Electronic Supplementary Information

Mechanism of nickel-catalyzed direct carbonyl-Heck coupling reaction: the crucial role of second-sphere interactions

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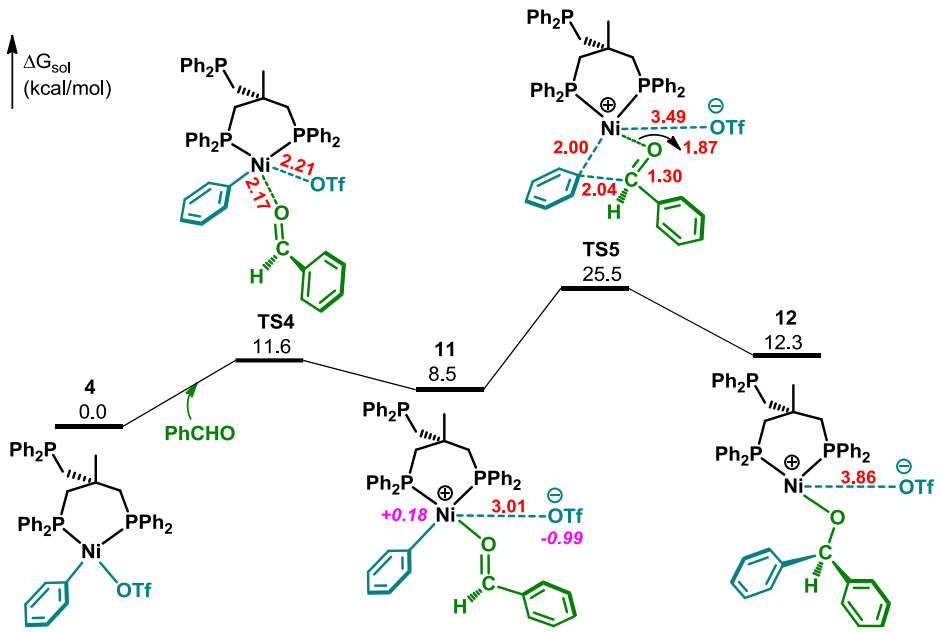

Fig. S1 Free energy profile for benzaldehyde ligation and insertion obtained with M06/6-311++G(d,p)–SDD/SMD(toluene)//M06/6-31G(d)–SDD for benchmarking with Fig. 3. The structures and relative energies are consistent with those shown in Fig. 3.

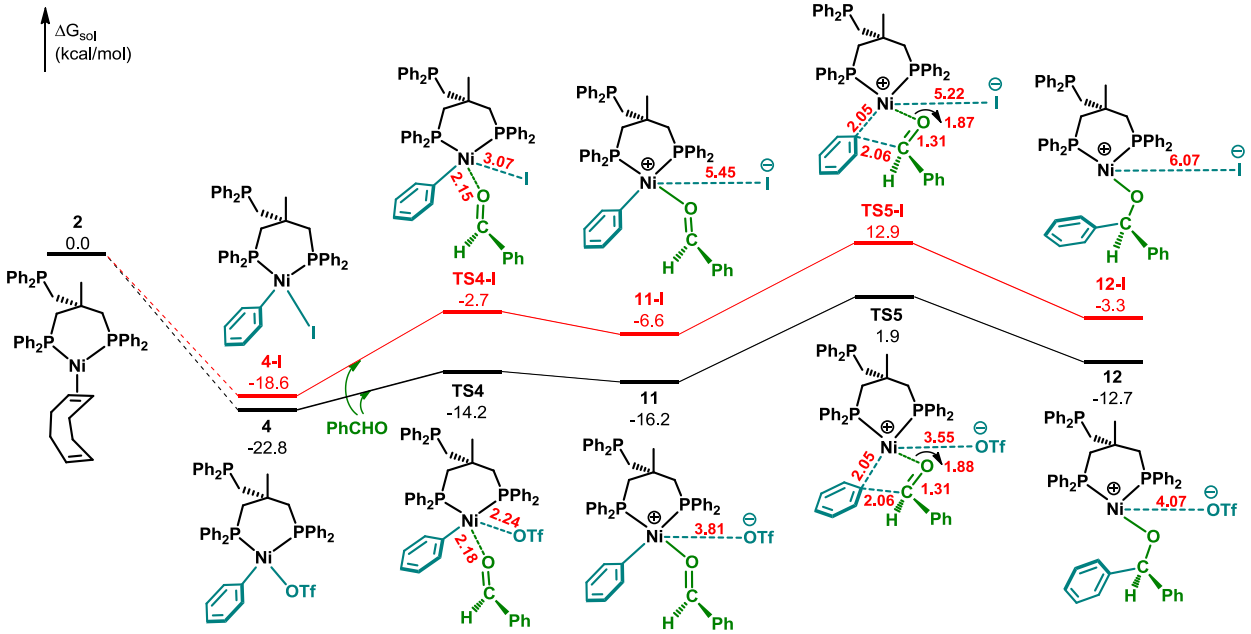

Fig. S2 Free energy profile for the pathways in Fig. 6 computed with reoptimization including the solvent correction. These M06/BS2/SMD(toluene)//B3LYP/BS1/SMD(toluene) outcomes are consistent with the M06/BS2/SMD(toluene)//B3LYP/BS1 results shown in Fig. 6.

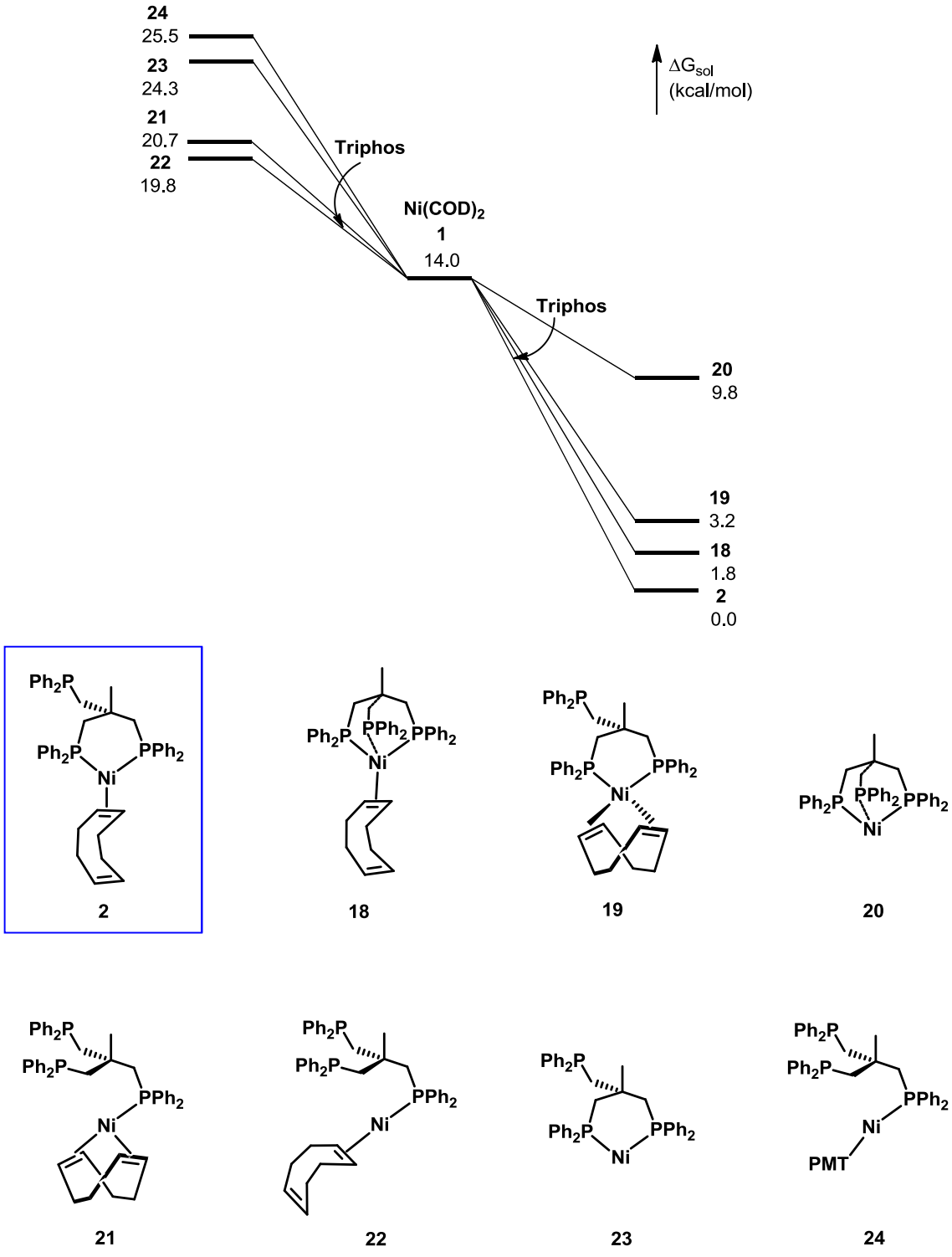

Fig. S3 Free energy profile for the precatalyst reacting with Triphos to form various possible products.

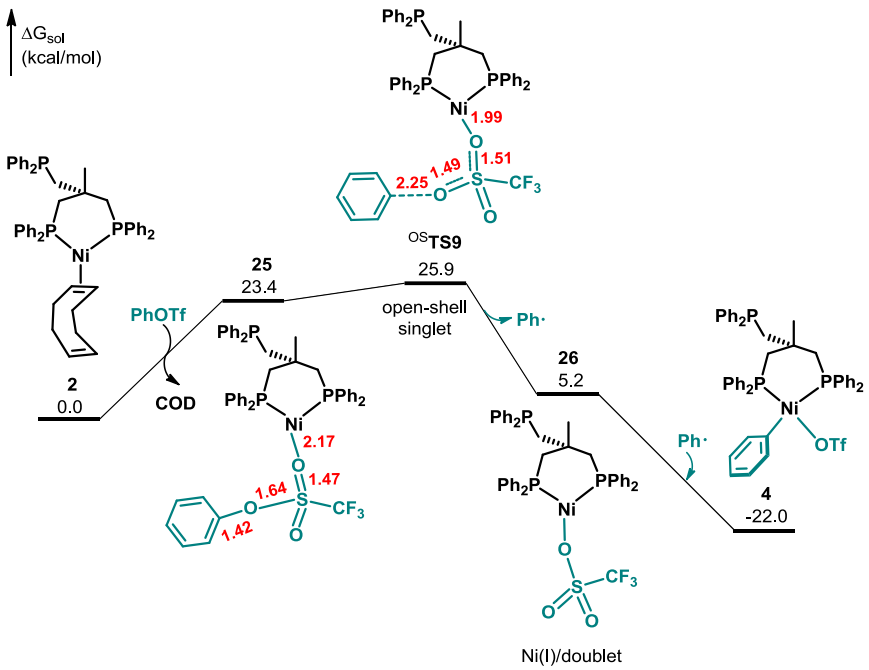

Fig. S4 Free energy profile for the disfavored SET pathway of oxidative addition. ^{OS}**TS9** is 12.4 kcal/mol higher than **TS1** of the two-electron concerted oxidative addition shown in Fig. 1.

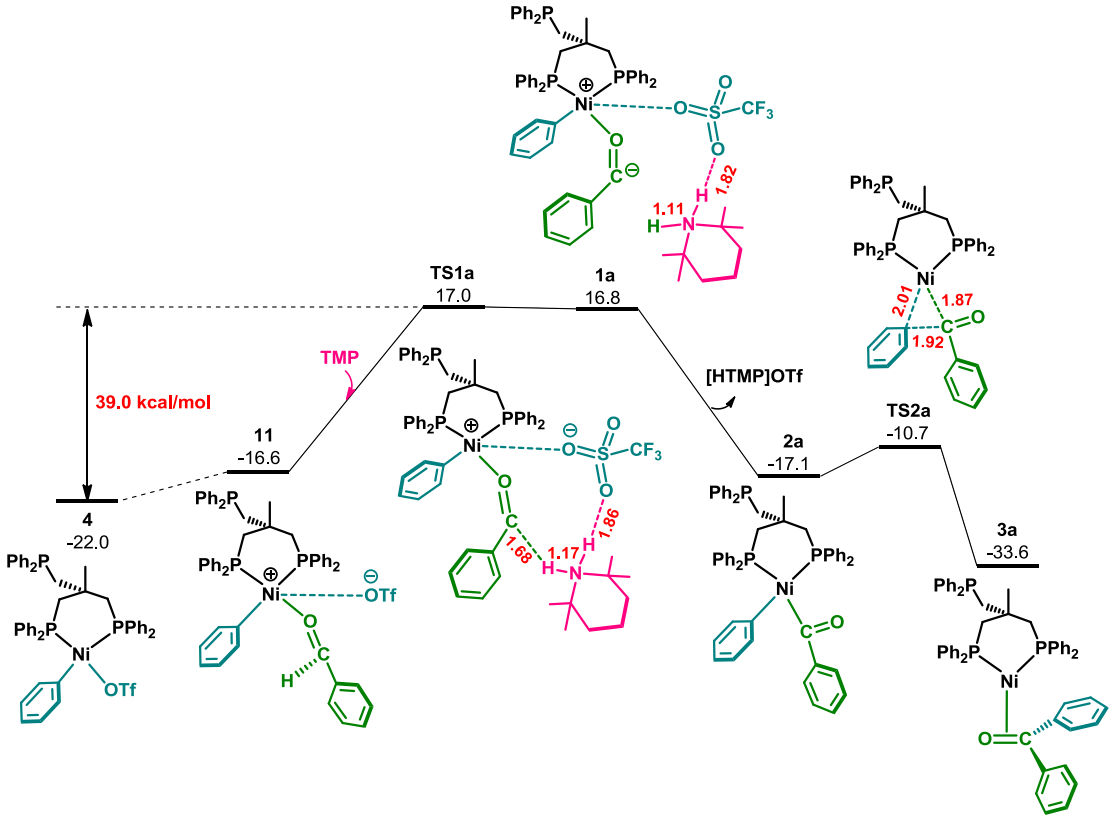

Fig. S5 Free energy profile for the disfavored C–H activation pathway. The energy span from **4** to **TS1a** is 39.0 kcal/mol, a much higher barrier than 25.7 kcal/mol of the favorable pathway (i.e., **TS5** – **4** in Fig. 3).

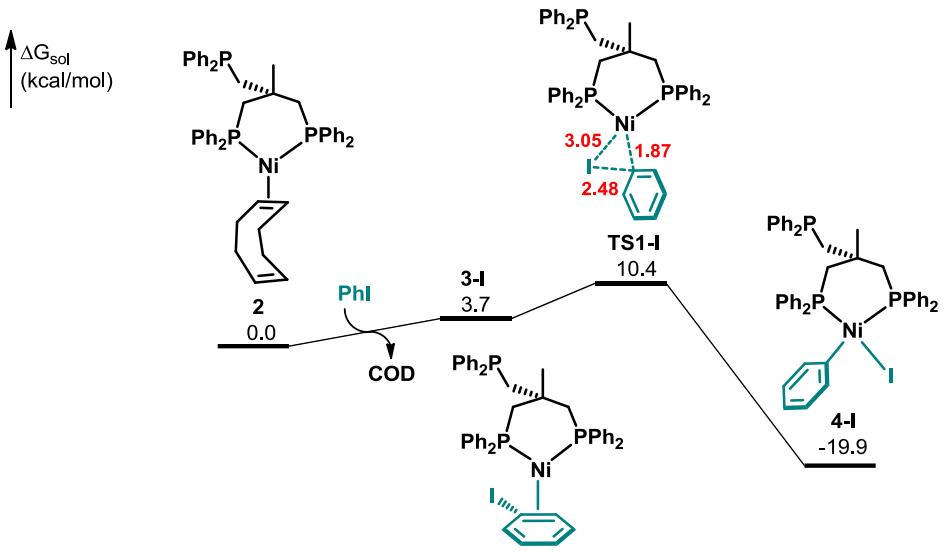

Fig. S6 Free energy profile for the reaction using PhI as substrate: part A (oxidative addition).

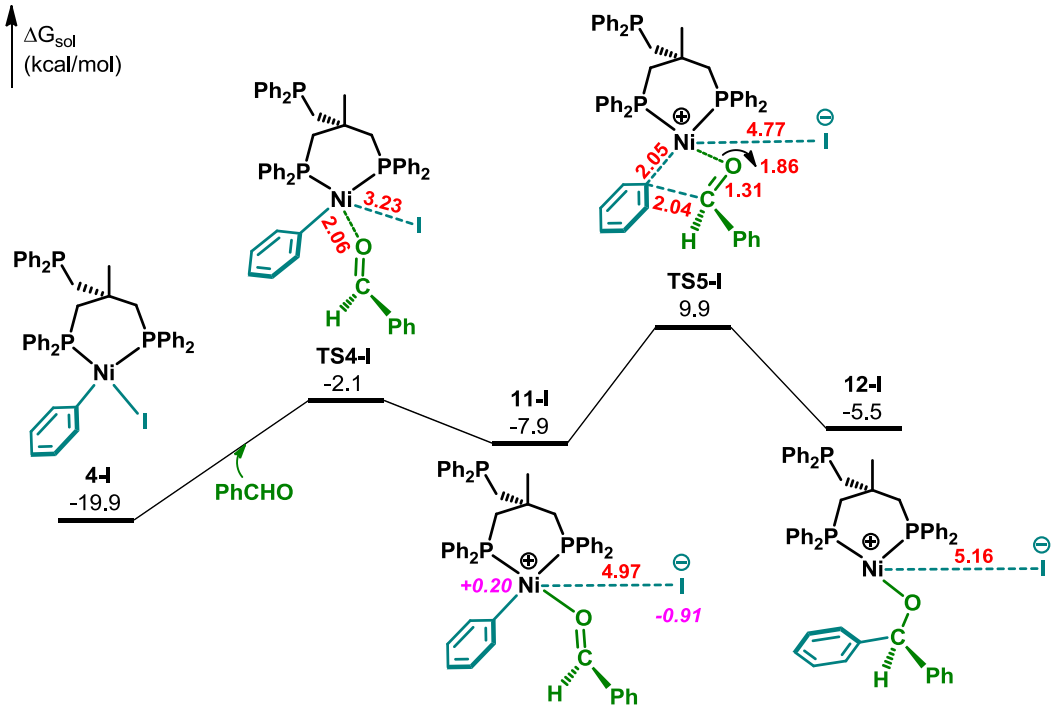

Fig. S7 Free energy profile for the reaction using PhI as substrate: part B (the interchange pathway of benzaldehyde ligation and insertion).

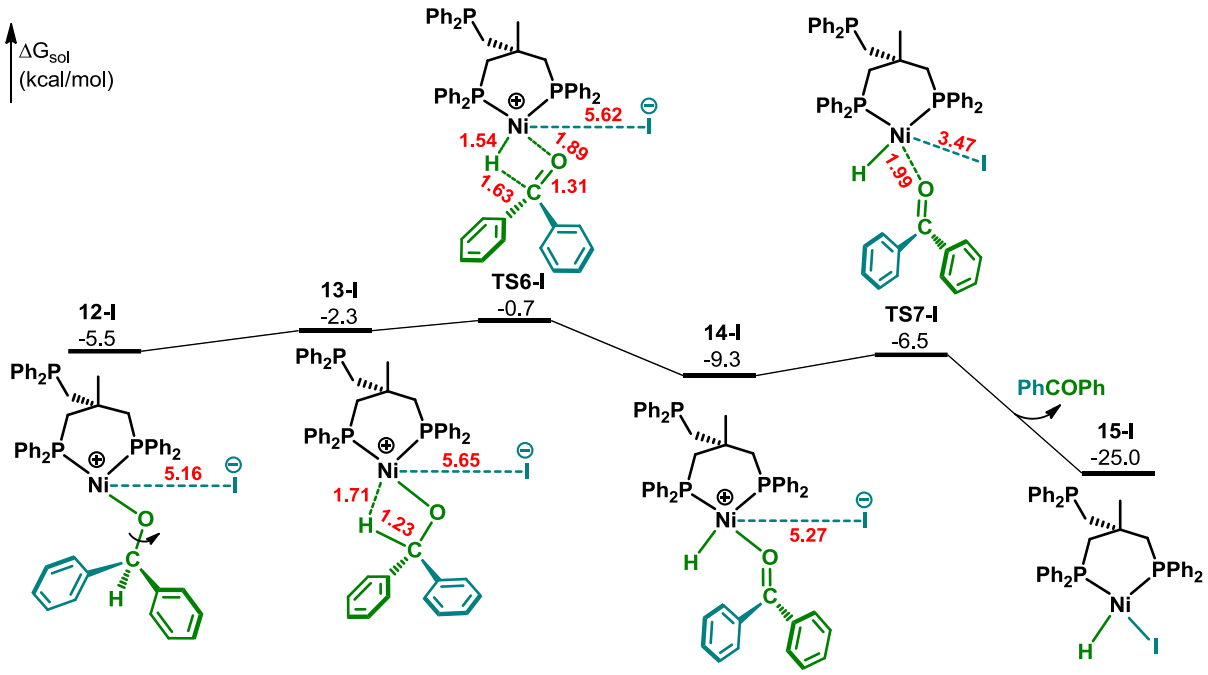

Fig. S8 Free energy profile for the reaction using PhI as substrate: part C (the β-hydride elimination and ketone product release).

