	-1.08600
H	-2.09348	4.11987	-0.32101
H	-2.27770	3.98050	-1.81194
O	-4.29800	2.57649	-0.53829
H	-3.58115	2.35209	0.08781

H	-4.04475	3.49341	-0.74802
O	-0.42186	1.37733	-1.04652
H	-1.22750	2.05389	0.08153
H	0.30952	1.97915	-1.23295
O	-2.39074	2.26150	-2.64603
H	-1.63485	1.86992	-2.13801
H	-3.13508	2.19038	-2.02145

1_{C2}(I10)

Energy	=	-2710.591712
Enthalpy 0K	=	-2710.128987
Enthalpy 298K	=	-2710.092155
Free Energy 298K	=	-2710.197831
Nimag	=	0 (16.2577 cm ⁻¹)

C	2.54302	3.26776	0.14896
C	2.18664	1.93092	0.30678
N	2.96016	0.92118	-0.14695
C	4.18202	1.20396	-0.63756
C	4.60327	2.53016	-0.79731
C	3.76486	3.57196	-0.43882
C	0.97710	1.52703	1.06118
N	0.70018	0.20730	1.09259
C	-0.30193	-0.21072	1.88660
C	-1.07825	0.67271	2.63543
C	-0.82455	2.03342	2.56734
C	0.22333	2.46376	1.77066
C	-0.61329	-1.67894	2.01070
N	-1.70583	-2.09148	1.12983
C	-2.22233	-1.38721	0.11685
N	-3.14099	-2.15088	-0.47526
C	-3.21359	-3.36620	0.16861
C	-2.30607	-3.33079	1.18054
C	-3.96496	-1.74434	-1.60383
Mn	1.88802	-0.90536	-0.28809
C	0.79096	-2.27235	-0.62799
O	0.15224	-3.17161	-0.97035
C	5.12842	0.10281	-1.01082
C	2.76914	-1.55046	-1.70175
O	3.22340	-2.00333	-2.66009
C	2.86260	-1.78314	0.98057
O	3.47662	-2.40455	1.72988
H	0.26982	-2.29082	1.79412
H	-0.92766	-1.89295	3.04009
H	1.88475	4.06744	0.48319
H	-1.87539	0.27551	3.26581
H	0.46748	3.52314	1.72225
H	-1.41955	2.74899	3.13759
H	5.59499	2.72364	-1.20885
H	4.06678	4.61081	-0.58356
H	-3.90091	-4.14601	-0.14759
H	-2.02970	-4.07462	1.92241
H	-4.97045	-1.47496	-1.25551
H	-4.02188	-2.57152	-2.32149
H	-3.51291	-0.86819	-2.08210
H	6.16309	0.45616	-0.90788
H	4.99136	-0.78134	-0.37656

H	4.99038	-0.19820	-2.05945
H	-1.95497	-0.32974	-0.19529
H	-3.37966	2.04641	1.71474
O	-3.63286	2.06854	0.78765
H	1.04639	-0.16580	-1.43766
O	-4.82562	3.64298	-1.13656
H	-4.37933	3.33525	-0.32333
H	-4.35931	3.11356	-1.81317
O	-5.70801	1.01474	-0.60132
H	-4.99373	1.15712	0.05715
H	-5.85723	1.94173	-0.85860
O	-1.84899	1.25090	-0.71842
H	-2.79662	1.77008	0.21870
H	-1.01395	1.72631	-0.76746
O	-3.67805	1.51102	-2.57267
H	-2.89184	1.43742	-1.95270
H	-4.39334	1.14040	-2.02595

1_{C2}⁺(I11)

Energy	=	-2329.272994
Enthalpy 0K	=	-2328.925900
Enthalpy 298K	=	-2328.900231
Free Energy 298K	=	-2328.982041
Nimag	=	1 (20.1967 cm ⁻¹)

