SUPPORTING INFORMATION

Comparison of the Photochemistry of Organometallic N-Heterocyclic Carbene and Phosphine Complexes

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Computational Details.

Calculations used Gaussian 03, Revision C.02[1] for the BP86, BLYP, B3P86, B3LYP, TPSS functionals) and Gaussian 09, Revision A.02[2] for the B97D and M06 functionals. Mn and P were described using SDD RECPs and basis sets[3] with a polarisation function was added for P (ζ = 0.387).[4] 6-31G** basis sets were used for C, N, O, and H atoms.[5] All stationary points computed with the BP86 functional were characterized as minima via analytical frequency calculations. Density functionals were tested by computing the structure of **2-CO** and an agostic structure was located in all cases.

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Computed Structures and Energies

$CpMn(CO)_2(IEt_2Me_2)$

BP86 Energy = -986.822357503
Enthalpy 0K= -986.487492
Enthalpy 298K= -986.464353
Free Energy 298K= -986.539791

Mn	1.42366	0.05154	0.10027
O	1.75259	-1.33914	2.67082
O	1.73098	2.60954	1.51386
N	-1.42439	-1.07335	0.30208
N	-1.46012	1.00930	-0.29162
C	1.56914	-0.78045	1.64066
C	1.54386	1.58519	0.94492
C	-0.57624	-0.00253	0.05504
C	-2.77577	-0.73528	0.12155
C	-2.79811	0.58294	-0.26093
C	-1.07155	2.37867	-0.65946
H	-1.62379	2.65063	-1.57736
H	-0.00216	2.33184	-0.90957
C	-1.31838	3.41354	0.44696
H	-2.38295	3.48028	0.72445
H	-0.99979	4.40864	0.09308
H	-0.73218	3.17063	1.34515
C	-0.99710	-2.43997	0.62796
H	-1.65963	-2.82340	1.42342
H	0.01483	-2.36522	1.04515
C	-1.00754	-3.38481	-0.58272
H	-2.01449	-3.49668	-1.01738
H	-0.65896	-4.38582	-0.27674
H	-0.33671	-3.01219	-1.37245
C	-3.90877	-1.67713	0.38506
H	-4.86882	-1.17056	0.20122
H	-3.91965	-2.02417	1.43459
H	-3.88140	-2.57528	-0.25699
C	-3.95998	1.45462	-0.62152
H	-4.88501	0.85785	-0.64209
H	-3.84153	1.90744	-1.62259
H	-4.11561	2.28071	0.09484
C	2.17847	-1.55042	-1.19771
H	1.98297	-2.61393	-1.06523
C	3.26132	-0.81018	-0.59986
H	4.02256	-1.21537	0.06664
C	3.16927	0.54505	-1.04501
H	3.85003	1.35310	-0.77684
C	2.02914	0.65464	-1.91935
H	1.70553	1.55143	-2.44705
C	1.42179	-0.63910	-1.99577
H	0.52092	-0.88206	-2.56058

$CpMn(CO)_2(PPh_3)$

BP86 Energy = -1226.23997714
Enthalpy 0K= -1225.872738
Enthalpy 298K= -1225.845915
Free Energy 298K= -1225.932008