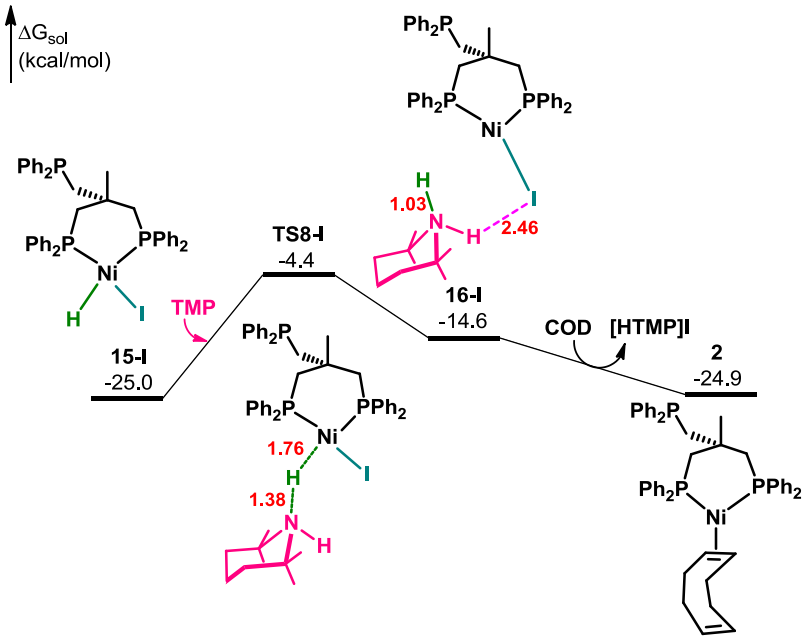

Fig. S9 Free energy profile for the reaction using PhI as substrate: part D (the base-induced reduction and catalyst regeneration).

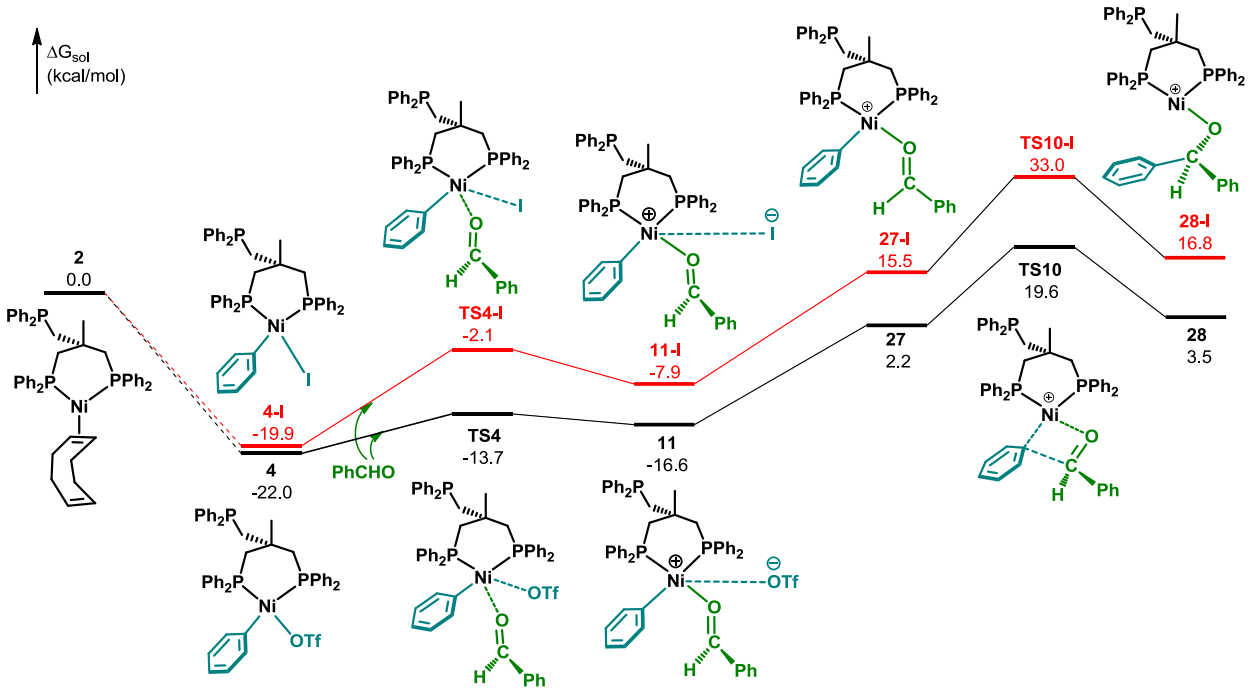

Fig. S10 Free energy profile for the two alternative parallel pathways with the dissociation of OTf^-/I^- from **11**/**11-I**. This is to be viewed in comparison with Fig. 6.

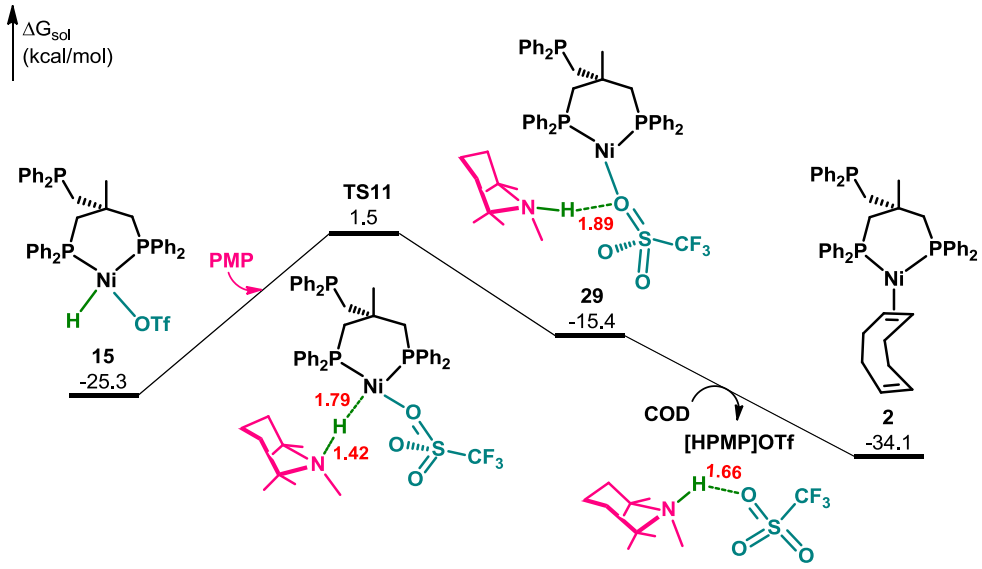

Fig. S11 Free energy profile for the base-induced reduction and catalyst regeneration using PMP.

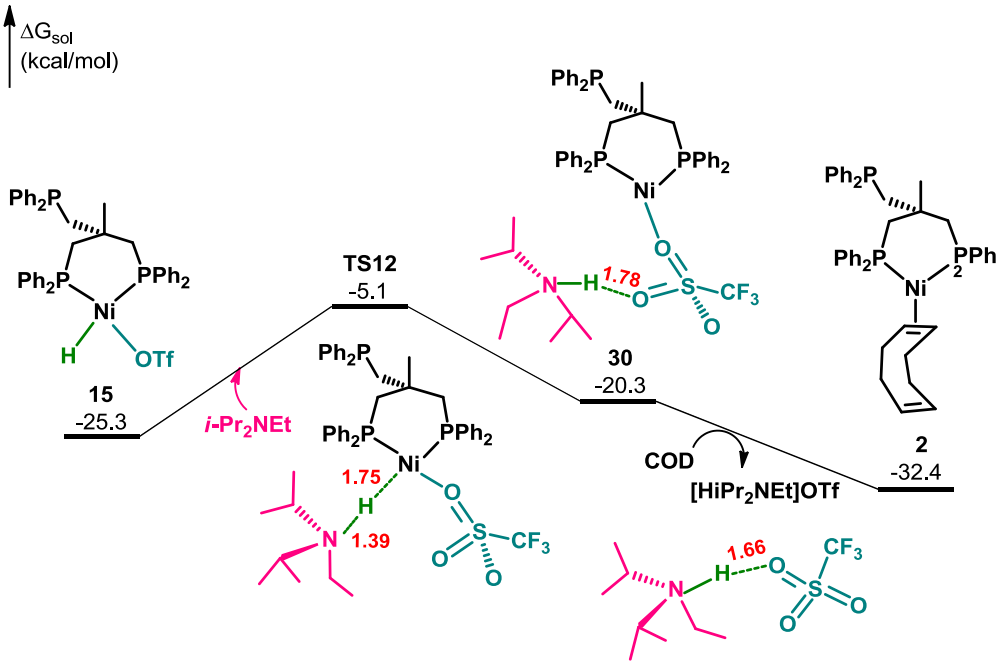

Fig. S12 Free energy profile for the base-induced reduction and catalyst regeneration using *i*-Pr$_2$NEt.

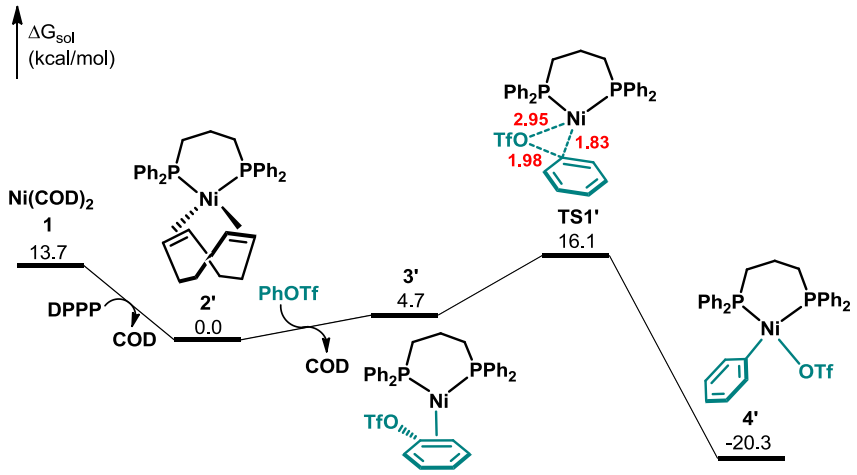

Fig. S13 Free energy profile for the dppp-enabled reaction: part A (oxidative addition).

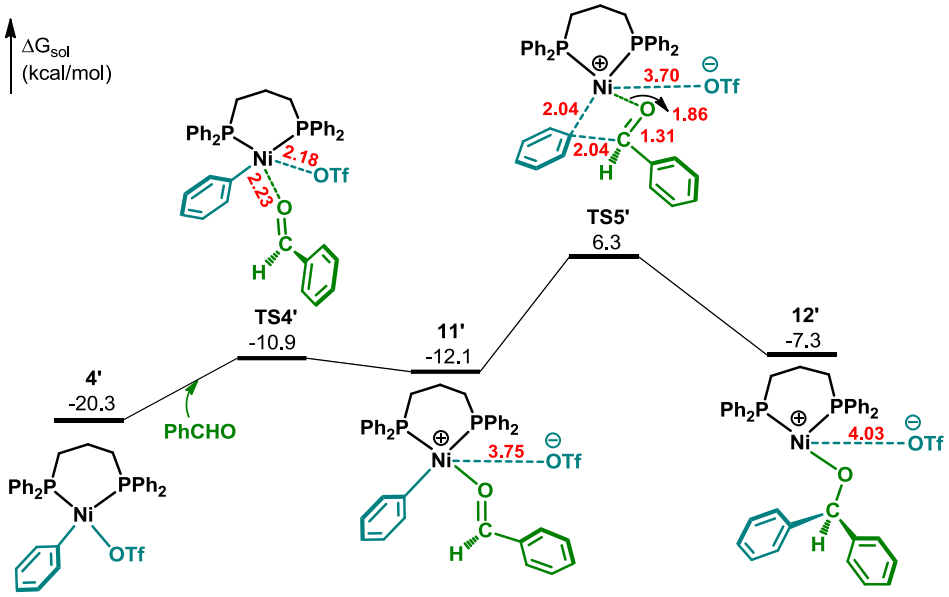

Fig. S14 Free energy profile for the dppp-enabled reaction: part B (ligand interchange and benzaldehyde C=O insertion).

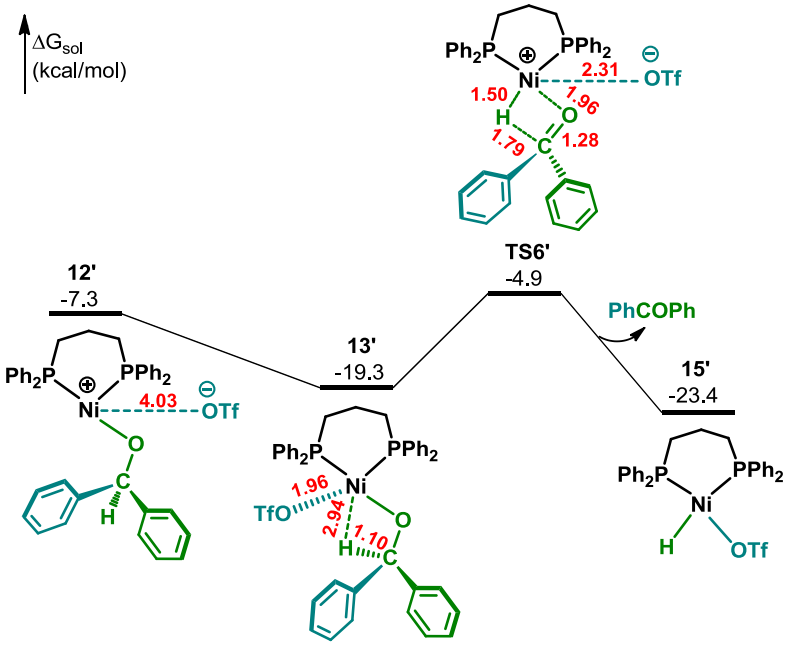

Fig. S15 Free energy profile for the dppp-enabled reaction: part C (β-hydride elimination and ketone product release).

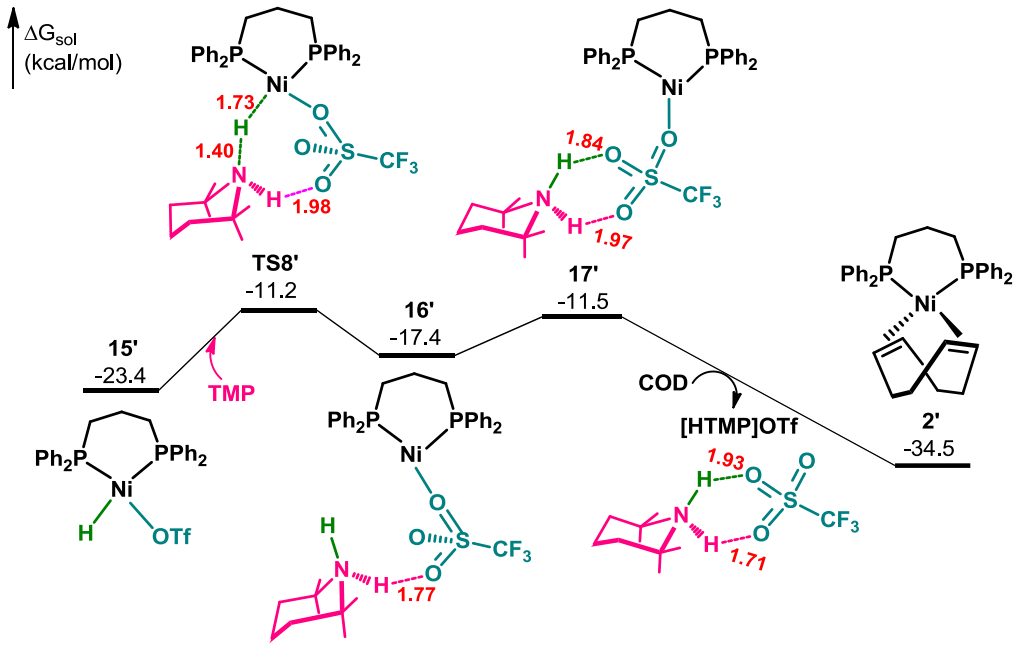

Fig. S16 Free energy profile for the dppp-enabled reaction: part D (base-induced reduction and catalyst regeneration).

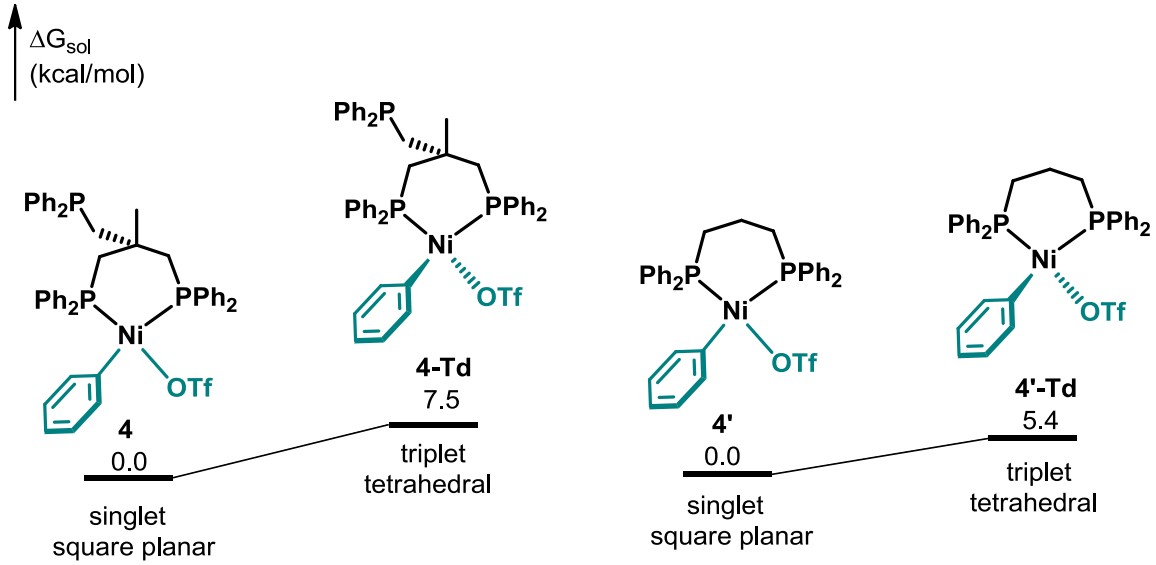

Fig. S17 Free energy profile comparing the relative energies of the square planar and tetrahedral Ni(II) complexes. Isomerization of **4** to **4-Td** is more uphill than is isomerization of **4'** to **4'-Td**.

Cartesian Coordinates (Å), SCF Energies, and Free Energies at 298.15 K and 1 atm for the Optimized Structures

COD

B3LYP/BS1 SCF energy: -312.024465 a.u.

M06/BS2 SCF energy in PhMe: -311.86187955 a.u.

M06/BS2 Free energy in PhMe: -311.71220855 a.u.

C	-1.083220	-1.107300	0.665617
C	-1.923436	-0.010506	-0.024042
C	-1.214901	1.236156	-0.495523
C	-0.008464	-1.704541	-0.218391
C	0.008464	1.704541	-0.218390
C	1.214901	-1.236156	-0.495525
C	1.083220	1.107299	0.665617
C	1.923436	0.010507	-0.024045
H	1.771774	1.909493	0.959659
H	2.741036	-0.284292	0.653831
H	-0.665916	-0.724044	1.600204
H	-2.425669	-0.455434	-0.896040
H	-2.741033	0.284293	0.653837
H	0.665916	0.724040	1.600203
H	2.425665	0.455436	-0.896044
H	-1.771774	-1.909494	0.959657
H	0.292254	2.634539	-0.712204
H	1.821457	-1.841621	-1.171407
H	-0.292254	-2.634540	-0.712205
H	-1.821457	1.841621	-1.171405

Triphos

B3LYP/BS1 SCF energy: -2609.857604 a.u.