N	2.63020	0.47464	0.21513
C	2.20554	1.70341	-0.15347
C	3.04639	2.81317	-0.14785
C	4.35305	2.66337	0.30045
C	4.75487	1.42231	0.76411
C	3.87263	0.33547	0.71629
C	0.76458	1.81731	-0.48129
N	0.04395	0.68100	-0.37726
C	-1.29417	0.75422	-0.47953
C	-1.94665	1.94603	-0.79089
C	-1.20027	3.10024	-0.97774
C	0.17324	3.04085	-0.79645
C	-2.09895	-0.50484	-0.23695
N	-3.43647	-0.22554	0.26417
C	-3.73823	0.26407	1.51711
C	-5.09250	0.37793	1.57813
N	-5.58866	-0.04562	0.36401
C	-4.57194	-0.40575	-0.41100
H	-2.96564	0.48524	2.24853
H	-5.74594	0.71737	2.37707
Mn	1.27494	-1.04974	-0.36239
C	0.15700	-2.15852	-1.20439
O	-0.47710	-2.90866	-1.81074
C	4.33779	-0.98847	1.24285
C	2.48630	-2.32857	-0.67435
O	3.20392	-3.17920	-0.97481
C	0.86656	-1.58832	1.33206
O	0.61315	-2.00513	2.37490
H	-4.64806	-0.78267	-1.42855
C	-6.99775	-0.09680	-0.00101
H	-2.21337	-1.07609	-1.16694

H	-1.59214	-1.14222	0.49612
H	2.69132	3.78837	-0.47524
H	-3.03240	1.96900	-0.88440
H	0.77263	3.94402	-0.89226
H	-1.68621	4.04201	-1.23764
H	5.75643	1.27247	1.16982
H	5.03601	3.51471	0.31172
H	5.14606	-0.83486	1.96979
H	3.52455	-1.54017	1.72994
H	4.74134	-1.61363	0.43317
H	1.64827	-0.62196	-1.86663
H	-7.43187	0.90581	0.09492
H	-7.08186	-0.43905	-1.03796
H	-7.52040	-0.79495	0.66441

1_{C2}(I11-R)

Energy	=	-2329.366159
Enthalpy 0K	=	-2329.022727
Enthalpy 298K	=	-2328.996647
Free Energy 298K	=	-2329.080227
Nimag	=	0 (20.8806 cm ⁻¹)

N	2.65244	0.45823	0.18508
C	2.18941	1.70731	-0.18965
C	3.07701	2.82453	-0.20067
C	4.35996	2.67948	0.26067
C	4.77374	1.42670	0.75779
C	3.89586	0.34541	0.69394
C	0.80305	1.81551	-0.48217
N	0.04148	0.66269	-0.34311
C	-1.29856	0.77232	-0.37360
C	-1.96435	1.95869	-0.64675
C	-1.19435	3.11676	-0.91990
C	0.16851	3.04817	-0.82813
C	-2.09063	-0.49196	-0.10196
N	-3.45909	-0.23087	0.32297
C	-3.83694	0.26056	1.55277
C	-5.19269	0.37542	1.53205
N	-5.61369	-0.04765	0.29015
C	-4.54997	-0.40909	-0.42049
H	-3.11036	0.48425	2.32905
H	-5.89389	0.71614	2.28872
Mn	1.28138	-1.05745	-0.37625
C	0.13498	-2.17121	-1.16166
O	-0.52450	-2.93466	-1.72866
C	4.36868	-0.98594	1.20879
C	2.48611	-2.33370	-0.70274
O	3.19901	-3.19062	-1.00714
C	0.92044	-1.58149	1.32581
O	0.69387	-1.98823	2.38132
H	-4.56415	-0.78521	-1.44086
C	-6.99709	-0.09704	-0.16007
H	-2.15157	-1.11609	-1.00130
H	-1.60476	-1.08088	0.68506
H	2.73125	3.79457	-0.55720
H	-3.05300	1.99968	-0.66308