C	-2.86905	1.43462	0.14264
C	-2.44428	0.85724	1.38550
C	-3.11502	-0.39341	1.55600
C	-3.95239	-0.60698	0.40329
C	-3.79980	0.52090	-0.46238
Mn	-1.90699	-0.47033	-0.25678
C	-1.72924	-0.39675	-2.01095
O	-1.68517	-0.31591	-3.18883
H	-1.73509	1.30424	2.08276
P	0.28154	0.00113	0.02654
C	1.13792	-0.61416	1.57961
C	-1.68382	-2.21949	-0.20665
O	-1.61900	-3.40017	-0.15904
C	0.60195	1.84654	0.07642
H	-3.01949	-1.06844	2.40642
H	-4.58498	-1.47543	0.22119
H	-4.30002	0.65940	-1.42111
H	-2.53668	2.38630	-0.26951
C	1.48931	-0.58603	-1.28066
C	1.03954	2.51534	1.23714
C	1.16898	3.91583	1.24635
C	0.87150	4.66145	0.09631
C	0.43563	4.00211	-1.06677
C	0.29139	2.60697	-1.07490
H	1.28646	1.94325	2.13677
H	1.50793	4.42091	2.15722
H	0.97701	5.75132	0.10373
H	0.20253	4.57588	-1.97009
H	-0.06125	2.10229	-1.98089
C	2.53360	0.22573	-1.77126
C	3.43470	-0.27511	-2.72583
C	3.30703	-1.59068	-3.19651
C	2.27246	-2.40573	-2.70895
C	1.36716	-1.90812	-1.75993
H	2.64107	1.25544	-1.41720
H	4.23689	0.36910	-3.10167
H	4.00825	-1.97869	-3.94274
H	2.16259	-3.43289	-3.07205
H	0.56464	-2.55339	-1.39195
C	2.53187	-0.47859	1.76165
C	3.14341	-0.95516	2.93060
C	2.37302	-1.57852	3.92779
C	0.98929	-1.72658	3.74952
C	0.37597	-1.24733	2.57976
H	3.14228	-0.01027	0.98247
H	4.22558	-0.84668	3.05984
H	2.85396	-1.95539	4.83659
H	0.38515	-2.22280	4.51648
H	-0.69861	-1.37874	2.42133

$CpMn(CO)(IEt_2Me_2)$

BP86 Energy = -873.427414353
Enthalpy 0K= -873.102841
Enthalpy 298K= -873.082038
Free Energy 298K= -873.151635

C	-1.66475	0.64847	-1.80778
C	-2.22092	1.48373	-0.77922

C	-3.25127	0.71698	-0.11834
C	-3.31223	-0.58204	-0.71940
C	-2.32658	-0.61196	-1.77895
Mn	-1.39839	-0.23653	0.16002
C	0.53613	-0.11698	0.06299
N	1.47514	0.89044	0.17301
C	2.79005	0.40239	0.04019
C	2.68720	-0.95451	-0.16314
N	1.31434	-1.24411	-0.14096
C	1.12057	2.28524	0.44893
C	1.15565	3.18789	-0.79259
C	0.68173	-2.54953	-0.31557
C	-0.56111	-2.66784	0.56888
C	4.00389	1.26776	0.16518
C	3.74368	-1.99479	-0.36099
H	-0.84806	0.91782	-2.47923
C	-1.47645	0.16365	1.86792
O	-1.59103	0.50267	3.00398
H	1.41565	-3.32873	-0.04456
H	0.41173	-2.70054	-1.37878
H	-0.32222	-2.52138	1.63105
H	-1.00634	-3.67155	0.44584
H	-1.46414	-2.01765	0.28925
H	1.80198	2.67090	1.22825
H	0.10325	2.24861	0.87049
H	2.16041	3.23425	-1.24479
H	0.86229	4.21541	-0.51742
H	0.45283	2.82240	-1.55805
H	4.91536	0.65794	0.06544
H	4.05410	1.77225	1.14773
H	4.04702	2.05489	-0.60923
H	4.74101	-1.52788	-0.36702
H	3.62621	-2.53294	-1.31953
H	3.74217	-2.75253	0.44473
H	-1.96601	2.52407	-0.57829
H	-3.87570	1.06911	0.70342
H	-4.01199	-1.37799	-0.46274
H	-2.11158	-1.45978	-2.43186

CpMn(CO)(PPh_3)

BP86 Energy = -1112.83201779
Enthalpy 0K= -1112.475497
Enthalpy 298K= -1112.450583
Free Energy 298K= -1112.532867