M06/BS2 SCF energy in PhMe: -2609.04764540 a.u.

M06/BS2 Free energy in PhMe: -2608.44853340 a.u.

P	-0.404105	2.930921	-0.109164
P	-2.331992	-1.761178	-0.241786
P	2.711991	-1.120285	-0.138048
C	0.002080	0.020069	-0.151052
C	-0.845266	1.196136	-0.719470
C	-0.567167	-1.309127	-0.729416
C	1.462777	0.189008	-0.665012
C	-0.037830	0.012512	1.388285
C	-1.184973	3.937672	-1.460133
C	-1.561637	3.172933	1.318017
C	-2.733332	-3.045396	-1.521140
C	-2.077429	-2.819752	1.266188
C	4.090209	-0.794663	-1.339862
C	3.420807	-0.404451	1.425208
C	-2.205966	4.876622	-1.248843
C	-1.041749	3.789792	2.466661
C	-4.095113	-3.334845	-1.714159
C	-2.724936	-2.431215	2.448492
C	5.035332	-1.822066	-1.503487
C	3.383086	-1.201450	2.578965
C	-0.641267	3.831800	-2.753715
C	-2.909648	2.774335	1.327265
C	-1.792636	-3.730463	-2.307851
C	-1.292312	-3.983783	1.284920
C	4.249583	0.377817	-2.096703
C	3.997009	0.873031	1.512450
C	-2.682423	5.665042	-2.299841
C	-1.839713	4.001779	3.593790
C	-4.504678	-4.287913	-2.647029
C	-2.583950	-3.175265	3.622751
C	6.112341	-1.678895	-2.378571
C	3.896005	-0.733664	3.791708
C	-1.122967	4.610620	-3.804646
C	-3.708474	2.982872	2.452034
C	-2.201024	-4.677387	-3.250174
C	-1.150687	-4.729774	2.454964
C	5.321051	0.519181	-2.981727
C	4.511150	1.342394	2.720992
C	-2.149105	5.532258	-3.581657
C	-3.174494	3.596341	3.588827
C	-3.556925	-4.961446	-3.420382
C	-1.795426	-4.325990	3.627815
C	6.257217	-0.506354	-3.123007
C	4.460460	0.539847	3.864582
H	-0.724677	1.222187	-1.809831
H	-1.906162	0.998938	-0.533007
H	-0.575590	-1.229363	-1.824718
H	0.114841	-2.128357	-0.474280
H	1.446550	0.148671	-1.762628

H	1.821082	1.187192	-0.386403
H	0.493023	0.876886	1.801376
H	0.431469	-0.889053	1.795013
H	-1.067828	0.046831	1.757646
H	-2.638318	4.994477	-0.260541
H	0.000285	4.099839	2.477664
H	-4.840843	-2.801763	-1.128841
H	-3.342493	-1.536237	2.448057
H	4.920404	-2.745685	-0.940723
H	2.944876	-2.195148	2.525772
H	0.173480	3.135892	-2.943703
H	-3.345058	2.305046	0.449542
H	-0.731587	-3.530011	-2.193298
H	-0.797502	-4.319871	0.377584
H	3.537341	1.192118	-2.003617
H	4.055691	1.504121	0.629592
H	-3.477343	6.382686	-2.112245
H	-1.416942	4.479092	4.473993
H	-5.563462	-4.496956	-2.776874
H	-3.091034	-2.856351	4.529789
H	6.832341	-2.486147	-2.486023
H	3.854975	-1.364582	4.675904
H	-0.691797	4.502840	-4.796795
H	-4.748751	2.667541	2.440889
H	-1.456492	-5.194728	-3.850182
H	-0.540076	-5.629259	2.451509
H	5.424446	1.434478	-3.559284
H	4.954227	2.333882	2.770782
H	-2.523263	6.143878	-4.398286
H	-3.797390	3.756259	4.465080
H	-3.872984	-5.698337	-4.154083
H	-1.685227	-4.908978	4.538570
H	7.090473	-0.394764	-3.811788
H	4.862180	0.906478	4.805678

PhCHO

B3LYP/BS1 SCF energy: -345.566491 a.u.

M06/BS2 SCF energy in PhMe: -345.42202777 a.u.

M06/BS2 Free energy in PhMe: -345.34227477 a.u.

C	-1.736492	1.060602	0.000001
C	-0.361386	1.292598	0.000003
C	0.534028	0.214912	0.000005
C	0.045638	-1.101087	0.000003
C	-1.326052	-1.331720	0.000002
C	-2.217111	-0.251216	0.000001
H	-2.431145	1.895876	0.000000
H	0.024464	2.310101	0.000004
H	0.759931	-1.918848	0.000004
H	-1.707454	-2.349097	0.000002
H	-3.288431	-0.434116	-0.000001
C	1.992525	0.468950	0.000006
H	2.274434	1.545926	-0.000016
O	2.847663	-0.396009	-0.000015

PhOTf

B3LYP/BS1 SCF energy: -1193.031241 a.u.

M06/BS2 SCF energy in PhMe: -1192.88463645 a.u.

M06/BS2 Free energy in PhMe: -1192.80754645 a.u.

C	3.509805	1.239816	-0.014763
C	4.213132	0.032745	0.002986
C	3.536822	-1.176734	-0.174684
C	2.155011	-1.187967	-0.372591
C	1.477902	0.028124	-0.388570
C	2.127724	1.245804	-0.210102
H	4.034814	2.180312	0.124307
H	5.288590	0.034688	0.155068
H	4.082940	-2.115387	-0.160364
H	1.606255	-2.112520	-0.514385
H	1.557434	2.168040	-0.226902
O	0.088814	0.033011	-0.659250
S	-0.915414	-0.111482	0.638434
O	-0.792446	1.049346	1.507099
O	-0.873992	-1.467498	1.164684
C	-2.468230	0.075336	-0.384718
F	-2.475599	1.260988	-0.985260
F	-3.502916	-0.014369	0.449543
F	-2.534308	-0.894735	-1.290758

OTf^-

B3LYP/BS1 SCF energy: -961.487296 a.u.

M06/BS2 SCF energy in PhMe: -961.52703821 a.u.

M06/BS2 Free energy in PhMe: -961.53224121 a.u.

O	-1.241413	1.351932	0.513953

S	-0.924683	0.000010	0.000051
O	-1.241739	-0.230972	-1.427604
O	-1.241324	-1.121000	0.913936
C	0.939068	0.000010	-0.000056
F	1.442683	0.972078	-0.793257
F	1.442767	-1.172914	-0.445353
F	1.443031	0.200847	1.238302

PhI

B3LYP/BS1 SCF energy: -243.053411 a.u.

M06/BS2 SCF energy in PhMe: -242.907454260 a.u.

M06/BS2 Free energy in PhMe: -242.848966260 a.u.

C	-2.665303	-1.207251	0.000001
C	-1.267558	-1.216331	-0.000002
C	-0.587018	-0.000024	-0.000004
C	-1.267543	1.216319	-0.000003
C	-2.665263	1.207275	0.000001
C	-3.365557	0.000009	0.000001
H	-3.202446	-2.151952	0.000007
H	-0.725922	-2.155860	-0.000005
H	-0.725854	2.155818	-0.000004
H	-3.202421	2.151968	0.000007
H	-4.451802	0.000042	0.000000
I	1.570149	0.000000	0.000001

PhCOPh

B3LYP/BS1 SCF energy: -576.620608 a.u.

M06/BS2 SCF energy in PhMe: -576.35713087 a.u.

M06/BS2 Free energy in PhMe: -576.20256087 a.u.

C	-2.709273	-1.535464	-0.668879
C	-1.454288	-0.926782	-0.616044
C	-1.303911	0.336973	-0.023720
C	-2.434645	0.984237	0.501043
C	-3.681781	0.367579	0.465456
C	-3.821646	-0.894907	-0.120277
H	-2.817669	-2.508003	-1.141278
H	-0.596563	-1.422877	-1.058739
H	-2.310679	1.973089	0.930578
H	-4.547709	0.870888	0.886930
H	-4.796627	-1.373899	-0.154361
C	-0.000047	1.080292	0.000545
O	-0.000043	2.306847	-0.000057
C	1.303863	0.337022	0.024208
C	1.454625	-0.926579	0.616761
C	2.434273	0.984212	-0.501337
C	2.709675	-1.535175	0.669080
H	0.597163	-1.422608	1.060038
C	3.681462	0.367627	-0.466274
H	2.310039	1.972957	-0.931042
C	3.821715	-0.894699	0.119707
H	2.818381	-2.507583	1.141676
H	4.547133	0.870874	-0.888349
H	4.796741	-1.373627	0.153386

TMP

B3LYP/BS1 SCF energy: -409.152527 a.u.

M06/BS2 SCF energy in PhMe: -408.95815891 a.u.

M06/BS2 Free energy in PhMe: -408.72142191 a.u.

C	0.261526	0.019580	1.293225
C	-1.179864	0.574483	1.257378
C	-1.949346	0.151366	0.000000
C	-1.179864	0.574483	-1.257378
C	0.261526	0.019580	-1.293225
N	0.903667	0.331247	0.000000
H	-2.119056	-0.933388	0.000000
H	-1.711564	0.258662	2.164051
H	-1.711564	0.258662	-2.164051
H	-2.944500	0.614085	0.000000
H	-1.126561	1.671285	-1.281268
H	-1.126561	1.671285	1.281268
H	1.860181	-0.019752	0.000000
C	1.070402	0.777053	2.363532
H	0.618251	0.659751	3.355624
H	2.098322	0.394694	2.420597
H	1.118966	1.842773	2.119539
C	0.261526	-1.483106	1.674759
H	1.273260	-1.899481	1.591240
H	-0.066802	-1.617150	2.713164
H	-0.398521	-2.082527	1.042606
C	1.070402	0.777053	-2.363532
H	2.098322	0.394694	-2.420597
H	0.618251	0.659751	-3.355624
H	1.118966	1.842773	-2.119539

C	0.261526	-1.483106	-1.674759
H	-0.066802	-1.617150	-2.713164
H	1.273260	-1.899481	-1.591240
H	-0.398521	-2.082527	-1.042606

PMP

B3LYP/BS1 SCF energy: -448.449055 a.u.

M06/BS2 SCF energy in PhMe: -448.23420684 a.u.

M06/BS2 Free energy in PhMe: -447.97022984 a.u.

C	1.292834	-0.049573	-0.027796
C	1.240318	1.427066	-0.485063
C	-0.000105	2.173400	-0.001398
C	-1.240492	1.426934	-0.484950
C	-1.292858	-0.049743	-0.027767
N	0.000038	-0.719296	-0.365010
H	-0.000060	2.262015	1.092705
H	2.156434	1.927626	-0.146692
H	-2.156627	1.927389	-0.146474
H	-0.000184	3.199230	-0.391711
H	-1.252789	1.446997	-1.583522
H	1.252503	1.447077	-1.583638
C	2.426649	-0.713513	-0.845803
H	3.314313	-0.070948	-0.827740
H	2.729437	-1.686474	-0.445548
H	2.116553	-0.844954	-1.887863
C	1.690432	-0.124055	1.470365
H	1.652227	-1.153800	1.841543
H	2.718988	0.232758	1.603850
H	1.047306	0.485439	2.110228
C	-2.426675	-0.713604	-0.845851
H	-2.729876	-1.686353	-0.445403
H	-3.314156	-0.070775	-0.828162
H	-2.116380	-0.845417	-1.887804
C	-1.690448	-0.124389	1.470382
H	-2.719024	0.232343	1.603930
H	-1.652157	-1.154178	1.841431
H	-1.047345	0.485071	2.110303
C	0.000271	-2.155588	-0.106224
H	0.874294	-2.620194	-0.566512
H	0.000893	-2.439058	0.962287
H	-0.874181	-2.620324	-0.565518

***i*-Pr2NEt**

B3LYP/BS1 SCF energy: -371.031279 a.u.

M06/BS2 SCF energy in PhMe: -370.84450255 a.u.

M06/BS2 Free energy in PhMe: -370.61842655 a.u.

N	0.000051	0.077116	-0.180535
C	1.255186	-0.628404	-0.474757
C	-1.255068	-0.628484	-0.474662
C	2.357101	0.358229	-0.898730
H	2.667376	0.999555	-0.065038
H	3.246386	-0.184282	-1.241052
H	2.005469	1.001601	-1.711409
C	1.785755	-1.568627	0.632721
H	2.708356	-2.061484	0.302564
H	2.021880	-1.018730	1.551402
H	1.062290	-2.349468	0.884274
C	-1.785985	-1.568261	0.633042
H	-1.062676	-2.349060	0.885157
H	-2.022357	-1.018022	1.551453
H	-2.708543	-2.061159	0.302808
C	-2.356910	0.358033	-0.899186
H	-2.005279	1.000769	-1.712357
H	-3.246358	-0.184539	-1.240993
H	-2.666927	0.999982	-0.065871
C	0.000078	1.009555	0.948033
H	-0.871146	0.821388	1.589374
H	0.871492	0.821570	1.589183
C	-0.000148	2.491610	0.539213
H	-0.883816	2.735968	-0.058854
H	-0.000138	3.136200	1.428350
H	0.883352	2.736128	-0.059026
H	1.036168	-1.253832	-1.350333
H	-1.035940	-1.254307	-1.349929

[HTMP]OTf

B3LYP/BS1 SCF energy: -1371.192960 a.u.

M06/BS2 SCF energy in PhMe: -1370.99030498 a.u.

M06/BS2 Free energy in PhMe: -1370.72362898 a.u.

O	1.112130	-0.431693	-1.307945
S	1.879473	-0.786366	-0.073872
O	2.587536	-2.067243	-0.093475
O	1.079232	-0.509934	1.171567

C	3.206705	0.510915	0.004510
F	3.994905	0.441578	-1.073450
F	3.955310	0.349138	1.100370
F	2.657803	1.741857	0.046518
H	-0.744461	-0.116921	-0.873923
C	-1.823220	1.418215	0.068557
C	-3.067192	1.535018	-0.832760
C	-4.103092	0.427773	-0.603086
C	-3.468039	-0.950984	-0.820365
C	-2.251677	-1.222401	0.085529
N	-1.306018	-0.020453	-0.006329
H	-4.533981	0.501833	0.402880
H	-3.510940	2.524715	-0.673151
H	-4.200241	-1.749374	-0.652755
H	-4.937032	0.559203	-1.301894
H	-3.150754	-1.034184	-1.869465
H	-2.743440	1.504577	-1.882617
H	-0.522474	-0.149553	0.687716
C	-0.686415	2.307862	-0.461416
H	-1.023372	3.349725	-0.468339
H	0.205891	2.236021	0.165733
H	-0.399403	2.032710	-1.481227
C	-2.114041	1.800196	1.528365
H	-1.256887	1.570213	2.170220
H	-2.286645	2.880018	1.579403
H	-2.996859	1.307323	1.939192
C	-1.457864	-2.437055	-0.424901
H	-0.607617	-2.662045	0.225539
H	-2.118188	-3.310459	-0.442013
H	-1.073887	-2.276755	-1.437073
C	-2.649220	-1.470987	1.549243
H	-3.147489	-2.443617	1.614471
H	-1.762911	-1.508378	2.191427
H	-3.337765	-0.723522	1.947963

[HPMP]OTf

B3LYP/BS1 SCF energy: -1410.486805 a.u.

M06/BS2 SCF energy in PhMe: -1410.26577813 a.u.

M06/BS2 Free energy in PhMe: -1409.97190913 a.u.

O	-0.827725	-0.727207	0.586550
S	-2.027648	-0.816176	-0.332875
O	-2.782958	-2.066000	-0.226719
O	-1.709769	-0.314494	-1.690027
C	-3.129837	0.493922	0.388647
F	-3.489913	0.179574	1.638575
F	-4.232543	0.647605	-0.351782
F	-2.478245	1.676488	0.425518
H	0.581390	-0.350286	-0.210226
C	1.736462	1.371809	-0.402469
C	1.538539	1.674001	1.096799
C	2.457241	0.859381	2.010813
C	2.237844	-0.637965	1.785618
C	2.421652	-1.111796	0.326260
N	1.561386	-0.172236	-0.578291
H	3.508401	1.132180	1.852038
H	1.703476	2.748335	1.240267
H	2.923474	-1.226596	2.406725
H	2.236559	1.100473	3.056939
H	1.219412	-0.896597	2.097965
H	0.491808	1.472139	1.353756
C	0.624922	2.069314	-1.209209
H	0.591586	3.117749	-0.895033
H	0.826749	2.058737	-2.284534
H	-0.359242	1.629980	-1.038403
C	3.095978	1.885968	-0.905067
H	3.329634	1.543810	-1.917308
H	3.037648	2.978546	-0.946003
H	3.932550	1.633100	-0.253343
C	1.837435	-2.536883	0.223353
H	2.118165	-3.047902	-0.702454
H	2.248789	-3.126712	1.049101
H	0.749044	-2.530988	0.324332
C	3.895525	-1.147538	-0.102575
H	4.375953	-1.984945	0.414009
H	4.005624	-1.327302	-1.176775
H	4.451476	-0.245708	0.155539
C	1.520949	-0.586042	-2.018678
H	1.497797	-1.671301	-2.078555
H	0.597414	-0.208704	-2.454570
H	2.394628	-0.209967	-2.549631

[HTMP]I

B3LYP/BS1 SCF energy: -421.206716 a.u.

M06/BS2 SCF energy in PhMe: -420.99551738 a.u.

M06/BS2 Free energy in PhMe: -420.74980338 a.u.

H	-0.859835	-0.000023	-1.545453
C	-1.439615	1.341395	-0.074919
C	-2.966012	1.262226	-0.265290
C	-3.596969	0.000239	0.338741
C	-2.966269	-1.262013	-0.265034
C	-1.439818	-1.341396	-0.074904
N	-0.836801	-0.000045	-0.520750
H	-3.489227	0.000345	1.429780
H	-3.408455	2.166029	0.169678
H	-3.408837	-2.165639	0.170183
H	-4.674284	0.000356	0.138128
H	-3.193955	-1.292420	-1.340803
H	-3.193568	1.292404	-1.341096
H	0.215118	-0.000128	-0.293331
C	-0.817205	2.392125	-1.008445
H	-1.212507	3.381355	-0.757115
H	0.272403	2.414672	-0.902759
H	-1.064769	2.194130	-2.059531
C	-1.033883	1.650177	1.374132
H	0.043140	1.513058	1.513588
H	-1.274721	2.697602	1.582448
H	-1.564051	1.039799	2.107394
C	-0.817707	-2.392198	-1.008510
H	0.271944	-2.414740	-0.903161
H	-1.212914	-3.381421	-0.756979
H	-1.065540	-2.194328	-2.059554
C	-1.033888	-1.650249	1.374065
H	-1.274831	-2.697637	1.582420
H	0.043180	-1.513290	1.513342
H	-1.563835	-1.039798	2.107415
I	2.530969	-0.000035	0.017956
F	-3.914098	-0.131552	-0.988420
F	-3.624468	-0.522544	1.132001
F	-2.558968	-1.709762	-0.348190
H	0.816943	-0.002765	0.395167
N	1.845623	-0.008552	0.131719
C	2.050410	1.392440	-0.481186
C	2.021761	-1.122938	-0.920762
C	1.648409	2.498269	0.500904
H	2.428166	2.706038	1.242221
H	1.493255	3.416732	-0.073971
H	0.710782	2.271451	1.014237
C	3.460132	1.609963	-1.029472
H	3.513007	2.623815	-1.439132
H	4.223832	1.536073	-0.246833
H	3.715549	0.920522	-1.838285
C	3.405771	-1.778214	-0.893317
H	4.226980	-1.058310	-0.939861
H	3.546786	-2.410138	-0.010978
H	3.487707	-2.426708	-1.771618
C	0.895393	-2.157363	-0.831892
H	-0.082169	-1.688714	-0.945522
H	1.025718	-2.873049	-1.651224
H	0.914964	-2.717800	0.106270
C	2.570034	-0.212361	1.440219
H	3.632993	-0.347024	1.231482
H	2.453713	0.720470	1.991304
C	2.003782	-1.352587	2.284815
H	2.210478	-2.338829	1.861997
H	2.471204	-1.312865	3.274510
H	0.923293	-1.239905	2.411227
H	1.321815	1.393235	-1.296212
H	1.901289	-0.597272	-1.871155

[HiPr2NEt]OTf

B3LYP/BS1 SCF energy: -1333.067019 a.u.