H	0.77077	3.93868	-1.00821
H	-1.68695	4.05586	-1.18228
H	5.77036	1.28699	1.17879
H	5.04570	3.53053	0.26309
H	5.21436	-0.84607	1.89572
H	3.57063	-1.52198	1.73920
H	4.71652	-1.62948	0.38771
H	1.61183	-0.61399	-1.90172
H	-7.43475	0.90661	-0.09545
H	-7.01825	-0.44302	-1.19884
H	-7.56226	-0.79149	0.47386

1_{C2}(I12-R)

Energy	=	-2711.185371
Enthalpy 0K	=	-2710.710700
Enthalpy 298K	=	-2710.672915
Free Energy 298K	=	-2710.779593
Nimag	=	1 (23.1979 cm ⁻¹)

C	-1.00811	-3.76329	-0.23575
N	-1.12719	-2.67299	0.59396
C	-2.06917	-1.86688	0.10859
N	-2.55520	-2.40365	-1.00823
C	-1.90323	-3.59068	-1.24730
C	-0.39431	-2.46824	1.84537
C	-0.19775	-1.01046	2.18218
N	0.54063	-0.22327	1.36850
C	0.62938	1.12909	1.67850
C	0.05315	1.62589	2.89024
C	-0.65905	0.79842	3.71316
C	-0.81803	-0.55944	3.33577
C	1.24204	1.98885	0.72496
C	1.36099	3.39678	0.92325
C	1.81237	4.19461	-0.09502
C	2.14086	3.60623	-1.33224
C	2.07269	2.22244	-1.46769
N	1.67473	1.41745	-0.45704
Mn	1.83374	-0.69881	-0.25614
C	3.29879	-0.40816	0.79414
O	4.24906	-0.25783	1.42170
C	2.43361	1.61811	-2.79309
C	-3.58788	-1.81963	-1.85271
C	1.98324	-2.45752	-0.02466
O	2.20329	-3.59237	0.04083
C	2.80146	-1.06567	-1.71480
O	3.40083	-1.45255	-2.62182
O	-1.13052	1.04305	-1.28189
O	-2.63103	1.31136	0.94862
O	-3.66146	1.52762	-2.36408
O	-5.14854	0.71572	-0.08492
O	-4.26328	3.34888	-0.31910
H	0.55971	-2.99677	1.76059
H	-0.96368	-2.95316	2.64793
H	1.08480	3.84175	1.87816
H	-1.41534	-1.24584	3.93587
H	0.16562	2.67699	3.15234

H	-1.10861	1.17802	4.63287
H	2.45972	4.21414	-2.17962
H	1.90092	5.27437	0.04671
H	-2.13516	-4.20991	-2.10930
H	-0.30545	-4.56654	-0.03630
H	-4.26975	-1.22769	-1.23105
H	-4.14496	-2.63192	-2.33253
H	-3.13261	-1.18122	-2.62030
H	2.45572	2.39458	-3.56909
H	3.43006	1.15471	-2.76086
H	1.70668	0.84858	-3.08792
H	-2.37177	-0.91265	0.54053
H	-2.11491	1.36744	1.76526
H	0.52177	-0.90311	-1.21484
H	-3.62024	2.94981	0.28924
H	-3.98973	2.96554	-1.17525
H	-4.34366	0.65053	0.45932
H	-5.25454	1.68530	-0.10869
H	-1.97522	1.25038	0.21658
H	-0.58449	1.82961	-1.41995
H	-2.75097	1.27369	-2.12957
H	-4.20520	1.03747	-1.72003
H	-0.46630	0.30986	-1.21900

1c2(TS6)

Energy = -2711.159466
 Enthalpy 0K = -2710.689612
 Enthalpy 298K = -2710.653032
 Free Energy 298K = -2710.756643
 Nimag = 1 (-179.1310 cm⁻¹)