C	-1.73882	1.51903	-2.07967
C	-2.13879	2.14403	-0.84225
C	-3.36539	1.52069	-0.42753
C	-3.74400	0.54342	-1.39838
C	-2.72404	0.53595	-2.42389
Mn	-1.81997	0.03741	-0.59381
C	-1.96451	-1.68082	-0.97379
O	-2.14273	-2.80362	-1.31844
H	-1.60896	2.94075	-0.32078
P	0.35584	0.00581	-0.04919
C	-0.02684	-0.66532	1.63721
C	1.25996	1.61324	0.23916
H	-3.91562	1.74655	0.48883
H	-4.62894	-0.09151	-1.36302
H	-2.71010	-0.10090	-3.30846
H	-0.85313	1.76375	-2.66612
C	1.71575	-1.08489	-0.71807
C	1.26908	2.24905	1.49779
C	1.87283	3.50792	1.65313
C	2.47236	4.14583	0.55530
C	2.46892	3.51830	-0.70188
C	1.86633	2.26099	-0.86033
H	0.80783	1.75460	2.35902
H	1.87784	3.98807	2.63762
H	2.94317	5.12669	0.67856
H	2.93850	4.00752	-1.56198
H	1.87934	1.77382	-1.84198
C	3.05954	-0.92918	-0.31149
C	4.05243	-1.78805	-0.80778
C	3.71491	-2.80403	-1.71785
C	2.38191	-2.95919	-2.12992
C	1.38475	-2.10274	-1.63531
H	3.33159	-0.12766	0.38336
H	5.09179	-1.66004	-0.48662
H	4.49157	-3.47076	-2.10742
H	2.11399	-3.74733	-2.84143
H	0.34548	-2.22750	-1.95276
C	0.76596	-1.42833	2.51015
C	0.19306	-1.97196	3.67454
C	-1.17133	-1.78216	3.95157
C	-1.98285	-1.05285	3.06368
C	-1.40661	-0.49840	1.91121
H	1.82067	-1.60707	2.27603
H	0.81377	-2.55285	4.36500
H	-1.60956	-2.21443	4.85717
H	-3.05103	-0.92418	3.26466
H	-2.06230	0.16579	1.27740

CpMn(CO)$_2$

BP86 Energy = -524.668040712
Enthalpy 0K= -524.569227
Enthalpy 298K= -524.560016
Free Energy 298K= -524.604670

Mn	0.13323	-0.00000	-0.40371
C	1.31476	1.29949	-0.13033
C	-2.00095	-0.00002	-0.81786
H	-2.40833	-0.00003	-1.83195
C	-1.65538	-1.16685	-0.06793
H	-1.80986	-2.20130	-0.37252
C	-1.05949	-0.71746	1.17007
H	-0.68579	-1.35449	1.97151
C	-1.05950	0.71745	1.17007
H	-0.68580	1.35449	1.97149
C	-1.65539	1.16683	-0.06794
H	-1.80988	2.20127	-0.37254
C	1.31479	-1.29947	-0.13033
O	2.05472	2.18023	0.12326
O	2.05478	-2.18018	0.12326

CpMn(CO)(IEt$_2$Me$_2$)(*c*-C$_5$H$_{10}$)

BP86 Energy = -1069.97389829
Enthalpy 0K= -1069.511557
Enthalpy 298K= -1069.483410
Free Energy 298K= -1069.572938

Mn	0.61260	-0.89223	0.60790
C	2.08771	0.90075	-0.98994
O	0.88604	-2.88773	-1.53375
N	-1.41221	1.35069	0.22257
N	-2.22252	-0.52251	-0.50565
H	1.99827	0.11813	-0.16781
C	0.73090	-2.02365	-0.72391
C	-1.06902	0.00675	0.06436
C	-2.70655	1.63524	-0.24406
C	-3.22114	0.44488	-0.69662
C	-2.40793	-1.93852	-0.85105
H	-3.40865	-2.24389	-0.49495
H	-1.65522	-2.49116	-0.26977
C	-2.25381	-2.23631	-2.34881
H	-2.98138	-1.67732	-2.96070
H	-2.41663	-3.31260	-2.52770
H	-1.23770	-1.98932	-2.68922
C	-0.54958	2.34598	0.86448
H	-0.49406	3.24055	0.21709
H	0.45236	1.89308	0.90474
C	-0.99806	2.73604	2.28093
H	-1.98941	3.21688	2.29066
H	-0.27680	3.44918	2.71593
H	-1.04206	1.84913	2.93245
C	-3.30701	3.00631	-0.25901
H	-4.25158	2.99681	-0.82500
H	-2.64253	3.74147	-0.74850
H	-3.53386	3.39303	0.75118
C	-4.57493	0.14180	-1.25792
H	-5.19346	1.05278	-1.26468
H	-5.11268	-0.61271	-0.65474
H	-4.53266	-0.23922	-2.29364
C	1.10368	-0.21934	2.61902
H	1.21777	0.80679	2.96944
C	2.15246	-1.05725	2.07915
H	3.19661	-0.77165	1.94208
C	1.59534	-2.34498	1.80964
H	2.13313	-3.20265	1.40443
C	0.19082	-2.30874	2.14268
H	-0.51207	-3.13829	2.06644
C	-0.09638	-0.99475	2.64201
H	-1.07864	-0.64718	2.96593
C	2.93027	2.09739	-0.45003
C	2.91987	0.26865	-2.14880
H	1.08586	1.20777	-1.31865
C	4.07320	1.26579	-2.41206
H	3.32813	-0.70552	-1.82717
H	2.30761	0.07266	-3.04397
C	4.34828	1.87348	-1.02198
H	2.52171	3.04899	-0.83889
H	2.92027	2.16798	0.65124
H	4.95890	0.78739	-2.86398
H	3.74161	2.06323	-3.10452
H	4.89658	1.14187	-0.39816
H	4.95169	2.79698	-1.05421