M06/BS2 SCF energy in PhMe: -1332.87604521 a.u.

M06/BS2 Free energy in PhMe: -1332.61736321 a.u.

O	-0.997492	0.627930	-1.375799
S	-1.612406	0.741458	-0.029424
O	-2.219807	2.026698	0.328329
O	-0.709896	0.156316	1.032888
C	-3.015993	-0.475750	-0.058762

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B3LYP/BS1 SCF energy: -795.042155 a.u.

M06/BS2 SCF energy in PhMe: -794.75520352 a.u.

M06/BS2 Free energy in PhMe: -794.43202852 a.u.

C	-2.621354	0.591907	-1.417042
C	-2.238695	1.840905	-0.588783
C	-1.370019	1.527756	0.613403
C	-1.510482	-0.451168	-1.473072
C	-1.511420	0.451103	1.473110

C	-1.369045	-1.527858	-0.613012
C	-2.621839	-0.592303	1.416583
C	-2.238177	-1.841288	0.588789
H	-2.867941	-0.906239	2.438376
H	-3.148209	-2.385669	0.285825
H	-3.537153	0.140723	-1.020989
H	-1.679347	2.532387	-1.232303
H	-3.149116	2.384783	-0.286097
H	-3.537485	-0.141478	1.019796
H	-1.678805	-2.532358	1.232753
H	-2.866879	0.906020	-2.438917
H	-0.981909	0.513336	2.420829
H	-0.761617	-2.360749	-0.964323
H	-0.981683	-0.514131	-2.421159
H	-0.762045	2.360348	0.964407
C	2.621912	-0.591732	-1.416348
C	2.239085	-1.840784	-0.588248
C	1.369930	-1.527745	0.613627
C	1.510967	0.451232	-1.472746
C	1.510929	-0.451071	1.473428
C	1.369126	1.527882	-0.612754
C	2.621277	0.592445	1.417290
C	2.237784	1.841394	0.589362
H	2.866996	0.906414	2.439165
H	3.147863	2.385880	0.286730
H	3.537527	-0.140463	-1.019968
H	1.680050	-2.532319	-1.231984
H	3.149460	-2.384562	-0.285241
H	3.537106	0.141711	1.020822
H	1.678103	2.532398	1.233127
H	2.867821	-0.905793	-2.438147
H	0.981238	-0.513476	2.421038
H	0.761597	2.360637	-0.964203
H	0.982352	0.514047	-2.420944
H	0.762064	-2.360485	0.964475
Ni	0.000005	-0.000179	-0.000878

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B3LYP/BS1 SCF energy: -3092.889105 a.u.

M06/BS2 SCF energy in PhMe: -3091.96646985 a.u.

M06/BS2 Free energy in PhMe: -3091.19066685 a.u.

C	1.243412	0.425964	-1.875333
C	2.204883	0.682569	-3.061384
H	2.860817	-0.176661	-3.238019
H	1.639960	0.862441	-3.984315
H	2.839692	1.556245	-2.875691
C	0.298088	1.666747	-1.842011
H	-0.292872	1.635357	-2.766041
H	0.912613	2.574617	-1.896767
C	0.470498	-0.880367	-2.215767
H	1.194943	-1.690606	-2.355580
H	-0.016915	-0.736366	-3.188142
C	2.040731	0.318207	-0.546207
H	1.367967	-0.021581	0.248102
H	2.386823	1.317064	-0.257122
P	-0.964835	1.859665	-0.466603
P	3.501697	-0.878515	-0.549924
P	-0.903964	-1.475718	-1.065465
Ni	-2.133419	0.055230	-0.113093
C	4.916757	0.242643	-1.012820
C	5.723426	-0.134917	-2.096324
C	5.231295	1.427212	-0.327270
C	6.807261	0.652173	-2.494945
H	5.498856	-1.054019	-2.632471
C	6.312322	2.215467	-0.721778
H	4.637669	1.731372	0.531088
C	7.102467	1.830351	-1.808884
H	7.419577	0.343218	-3.338324
H	6.542584	3.128442	-0.178168
H	7.945678	2.444285	-2.114684
C	3.819850	-1.082085	1.267075
C	4.632390	-2.166375	1.640135
C	3.320640	-0.247358	2.279559
C	4.952724	-2.400556	2.977403
H	5.015053	-2.834483	0.871952
C	3.631301	-0.487494	3.620412
H	2.683846	0.597161	2.036633
C	4.450278	-1.560751	3.973746
H	5.587696	-3.242385	3.241975
H	3.233114	0.171381	4.388215
H	4.692424	-1.743996	5.017431
C	0.016027	2.636657	0.909502
C	-0.016016	2.040122	2.177636
C	0.767620	3.810628	0.736633
C	0.693157	2.595173	3.247470

H	-0.607038	1.140033	2.322784
C	1.481694	4.362348	1.800211
H	0.783913	4.307089	-0.230480
C	1.446875	3.754410	3.059053
H	0.650760	2.123707	4.226085
H	2.058782	5.271302	1.650423
H	1.998521	4.188521	3.888807
C	-1.909336	3.349338	-1.066070
C	-2.796168	3.954066	-0.156185
C	-1.845936	3.870725	-2.367506
C	-3.583501	5.040954	-0.529491
H	-2.865559	3.569755	0.857174
C	-2.641220	4.957307	-2.745658
H	-1.173189	3.444999	-3.103969
C	-3.511601	5.546641	-1.830531
H	-4.257169	5.491427	0.194935
H	-2.572358	5.342735	-3.759878
H	-4.128624	6.391114	-2.125634
C	-1.798974	-2.607860	-2.236232
C	-2.472770	-2.018816	-3.321987
C	-1.925034	-3.992047	-2.050048
C	-3.221449	-2.791091	-4.208257
H	-2.425099	-0.941550	-3.466953
C	-2.683902	-4.765616	-2.933261
H	-1.431187	-4.475438	-1.213826
C	-3.329367	-4.171377	-4.016968
H	-3.729214	-2.313757	-5.042551
H	-2.767042	-5.837209	-2.769852
H	-3.917302	-4.774705	-4.703497
C	-0.033700	-2.634859	0.087910
C	-0.333412	-2.546809	1.456257
C	0.898063	-3.598895	-0.332587
C	0.277404	-3.396488	2.381138
H	-1.052772	-1.803407	1.789663
C	1.506254	-4.451420	0.589507
H	1.147250	-3.695146	-1.385300
C	1.198061	-4.350971	1.948558
H	0.034090	-3.310750	3.436772
H	2.224856	-5.191120	0.246533
H	1.677618	-5.011619	2.665763
C	-5.825358	-0.290062	3.257555
C	-5.464931	-1.566049	3.071359
C	-3.835219	0.534856	0.822615
C	-4.168075	-2.140268	2.543346
C	-3.907168	-0.781307	0.293609
C	-4.074047	-2.127755	1.000744
H	-3.295609	-1.646753	2.982113
H	-4.107546	-3.187764	2.866418
H	-3.272137	-2.815725	0.701670
H	-5.000295	-2.586000	0.621548
C	-5.058782	0.991723	3.050227
H	-4.882891	1.451898	4.037640
H	-5.722942	1.696869	2.526069
C	-3.719224	0.934004	2.286832
H	-3.282616	1.941017	2.335792
H	-3.015265	0.293585	2.826554
H	-6.838184	-0.126217	3.631637
H	-6.228064	-2.314837	3.289611
H	-4.301278	1.317019	0.216033
H	-4.339382	-0.820631	-0.711595

3

B3LYP/BS1 SCF energy: -3973.886193 a.u.

M06/BS2 SCF energy in PhMe: -3972.98482554 a.u.

M06/BS2 Free energy in PhMe: -3972.28028154 a.u.

C	-1.873895	1.435462	1.505288
C	-2.954395	2.113173	2.383387
H	-3.662940	2.682842	1.771588
H	-2.492652	2.803247	3.100070
H	-3.525803	1.374850	2.956230
C	-0.987037	0.602114	2.474601
H	-0.572100	1.289896	3.220851
H	-1.633203	-0.090414	3.024916
C	-1.086135	2.608956	0.848930
H	-1.805979	3.297212	0.388664
H	-0.594814	3.179379	1.647470
C	-2.537216	0.564210	0.403782
H	-1.761279	-0.013081	-0.110364
P	0.483015	-0.377385	1.809273
P	0.282223	2.250005	-0.386778
Ni	1.628488	0.629146	0.212641
C	-0.218127	-2.061710	1.512702
C	0.078784	-2.709988	0.305334
C	-1.009808	-2.732216	2.461271
C	-0.401353	-3.996289	0.048360

H	0.706032	-2.213658	-0.425357
C	-1.486467	-4.017471	2.206548
H	-1.245665	-2.259588	3.410485
C	-1.184157	-4.651586	0.997849
H	-0.154732	-4.481842	-0.891460
H	-2.094703	-4.523757	2.951476
H	-1.557433	-5.652946	0.800759
C	1.464331	-0.593899	3.368128
C	1.915962	-1.849808	3.802272
C	1.888675	0.545658	4.073859
C	2.742048	-1.963102	4.923262
H	1.623181	-2.746870	3.267086
C	2.706699	0.431883	5.197313
H	1.590147	1.536301	3.739822
C	3.135060	-0.825459	5.628825
H	3.076153	-2.946540	5.243678
H	3.015570	1.327219	5.730732
H	3.774731	-0.915761	6.502608
C	1.034332	3.938228	-0.517932
C	1.654834	4.470320	0.626800
C	1.113688	4.664123	-1.715840
C	2.300608	5.704847	0.584360
H	1.648643	3.908306	1.557639
C	1.770635	5.896758	-1.760523
H	0.662382	4.271826	-2.621174
C	2.359397	6.424852	-0.611433
H	2.768097	6.098946	1.482933
H	1.817916	6.444292	-2.698389
H	2.867114	7.384897	-0.647623
C	-0.602501	2.033415	-1.998893
C	-0.222354	0.965556	-2.826134
C	-1.636980	2.881163	-2.431215
C	-0.858991	0.746943	-4.051205
H	0.573302	0.299071	-2.505719
C	-2.275401	2.662951	-3.652580
H	-1.942851	3.725357	-1.818984
C	-1.888268	1.593268	-4.465354
H	-0.547232	-0.083845	-4.678570
H	-3.072810	3.329112	-3.971433
H	-2.385042	1.425118	-5.417146
C	4.993692	0.920171	1.374548
C	4.292798	-0.229013	1.117852
C	3.382563	-0.282432	0.008290
C	3.292659	0.835692	-0.902978
C	4.118171	1.981870	-0.627101
C	4.912048	2.039100	0.489404
H	5.645784	0.968544	2.242595
H	4.386568	-1.105243	1.752881
H	2.987812	0.663628	-1.932298
H	4.116975	2.800910	-1.341864
H	5.521640	2.917999	0.681247
O	3.081830	-1.621527	-0.492970
S	4.135310	-2.409027	-1.460929
O	4.321766	-3.758886	-0.950192
O	5.250131	-1.568355	-1.870806
C	2.998159	-2.572152	-2.935190
F	3.629368	-3.244633	-3.896742
F	2.657131	-1.361792	-3.399716
F	1.885499	-3.229638	-2.592598
H	-2.985466	1.222409	-0.349115
P	-3.828962	-0.684288	0.987390
C	-5.409621	0.282501	0.790267
C	-6.243556	0.405518	1.911401
C	-5.822482	0.870801	-0.416320
C	-7.449936	1.107088	1.837332
H	-5.944224	-0.053636	2.850606
C	-7.026368	1.571016	-0.494646
H	-5.208770	0.767177	-1.307611
C	-7.842683	1.692691	0.633713
H	-8.081681	1.192283	2.717801
H	-7.332224	2.016997	-1.437845
H	-8.781673	2.236512	0.571273
C	-3.931488	-1.806886	-0.487491
C	-4.549605	-3.052368	-0.284327
C	-3.441641	-1.510580	-1.769894
C	-4.689926	-3.966289	-1.328827
H	-4.918489	-3.309292	0.705855
C	-3.570612	-2.429888	-2.813891
H	-2.951391	-0.563088	-1.970520
C	-4.197463	-3.658002	-2.598690
H	-5.175173	-4.922266	-1.148934
H	-3.180709	-2.180303	-3.797611
H	-4.297624	-4.371290	-3.412646

TS1

B3LYP/BS1 SCF energy: -3973.870108 a.u.

M06/BS2 SCF energy in PhMe: -3972.96984700 a.u.

M06/BS2 Free energy in PhMe: -3972.26445200 a.u.

C	-1.953036	1.171492	1.595256
C	-3.005912	1.692814	2.604657
H	-3.757817	2.313266	2.105197
H	-2.529577	2.298621	3.384876
H	-3.529063	0.867085	3.097485
C	-0.984930	0.268158	2.416062
H	-0.561890	0.902070	3.204852
H	-1.574653	-0.506367	2.919928
C	-1.244347	2.451724	1.059979
H	-2.005176	3.140563	0.672944
H	-0.777015	2.968106	1.909065
C	-2.651262	0.422798	0.426478
H	-1.898443	-0.080912	-0.187538
P	0.500984	-0.566207	1.626657
P	0.136430	2.304869	-0.192187
Ni	1.680740	0.790503	0.345484
C	-0.156020	-2.092465	0.830298
C	0.194169	-2.382473	-0.494599
C	-0.944645	-3.008569	1.546496
C	-0.251330	-3.558947	-1.102223
H	0.841869	-1.705542	-1.039823
C	-1.389452	-4.180256	0.937586
H	-1.200821	-2.817620	2.584759
C	-1.046167	-4.454928	-0.389515
H	0.044272	-3.777079	-2.123298
H	-1.999581	-4.881429	1.500373
H	-1.391534	-5.370695	-0.861127
C	1.373348	-1.268451	3.102642
C	2.408997	-2.187709	2.850714
C	1.076451	-0.936224	4.432866
C	3.119616	-2.759623	3.905205
H	2.672418	-2.443129	1.828327
C	1.795069	-1.509290	5.486405
H	0.280682	-0.239769	4.672662
C	2.816293	-2.422025	5.227044
H	3.914804	-3.467663	3.688541
H	1.547838	-1.240847	6.510287
H	3.372719	-2.867412	6.047393
C	0.791264	4.033592	-0.160592
C	1.558355	4.403997	0.958250
C	0.604930	4.967678	-1.188843
C	2.097621	5.685229	1.059539
H	1.753149	3.679267	1.745817
C	1.156145	6.248134	-1.090449
H	0.036449	4.702095	-2.073822
C	1.896560	6.612550	0.034003
H	2.687219	5.953483	1.931906
H	1.003986	6.959799	-1.897632
H	2.323380	7.609047	0.107786
C	-0.685033	2.124952	-1.832878
C	-0.142731	1.215767	-2.754642
C	-1.826811	2.857993	-2.201293
C	-0.725332	1.042579	-4.012844
H	0.734026	0.632653	-2.489570
C	-2.409358	2.684219	-3.457013
H	-2.263507	3.575062	-1.511660
C	-1.859473	1.774823	-4.365516
H	-0.290035	0.334431	-4.712245
H	-3.290940	3.259445	-3.726978
H	-2.313556	1.641377	-5.343622
C	5.167474	1.587719	1.553402
C	4.351649	0.470694	1.523989
C	3.453002	0.330414	0.445734
C	3.469814	1.229343	-0.654106
C	4.361283	2.339465	-0.604463
C	5.176585	2.526135	0.491811
H	5.811017	1.749809	2.415308
H	4.354155	-0.253501	2.331552
H	3.071244	0.931921	-1.620773
H	4.440362	2.992922	-1.469666
H	5.862478	3.367801	0.527633
O	3.533859	-1.600546	-0.151251
S	4.545069	-2.052490	-1.210747
O	5.041278	-3.408231	-0.963696
O	5.490732	-1.004794	-1.606617
C	3.432852	-2.233881	-2.698615
F	4.149227	-2.445689	-3.805247
F	2.695608	-1.107222	-2.892428
F	2.570503	-3.251503	-2.547434
H	-3.142938	1.159169	-0.218696
P	-3.909825	-0.901935	0.910601
C	-5.497304	0.074707	0.920330
C	-6.275755	0.047389	2.086973

C	-5.966839	0.813258	-0.178195
C	-7.481240	0.750144	2.164132
H	-5.933950	-0.530246	2.942673
C	-7.169486	1.515997	-0.105041
H	-5.399702	0.825412	-1.105630
C	-7.928879	1.488303	1.068414
H	-8.069384	0.717385	3.077617
H	-7.519625	2.080099	-0.965984
H	-8.867064	2.034161	1.123599
C	-4.096911	-1.820717	-0.690307
C	-4.751118	-3.062812	-0.623986
C	-3.643246	-1.375490	-1.942038
C	-4.961368	-3.828097	-1.770820
H	-5.096412	-3.434021	0.338234
C	-3.842737	-2.146512	-3.089928
H	-3.127746	-0.425196	-2.038418
C	-4.504174	-3.372393	-3.009355
H	-5.474055	-4.783677	-1.696152
H	-3.478738	-1.783612	-4.047839
H	-4.658982	-3.970432	-3.903510

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B3LYP/BS1 SCF energy: -3973.931787 a.u.

M06/BS2 SCF energy in PhMe: -3973.02843981 a.u.

M06/BS2 Free energy in PhMe: -3972.32111781 a.u.

C	-1.752695	0.364999	-1.973058
C	-2.748719	0.564395	-3.141097
H	-3.451308	1.377926	-2.933865
H	-2.216682	0.812238	-4.067623
H	-3.333796	-0.344777	-3.317312
C	-0.743284	-0.709603	-2.468562
H	-0.224762	-0.304560	-3.345334
H	-1.300798	-1.584656	-2.821654
C	-1.052937	1.732832	-1.759129
H	-1.810736	2.477192	-1.489429
H	-0.645348	2.050606	-2.724768
C	-2.498341	-0.134538	-0.705121
H	-1.811745	-0.124406	0.147810
H	-2.794352	-1.178753	-0.857109
P	0.584835	-1.296627	-1.295407
P	-4.000161	0.881685	-0.172803
P	0.356363	1.963027	-0.527133
Ni	1.774886	0.335819	-0.185287
C	-5.389311	0.020406	-1.065517
C	-6.232727	0.802349	-1.868539
C	-5.652066	-1.355291	-0.961277
C	-7.301592	0.227661	-2.561483
H	-6.049710	1.871152	-1.951305
C	-6.717551	-1.932508	-1.652149
H	-5.031871	-1.980104	-0.323498
C	-7.544074	-1.142016	-2.456181
H	-7.943355	0.850083	-3.179712
H	-6.908144	-2.998707	-1.558749
H	-8.375238	-1.592550	-2.992283
C	-4.268472	0.258303	1.552764
C	-5.135820	1.013501	2.360743
C	-3.678706	-0.890445	2.103273
C	-5.419684	0.626110	3.670152
H	-5.591524	1.915375	1.958362
C	-3.952662	-1.272536	3.419018
H	-2.997809	-1.499625	1.517566
C	-4.825159	-0.519079	4.205067
H	-6.098204	1.222252	4.275053
H	-3.482021	-2.163847	3.826095
H	-5.037990	-0.819316	5.227662
C	-0.229883	-2.668450	-0.374796
C	-0.211469	-2.676420	1.026710
C	-0.885064	-3.709582	-1.056475
C	-0.850964	-3.701090	1.731949
H	0.325228	-1.908565	1.574556
C	-1.523592	-4.727279	-0.350012
H	-0.884687	-3.738322	-2.143028
C	-1.511112	-4.721878	1.048442
H	-0.814683	-3.702213	2.817846
H	-2.024337	-5.526958	-0.889304
H	-2.004947	-5.518021	1.599235
C	1.770479	-2.143851	-2.428141
C	2.369466	-3.355932	-2.050391
C	2.186085	-1.529706	-3.621215
C	3.335485	-3.950557	-2.862832
H	2.097373	-3.828505	-1.113623
C	3.150328	-2.128120	-4.432604
H	1.770769	-0.573021	-3.925590
C	3.724973	-3.343561	-4.057431
H	3.790013	-4.887544	-2.553161

H	3.454728	-1.640188	-5.354674
H	4.478157	-3.808810	-4.687332
C	1.023191	3.569973	-1.149322
C	1.400289	3.680584	-2.497713
C	1.239583	4.663147	-0.299211
C	1.951531	4.862738	-2.990118
H	1.285205	2.836906	-3.173387
C	1.792677	5.845682	-0.793378
H	0.991472	4.590428	0.753347
C	2.144563	5.952177	-2.138879
H	2.235957	4.928580	-4.036841
H	1.954282	6.681999	-0.118912
H	2.575513	6.873710	-2.520470
C	-0.498448	2.342926	1.058594
C	-0.238421	1.549239	2.187260
C	-1.428904	3.391255	1.161857
C	-0.894986	1.801674	3.394115
H	0.483381	0.738218	2.135770
C	-2.076159	3.644472	2.370587
H	-1.644162	4.021055	0.303380
C	-1.811451	2.848553	3.488229
H	-0.681952	1.177922	4.257195
H	-2.790792	4.460210	2.436887
H	-2.322055	3.043347	4.427160
C	5.055352	2.856098	-0.267184
C	5.141232	3.446515	0.995996
C	4.174976	3.149879	1.956103
C	3.123969	2.274579	1.656843
C	3.022132	1.680346	0.392906
C	4.003864	1.985495	-0.564142
H	5.808916	3.069717	-1.022498
H	5.958990	4.123688	1.230327
H	4.240261	3.587869	2.949907
H	2.402488	2.046022	2.435321
H	3.964000	1.534040	-1.554686
O	2.988026	-1.104824	0.374348
S	3.349234	-1.303377	1.850133
O	2.175286	-1.127685	2.731822
O	4.620045	-0.711675	2.261658
C	3.679155	-3.138215	1.819515
F	2.584247	-3.823830	1.434928
F	4.022658	-3.553760	3.043678
F	4.670746	-3.424096	0.969296

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B3LYP/BS1 SCF energy: -3012.302606 a.u.