C	-0.85150	-3.77049	-0.36555
N	-0.98266	-2.74247	0.54260
C	-1.95650	-1.93004	0.13464
N	-2.44577	-2.39855	-1.00904
C	-1.76907	-3.54862	-1.34618
C	-0.22345	-2.59579	1.78517
C	-0.04482	-1.15587	2.20024
N	0.60331	-0.28779	1.38515
C	0.64810	1.04861	1.76297
C	0.16995	1.44592	3.04874
C	-0.43703	0.54089	3.87291
C	-0.58760	-0.79474	3.41870
C	1.11610	1.98602	0.80132
C	1.14132	3.39058	1.03940
C	1.44455	4.25019	0.01708
C	1.70848	3.72546	-1.26440
C	1.73157	2.34847	-1.44750
N	1.49164	1.48606	-0.43101
Mn	1.76220	-0.59482	-0.33953
C	3.26082	-0.26713	0.63839
O	4.19954	-0.05214	1.25351
C	2.00189	1.81635	-2.82469
C	-3.48266	-1.75603	-1.80174
C	2.06342	-2.36588	-0.18008
O	2.39806	-3.46671	-0.16250

C	2.74921	-0.81198	-1.84707
O	3.40508	-1.09820	-2.74401
O	-1.35223	0.75944	-1.11363
O	-2.59404	1.02417	0.97312
O	-3.58034	1.49603	-2.32607
O	-5.12171	0.74147	0.01913
O	-3.88365	3.25608	-0.18160
H	0.73848	-3.10112	1.65115
H	-0.75932	-3.13565	2.57562
H	0.89983	3.78356	2.02591
H	-1.11933	-1.53550	4.01581
H	0.27316	2.48225	3.36791
H	-0.81576	0.84223	4.85146
H	1.89794	4.38252	-2.11381
H	1.45733	5.32916	0.18759
H	-2.00253	-4.11075	-2.24612
H	-0.12993	-4.57132	-0.23417
H	-4.17224	-1.22727	-1.13343
H	-4.02827	-2.52830	-2.35554
H	-3.03178	-1.03691	-2.49588
H	1.85864	2.61128	-3.56826
H	3.03915	1.46478	-2.92074
H	1.32513	0.98678	-3.07181
H	-2.26653	-1.00056	0.62126
H	-2.02135	1.08677	1.74571
H	0.39518	-1.06346	-1.33232
H	-3.33150	2.67430	0.37472
H	-3.72103	2.87328	-1.06720
H	-4.28691	0.61569	0.51575
H	-5.12925	1.71459	-0.01747
H	-1.96811	0.92680	0.08064
H	-0.76975	1.52353	-1.18562
H	-2.69578	1.19929	-1.96610
H	-4.19787	1.05148	-1.72136
H	-0.02081	-0.38404	-1.10701

1c2(I13-R)

Energy = -2711.164471
 Enthalpy 0K = -2710.691974
 Enthalpy 298K = -2710.654739
 Free Energy 298K = -2710.759747
 Nimag = 0 (24.0364 cm⁻¹)

C	-0.50962	-3.76320	-0.48153
N	-0.75643	-2.77759	0.44924
C	-1.76864	-2.01949	0.02441
N	-2.17020	-2.48905	-1.15472
C	-1.39822	-3.57633	-1.49595
C	-0.05940	-2.61243	1.72452
C	0.01286	-1.16966	2.16128
N	0.59976	-0.24949	1.35624
C	0.50825	1.08556	1.72119
C	-0.02424	1.44711	2.99443
C	-0.54526	0.49228	3.82088
C	-0.57066	-0.85337	3.37219
C	0.90885	2.04864	0.75618