CpMn(CO)(PPh_3)(*c*-C_5H_{10})

BP86 Energy = -1309.39304760
Enthalpy 0K= -1308.897492
Enthalpy 298K= -1308.865997
Free Energy 298K= -1308.963506

C	-0.69378	-2.65285	1.42980
C	0.36093	-2.95580	0.49240
C	-0.24175	-3.45971	-0.70785
C	-1.67399	-3.46624	-0.52409
C	-1.93411	-2.96449	0.78543
Mn	-0.86249	-1.46662	-0.37645
H	-2.20085	-0.19522	-0.53696
C	-2.95500	0.02969	0.28772
H	1.43092	-2.86260	0.68127
P	0.70430	0.08711	0.02158
C	2.32370	-0.04333	-0.93006
C	-0.87676	-1.17129	-2.10809
O	-0.88299	-1.07980	-3.29530
C	1.30627	0.14792	1.80143
H	0.28576	-3.79843	-1.60031
H	-2.41638	-3.78640	-1.25461
H	-2.92696	-2.80569	1.20940
H	-0.56415	-2.26545	2.43964
C	0.31154	1.89321	-0.34220
C	2.61495	-0.20924	2.18444
C	2.97755	-0.25087	3.54273
C	2.04318	0.07497	4.53646
C	0.73493	0.43403	4.16710
C	0.36777	0.45697	2.81344
H	3.35819	-0.45474	1.42001
H	3.99777	-0.53713	3.82037
H	2.32858	0.04661	5.59324
H	-0.00323	0.68983	4.93502
H	-0.66012	0.71653	2.53571
C	0.45429	2.93855	0.59309
C	0.13727	4.26166	0.23799
C	-0.31602	4.55869	-1.05610
C	-0.45054	3.52442	-1.99820
C	-0.14469	2.20158	-1.64455
H	0.81695	2.72486	1.60310
H	0.25293	5.06173	0.97745
H	-0.55960	5.59023	-1.33159
H	-0.79637	3.74600	-3.01360
H	-0.25275	1.40542	-2.38835
C	3.29404	0.98155	-0.87318
C	4.49452	0.86456	-1.58933
C	4.73874	-0.27426	-2.37667
C	3.77606	-1.29249	-2.44624
C	2.57466	-1.17657	-1.72639
H	3.10504	1.87871	-0.27405
H	5.23799	1.66741	-1.53841
H	5.67384	-0.36137	-2.94014
H	3.95406	-2.17666	-3.06769
H	1.80937	-1.95517	-1.79360
C	-3.16442	1.57457	0.31240

C	-4.33400	-0.59315	-0.10402
H	-2.60754	-0.33598	1.26379
C	-5.24809	0.61085	-0.43959
H	-4.24248	-1.30405	-0.94134
H	-4.74976	-1.15364	0.75305
C	-4.69299	1.74752	0.44208
H	-2.59544	2.06684	1.11800
H	-2.81985	2.02289	-0.63572
H	-5.13697	0.88462	-1.50556
H	-6.31671	0.39926	-0.26496
H	-5.03735	2.74979	0.13464
H	-5.00876	1.59638	1.49250

$CpMn(CO)_2(c\text{-}C_5H_{10})$

BP86 Energy = -721.238333764
Enthalpy 0K= -721.001422
Enthalpy 298K= -720.985599
Free Energy 298K= -721.047624