M06/BS2 SCF energy in PhMe: -3011.42542826 a.u.

M06/BS2 Free energy in PhMe: -3010.73785926 a.u.

C	-0.882708	0.452607	1.789131
C	-1.636160	0.606926	3.133777
H	-2.227852	-0.283529	3.365204
H	-0.933736	0.766082	3.960436
H	-2.322549	1.459356	3.099964
C	-0.015759	1.739606	1.664647
H	0.677796	1.784052	2.514118
H	-0.664949	2.617524	1.761118
C	-0.007711	-0.824148	1.934567
H	-0.666694	-1.675141	2.142009
H	0.625803	-0.711308	2.822868
C	-1.886911	0.363344	0.608031
H	-1.348455	0.114552	-0.313133
H	-2.334334	1.351458	0.450965
P	1.060744	1.976129	0.166589
P	-3.259935	-0.927089	0.774891
P	1.182875	-1.410635	0.609399
Ni	2.317552	0.163387	-0.321339
C	-4.618339	0.040768	1.590664
C	-5.154385	-0.464983	2.784360
C	-5.153793	1.226672	1.062123
C	-6.188609	0.203491	3.444644
H	-4.761983	-1.390862	3.198315
C	-6.185636	1.895990	1.719622
H	-4.780121	1.619294	0.119511
C	-6.703584	1.386541	2.914331
H	-6.592976	-0.202651	4.367733
H	-6.593996	2.809946	1.296379
H	-7.510368	1.906645	3.423169
C	-3.879944	-1.012989	-0.969316
C	-4.745003	-2.080730	-1.267096
C	-3.559707	-0.110713	-1.996134
C	-5.285465	-2.234380	-2.543406
H	-5.001637	-2.796161	-0.488870
C	-4.091003	-0.271495	-3.278595
H	-2.898715	0.730322	-1.810048
C	-4.956303	-1.330265	-3.555982

H	-5.959466	-3.061716	-2.748464
H	-3.831125	0.439056	-4.059098
H	-5.372074	-1.450272	-4.552522
C	0.004206	2.631612	-1.179067
C	0.168072	2.123356	-2.477084
C	-0.953438	3.637021	-0.956665
C	-0.609094	2.606809	-3.532252
H	0.900399	1.342315	-2.665050
C	-1.729590	4.117379	-2.011081
H	-1.091692	4.057237	0.035725
C	-1.559218	3.602216	-3.299871
H	-0.470775	2.205444	-4.531910
H	-2.465029	4.895348	-1.827892
H	-2.163994	3.979785	-4.119228
C	2.167480	3.360127	0.674514
C	2.171006	4.609342	0.037207
C	3.087602	3.120277	1.711834
C	3.065511	5.602820	0.443276
H	1.480077	4.813808	-0.773660
C	3.974112	4.116417	2.117390
H	3.119270	2.149988	2.203289
C	3.963776	5.361553	1.483082
H	3.056040	6.567403	-0.056036
H	4.675396	3.918903	2.922916
H	4.656403	6.137225	1.796080
C	2.194854	-2.605914	1.574970
C	3.067338	-2.099094	2.553687
C	2.135596	-3.990448	1.363978
C	3.850250	-2.961144	3.318205
H	3.149116	-1.025955	2.710981
C	2.926618	-4.851664	2.130134
H	1.478005	-4.403046	0.606659
C	3.780270	-4.341443	3.107703
H	4.519435	-2.556671	4.072000
H	2.871459	-5.922775	1.958619
H	4.393005	-5.013654	3.701104
C	0.244394	-2.381337	-0.627216
C	0.565791	-2.258852	-1.989204
C	-0.766657	-3.279707	-0.241238
C	-0.111119	-3.015898	-2.946120
H	1.354040	-1.579759	-2.298507
C	-1.437170	-4.036366	-1.202073
H	-1.038531	-3.397229	0.802462
C	-1.112817	-3.904594	-2.554081
H	0.146992	-2.911212	-3.995856
H	-2.218260	-4.723753	-0.892170
H	-1.642068	-4.491719	-3.298694
C	5.415347	0.330171	-2.194603
C	6.106065	-0.873511	-2.342325
C	5.602729	-2.058641	-1.790246
C	4.398380	-2.068284	-1.078367
C	3.708671	-0.867219	-0.936175
C	4.207705	0.309586	-1.484940
H	5.802139	1.253825	-2.614458
H	7.044800	-0.889478	-2.888209
H	6.157567	-2.984924	-1.913589
H	4.026746	-2.992343	-0.645832
H	3.656251	1.268822	-1.356548

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B3LYP/BS1 SCF energy: -3357.904552 a.u.

M06/BS2 SCF energy in PhMe: -3356.88215466 a.u.

M06/BS2 Free energy in PhMe: -3356.09257266 a.u.

C	1.833237	0.104736	-1.865381
C	2.801007	0.145451	-3.074029
H	3.597761	-0.597416	-2.973286
H	2.267353	-0.062246	-4.009226
H	3.274970	1.128743	-3.163112
C	0.692883	1.099073	-2.219088
H	0.192802	0.749937	-3.131987
H	1.129321	2.071750	-2.472782
C	1.302643	-1.351046	-1.791057
H	2.149558	-2.024479	-1.615758
H	0.906639	-1.608842	-2.778745
C	2.564707	0.557393	-0.573432
H	1.906170	0.420221	0.290800
H	2.768688	1.632089	-0.644294
P	-0.696796	1.370368	-1.010062
P	4.165576	-0.359077	-0.151140
P	-0.015336	-1.901237	-0.568225
Ni	-1.682566	-0.532401	-0.136259
C	5.448105	0.678493	-1.005924
C	6.309974	0.037041	-1.908048
C	5.614157	2.054949	-0.781637
C	7.301718	0.752755	-2.583936

H	6.205021	-1.031478	-2.080822
C	6.603150	2.771733	-1.454918
H	4.982243	2.568200	-0.060843
C	7.447515	2.121937	-2.360325
H	7.960485	0.239927	-3.279426
H	6.722898	3.835693	-1.267797
H	8.219886	2.680715	-2.881539
C	4.407885	0.159164	1.612565
C	5.357427	-0.570574	2.348599
C	3.728616	1.205273	2.257511
C	5.631423	-0.258083	3.680101
H	5.888755	-1.391077	1.871871
C	3.992835	1.510724	3.595258
H	2.990154	1.797706	1.725572
C	4.945611	0.783186	4.309749
H	6.376633	-0.829799	4.226711
H	3.456625	2.325785	4.074908
H	5.154009	1.026118	5.348084
C	-0.107788	2.613605	0.209210
C	-0.466065	2.458022	1.557542
C	0.683085	3.716941	-0.156999
C	-0.041611	3.378135	2.518632
H	-1.082224	1.615391	1.856400
C	1.106850	4.635759	0.803578
H	0.967419	3.871330	-1.193843
C	0.746898	4.466913	2.143648
H	-0.327475	3.243280	3.557957
H	1.716728	5.483744	0.505394
H	1.078106	5.183533	2.889705
C	-1.921399	2.248186	-2.075117
C	-2.224623	3.610647	-1.942867
C	-2.592168	1.495560	-3.054905
C	-3.167994	4.208328	-2.783727
H	-1.726729	4.211996	-1.189391
C	-3.529931	2.094996	-3.894668
H	-2.387491	0.432082	-3.161222
C	-3.819946	3.455184	-3.760665
H	-3.387038	5.267064	-2.675554
H	-4.036470	1.500150	-4.649398
H	-4.550632	3.923348	-4.413771
C	-0.487743	-3.520226	-1.315344
C	-0.836151	-3.580799	-2.675100
C	-0.596205	-4.683492	-0.538637
C	-1.255677	-4.780657	-3.249535
H	-0.794564	-2.692854	-3.300143
C	-1.014298	-5.882767	-1.116686
H	-0.364919	-4.657014	0.520135
C	-1.340474	-5.936909	-2.472388
H	-1.515498	-4.809675	-4.303907
H	-1.087490	-6.775093	-0.501718
H	-1.663763	-6.872319	-2.919771
C	0.915803	-2.284873	0.967582
C	0.655856	-1.562053	2.141728
C	1.921116	-3.266779	0.982555
C	1.377207	-1.817579	3.308849
H	-0.112542	-0.793683	2.141798
C	2.632607	-3.528668	2.152867
H	2.145203	-3.837922	0.086620
C	2.362699	-2.805044	3.316811
H	1.171571	-1.244297	4.207876
H	3.403071	-4.294076	2.152152
H	2.924637	-3.005226	4.224085
C	-4.561865	-3.528470	-0.092291
C	-4.552308	-4.038965	1.208712
C	-3.605574	-3.571932	2.120783
C	-2.674282	-2.596892	1.736474
C	-2.675100	-2.068547	0.436076
C	-3.630290	-2.558111	-0.472798
H	-5.291798	-3.888209	-0.813601
H	-5.272135	-4.797036	1.505097
H	-3.583717	-3.966218	3.134215
H	-1.944431	-2.262130	2.468937
H	-3.654429	-2.186556	-1.496053
O	-3.190040	0.664988	0.385914
C	-4.196450	0.458154	1.088485
H	-4.339448	-0.532427	1.539412
C	-5.207235	1.464261	1.355070
C	-6.280393	1.119762	2.199427
C	-5.137623	2.754868	0.791496
C	-7.270940	2.054814	2.483252
H	-6.329073	0.120664	2.625508
C	-6.131172	3.681609	1.077285
H	-4.311827	3.003584	0.132768
C	-7.194350	3.333192	1.922331
H	-8.098993	1.792803	3.134342
H	-6.087655	4.676794	0.645229

H	-7.967976	4.063662	2.141721

TS2

B3LYP/BS1 SCF energy: -3357.877084 a.u.

M06/BS2 SCF energy in PhMe: -3356.85749707 a.u.

M06/BS2 Free energy in PhMe: -3356.06481807 a.u.

C	1.847100	0.297872	-1.865812
C	2.807414	0.365942	-3.078097
H	3.458315	-0.512322	-3.121484
H	2.246703	0.412477	-4.019350
H	3.449773	1.250984	-3.019569
C	0.900105	1.520262	-2.019433
H	0.342777	1.412507	-2.957455
H	1.502401	2.428982	-2.129983
C	1.058131	-1.030013	-2.010634
H	1.767869	-1.864817	-1.996846
H	0.590727	-1.040543	-3.001479
C	2.642378	0.391591	-0.536031
H	1.965501	0.225283	0.309360
H	3.032191	1.410712	-0.429557
P	-0.372630	1.851956	-0.702742
P	4.050332	-0.854768	-0.324185
P	-0.307889	-1.502898	-0.812502
Ni	-1.576002	0.112935	0.073922
C	5.505715	0.076917	-1.004240
C	6.248658	-0.532761	-2.026268
C	5.913604	1.337110	-0.536892
C	7.361284	0.104871	-2.581288
H	5.955040	-1.515302	-2.388240
C	7.023700	1.975564	-1.089270
H	5.375634	1.816102	0.277552
C	7.748536	1.361292	-2.115033
H	7.925469	-0.381644	-3.372263
H	7.330213	2.948633	-0.714515
H	8.615370	1.858233	-2.541730
C	4.362782	-0.729534	1.498978
C	5.152882	-1.745272	2.064712
C	3.879212	0.283445	2.342790
C	5.463155	-1.742893	3.424691
H	5.530613	-2.545077	1.431951
C	4.178142	0.279202	3.707880
H	3.268819	1.090051	1.948039
C	4.972315	-0.730712	4.252650
H	6.084373	-2.532829	3.838291
H	3.796277	1.074584	4.343051
H	5.209383	-0.728335	5.312996
C	0.474445	2.873668	0.565636
C	0.361091	2.548716	1.925440
C	1.246234	3.987957	0.191632
C	1.018663	3.314256	2.891593
H	-0.257259	1.710813	2.227460
C	1.901476	4.749778	1.158190
H	1.328043	4.276459	-0.852641
C	1.791798	4.411573	2.509989
H	0.919209	3.055638	3.941965
H	2.493916	5.608635	0.856395
H	2.301457	5.007188	3.261847
C	-1.557277	2.983030	-1.543396
C	-1.990556	4.167335	-0.928432
C	-2.116832	2.614453	-2.779498
C	-2.945139	4.975648	-1.549535
H	-1.584551	4.462567	0.032927
C	-3.068186	3.425357	-3.397414
H	-1.818118	1.691182	-3.269707
C	-3.483202	4.609908	-2.784128
H	-3.265026	5.893886	-1.065336
H	-3.483746	3.132365	-4.357382
H	-4.221960	5.243013	-3.266906
C	-1.200434	-2.758617	-1.826230
C	-1.718042	-2.366148	-3.073601
C	-1.406585	-4.076030	-1.395070
C	-2.398754	-3.275634	-3.880647
H	-1.594924	-1.344159	-3.424260
C	-2.089539	-4.986006	-2.206047
H	-1.034822	-4.399782	-0.429663
C	-2.581407	-4.592055	-3.449922
H	-2.784278	-2.957025	-4.844953
H	-2.232066	-6.006310	-1.861454
H	-3.105549	-5.304079	-4.080809
C	0.548831	-2.409983	0.535243
C	0.421724	-1.961356	1.859169
C	1.364190	-3.524156	0.272029
C	1.084872	-2.613521	2.899633
H	-0.193384	-1.090996	2.074009
C	2.016710	-4.182195	1.314111

H	1.489730	-3.885847	-0.744256
C	1.878715	-3.728324	2.628124
H	0.987349	-2.247380	3.917337
H	2.641106	-5.043787	1.096883
H	2.396372	-4.236798	3.435933
C	-4.871495	-2.230173	-0.752731
C	-4.808800	-3.355880	0.074542
C	-3.899785	-3.397086	1.137205
C	-3.049548	-2.316346	1.366568
C	-3.094566	-1.170800	0.546774
C	-4.035762	-1.143357	-0.504438
H	-5.587628	-2.192711	-1.568943
H	-5.478318	-4.193846	-0.098681
H	-3.859889	-4.268021	1.786243
H	-2.356252	-2.360002	2.203384
H	-4.139313	-0.245837	-1.111869
O	-2.541573	1.363160	1.092004
C	-3.301917	0.522774	1.732537
H	-2.877026	0.015112	2.608369
C	-4.758220	0.773265	1.827674
C	-5.527606	0.045244	2.747802
C	-5.362650	1.769665	1.045586
C	-6.889904	0.302639	2.879238
H	-5.056925	-0.725406	3.353794
C	-6.724528	2.026627	1.183085
H	-4.752575	2.342621	0.354581
C	-7.489932	1.292232	2.094962
H	-7.482871	-0.262080	3.592618
H	-7.191869	2.803544	0.584703
H	-8.551981	1.495513	2.198996

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B3LYP/BS1 SCF energy: -3357.905729 a.u.

M06/BS2 SCF energy in PhMe: -3356.88500903 a.u.

M06/BS2 Free energy in PhMe: -3356.09053103 a.u.

C	1.796377	0.676327	-1.851831
C	2.758030	1.059351	-3.003021
H	3.521567	0.291034	-3.156312
H	2.211180	1.178241	-3.946006
H	3.274105	2.000546	-2.786354
C	0.701545	1.776697	-1.849922
H	0.198212	1.766432	-2.823544
H	1.182312	2.758905	-1.771993
C	1.184222	-0.697052	-2.233639
H	1.994549	-1.421820	-2.367359
H	0.693305	-0.598983	-3.209357
C	2.548077	0.652112	-0.494075
H	1.885518	0.259222	0.285792
H	2.789415	1.682070	-0.206711
P	-0.662811	1.755056	-0.584964
P	4.115821	-0.406372	-0.438725
P	-0.086329	-1.516451	-1.128158
Ni	-1.608957	-0.176710	-0.118298
C	5.431638	0.825213	-0.884811
C	6.275667	0.515628	-1.961801
C	5.641559	2.027839	-0.190139
C	7.294082	1.390870	-2.348163
H	6.136799	-0.419026	-2.500039
C	6.657463	2.902950	-0.573776
H	5.023006	2.274819	0.669357
C	7.484424	2.586977	-1.656074
H	7.939067	1.135454	-3.184432
H	6.811325	3.827756	-0.023994
H	8.277791	3.267883	-1.951537
C	4.374670	-0.569753	1.389050
C	5.295603	-1.549989	1.797983
C	3.735466	0.195479	2.377847
C	5.582683	-1.749096	3.148319
H	5.794978	-2.160833	1.049405
C	4.012910	-0.012252	3.731595
H	3.019312	0.965642	2.107287
C	4.938283	-0.981428	4.121061
H	6.306061	-2.505393	3.440962
H	3.509963	0.593212	4.481443
H	5.157413	-1.136678	5.173849
C	0.009565	2.581251	0.906509
C	-0.146471	2.000736	2.173227
C	0.691753	3.805476	0.794043
C	0.380338	2.625155	3.305839
H	-0.688395	1.066578	2.273357
C	1.213492	4.428183	1.927510
H	0.803991	4.288693	-0.172345
C	1.061885	3.837150	3.184780
H	0.251115	2.167003	4.282193
H	1.734168	5.376154	1.828684

H	1.468148	4.324387	4.066369
C	-1.898937	2.891798	-1.318351
C	-2.451227	3.944101	-0.574299
C	-2.345987	2.673950	-2.632780
C	-3.411492	4.779456	-1.146548
H	-2.137685	4.111861	0.449760
C	-3.307443	3.509012	-3.199505
H	-1.954088	1.848820	-3.222405
C	-3.839386	4.566620	-2.457596
H	-3.828985	5.593815	-0.561800
H	-3.640444	3.333769	-4.218418
H	-4.586969	5.218737	-2.899676
C	-0.908450	-2.641336	-2.337184
C	-1.740000	-2.056323	-3.308843
C	-0.764243	-4.035425	-2.318199
C	-2.400216	-2.846743	-4.248902
H	-1.881088	-0.977533	-3.331173
C	-1.427176	-4.824956	-3.261632
H	-0.142440	-4.511568	-1.568109
C	-2.243589	-4.235117	-4.227569
H	-3.038391	-2.380055	-4.993728
H	-1.302497	-5.903824	-3.238847
H	-2.757419	-4.852310	-4.958598
C	0.863580	-2.560514	0.038421
C	0.558311	-2.503786	1.406479
C	1.897084	-3.410340	-0.395081
C	1.268921	-3.278570	2.324499
H	-0.239544	-1.856332	1.756663
C	2.598029	-4.190630	0.523175
H	2.159434	-3.469757	-1.446862
C	2.287501	-4.123373	1.883943
H	1.027966	-3.218275	3.381672
H	3.393952	-4.842894	0.176288
H	2.843560	-4.724023	2.597595
C	-3.102408	-3.247843	0.233700
C	-2.809647	-3.978159	1.379374
C	-2.724799	-3.325652	2.618272
C	-2.931436	-1.951612	2.708565
C	-3.258237	-1.203706	1.565499
C	-3.320791	-1.859194	0.317120
H	-3.191585	-3.746622	-0.725528
H	-2.658467	-5.051772	1.319946
H	-2.502174	-3.897724	3.514918
H	-2.876748	-1.454203	3.673791
H	-3.710061	-1.326376	-0.549923
O	-2.860409	0.936610	0.607197
C	-3.571733	0.291454	1.636729
H	-3.231117	0.652826	2.622687
C	-5.072703	0.559944	1.534753
C	-5.897357	0.335371	2.644829
C	-5.644112	1.008078	0.339593
C	-7.273831	0.541227	2.558676
H	-5.462047	-0.000508	3.584205
C	-7.022584	1.219065	0.254796
H	-4.999893	1.212457	-0.509196
C	-7.841017	0.982899	1.360324
H	-7.902313	0.364180	3.427177
H	-7.456722	1.573793	-0.676412
H	-8.912594	1.148644	1.293096

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B3LYP/BS1 SCF energy: -3973.882142 a.u.