C	0.78222	3.45285	0.95898
C	1.01691	4.31461	-0.07890
C	1.36502	3.78988	-1.34238
C	1.54446	2.42103	-1.48894
N	1.37184	1.56219	-0.45406
Mn	1.88329	-0.46101	-0.29341
C	3.26391	0.03427	0.78715
O	4.12038	0.35574	1.46968
C	1.91172	1.88628	-2.84286
C	-3.21834	-1.89274	-1.97002
C	2.35045	-2.19435	-0.07377
O	2.77986	-3.25800	-0.00391
C	3.01654	-0.56495	-1.71381
O	3.78593	-0.75578	-2.54173
O	-1.50831	0.83100	-1.27552
O	-2.75278	0.59475	0.91379
O	-4.03098	1.36395	-2.23333
O	-5.16586	0.12273	0.05492
O	-4.21858	2.81323	0.21396
H	0.93385	-3.06155	1.62258
H	-0.59397	-3.19429	2.48564
H	0.47563	3.83830	1.93047
H	-1.04852	-1.63406	3.96421
H	-0.02734	2.49251	3.30140
H	-0.96109	0.76150	4.79379
H	1.50159	4.44333	-2.20463
H	0.91070	5.39258	0.06247
H	-1.55116	-4.12539	-2.42093
H	0.26278	-4.51365	-0.34014
H	-3.98317	-1.46182	-1.31292
H	-3.66656	-2.67528	-2.59257
H	-2.79485	-1.10231	-2.60124
H	1.65715	2.62155	-3.61749
H	2.99285	1.69914	-2.91732
H	1.37825	0.95186	-3.06447
H	-2.17103	-1.10293	0.51102
H	-2.34996	0.65754	1.78652
H	0.64570	-1.11624	-1.42074
H	-3.61122	2.13084	0.58479
H	-4.16326	2.60322	-0.73442
H	-4.26806	0.15372	0.49552
H	-5.43051	1.04517	0.19388
H	-1.90945	0.78489	-0.33240
H	-0.91547	1.59014	-1.25249
H	-3.08564	1.20720	-2.02522
H	-4.47928	0.79684	-1.57648
H	0.25689	-0.47686	-1.14185

1_{C2}⁺(I14)

Energy	= -2329.83578878
Enthalpy 0K	= -2329.481846
Enthalpy 298K	= -2329.455155
Free Energy 298K	= -2329.538267
Nimag	= 0 (27.8293 cm ⁻¹)

C	-4.58491	-0.39582	-0.42243
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N	-3.46066	-0.23280	0.27414
C	-3.78070	0.23615	1.52955
C	-5.13548	0.35430	1.57156
N	-5.61351	-0.04513	0.34201
C	-2.11555	-0.50052	-0.21245
C	-1.30598	0.76069	-0.44264
N	0.04317	0.65207	-0.39941
C	0.80163	1.81150	-0.49913
C	0.17162	3.04934	-0.82208
C	-1.18861	3.11866	-0.93155
C	-1.95840	1.95115	-0.69592
C	2.18497	1.70029	-0.18829
N	2.64469	0.44488	0.16903
C	3.88777	0.32332	0.69676
C	4.75238	1.40583	0.78961
C	4.34298	2.66771	0.30965
C	3.06751	2.81781	-0.16617
Mn	1.28900	-1.02625	-0.42677
C	0.89563	-1.45225	1.29337
O	0.65300	-1.68068	2.38632
C	4.36578	-1.01182	1.19239
C	-7.01619	-0.08203	-0.04728
C	0.10577	-2.21403	-1.12368
O	-0.55634	-3.03370	-1.57628
C	2.46748	-2.40215	-0.59907
O	3.11360	-3.33445	-0.75957
H	-3.01914	0.44295	2.27646
H	-5.80053	0.68237	2.36561
H	-4.64613	-0.75346	-1.44780
H	-2.22304	-1.06828	-1.14551
H	-1.62597	-1.14451	0.52709
H	2.72216	3.79288	-0.50755
H	-3.04674	1.99285	-0.72337
H	0.77551	3.94482	-0.96580
H	-1.68062	4.06248	-1.17517
H	5.74296	1.26349	1.22293
H	5.02645	3.51941	0.33879
H	5.20667	-0.87316	1.88450
H	3.57785	-1.56529	1.72020
H	4.73041	-1.63524	0.36300
H	2.08314	-0.49536	-1.98206
H	-7.44567	0.92216	0.05341
H	-7.08509	-0.41092	-1.08959
H	-7.55519	-0.78461	0.60024
H	1.31390	-0.40750	-2.14343