Mn	-0.86878	0.10762	0.02025
C	-0.90544	1.48177	-1.09882
C	-1.11386	-2.04677	-0.27738
H	-0.28003	-2.72725	-0.45790
C	-1.61284	-1.67625	1.01097
H	-1.27143	-2.05869	1.97209
C	-2.65899	-0.70543	0.80008
H	-3.25118	-0.22164	1.57686
C	-2.79635	-0.49462	-0.61081
H	-3.51066	0.17523	-1.08921
C	-1.83655	-1.33755	-1.28435
H	-1.69097	-1.41433	-2.36146
C	-0.74970	1.16556	1.43392
H	0.87852	-0.03328	0.37540
O	-1.01223	2.38258	-1.85265
O	-0.74930	1.85077	2.39465
C	1.63875	-0.23212	-0.46198
H	1.16928	-0.41221	-1.43722
C	2.59941	0.99355	-0.49769
C	2.48543	-1.45199	0.02934
C	3.81681	0.55782	0.34595
H	2.91246	1.18254	-1.54059
H	2.11979	1.91481	-0.13060
C	3.94890	-0.94526	0.02730
H	2.18884	-1.73653	1.05499
H	2.34342	-2.34275	-0.60565
H	3.60156	0.69540	1.42268
H	4.72822	1.13476	0.11582
H	4.58770	-1.49216	0.74118
H	4.39276	-1.07349	-0.97785

Functional Tests on $CpMn(CO)_2(IEt_2Me_2)$

(i) BLYP

Energy = -872.955150918

C	-1.76266	0.66653	-1.82760
C	-2.30350	1.49169	-0.78049
C	-3.30841	0.70951	-0.09710
C	-3.36583	-0.58984	-0.69993
C	-2.40473	-0.60444	-1.78197
Mn	-1.40524	-0.23298	0.17261
C	0.56044	-0.11356	0.05652
N	1.48971	0.90730	0.17645
C	2.81620	0.43319	0.04231
C	2.72996	-0.92300	-0.17214
N	1.35416	-1.23519	-0.15447
C	1.11894	2.30589	0.46041
C	1.13584	3.21906	-0.78270
C	0.75778	-2.56182	-0.37458
C	-0.47348	-2.78375	0.51722
C	4.02512	1.31513	0.17365
C	3.80655	-1.94947	-0.38009
H	-0.97245	0.95091	-2.52095
C	-1.48585	0.11777	1.90616
O	-1.60998	0.41443	3.05383
H	1.52229	-3.32144	-0.15002
H	0.48056	-2.67479	-1.43859
H	-0.22657	-2.69591	1.58293
H	-0.88677	-3.78884	0.33057
H	-1.35775	-2.11518	0.29478
H	1.80258	2.69562	1.23259
H	0.10831	2.26264	0.88861
H	2.13619	3.28155	-1.23872
H	0.83135	4.23929	-0.49766
H	0.43411	2.85087	-1.54526
H	4.94290	0.71812	0.07393
H	4.06686	1.81667	1.15637
H	4.06007	2.10453	-0.59655
H	4.79570	-1.46968	-0.37460
H	3.70207	-2.47557	-1.34526
H	3.81181	-2.71806	0.41321
H	-2.06155	2.53430	-0.58681
H	-3.91989	1.05264	0.73556
H	-4.04719	-1.39451	-0.42976
H	-2.19709	-1.44628	-2.44205

(ii) B3P86

Energy = -876.086438079

C	-1.66132	0.70281	-1.76922
C	-2.24029	1.49079	-0.73567
C	-3.25201	0.69449	-0.11552
C	-3.29011	-0.57115	-0.75567
C	-2.29903	-0.55789	-1.78864
Mn	-1.38946	-0.25212	0.15666
C	0.55133	-0.12540	0.06902
N	1.45710	0.88757	0.18485
C	2.76950	0.43184	0.04587
C	2.69238	-0.91055	-0.16617
N	1.33656	-1.22362	-0.14202
C	1.08008	2.25992	0.47717
C	1.09661	3.17071	-0.74309
C	0.74705	-2.53296	-0.34119
C	-0.51318	-2.68972	0.49038
C	3.95805	1.31518	0.17453