M06/BS2 SCF energy in PhMe: -3972.95813855 a.u.

M06/BS2 Free energy in PhMe: -3972.26018855 a.u.

C	1.683016	0.454749	1.572359
C	2.695780	0.805149	2.683965
H	3.565269	1.332238	2.274755
H	2.246858	1.452929	3.442362
H	3.061325	-0.104096	3.175083
C	0.424554	-0.140388	2.277668
H	-0.138730	0.673266	2.750659
H	0.734878	-0.799294	3.097128
C	1.308294	1.715744	0.743058
H	0.510480	1.470306	0.026940
H	2.177073	1.995900	0.139605
C	2.299517	-0.609419	0.619844
H	1.600511	-0.791284	-0.205858
H	2.408849	-1.558183	1.156170
P	-0.853431	-1.057026	1.251426
P	3.937008	-0.152072	-0.204811
P	0.824852	3.266325	1.721585
Ni	-1.315480	-0.193811	-0.925894
C	5.176129	-0.980706	0.907888
C	6.192230	-0.181963	1.453279
C	5.161697	-2.350159	1.219636

C	7.161412	-0.729867	2.297844
H	6.223916	0.878017	1.213095
C	6.128860	-2.900520	2.060494
H	4.399728	-2.997105	0.792792
C	7.130400	-2.090391	2.603676
H	7.939534	-0.094410	2.712558
H	6.105581	-3.963235	2.288481
H	7.884319	-2.520630	3.257642
C	3.918401	-1.296064	-1.666556
C	4.714290	-0.924768	-2.763339
C	3.166034	-2.479657	-1.762013
C	4.768954	-1.714117	-3.913707
H	5.290245	-0.003615	-2.716203
C	3.209924	-3.264214	-2.917111
H	2.534161	-2.799931	-0.938757
C	4.012842	-2.885276	-3.994796
H	5.393977	-1.408991	-4.748926
H	2.615368	-4.172397	-2.972171
H	4.044933	-3.496098	-4.892902
C	-0.304209	-2.815615	1.149102
C	-0.819148	-3.587860	0.092426
C	0.568498	-3.421887	2.068156
C	-0.460454	-4.931568	-0.039762
H	-1.514024	-3.152942	-0.622672
C	0.928110	-4.763752	1.928755
H	0.976294	-2.856579	2.900491
C	0.416094	-5.520921	0.872592
H	-0.871399	-5.513257	-0.860142
H	1.606021	-5.215999	2.647798
H	0.697145	-6.565104	0.764966
C	-2.292157	-1.081601	2.400853
C	-2.476522	-2.093140	3.355294
C	-3.219409	-0.031017	2.325583
C	-3.565464	-2.047665	4.226578
H	-1.779843	-2.923637	3.413257
C	-4.302789	0.012950	3.203630
H	-3.106678	0.744753	1.575543
C	-4.478736	-0.993841	4.154121
H	-3.701164	-2.839007	4.958974
H	-5.013852	0.831088	3.132970
H	-5.328611	-0.962761	4.830694
C	1.462982	4.586408	0.584137
C	2.829389	4.589422	0.249226
C	0.673934	5.664506	0.153486
C	3.379085	5.615939	-0.517652
H	3.477263	3.784551	0.588795
C	1.226985	6.696333	-0.608707
H	-0.380759	5.700323	0.406381
C	2.578694	6.674858	-0.952232
H	4.435471	5.589204	-0.772459
H	0.593996	7.516944	-0.936968
H	3.006450	7.476542	-1.548172
C	-1.008804	3.381068	1.485097
C	-1.783586	3.678590	2.617417
C	-1.662045	3.219259	0.249721
C	-3.171832	3.813102	2.523255
H	-1.292823	3.810352	3.578561
C	-3.049159	3.342921	0.155179
H	-1.089424	3.012810	-0.650151
C	-3.806445	3.643690	1.292058
H	-3.753296	4.049420	3.410561
H	-3.538238	3.201487	-0.804240
H	-4.885654	3.745514	1.213969
C	-0.904628	2.088834	-4.382570
C	0.344597	1.589283	-4.770048
C	0.909203	0.505324	-4.097557
C	0.218586	-0.079138	-3.025601
C	-1.004712	0.461710	-2.608452
C	-1.591933	1.518940	-3.307949
H	-1.344477	2.924734	-4.921177
H	0.867883	2.035500	-5.611693
H	1.864039	0.092316	-4.411756
H	0.643461	-0.961883	-2.543857
H	-2.570908	1.888233	-3.018641
O	-3.181434	-0.178444	-1.013492
S	-3.893148	-1.175238	-1.964898
O	-3.201219	-2.471579	-2.029137
O	-4.359693	-0.555719	-3.204034
C	-5.415834	-1.463974	-0.929855
F	-5.087839	-2.034322	0.235030
F	-6.246536	-2.276723	-1.590565
F	-6.041487	-0.307144	-0.685648

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B3LYP/BS1 SCF energy: -4319.479211 a.u.

M06/BS2 SCF energy in PhMe: -4318.42241835 a.u.

M06/BS2 Free energy in PhMe: - 4317.61559835 a.u.

C	1.484763	-0.803668	1.649194
C	2.076609	-1.264120	2.999896
H	2.860371	-0.585611	3.348500
H	1.306275	-1.295815	3.778191
H	2.512198	-2.265794	2.912127
C	0.289698	-1.764933	1.370210
H	-0.458717	-1.607769	2.154713
H	0.635316	-2.798614	1.495848
C	1.030379	0.687512	1.706591
H	0.252120	0.868742	0.959594
H	1.884360	1.311201	1.415513
C	2.544916	-0.975988	0.520226
H	2.131240	-0.578854	-0.414392
H	2.720525	-2.044938	0.356965
P	-0.746182	-1.742660	-0.216885
P	4.195004	-0.093856	0.751939
P	0.551125	1.475041	3.359280
Ni	-1.823318	0.346658	-1.010060
C	5.196724	-1.329232	1.717515
C	5.786908	-0.900401	2.915507
C	5.411198	-2.653273	1.301512
C	6.559606	-1.772512	3.687025
H	5.636804	0.124107	3.247300
C	6.181018	-3.526507	2.069766
H	4.988077	-3.002435	0.362886
C	6.755840	-3.087916	3.266284
H	7.006981	-1.423161	4.613892
H	6.338453	-4.548165	1.733165
H	7.357067	-3.768493	3.863345
C	4.956871	-0.309350	-0.929494
C	6.108112	0.452552	-1.196107
C	4.480431	-1.163756	-1.936859
C	6.773871	0.350805	-2.417539
H	6.485950	1.132450	-0.435867
C	5.139087	-1.257894	-3.166443
H	3.594532	-1.769234	-1.776734
C	6.289495	-0.505787	-3.410078
H	7.667883	0.942845	-2.596370
H	4.751151	-1.928622	-3.929082
H	6.805649	-0.586922	-4.363233
C	0.285841	-2.517802	-1.538711
C	0.148873	-2.036045	-2.849889
C	1.143202	-3.607951	-1.309316
C	0.859628	-2.619211	-3.903042
H	-0.524861	-1.208991	-3.051435
C	1.856204	-4.187874	-2.359036
H	1.243698	-4.022949	-0.310530
C	1.717156	-3.692446	-3.659579
H	0.732263	-2.238406	-4.912679
H	2.511581	-5.032688	-2.164201
H	2.265355	-4.151061	-4.478315
C	-1.906303	-3.110862	0.245578
C	-2.015703	-4.293156	-0.501248
C	-2.706408	-2.963417	1.391080
C	-2.879516	-5.312563	-0.095218
H	-1.431564	-4.427875	-1.404452
C	-3.564997	-3.984307	1.795596
H	-2.676269	-2.045757	1.968844
C	-3.649679	-5.166166	1.057644
H	-2.949234	-6.221002	-0.687693
H	-4.174473	-3.848921	2.684884
H	-4.320326	-5.961053	1.372730
C	0.455990	3.226201	2.732309
C	1.576430	4.042781	2.958630
C	-0.629002	3.764369	2.022410
C	1.621085	5.351721	2.473354
H	2.419448	3.649536	3.522076
C	-0.589073	5.074497	1.538099
H	-1.516613	3.165766	1.845732
C	0.537774	5.871272	1.760739
H	2.496854	5.967748	2.661471
H	-1.439910	5.464914	0.985658
H	0.565197	6.893775	1.392546
C	-1.227813	1.037900	3.636692
C	-1.670220	1.061864	4.970917
C	-2.156453	0.697825	2.639510
C	-2.997607	0.773854	5.293968
H	-0.965100	1.306977	5.761777
C	-3.484702	0.399153	2.956962
H	-1.857023	0.665592	1.595598
C	-3.906923	0.440177	4.288079
H	-3.318695	0.802863	6.332020
H	-4.173896	0.131533	2.160660
H	-4.939092	0.210260	4.538695

C	-3.763280	4.062593	-0.851208
C	-3.592627	4.584522	-2.135229
C	-2.947253	3.818615	-3.107640
C	-2.454207	2.548116	-2.789045
C	-2.608180	2.016866	-1.498493
C	-3.287921	2.783318	-0.540871
H	-4.291523	4.638552	-0.094132
H	-3.975503	5.572051	-2.380616
H	-2.830638	4.204370	-4.118203
H	-1.961611	1.965946	-3.565419
H	-3.480057	2.376489	0.448199
O	-3.498137	-0.370298	-0.522062
S	-4.652936	-0.425393	-1.558170
O	-4.183832	-0.823535	-2.891145
O	-5.603982	0.678456	-1.430355
C	-5.562919	-1.901797	-0.873819
F	-4.893037	-3.033297	-1.113264
F	-6.761596	-1.984359	-1.462774
F	-5.744688	-1.775245	0.450383
O	-0.113669	0.993956	-1.591973
C	0.330350	2.148937	-1.435102
H	-0.233765	2.865322	-0.828888
C	1.579164	2.610607	-2.014434
C	2.010157	3.913689	-1.701776
C	2.345558	1.799309	-2.873763
C	3.195424	4.400583	-2.244920
H	1.417074	4.528040	-1.029097
C	3.527706	2.292114	-3.411005
H	2.003937	0.795228	-3.102752
C	3.950374	3.590584	-3.097817
H	3.532555	5.404253	-2.004066
H	4.131575	1.664760	-4.058363
H	4.877351	3.969402	-3.519725

TS3

B3LYP/BS1 SCF energy: -4319.463362 a.u.

M06/BS2 SCF energy in PhMe: -4318.40371330 a.u.

M06/BS2 Free energy in PhMe: -4317.59776130 a.u.

C	-1.451834	1.605004	1.169141
C	-2.066011	2.640807	2.136525
H	-2.788697	2.176982	2.813623
H	-1.296394	3.115474	2.755364
H	-2.585807	3.428024	1.578171
C	-0.344172	2.367539	0.378892
H	0.466696	2.602458	1.076309
H	-0.741294	3.333845	0.045346
C	-0.843577	0.383545	1.930555
H	-0.005869	-0.032473	1.357751
H	-1.605296	-0.401685	1.973353
C	-2.542020	1.105581	0.175710
H	-2.097101	0.342313	-0.470369
H	-2.851997	1.937551	-0.467028
P	0.532778	1.607089	-1.107889
P	-4.059677	0.289277	0.938001
P	-0.355412	0.573476	3.748005
Ni	1.270851	-0.622398	-0.796350
C	-5.237851	1.714439	1.139861
C	-5.768171	1.953431	2.416183
C	-5.635016	2.549106	0.082519
C	-6.661000	3.005716	2.636949
H	-5.477548	1.310723	3.243668
C	-6.526490	3.599628	0.299431
H	-5.258177	2.368869	-0.921164
C	-7.040271	3.831666	1.578793
H	-7.059575	3.176874	3.633557
H	-6.825870	4.235233	-0.530296
H	-7.736134	4.649581	1.746384
C	-4.794107	-0.558482	-0.540797
C	-5.793208	-1.513295	-0.282302
C	-4.428765	-0.325424	-1.876804
C	-6.420794	-2.199403	-1.321756
H	-6.079794	-1.721561	0.746157
C	-5.049358	-1.020479	-2.918124
H	-3.656624	0.396777	-2.121362
C	-6.048655	-1.955406	-2.645664
H	-7.193454	-2.930352	-1.097544
H	-4.748920	-0.824048	-3.944362
H	-6.530820	-2.493741	-3.457480
C	-0.612174	1.798510	-2.542786
C	-0.624877	0.803592	-3.531826
C	-1.420845	2.934413	-2.719700
C	-1.434375	0.934255	-4.663760
H	-0.002836	-0.077721	-3.415866
C	-2.234184	3.061457	-3.845520
H	-1.409951	3.734461	-1.985543

C	-2.244324	2.059324	-4.820212
H	-1.427450	0.156002	-5.422079
H	-2.854121	3.945884	-3.965513
H	-2.875248	2.161076	-5.699119
C	1.796030	2.920655	-1.415399
C	1.950194	3.515525	-2.676944
C	2.639211	3.330265	-0.369657
C	2.906719	4.512106	-2.879074
H	1.323078	3.208581	-3.506796
C	3.587036	4.332054	-0.572990
H	2.577826	2.859169	0.605130
C	3.720908	4.930493	-1.826684
H	3.010489	4.961798	-3.862975
H	4.227994	4.634584	0.250495
H	4.461357	5.710023	-1.984724
C	0.036446	-1.210743	4.090203
C	-1.014054	-2.145272	4.002604
C	1.286890	-1.665208	4.538577
C	-0.810013	-3.489660	4.314149
H	-2.007701	-1.820584	3.701242
C	1.487489	-3.010424	4.863311
H	2.114348	-0.969950	4.633743
C	0.444639	-3.929426	4.744880
H	-1.637124	-4.190964	4.235072
H	2.465473	-3.336299	5.208672
H	0.602785	-4.974747	4.996268
C	1.317129	1.370134	3.708246
C	1.553060	2.385940	4.649666
C	2.355206	1.024200	2.824652
C	2.787942	3.036775	4.711322
H	0.760700	2.665111	5.340039
C	3.590667	1.673180	2.883087
H	2.220291	0.240768	2.084928
C	3.807888	2.680867	3.827974
H	2.950876	3.819004	5.448224
H	4.371695	1.393634	2.182789
H	4.770159	3.184270	3.874430
C	2.871473	-4.119638	1.018132
C	3.281961	-4.859122	-0.095379
C	2.926679	-4.446723	-1.382591
C	2.155523	-3.298560	-1.554733
C	1.754111	-2.526638	-0.447894
C	2.111229	-2.965419	0.842305
H	3.144638	-4.439939	2.020271
H	3.875100	-5.759957	0.040605
H	3.248179	-5.020360	-2.247974
H	1.870106	-2.996006	-2.558967
H	1.795179	-2.405272	1.719771
O	3.045772	0.004684	-0.465055
S	4.258657	-0.580140	-1.223439
O	3.943954	-0.900058	-2.622280
O	5.025825	-1.535078	-0.422184
C	5.339645	0.937223	-1.307937
F	4.849896	1.825549	-2.177477
F	6.563033	0.575117	-1.710625
F	5.446113	1.525304	-0.103042
O	-0.478544	-1.239884	-1.108206
C	-0.454359	-2.363359	-0.480588
H	-0.456703	-2.357270	0.615098
C	-0.963238	-3.598061	-1.096899
C	-1.115983	-4.745563	-0.302509
C	-1.340193	-3.628428	-2.448941
C	-1.629851	-5.914648	-0.857174
H	-0.819358	-4.715614	0.743136
C	-1.859093	-4.797179	-2.997442
H	-1.232313	-2.728614	-3.045324
C	-2.000386	-5.941538	-2.204850
H	-1.743077	-6.803246	-0.242745
H	-2.156790	-4.820462	-4.042046
H	-2.402966	-6.853484	-2.637529

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B3LYP/BS1 SCF energy: -4319.507118 a.u.

M06/BS2 SCF energy in PhMe: -4318.44482059 a.u.

M06/BS2 Free energy in PhMe: -4317.63468859 a.u.

C	1.432578	-0.941386	-1.731966
C	2.119942	-1.585679	-2.957099
H	2.926709	-2.257867	-2.649437
H	1.417037	-2.179108	-3.550299
H	2.554038	-0.815373	-3.604390
C	0.174348	-0.218535	-2.296868
H	-0.564540	-0.975816	-2.580425
H	0.442136	0.289827	-3.231576
C	1.028674	-2.016159	-0.679421
H	0.314023	-1.591028	0.033720

H	1.926765	-2.263039	-0.103689
C	2.388274	0.095065	-1.070170
H	1.888285	0.489805	-0.180078
H	2.543379	0.939580	-1.751285
P	-0.842370	1.060102	-1.365532
P	4.066138	-0.563775	-0.513894
P	0.430505	-3.697689	-1.314782
Ni	-1.450468	0.629263	0.753922
C	5.119508	-0.331201	-2.028103
C	5.805717	-1.442369	-2.538938
C	5.273037	0.906635	-2.675423
C	6.613003	-1.328334	-3.674494
H	5.705874	-2.404882	-2.042857
C	6.076307	1.023391	-3.809404
H	4.774095	1.787783	-2.279670
C	6.746697	-0.095669	-4.313280
H	7.136486	-2.201026	-4.056277
H	6.186277	1.988473	-4.297934
H	7.374196	-0.003103	-5.195890
C	4.704603	0.824902	0.539203
C	6.093586	0.876238	0.765679
C	3.889853	1.747241	1.213415
C	6.648165	1.825538	1.621200
H	6.748781	0.170941	0.260380
C	4.447125	2.693011	2.080016
H	2.813875	1.745747	1.079981
C	5.824896	2.739560	2.284791
H	7.724473	1.848579	1.773246
H	3.790578	3.385394	2.599642
H	6.255102	3.475669	2.958846
C	0.038969	2.669204	-1.441795
C	-0.180425	3.604400	-0.419164
C	0.855193	3.028776	-2.527066
C	0.408444	4.868684	-0.477739
H	-0.805534	3.340647	0.427370
C	1.447868	4.290487	-2.579733
H	1.027167	2.335155	-3.344268
C	1.227109	5.212320	-1.553892
H	0.228707	5.581257	0.322241
H	2.078800	4.552888	-3.424482
H	1.689903	6.194431	-1.595785
C	-2.220588	1.231494	-2.577252
C	-2.452957	2.422794	-3.280082
C	-3.036356	0.116915	-2.833845
C	-3.469311	2.490287	-4.234977
H	-1.846002	3.300297	-3.087655
C	-4.044960	0.188274	-3.792567
H	-2.904289	-0.803278	-2.275166
C	-4.263129	1.373737	-4.497598
H	-3.637458	3.419711	-4.772255
H	-4.665584	-0.683801	-3.977288
H	-5.052303	1.428408	-5.242608
C	0.628080	-4.697732	0.238149
C	1.900768	-4.781808	0.834594
C	-0.400702	-5.493925	0.767524
C	2.124734	-5.600152	1.942101
H	2.733431	-4.210599	0.430742
C	-0.172579	-6.323073	1.869245
H	-1.389936	-5.467476	0.322330
C	1.087244	-6.374234	2.467162
H	3.114828	-5.638118	2.389167
H	-0.985990	-6.930548	2.258713
H	1.262410	-7.016414	3.326038
C	-1.410272	-3.527162	-1.455221
C	-2.008818	-4.028322	-2.623216
C	-2.239808	-2.965471	-0.467930
C	-3.394639	-3.975629	-2.799267
H	-1.382786	-4.469079	-3.395250
C	-3.623991	-2.906823	-0.641179
H	-1.809689	-2.584015	0.452806
C	-4.203268	-3.416520	-1.807946
H	-3.839384	-4.374541	-3.707397
H	-4.241923	-2.450198	0.126160
H	-5.281220	-3.374961	-1.940878
C	-1.602989	-2.737712	3.348711
C	-2.798833	-2.101638	3.706189
C	-2.886457	-0.712774	3.660908
C	-1.776392	0.048466	3.263781
C	-0.575135	-0.585704	2.894528
C	-0.503345	-1.987514	2.935480
H	-1.527749	-3.821107	3.379279
H	-3.655603	-2.690478	4.021468
H	-3.808160	-0.209459	3.932704
H	-1.828137	1.132155	3.321255
H	0.417791	-2.489177	2.651297
O	-3.277449	0.337746	0.336358

S	-4.365709	1.114957	1.107720
O	-3.788174	2.076893	2.059801
O	-5.444702	0.228497	1.543678
C	-5.103646	2.179470	-0.229063
F	-4.175248	3.021867	-0.708541
F	-6.105417	2.897501	0.287496
F	-5.574858	1.433445	-1.231014
O	0.231459	1.004917	1.294446
C	0.610365	0.263623	2.437140
H	1.429660	-0.427278	2.176055
C	1.116893	1.174979	3.555509
C	1.901270	0.635290	4.583554
C	0.796500	2.535812	3.592350
C	2.347150	1.435943	5.634073
H	2.166373	-0.419808	4.559398
C	1.243615	3.340549	4.644376
H	0.208527	2.959911	2.785718
C	2.018118	2.793864	5.668617
H	2.956757	1.002216	6.422547
H	0.984360	4.396361	4.662170
H	2.366240	3.419828	6.486041

TS4

B3LYP/BS1 SCF energy: -4319.500738 a.u.