1_{C2}⁺(I11-P)

Energy	= -2711.084269
Enthalpy 0K	= -2710.606350
Enthalpy 298K	= -2710.568586
Free Energy 298K	= -2710.675518
Nimag	= 0 (14.2219 cm ⁻¹)

C	-0.94084	-3.81012	-0.23866
N	-1.00641	-2.71954	0.59860
C	-1.98117	-1.91312	0.17593

N	-2.53350	-2.45026	-0.90893
C	-1.89705	-3.63600	-1.19070
C	-0.19835	-2.55197	1.80592
C	0.00792	-1.11390	2.20666
N	0.63479	-0.24304	1.38806
C	0.71084	1.04826	1.77101
C	0.26978	1.47869	3.02675
C	-0.32004	0.57125	3.88976
C	-0.48389	-0.73630	3.45451
C	1.23533	2.01313	0.77284
C	1.22051	3.38365	1.02272
C	1.62709	4.25717	0.02411
C	2.00902	3.72980	-1.19705
C	2.01292	2.34411	-1.39415
N	1.65183	1.49903	-0.40543
Mn	1.83120	-0.62852	-0.35088
C	3.38255	-0.41465	0.59601
O	4.38149	-0.30928	1.14930
C	2.39358	1.81655	-2.74107
C	-3.61531	-1.87026	-1.69303
C	1.99919	-2.40233	-0.23695
O	2.23518	-3.53265	-0.26018
C	2.67323	-0.93078	-1.90310
O	3.17758	-1.28236	-2.87642
O	-1.20900	1.17889	-1.24590
O	-2.74888	1.37029	0.95947
O	-3.80892	1.45074	-2.30441
O	-5.22595	0.56767	-0.00542
O	-4.56159	3.26193	-0.30006
H	0.75784	-3.05965	1.64599
H	-0.70573	-3.07804	2.62370
H	0.88260	3.77835	1.97780
H	-0.98824	-1.47527	4.07742
H	0.37992	2.51700	3.33149
H	-0.67015	0.88445	4.87434
H	2.30528	4.38083	-2.02020
H	1.62502	5.33485	0.19565
H	-2.18257	-4.25422	-2.03719
H	-0.23001	-4.61591	-0.08218
H	-4.27801	-1.29893	-1.03317
H	-4.17953	-2.68556	-2.15891
H	-3.20655	-1.21409	-2.47165
H	2.43218	2.63770	-3.46754
H	3.38764	1.34856	-2.71446
H	1.66310	1.07487	-3.09160
H	-2.26426	-0.95985	0.62323
H	-2.25297	1.44208	1.78533
H	0.46721	-0.77056	-1.22662
H	-3.88044	2.93477	0.30885
H	-4.26095	2.88747	-1.15080
H	-4.40551	0.58161	0.51919
H	-5.41750	1.52333	-0.04287
H	-2.08226	1.34705	0.23655
H	-0.71976	1.97200	-1.50898
H	-2.88227	1.26678	-2.07159
H	-4.31498	0.93497	-1.64969
H	-0.53728	0.45391	-1.24613

1_{C2}⁺(TS7)

Energy	=	-2711.054803
Enthalpy 0K	=	-2710.582603
Enthalpy 298K	=	-2710.546056
Free Energy 298K	=	-2710.649700
Nimag	=	1 (-430.6366 cm ⁻¹)