C	3.75876	-1.92461	-0.37419
H	-0.85023	1.00248	-2.41983
C	-1.49018	0.08017	1.87218
O	-1.62231	0.37637	2.99943
H	1.48193	-3.28917	-0.04868
H	0.52303	-2.68474	-1.40498
H	-0.32147	-2.52419	1.55009
H	-0.91316	-3.70149	0.36654
H	-1.38833	-2.06944	0.15359
H	1.74962	2.64529	1.25375
H	0.07315	2.20306	0.89659
H	2.09054	3.23586	-1.19481
H	0.79226	4.18212	-0.45731
H	0.40139	2.80707	-1.50320
H	4.87381	0.73015	0.06777
H	3.99771	1.80641	1.15356
H	3.97984	2.10201	-0.58723
H	4.73929	-1.44436	-0.38419
H	3.64317	-2.45405	-1.32686
H	3.77282	-2.67851	0.42191
H	-2.00275	2.51798	-0.49721
H	-3.88562	1.00695	0.70376
H	-3.97119	-1.37978	-0.52740
H	-2.07228	-1.37103	-2.46633

(iii) B3LYP

Energy = -873.329028983

C	-1.75342	0.71923	-1.78752
C	-2.33398	1.49588	-0.74267
C	-3.31980	0.67732	-0.10554
C	-3.33925	-0.59165	-0.74506
C	-2.36306	-0.55848	-1.79416
Mn	-1.39822	-0.24920	0.17239
C	0.57609	-0.12147	0.06374
N	1.47462	0.90296	0.18747
C	2.79764	0.45810	0.04611
C	2.73335	-0.88490	-0.17602
N	1.37362	-1.21583	-0.15506
C	1.08359	2.28054	0.48310
C	1.08433	3.19752	-0.74242
C	0.81073	-2.54189	-0.39023
C	-0.43167	-2.78739	0.45985
C	3.98405	1.35522	0.18110
C	3.81746	-1.88851	-0.39332
H	-0.96376	1.03954	-2.45469
C	-1.49710	0.05254	1.91094
O	-1.63286	0.31824	3.04638
H	1.57541	-3.28432	-0.14543
H	0.56877	-2.65811	-1.45477
H	-0.22291	-2.67126	1.52396
H	-0.80032	-3.80391	0.28523
H	-1.30875	-2.15635	0.18426
H	1.75589	2.67226	1.25414
H	0.08066	2.21915	0.90884
H	2.07600	3.27596	-1.19817
H	0.76917	4.20488	-0.45081
H	0.38931	2.82789	-1.50025
H	4.90587	0.77967	0.07121
H	4.01872	1.84181	1.16330
H	3.99863	2.14728	-0.57612
H	4.79275	-1.39684	-0.39372
H	3.71221	-2.40841	-1.35325
H	3.83767	-2.65286	0.39351
H	-2.11561	2.52855	-0.50913
H	-3.94937	0.97754	0.72164
H	-3.99966	-1.41469	-0.50670
H	-2.13348	-1.36605	-2.47802

(iv) Energy = -873.463915638

C	-1.65275	0.65766	-1.79460
C	-2.23198	1.47763	-0.77150
C	-3.25910	0.69484	-0.13120
C	-3.29566	-0.59836	-0.73949
C	-2.29683	-0.61017	-1.78297
Mn	-1.40621	-0.23992	0.15035
C	0.54214	-0.12269	0.05872
N	1.47245	0.88909	0.16757
C	2.78998	0.41053	0.04251
C	2.69775	-0.94312	-0.15599
N	1.32783	-1.24218	-0.13856
C	1.10008	2.28007	0.45465
C	1.15021	3.19482	-0.77758
C	0.70613	-2.55655	-0.30683
C	-0.54456	-2.66593	0.56772
C	3.99744	1.28694	0.16745
C	3.76078	-1.97940	-0.34770
H	-0.83391	0.93882	-2.44834
C	-1.50140	0.15737	1.86741
O	-1.63232	0.49812	2.99788
H	1.43753	-3.32106	-0.01594
H	0.45085	-2.71671	-1.36492
H	-0.32010	-2.47330	1.61910
H	-0.97006	-3.67489	0.47705
H	-1.43139	-2.03650	0.23935
H	1.76328	2.65861	1.24383
H	0.08095	2.22540	0.85217
H	2.15878	3.25469	-1.20450
H	0.84205	4.20997	-0.49570
H	0.46939	2.83088	-1.55476
H	4.90733	0.68092	0.10031
H	4.02191	1.81200	1.13317
H	4.04671	2.04884	-0.62306
H	4.74953	-1.50829	-0.34840
H	3.64709	-2.51374	-1.30198
H	3.75382	-2.73101	0.45550
H	-1.99345	2.51361	-0.56050
H	-3.89179	1.02977	0.68336
H	-3.98417	-1.40032	-0.49671
H	-2.06572	-1.44480	-2.43743