M06/BS2 SCF energy in PhMe: -4318.45962382 a.u.

M06/BS2 Free energy in PhMe: -4317.65008682 a.u.

C	-2.122890	0.016904	-2.050504
C	-2.909744	0.005794	-3.385246
H	-3.711300	0.751459	-3.383679
H	-2.247115	0.231561	-4.229568
H	-3.366443	-0.973911	-3.563037
C	-0.949742	-0.982885	-2.267140
H	-0.351522	-0.598156	-3.103245
H	-1.361409	-1.945154	-2.594378
C	-1.606321	1.466680	-1.865833
H	-2.469075	2.135622	-1.770485
H	-1.104090	1.753096	-2.795840
C	-3.045935	-0.441618	-0.887372
H	-2.540153	-0.277223	0.067986
H	-3.214500	-1.520723	-0.970522
P	0.281768	-1.278904	-0.900615
P	-4.706409	0.451185	-0.760671
P	-0.391588	1.974438	-0.514882
Ni	1.346915	0.691007	-0.192938
C	-5.822714	-0.654415	-1.761023
C	-6.573276	-0.070897	-2.792182
C	-5.971321	-2.030402	-1.521830
C	-7.439197	-0.839822	-3.574553
H	-6.478038	0.995450	-2.983275
C	-6.833909	-2.801138	-2.301257
H	-5.422500	-2.501830	-0.710359
C	-7.568675	-2.207395	-3.331853
H	-8.012061	-0.369684	-4.369746
H	-6.938835	-3.864572	-2.101212
H	-8.242230	-2.808397	-3.937154
C	-5.248214	0.000397	0.954540
C	-6.344269	0.716130	1.467408
C	-4.655253	-0.979469	1.765461
C	-6.843511	0.451879	2.742316
H	-6.809097	1.489713	0.859982
C	-5.146646	-1.235412	3.048344
H	-3.804039	-1.552688	1.413338
C	-6.242376	-0.525229	3.539542
H	-7.695566	1.013812	3.116420
H	-4.668027	-1.995024	3.661058
H	-6.623471	-0.728014	4.536994
C	-0.614705	-2.382977	0.282505
C	-0.657953	-2.090234	1.650897
C	-1.245682	-3.550973	-0.183406
C	-1.334583	-2.938253	2.534153
H	-0.138971	-1.223436	2.037567
C	-1.925113	-4.390818	0.696577
H	-1.193382	-3.818239	-1.235639
C	-1.973313	-4.083345	2.060714
H	-1.341516	-2.703061	3.594602
H	-2.406578	-5.290206	0.321587
H	-2.494104	-4.743993	2.748897
C	1.452884	-2.482882	-1.675638
C	2.263487	-3.249442	-0.820031
C	1.606110	-2.633175	-3.061311
C	3.195505	-4.145152	-1.341048
H	2.172133	-3.141808	0.254768
C	2.538620	-3.536056	-3.580132
H	1.002472	-2.056555	-3.754259
C	3.335985	-4.293850	-2.723058

H	3.814405	-4.724792	-0.661654
H	2.635719	-3.645321	-4.657373
H	4.061531	-4.994519	-3.127462
C	-0.090292	3.708138	-1.100432
C	0.307100	3.940393	-2.427521
C	-0.190909	4.803035	-0.230899
C	0.564900	5.233646	-2.880564
H	0.440663	3.111149	-3.117003
C	0.073783	6.096748	-0.683607
H	-0.464596	4.648918	0.806618
C	0.444896	6.318125	-2.009774
H	0.867320	5.391161	-3.912532
H	-0.007804	6.931316	0.007438
H	0.647981	7.326236	-2.360830
C	-1.421297	2.186107	0.999795
C	-1.000347	1.601786	2.203096
C	-2.613218	2.932524	0.986035
C	-1.754490	1.756323	3.368947
H	-0.078983	1.032185	2.245468
C	-3.365132	3.082400	2.150516
H	-2.954819	3.407543	0.071401
C	-2.937370	2.493728	3.344163
H	-1.403480	1.299769	4.289786
H	-4.287690	3.655339	2.124332
H	-3.528341	2.610088	4.248457
C	3.837458	4.081175	-0.243154
C	3.889510	4.498575	1.089139
C	3.134270	3.819946	2.044146
C	2.331349	2.733480	1.674373
C	2.274997	2.294948	0.343431
C	3.033956	2.998135	-0.608304
H	4.418050	4.601570	-1.002416
H	4.512491	5.342009	1.377105
H	3.172120	4.122225	3.088294
H	1.777433	2.220525	2.453013
H	3.003571	2.701697	-1.654104
O	2.193192	-0.669731	1.340875
S	2.735501	-0.540730	2.743517
O	1.717482	-0.094911	3.715288
O	4.074623	0.065361	2.813642
C	3.037724	-2.329771	3.167365
F	1.899420	-3.043991	3.104298
F	3.540845	-2.443101	4.401164
F	3.910873	-2.875380	2.299177
O	3.128113	0.055336	-1.276483
C	4.215278	-0.025021	-0.698178
C	5.462867	-0.420841	-1.362401
C	6.635445	-0.471604	-0.591959
C	5.504071	-0.743532	-2.729518
C	7.843107	-0.837258	-1.184335
C	6.710833	-1.106756	-3.316575
C	7.879491	-1.151993	-2.545001
H	6.586006	-0.227287	0.466499
H	8.751446	-0.877087	-0.590106
H	8.820773	-1.436011	-3.008520
H	6.749294	-1.357352	-4.373177
H	4.584068	-0.710848	-3.304288
H	4.285147	0.203662	0.373471

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B3LYP/BS1 SCF energy: -4319.512054 a.u.

M06/BS2 SCF energy in PhMe: -4318.46302515 a.u.

M06/BS2 Free energy in PhMe: -4317.65470515 a.u.

C	-2.243552	1.874159	-1.464691
C	-3.425479	2.578974	-2.173962
H	-4.227134	2.819686	-1.468747
H	-3.096873	3.516268	-2.639743
H	-3.848620	1.940266	-2.956852
C	-1.140777	1.730151	-2.549424
H	-0.805797	2.732658	-2.841873
H	-1.579992	1.279678	-3.446373
C	-1.779521	2.826094	-0.332747
H	-2.613481	2.975354	0.361886
H	-1.570266	3.802560	-0.781141
C	-2.676298	0.479385	-0.930438
H	-1.886262	0.077025	-0.287813
H	-2.778623	-0.214016	-1.773155
P	0.388912	0.753349	-2.120378
P	-4.267529	0.468981	0.094217
P	-0.299216	2.409736	0.767185
Ni	1.327734	1.155824	-0.043168
C	-5.520747	-0.024967	-1.190885
C	-6.598057	0.839357	-1.434369
C	-5.455106	-1.231109	-1.908137
C	-7.576684	0.519538	-2.379616

H	-6.672948	1.769348	-0.875624
C	-6.430400	-1.553851	-2.851514
H	-4.646478	-1.931243	-1.713572
C	-7.492921	-0.677262	-3.091378
H	-8.404387	1.202201	-2.554492
H	-6.366533	-2.493136	-3.395190
H	-8.254307	-0.931372	-3.824288
C	-4.121927	-1.104876	1.058567
C	-5.111839	-1.311255	2.036315
C	-3.105082	-2.062933	0.928797
C	-5.093981	-2.444823	2.846985
H	-5.899617	-0.572277	2.166780
C	-3.071363	-3.188113	1.757924
H	-2.313221	-1.943776	0.196737
C	-4.067551	-3.383599	2.714105
H	-5.871408	-2.586412	3.593732
H	-2.252420	-3.893522	1.665711
H	-4.036563	-4.256259	3.360853
C	0.003025	-0.945881	-2.707259
C	0.150817	-2.030867	-1.832256
C	-0.465211	-1.176029	-4.014668
C	-0.167542	-3.325299	-2.257195
H	0.495936	-1.884602	-0.813528
C	-0.777526	-2.467716	-4.434353
H	-0.576064	-0.350577	-4.713387
C	-0.630027	-3.544625	-3.554007
H	-0.052821	-4.150372	-1.562101
H	-1.136430	-2.633576	-5.446713
H	-0.877210	-4.550824	-3.882057
C	1.618701	1.414691	-3.333082
C	2.349293	0.581366	-4.192753
C	1.907647	2.790173	-3.326578
C	3.324960	1.114377	-5.039068
H	2.157065	-0.486040	-4.207070
C	2.880076	3.321355	-4.173291
H	1.381197	3.457002	-2.648052
C	3.591393	2.483900	-5.035296
H	3.875088	0.453525	-5.703744
H	3.084937	4.388400	-4.155227
H	4.349642	2.896339	-5.695074
C	0.234895	4.111736	1.257034
C	0.439823	5.095543	0.276236
C	0.536845	4.422176	2.591383
C	0.908662	6.363585	0.621635
H	0.242490	4.881749	-0.771084
C	1.001931	5.691656	2.936141
H	0.418724	3.669993	3.363113
C	1.185898	6.667089	1.955287
H	1.056260	7.111968	-0.152441
H	1.227043	5.913228	3.975639
H	1.548287	7.654814	2.226668
C	-1.089905	1.680537	2.254325
C	-0.829950	0.347008	2.596181
C	-1.996225	2.426434	3.030584
C	-1.447954	-0.232488	3.708601
H	-0.156760	-0.264092	2.002374
C	-2.609633	1.846437	4.138840
H	-2.215381	3.461044	2.780640
C	-2.332977	0.518246	4.480601
H	-1.225368	-1.268426	3.946861
H	-3.305232	2.431509	4.734719
H	-2.814610	0.070386	5.345659
C	4.266227	3.165482	2.101375
C	4.378927	2.481656	3.314712
C	3.511871	1.423605	3.587672
C	2.533984	1.049844	2.656161
C	2.405791	1.731204	1.437282
C	3.286121	2.795078	1.176096
H	4.938809	3.990022	1.874058
H	5.137774	2.769756	4.038103
H	3.592928	0.875927	4.523730
H	1.886443	0.211497	2.892894
H	3.212075	3.350758	0.242743
O	0.830507	-2.090613	1.251076
S	1.217535	-3.085260	2.299040
O	0.229930	-3.260049	3.377657
O	2.638725	-2.991891	2.703803
C	1.143660	-4.683523	1.349763
F	-0.099898	-4.902941	0.861231
F	1.477954	-5.728149	2.113888
F	1.982503	-4.645079	0.294117
O	2.818717	0.011486	-0.626317
C	3.352077	-0.904209	0.029788
C	4.421180	-1.732289	-0.512800
C	4.869266	-2.818987	0.260726
C	4.997431	-1.466620	-1.770378

C	5.889664	-3.634101	-0.226971
C	6.018258	-2.281098	-2.242826
C	6.463009	-3.364404	-1.471511
H	4.396029	-3.018796	1.219158
H	6.235890	-4.478376	0.361860
H	7.261263	-3.999430	-1.847297
H	6.473925	-2.079883	-3.208419
H	4.638418	-0.621940	-2.350228
H	3.017742	-1.119303	1.047251

TS5

B3LYP/BS1 SCF energy: -4319.482249 a.u.

M06/BS2 SCF energy in PhMe: -4318.43369970 a.u.

M06/BS2 Free energy in PhMe: -4317.62232770 a.u.

C	-2.199132	-2.300344	0.511603
C	-3.333977	-3.338934	0.689026
H	-3.982636	-3.378795	-0.190659
H	-2.920062	-4.342944	0.845263
H	-3.961433	-3.090920	1.551606
C	-1.299156	-2.462458	1.768069
H	-0.904138	-3.484487	1.773442
H	-1.917598	-2.367277	2.667849
C	-1.431714	-2.721619	-0.769927
H	-2.128836	-2.704417	-1.613889
H	-1.119629	-3.764213	-0.644712
C	-2.779422	-0.859196	0.446100
H	-1.976642	-0.151915	0.211282
H	-3.146598	-0.578155	1.439833
P	0.144772	-1.303785	1.971528
P	-4.136645	-0.546278	-0.838595
P	0.092524	-1.783555	-1.371536
Ni	1.350112	-0.706848	0.164474
C	-5.662905	-1.083665	0.079123
C	-6.547820	-1.955213	-0.572739
C	-5.982431	-0.657570	1.379786
C	-7.712731	-2.402671	0.057530
H	-6.320854	-2.285649	-1.583719
C	-7.141214	-1.105669	2.013661
H	-5.331319	0.043656	1.895574
C	-8.008479	-1.982273	1.354141
H	-8.386436	-3.076761	-0.465186
H	-7.372977	-0.765736	3.019963
H	-8.912597	-2.328615	1.848044
C	-4.309337	1.300282	-0.740473
C	-5.587456	1.877923	-0.852287
C	-3.195473	2.156128	-0.715396
C	-5.744267	3.262481	-0.916938
H	-6.469341	1.244933	-0.883806
C	-3.352671	3.542978	-0.780894
H	-2.184400	1.769023	-0.654059
C	-4.628002	4.100144	-0.879188
H	-6.743175	3.684633	-0.997664
H	-2.470244	4.174375	-0.767018
H	-4.750064	5.178817	-0.932657
C	-0.520649	0.089333	2.962977
C	-0.446629	1.399814	2.472964
C	-1.132490	-0.152955	4.206376
C	-0.989638	2.454372	3.213238
H	0.026945	1.614438	1.521223
C	-1.667757	0.902892	4.941474
H	-1.178482	-1.161406	4.610369
C	-1.599100	2.208203	4.442813
H	-0.929003	3.461437	2.813301
H	-2.136073	0.708059	5.902692
H	-2.019550	3.029798	5.016718
C	1.272667	-2.207411	3.118660
C	1.989122	-1.493355	4.093380
C	1.523605	-3.581342	2.970958
C	2.914245	-2.144301	4.910366
H	1.826429	-0.427892	4.210191
C	2.447935	-4.230226	3.790640
H	1.003888	-4.161962	2.214167
C	3.144872	-3.513444	4.764691
H	3.455900	-1.576399	5.661811
H	2.621259	-5.295825	3.666555
H	3.863598	-4.018396	5.404206
C	1.056605	-3.160218	-2.144057
C	1.370141	-4.293811	-1.374693
C	1.554235	-3.079082	-3.451801
C	2.136506	-5.329953	-1.906384
H	1.021736	-4.372605	-0.347945
C	2.321000	-4.118355	-3.983851
H	1.349427	-2.204270	-4.058152
C	2.610495	-5.247041	-3.217632
H	2.362799	-6.200561	-1.296606

H	2.692782	-4.039805	-5.001809
H	3.204226	-6.055323	-3.635641
C	-0.574165	-0.794514	-2.766801
C	-0.519811	0.603183	-2.712400
C	-1.203183	-1.417092	-3.861704
C	-1.074388	1.374979	-3.738826
H	-0.065829	1.109357	-1.866522
C	-1.746991	-0.646040	-4.886297
H	-1.263293	-2.500614	-3.921819
C	-1.681715	0.750581	-4.826733
H	-1.024291	2.457387	-3.661077
H	-2.227975	-1.135181	-5.729238
H	-2.113034	1.347032	-5.626247
C	4.637052	-1.699275	-2.123561
C	4.586454	-0.926884	-3.288994
C	3.707049	0.156846	-3.376514
C	2.867295	0.464465	-2.305462
C	2.892970	-0.308690	-1.128272
C	3.809119	-1.379889	-1.049996
H	5.334323	-2.529703	-2.048129
H	5.249406	-1.155823	-4.119820
H	3.687983	0.774391	-4.270805
H	2.235029	1.343899	-2.359985
H	3.897042	-1.946163	-0.124476
O	0.442295	2.527377	-0.384083
S	0.857881	3.810795	-1.035682
O	-0.103000	4.323220	-2.031063
O	2.287510	3.840488	-1.414047
C	0.732714	5.009763	0.380861
F	-0.533575	5.051251	0.853851
F	1.077389	6.246520	0.006837
F	1.530954	4.632124	1.394605
O	2.421566	0.224036	1.383638
C	3.075042	0.926713	0.492075
C	4.533859	1.140413	0.667230
C	5.142871	2.193581	-0.031737
C	5.286659	0.360702	1.557141
C	6.502092	2.449244	0.146499
C	6.643078	0.622915	1.732904
C	7.253818	1.663039	1.023553
H	4.540373	2.811199	-0.693746
H	6.972654	3.266852	-0.392675
H	8.312774	1.865421	1.162667
H	7.226744	0.021923	2.425629
H	4.793989	-0.432413	2.111531
H	2.545522	1.755947	0.019917

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B3LYP/BS1 SCF energy: -4319.509090 a.u.

M06/BS2 SCF energy in PhMe: -4318.45954660 a.u.

M06/BS2 Free energy in PhMe: -4317.64719860 a.u.