C	-1.15459	-3.69104	-0.37252
N	-1.18081	-2.64784	0.52877
C	-2.13684	-1.78938	0.16652
N	-2.71124	-2.24537	-0.94193
C	-2.11330	-3.43161	-1.30176
C	-0.37703	-2.57148	1.74659
C	-0.08442	-1.15912	2.18571
N	0.57917	-0.30169	1.38423
C	0.72794	0.97555	1.79209
C	0.32760	1.39818	3.06220
C	-0.30458	0.50237	3.90832
C	-0.54602	-0.78337	3.44528
C	1.26815	1.93482	0.79690
C	1.31322	3.30005	1.06051
C	1.70573	4.16918	0.05040
C	2.00219	3.64496	-1.19467
C	1.95016	2.26171	-1.40524
N	1.62303	1.42262	-0.40270
Mn	1.72682	-0.68726	-0.37246
C	3.26486	-0.54116	0.61682
O	4.22646	-0.45853	1.22413
C	2.23021	1.73754	-2.77849
C	-3.78171	-1.58248	-1.67304
C	1.87086	-2.48982	-0.26988
O	2.09933	-3.61368	-0.30048
C	2.71170	-0.96131	-1.88144
O	3.34168	-1.28374	-2.78042
O	-1.24761	0.90616	-1.03856
O	-2.56298	1.17529	0.96320
O	-3.48848	1.59787	-2.34471
O	-5.08571	1.12920	0.01246
O	-3.59208	3.51235	-0.28979
H	0.54542	-3.13868	1.58715
H	-0.92358	-3.08194	2.54869
H	1.02898	3.69624	2.03257
H	-1.09021	-1.50626	4.05324
H	0.49459	2.42244	3.38804
H	-0.63005	0.81110	4.90269
H	2.27128	4.29535	-2.02755
H	1.75082	5.24417	0.23248
H	-2.42603	-3.99005	-2.17968
H	-0.47278	-4.53020	-0.26901
H	-4.34379	-0.94069	-0.98486
H	-4.44729	-2.34831	-2.08726
H	-3.36458	-0.96931	-2.48093
H	2.15380	2.55263	-3.50901
H	3.25142	1.33557	-2.84467
H	1.51391	0.95414	-3.05832
H	-2.37881	-0.83927	0.65909
H	-2.06845	1.30905	1.77842

H	0.35180	-1.00877	-1.37915
H	-3.12876	2.87915	0.28994
H	-3.48624	3.07922	-1.15866
H	-4.25502	0.97725	0.51409
H	-5.04991	2.09786	-0.06003
H	-1.86983	1.07478	0.06890
H	-0.75901	1.72249	-1.19440
H	-2.63200	1.27184	-1.96484
H	-4.13736	1.26248	-1.70166
H	-0.00933	-0.30567	-1.11457

1_{C2}⁺(I12-P)

Energy	=	-2711.059391
Enthalpy 0K	=	-2710.583501
Enthalpy 298K	=	-2710.546515
Free Energy 298K	=	-2710.650455
Nimag	=	0 (24.4073 cm ⁻¹)

C	-0.38401	-3.76246	-0.54249
N	-0.65590	-2.79319	0.40028
C	-1.70105	-2.06797	-0.00726
N	-2.09449	-2.54028	-1.18706
C	-1.28797	-3.59651	-1.54573
C	0.03056	-2.63643	1.67881
C	0.07737	-1.20252	2.14678
N	0.57710	-0.23352	1.35470
C	0.45906	1.04909	1.75405
C	-0.02078	1.38960	3.01945
C	-0.45482	0.38615	3.86963
C	-0.44603	-0.92263	3.40666
C	0.79449	2.08278	0.74513
C	0.48025	3.42206	0.95001
C	0.68257	4.32614	-0.08523
C	1.15863	3.85253	-1.29488
C	1.46998	2.49594	-1.44610
N	1.31937	1.63664	-0.41851
Mn	1.89285	-0.38575	-0.31401
C	3.27546	0.09278	0.79463
O	4.13367	0.39239	1.48096
C	1.93535	2.01285	-2.78337
C	-3.18089	-1.98770	-1.98370
C	2.39679	-2.12227	-0.13151
O	2.84548	-3.17533	-0.07851
C	3.06118	-0.43670	-1.72128
O	3.84094	-0.59393	-2.54185
O	-1.50712	0.87874	-1.23814
O	-2.72776	0.48897	0.94870
O	-4.09422	1.20111	-2.20758
O	-5.14371	-0.02465	0.09875
O	-4.21288	2.71153	0.21496
H	1.03525	-3.06191	1.58640
H	-0.49557	-3.23694	2.43092
H	0.05663	3.76349	1.89185
H	-0.84487	-1.73489	4.01483
H	-0.06455	2.42840	3.33941
H	-0.83113	0.62497	4.86536