(v) M06

Energy = -872.753741160

C	-1.62300	0.60171	-1.78668

C	-2.20281	1.43563	-0.78804
C	-3.23767	0.67792	-0.15342
C	-3.27581	-0.61463	-0.73628
C	-2.27001	-0.65202	-1.75785
Mn	-1.39964	-0.25303	0.16110
C	0.54407	-0.12460	0.09112
N	1.44414	0.89508	0.18969
C	2.76033	0.44366	0.04515
C	2.69047	-0.89863	-0.14640
N	1.33460	-1.22376	-0.10616
C	1.06422	2.27746	0.43072
C	1.03535	3.11033	-0.83767
C	0.75126	-2.53945	-0.28471
C	-0.48052	-2.70711	0.58069
C	3.93742	1.33928	0.15583
C	3.75650	-1.90944	-0.34776
H	-0.78904	0.86320	-2.43011
C	-1.49157	0.18795	1.86340
O	-1.61887	0.57870	2.96232
H	1.50461	-3.28956	-0.01345
H	0.49957	-2.69659	-1.34507
H	-0.25963	-2.52086	1.63447
H	-0.86622	-3.72858	0.48493
H	-1.37099	-2.09797	0.26799
H	1.75913	2.70612	1.16460
H	0.07150	2.24062	0.89326
H	2.01841	3.15301	-1.32108
H	0.72488	4.13701	-0.61522
H	0.32586	2.68735	-1.55736
H	4.86063	0.77197	0.00454
H	4.00312	1.80987	1.14568
H	3.92257	2.14627	-0.58787
H	4.73673	-1.42562	-0.39243
H	3.62264	-2.46710	-1.28398
H	3.79194	-2.64324	0.46861
H	-1.95096	2.47038	-0.58420
H	-3.87222	1.02950	0.65225
H	-3.96261	-1.41280	-0.48033
H	-2.02872	-1.50450	-2.38467

(vi) B97D

Energy = -873.060997980

C	-1.57975	0.62553	-1.80432
C	-2.13275	1.47466	-0.78756
C	-3.20908	0.74475	-0.16312
C	-3.29177	-0.55086	-0.76243
C	-2.27771	-0.61065	-1.79001
Mn	-1.39441	-0.25503	0.16987
C	0.52782	-0.13561	0.10073
N	1.42918	0.89395	0.21962
C	2.75294	0.45470	0.06127
C	2.69281	-0.89747	-0.15613
N	1.33399	-1.23487	-0.12027
C	1.02503	2.27599	0.47272
C	1.01488	3.12704	-0.80620
C	0.74913	-2.55646	-0.33236
C	-0.51389	-2.72857	0.51989
C	3.93303	1.36540	0.17882
C	3.78014	-1.90026	-0.37491
H	-0.72444	0.85889	-2.43227
C	-1.49917	0.10696	1.87930
O	-1.62128	0.43136	3.01590
H	1.50014	-3.31094	-0.05650
H	0.50709	-2.69147	-1.40056
H	-0.30529	-2.56177	1.58155
H	-0.92009	-3.74200	0.38342
H	-1.39454	-2.08469	0.20292
H	1.71019	2.70582	1.21896
H	0.01831	2.21484	0.90442
H	2.01352	3.17412	-1.26451
H	0.69374	4.15349	-0.57271
H	0.31701	2.69901	-1.53719
H	4.86119	0.79304	0.05005
H	3.97195	1.85329	1.16684
H	3.91792	2.16421	-0.58014
H	4.75669	-1.39816	-0.37783
H	3.66662	-2.42604	-1.33752
H	3.79810	-2.66615	0.41876
H	-1.83801	2.49563	-0.56866
H	-3.83096	1.11058	0.64879
H	-4.00887	-1.32881	-0.51783
H	-2.05192	-1.47264	-2.41335