H	1.28896	4.52117	-2.14624
H	0.44182	5.38218	0.04774
H	-1.43093	-4.14255	-2.47407
H	0.41123	-4.49101	-0.41449
H	-3.93167	-1.55466	-1.31246
H	-3.63417	-2.79715	-2.56691
H	-2.79570	-1.21142	-2.65578
H	1.68753	2.75493	-3.55250
H	3.02718	1.88396	-2.79544
H	1.45647	1.06230	-3.05264
H	-2.13166	-1.17205	0.49843
H	-2.43951	0.58471	1.86236
H	0.68824	-1.03224	-1.46206
H	-3.61281	2.02926	0.59055
H	-4.19746	2.46810	-0.72650
H	-4.24028	0.04682	0.52489
H	-5.46734	0.87417	0.25762
H	-1.89711	0.78510	-0.29931
H	-1.18822	1.78813	-1.27846
H	-3.14741	1.06094	-2.00484
H	-4.53041	0.64365	-1.53320
H	0.29139	-0.39035	-1.19092

1_{C2}²⁺(I13-P)

Energy	=	-2329.728765
Enthalpy 0K	=	-2329.370780
Enthalpy 298K	=	-2329.344672
Free Energy 298K	=	-2329.425926
Nimag	=	1 (28.5382 cm ⁻¹)

N	2.64251	0.47357	0.18433
C	2.20288	1.70587	-0.16264
C	3.03616	2.81870	-0.14863
C	4.34793	2.67041	0.28615
C	4.76375	1.42700	0.72708
C	3.89224	0.33250	0.66975
C	0.75650	1.82092	-0.47268
N	0.03320	0.68274	-0.38602
C	-1.30792	0.75831	-0.47191
C	-1.95864	1.96083	-0.73814
C	-1.21215	3.11700	-0.90697
C	0.16366	3.05114	-0.75061
C	-2.12304	-0.50102	-0.26525
N	-3.45823	-0.22742	0.24064
C	-3.75843	0.22934	1.50702
C	-5.11211	0.34469	1.57044
N	-5.60940	-0.04572	0.34544
C	-4.59483	-0.38758	-0.43938
C	-7.01917	-0.08388	-0.01991
Mn	1.29171	-1.02447	-0.42429
C	2.47802	-2.40928	-0.58024
O	3.12595	-3.33772	-0.73004
C	4.38298	-0.99290	1.16513
C	0.88672	-1.46416	1.31269
O	0.63724	-1.72460	2.39331
C	0.11006	-2.23355	-1.11355

O	-0.54271	-3.06210	-1.55462
H	-2.23964	-1.03953	-1.21505
H	-1.63215	-1.16367	0.45576
H	2.67273	3.79664	-0.45698
H	-3.04532	1.99095	-0.81179
H	0.76265	3.95531	-0.83359
H	-1.69996	4.06602	-1.13444
H	5.76982	1.27887	1.12116
H	5.02448	3.52652	0.30386
H	-5.76471	0.66451	2.37813
H	-2.98536	0.42896	2.24413
H	-7.44869	0.91855	0.09614
H	-7.54365	-0.79262	0.63266
H	-7.10495	-0.40573	-1.06323
H	5.20648	-0.83736	1.87360
H	3.59710	-1.56314	1.67530
H	4.78126	-1.59660	0.33656
H	-4.67205	-0.73822	-1.46623
H	2.08746	-0.53467	-1.95472
H	1.31380	-0.51578	-2.14411