C	-2.203508	-2.278333	0.686847
C	-3.361203	-3.241553	1.045318
H	-4.108814	-3.279558	0.247855
H	-2.985486	-4.260332	1.201575
H	-3.869735	-2.920595	1.960387
C	-1.164405	-2.448991	1.830387
H	-0.818283	-3.488499	1.818847
H	-1.667484	-2.304128	2.793368
C	-1.619787	-2.791283	-0.656009
H	-2.405241	-2.755759	-1.418398
H	-1.353142	-3.846795	-0.528871
C	-2.711460	-0.810751	0.617880
H	-1.911263	-0.163756	0.243719
H	-2.935479	-0.460194	1.631748
P	0.351196	-1.366624	1.869006
P	-4.206701	-0.499868	-0.503846
P	-0.113547	-1.975302	-1.432983
Ni	1.396476	-1.000263	-0.028768
C	-5.623458	-0.842247	0.651722
C	-6.626339	-1.723722	0.222227
C	-5.748943	-0.254935	1.922394
C	-7.718857	-2.024701	1.040840
H	-6.550362	-2.176984	-0.763510
C	-6.835114	-0.556518	2.743714
H	-5.003598	0.458316	2.264985
C	-7.822249	-1.444618	2.305095
H	-8.486771	-2.708971	0.689339
H	-6.917162	-0.092705	3.723504
H	-8.669945	-1.676022	2.944737
C	-4.257730	1.354735	-0.565760
C	-5.511550	1.987106	-0.660549
C	-3.104958	2.148605	-0.679194
C	-5.605597	3.366095	-0.844735
H	-6.422851	1.400737	-0.584293

C	-3.198899	3.530494	-0.867108
H	-2.111321	1.717139	-0.633153
C	-4.449626	4.142829	-0.947755
H	-6.585992	3.832127	-0.908817
H	-2.288955	4.114277	-0.959625
H	-4.522541	5.217101	-1.095301
C	-0.165330	0.118748	2.806397
C	-0.054012	1.397656	2.248020
C	-0.709308	-0.034484	4.095228
C	-0.497427	2.511805	2.966821
H	0.369909	1.548243	1.261643
C	-1.141918	1.081299	4.808737
H	-0.779312	-1.018236	4.552795
C	-1.039605	2.355763	4.241877
H	-0.413942	3.494860	2.516563
H	-1.555266	0.955925	5.805933
H	-1.380556	3.224857	4.798103
C	1.502663	-2.280442	2.974520
C	2.312386	-1.567049	3.873005
C	1.660184	-3.672847	2.877601
C	3.238755	-2.238415	4.671382
H	2.223598	-0.489301	3.940038
C	2.587517	-4.340546	3.677807
H	1.065486	-4.252812	2.177506
C	3.377552	-3.624357	4.578965
H	3.856755	-1.672620	5.362782
H	2.690803	-5.419136	3.596037
H	4.099286	-4.143907	5.203204
C	0.619638	-3.426211	-2.314926
C	1.086034	-4.504275	-1.542835
C	0.782958	-3.475007	-3.705585
C	1.682511	-5.610520	-2.146377
H	0.994990	-4.479696	-0.459024
C	1.376990	-4.586028	-4.310032
H	0.452394	-2.645806	-4.320571
C	1.826750	-5.655582	-3.535572
H	2.036321	-6.434492	-1.532665
H	1.488985	-4.610326	-5.390626
H	2.289176	-6.517470	-4.008454
C	-0.805812	-0.866266	-2.714500
C	-0.475617	0.495603	-2.693720
C	-1.701489	-1.343240	-3.691379
C	-1.024236	1.372901	-3.635245
H	0.180072	0.904728	-1.932125
C	-2.233019	-0.470388	-4.637277
H	-1.983848	-2.392331	-3.717936
C	-1.893966	0.887284	-4.610020
H	-0.776089	2.429165	-3.572663
H	-2.921795	-0.846924	-5.388728
H	-2.323185	1.566171	-5.341904
C	3.650045	-1.884183	-2.587770
C	3.487674	-1.098447	-3.723329
C	3.198920	0.268829	-3.594730
C	3.073092	0.851312	-2.338592
C	3.252984	0.071968	-1.177271
C	3.534273	-1.305973	-1.313238
H	3.880761	-2.941463	-2.679917
H	3.589864	-1.541752	-4.710320
H	3.074444	0.882047	-4.483180
H	2.866260	1.913499	-2.237419
H	3.769838	-1.894177	-0.430430
O	0.594170	2.637679	-0.582931
S	0.994408	3.919474	-1.240390
O	0.046786	4.392091	-2.270286
O	2.432831	3.995291	-1.582256
C	0.805916	5.147457	0.143213
F	-0.471065	5.171794	0.587190
F	1.132687	6.382832	-0.250625
F	1.586904	4.812172	1.186523
O	2.591475	-0.198946	1.087821
C	3.250131	0.710183	0.223617
C	4.660825	1.020610	0.708828
C	5.231326	2.260753	0.392086
C	5.404432	0.088574	1.440908
C	6.537597	2.554193	0.786164
C	6.708523	0.387476	1.840409
C	7.280688	1.617950	1.509526
H	4.645387	2.993817	-0.158800
H	6.971195	3.518917	0.535351
H	8.296262	1.849361	1.820905
H	7.278191	-0.340493	2.413583
H	4.946398	-0.857478	1.713230
H	2.697464	1.654134	0.153368

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B3LYP/BS1 SCF energy: -4319.498344 a.u.

M06/BS2 SCF energy in PhMe: -4318.45140554 a.u.

M06/BS2 Free energy in PhMe: -4317.64464654 a.u.

C	-1.750582	-2.674268	0.053693
C	-2.592969	-3.974588	0.052825
H	-3.214591	-4.046344	-0.844015
H	-1.944266	-4.858789	0.082953
H	-3.260754	-4.010291	0.919724
C	-0.831617	-2.800426	1.304013
H	-0.215678	-3.698591	1.179779
H	-1.459976	-2.981483	2.184046
C	-0.924737	-2.704806	-1.261032
H	-1.617171	-2.711121	-2.109719
H	-0.377751	-3.653939	-1.301392
C	-2.670783	-1.427890	0.162664
H	-2.075613	-0.516657	0.044348
H	-3.095224	-1.381814	1.171947
P	0.340588	-1.431045	1.773173
P	-4.068571	-1.316150	-1.116333
P	0.356035	-1.391007	-1.617548
Ni	1.543657	-0.648999	0.109339
C	-5.416919	-2.289679	-0.285159
C	-6.059866	-3.291881	-1.026570
C	-5.830733	-2.069219	1.039739
C	-7.077696	-4.065070	-0.460508
H	-5.759968	-3.467170	-2.057269
C	-6.842822	-2.841566	1.609333
H	-5.373739	-1.274450	1.623696
C	-7.467215	-3.844074	0.860501
H	-7.564731	-4.835994	-1.052034
H	-7.151520	-2.656927	2.635212
H	-8.257776	-4.443349	1.304467
C	-4.665779	0.418195	-0.850188
C	-6.045012	0.689649	-0.906979
C	-3.778696	1.501887	-0.738650
C	-6.517789	1.999799	-0.829273
H	-6.757020	-0.124460	-1.005242
C	-4.250829	2.814309	-0.652898
H	-2.703484	1.351565	-0.719035
C	-5.623706	3.063578	-0.696726
H	-7.588688	2.184974	-0.869497
H	-3.538160	3.629246	-0.552433
H	-5.992050	4.084042	-0.631472
C	-0.633466	-0.222785	2.732319
C	-0.626189	1.129353	2.370359
C	-1.395787	-0.646219	3.838256
C	-1.380641	2.053455	3.099864
H	-0.057215	1.490301	1.521568
C	-2.144426	0.278951	4.560658
H	-1.393189	-1.688736	4.146478
C	-2.137391	1.629284	4.190372
H	-1.358938	3.094743	2.798677
H	-2.730541	-0.051413	5.414113
H	-2.724595	2.347418	4.756247
C	1.467246	-2.232529	2.988682
C	1.893608	-1.510710	4.114622
C	1.991660	-3.516004	2.767412
C	2.804458	-2.072713	5.009955
H	1.516258	-0.509678	4.292468
C	2.898773	-4.076516	3.666578
H	1.707561	-4.089493	1.889847
C	3.305481	-3.357204	4.792024
H	3.122087	-1.501984	5.878023
H	3.288750	-5.074028	3.484118
H	4.011529	-3.794281	5.492692
C	1.487368	-2.280511	-2.777708
C	2.124934	-3.456852	-2.347310
C	1.780272	-1.778250	-4.054103
C	3.013565	-4.130033	-3.184199
H	1.939706	-3.849204	-1.350135
C	2.676178	-2.452060	-4.887865
H	1.307005	-0.866289	-4.401802
C	3.289498	-3.629670	-4.458918
H	3.496423	-5.038887	-2.836542
H	2.889389	-2.053699	-5.875903
H	3.982698	-4.153126	-5.111487
C	-0.433636	-0.077396	-2.607602
C	-0.105847	1.261797	-2.345796
C	-1.308644	-0.379394	-3.668625
C	-0.631129	2.288281	-3.135790
H	0.532249	1.531076	-1.511325
C	-1.835221	0.646614	-4.449740
H	-1.576667	-1.407465	-3.893240
C	-1.493566	1.977831	-4.186430
H	-0.368148	3.316668	-2.904551
H	-2.516963	0.406891	-5.260896

H	-1.911713	2.774077	-4.795797
C	6.117985	-2.561452	1.093727
C	6.603013	-2.993068	-0.142696
C	6.105314	-2.424950	-1.318139
C	5.133522	-1.425664	-1.254536
C	4.647064	-0.987451	-0.016239
C	5.140746	-1.566319	1.158361
H	6.499239	-3.000322	2.012054
H	7.363707	-3.767885	-0.191094
H	6.472381	-2.758457	-2.285033
H	4.752462	-0.983839	-2.172461
H	4.747252	-1.234426	2.113217
O	-0.217629	3.229813	0.214203
S	-0.446929	4.633891	-0.239213
O	-1.865439	5.034642	-0.319755
O	0.413579	5.045677	-1.371775
C	0.200175	5.630999	1.191236
F	-0.493245	5.358398	2.318175
F	0.096465	6.944684	0.953077
F	1.494125	5.348729	1.432478
O	2.825170	0.048113	1.205815
C	3.600589	0.120369	0.080852
C	4.075721	1.530225	-0.291136
C	5.414717	1.785486	-0.613681
C	3.153791	2.585567	-0.303120
C	5.821596	3.079659	-0.947030
C	3.557385	3.872673	-0.657137
C	4.894518	4.120833	-0.979321
H	6.144209	0.983445	-0.600725
H	6.865303	3.266426	-1.186994
H	5.209276	5.123720	-1.255843
H	2.817435	4.664550	-0.691817
H	2.115375	2.423168	-0.027908
H	2.839053	-0.122678	-0.852597

TS6

B3LYP/BS1 SCF energy: -4319.494045 a.u.

M06/BS2 SCF energy in PhMe: -4318.44753837 a.u.

M06/BS2 Free energy in PhMe: -4317.64187737 a.u.

C	-1.550505	-2.798998	0.100587
C	-2.351702	-4.124326	0.113239
H	-2.958703	-4.231663	-0.790476
H	-1.676167	-4.987011	0.167670
H	-3.027210	-4.164996	0.974098
C	-0.654654	-2.866503	1.371751
H	-0.004914	-3.744783	1.281014
H	-1.295174	-3.050813	2.241774
C	-0.697484	-2.824441	-1.196780
H	-1.372059	-2.895282	-2.057540
H	-0.096192	-3.740962	-1.197296
C	-2.509629	-1.576030	0.152808
H	-1.936821	-0.658664	-0.016999
H	-2.937917	-1.491912	1.157977
P	0.452931	-1.433619	1.810864
P	-3.901729	-1.611051	-1.130468
P	0.502387	-1.438491	-1.583481
Ni	1.586983	-0.553723	0.095682
C	-5.271063	-2.418407	-0.160501
C	-5.860341	-3.581431	-0.676793
C	-5.761917	-1.899229	1.049271
C	-6.901575	-4.221461	0.001440
H	-5.502919	-3.987103	-1.620565
C	-6.799502	-2.536181	1.729553
H	-5.343716	-0.979371	1.450565
C	-7.370438	-3.701214	1.207835
H	-7.347137	-5.121214	-0.415242
H	-7.169711	-2.119427	2.662859
H	-8.181815	-4.194507	1.736695
C	-4.511349	0.136389	-1.156871
C	-5.703715	0.349961	-1.875423
C	-3.861462	1.247501	-0.600710
C	-6.235917	1.629314	-2.014742
H	-6.223324	-0.494372	-2.323914
C	-4.387059	2.536304	-0.750784
H	-2.933778	1.144680	-0.047653
C	-5.576311	2.726567	-1.453518
H	-7.161881	1.769512	-2.567456
H	-3.849416	3.380201	-0.326277
H	-5.983411	3.727643	-1.569356
C	-0.563494	-0.328781	2.852950
C	-0.648388	1.033162	2.540186
C	-1.262976	-0.831561	3.967023
C	-1.431379	1.886613	3.324214
H	-0.130535	1.453188	1.685979
C	-2.039605	0.022747	4.745407

H	-1.191020	-1.881939	4.238170
C	-2.124736	1.382599	4.423018
H	-1.483371	2.936643	3.058925
H	-2.576721	-0.370375	5.604558
H	-2.733914	2.045231	5.031900
C	1.677752	-2.189127	2.966587
C	2.081021	-1.488943	4.114472
C	2.301923	-3.410942	2.667494
C	3.066624	-2.012139	4.953146
H	1.624585	-0.535139	4.356117
C	3.282963	-3.934430	3.509879
H	2.035794	-3.964147	1.771117
C	3.666476	-3.237317	4.657283
H	3.362692	-1.458839	5.840090
H	3.748080	-4.885771	3.266407
H	4.429019	-3.645737	5.314800
C	1.649856	-2.276582	-2.765147
C	2.327725	-3.439068	-2.362102
C	1.918783	-1.741822	-4.033353
C	3.233907	-4.066419	-3.216161
H	2.160963	-3.856730	-1.372311
C	2.831261	-2.369257	-4.885125
H	1.414155	-0.839313	-4.361069
C	3.486139	-3.533762	-4.482562
H	3.745936	-4.967268	-2.889494
H	3.024298	-1.945473	-5.866796
H	4.190922	-4.022667	-5.149467
C	-0.404516	-0.187476	-2.556848
C	-0.272622	1.169168	-2.223406
C	-1.210538	-0.554836	-3.650901
C	-0.924721	2.150701	-2.974799
H	0.312716	1.480647	-1.365222
C	-1.860897	0.425944	-4.396099
H	-1.325883	-1.598651	-3.928914
C	-1.715250	1.776636	-4.060636
H	-0.812329	3.192955	-2.689179
H	-2.486797	0.135192	-5.235145
H	-2.230711	2.536222	-4.641618
C	6.161008	-2.106736	1.125780
C	6.636609	-2.547013	-0.110809
C	6.106671	-2.012749	-1.288823
C	5.116168	-1.033635	-1.229384
C	4.639296	-0.583512	0.010383
C	5.161035	-1.135258	1.188213
H	6.564056	-2.521577	2.045548
H	7.413639	-3.305404	-0.158374
H	6.460831	-2.360832	-2.255082
H	4.698342	-0.629239	-2.147282
H	4.774919	-0.798829	2.144514
O	-0.445291	3.158685	0.371048
S	-0.841493	4.561692	0.047474
O	-2.276138	4.856939	0.229629
O	-0.208663	5.093772	-1.181242
C	-0.032141	5.530144	1.413891
F	-0.538444	5.178411	2.615108
F	-0.221945	6.846479	1.256438
F	1.294607	5.299665	1.449249
O	2.799201	0.413286	1.180754
C	3.578735	0.490305	0.134427
C	3.828459	1.838676	-0.488914
C	5.058755	2.145509	-1.094132
C	2.828166	2.823241	-0.430666
C	5.274384	3.409800	-1.643125
C	3.038204	4.076218	-1.001933
C	4.262693	4.370165	-1.609941
H	5.854994	1.410877	-1.122315
H	6.234077	3.638804	-2.098902
H	4.425990	5.348476	-2.054393
H	2.234679	4.804691	-0.981143
H	1.877632	2.619553	0.051893
H	2.536592	-0.040851	-0.993369

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B3LYP/BS1 SCF energy: -4319.515342 a.u.

M06/BS2 SCF energy in PhMe: -4318.46157074 a.u.

M06/BS2 Free energy in PhMe: -4317.65381974 a.u.

C	-2.283155	-2.251268	0.816732
C	-3.395219	-3.233076	1.259534
H	-4.135329	-3.386387	0.468046
H	-2.969695	-4.211960	1.513377
H	-3.925458	-2.854055	2.139662
C	-1.248602	-2.256463	1.983368
H	-0.823351	-3.264813	2.060749
H	-1.778858	-2.074848	2.925394
C	-1.679004	-2.847555	-0.485475

H	-2.462022	-2.865409	-1.250912
H	-1.415382	-3.892020	-0.286665
C	-2.864877	-0.825224	0.612061
H	-2.096791	-0.168929	0.188545
H	-3.118595	-0.396952	1.588175
P	0.191002	-1.072153	1.906896
P	-4.356622	-0.678502	-0.549645
P	-0.169163	-2.071593	-1.306246
Ni	1.187618	-0.905936	-0.125555
C	-5.780970	-0.987315	0.602612
C	-6.786103	-1.865072	0.169378
C	-5.911830	-0.399216	1.872668
C	-7.886165	-2.157939	0.980319
H	-6.703217	-2.323765	-0.813137
C	-7.006134	-0.692484	2.686768
H	-5.164155	0.307626	2.223003
C	-7.995587	-1.574940	2.242794
H	-8.654287	-2.840126	0.625252
H	-7.091339	-0.227612	3.665853
H	-8.848377	-1.801414	2.877465
C	-4.423691	1.163160	-0.764509
C	-5.604576	1.896618	-0.562984
C	-3.302923	1.836163	-1.281234
C	-5.650304	3.263432	-0.847207
H	-6.493937	1.405562	-0.181224
C	-3.344900	3.202674	-1.560673
H	-2.381019	1.301790	-1.487052
C	-4.522484	3.920727	-1.340465
H	-6.573622	3.813076	-0.679436
H	-2.456273	3.687881	-1.953042
H	-4.560907	4.984809	-1.558813
C	-0.431831	0.471214	2.678620
C	-0.332001	1.675921	1.968261
C	-1.034058	0.464593	3.950485
C	-0.834811	2.857927	2.521706
H	0.122408	1.712148	0.982176
C	-1.529208	1.646286	4.498132
H	-1.106305	-0.458258	4.521136
C	-1.431432	2.844282	3.781531
H	-0.759922	3.778132	1.952142
H	-1.990678	1.633426	5.482176
H	-1.823026	3.763801	4.208607
C	1.370536	-1.780306	3.142342
C	2.016795	-0.956810	4.077640
C	1.730401	-3.138203	3.084396
C	2.978303	-1.482411	4.943592
H	1.766689	0.097267	4.134614
C	2.687169	-3.662590	3.953700
H	1.268390	-3.799720	2.356082
C	3.313758	-2.835612	4.888463
H	3.463619	-0.828607	5.663152
H	2.943646	-4.717284	3.898518
H	4.059339	-3.243348	5.565429
C	0.713463	-3.567403	-1.948456
C	0.973594	-4.657375	-1.102499
C	1.220119	-3.595629	-3.255878
C	1.704310	-5.756414	-1.556520
H	0.609855	-4.657290	-0.078062
C	1.950234	-4.695497	-3.709607
H	1.042991	-2.758209	-3.922487
C	2.192504	-5.779685	-2.864454
H	1.887428	-6.594467	-0.889013
H	2.328416	-4.702411	-4.728242
H	2.756623	-6.636895	-3.221769
C	-0.825091	-1.215527	-2.786434
C	-0.486143	0.124847	-3.021623
C	-1.670215	-1.885510	-3.690506
C	-0.987866	0.789956	-4.145543
H	0.150505	0.668162	-2.328516
C	-2.156107	-1.222998	-4.815105
H	-1.937797	-2.926737	-3.528857
C	-1.816041	0.115374	-5.041555
H	-0.732477	1.836320	-4.282243
H	-2.804201	-1.748736	-5.511262
H	-2.205783	0.631483	-5.915018
C	4.988791	-3.062172	-0.877401
C	5.984825	-2.711506	-1.793703
C	6.297079	-1.367446	-2.009516
C	5.624672	-0.371662	-1.302530
C	4.612879	-0.715437	-0.388889
C	4.298013	-2.070306	-0.186949
H	4.741377	-4.106683	-0.712352
H	6.515246	-3.486165	-2.341024
H	7.061517	-1.093056	-2.730695
H	5.854990	0.673289	-1.481235
H	3.525900	-2.337666	0.527606

O	0.816411	2.439860	-0.905463
S	0.949238	3.606053	-1.831074
O	-0.095110	3.669620	-2.878021
O	2.329586	3.904681	-2.248038
C	0.510053	5.029628	-0.712628
F	-0.760254	4.926424	-0.264450
F	0.633041	6.207100	-1.335490
F	1.310358	5.051550	0.381187
O	2.620437	0.199034	0.550439
C	3.840636	0.337710	0.313571
C	4.492004	1.589339	0.748854
C	5.842696	1.620478	1.145596
C	3.723956	2.768067	0.781363
C	6.411404	2.814574	1.580047
C	4.310768	3.963164	1.188146
C	5.647910	3.986563	1.593448
H	6.432722	0.709336	1.135334
H	7.448630	2.834161	1.902780
H	6.100409	4.921136	1.914963
H	3.722049	4.874205	1.170068
H	2.693414	2.738762	0.444771
H	1.785110	-0.906564	-1.471618

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B3LYP/BS1 SCF energy: -4319.513985 a.u.

M06/BS2 SCF energy in PhMe: -4318.45993877 a.u.

M06/BS2 Free energy in PhMe: -4317.65151777 a.u.

C	2.443197	1.294598	1.733393
C	3.600473	1.831708	2.608506
H	4.338088	2.374578	2.008587
H	3.221890	2.518408	3.375967
H	4.122458	1.011817	3.114266
C	1.406060	0.683799	2.720572
H	0.930690	1.497180	3.282511
H	1.935334	0.070645	3.457578
C	1.854506	2.520550	0.986915
H	2.620907	2.905570	0.307381
H	1.665926	3.309986	1.721402
C	2.963716	0.205017	0.757406
H	2.148004	-0.108665	0.096925
H	3.251362	-0.683787	1.329552
P	0.032160	-0.362287	1.994160
P	4.384593	0.697440	-0.393711
P	0.290568	2.342155	-0.061162
Ni	-0.820639	0.518800	0.034454
C	5.878766	0.245511	0.612838
C	6.919666	1.183704	0.684486
C	6.027036	-0.969204	1.304711
C	8.072565	0.925040	1.431164
H	6.822906	2.126127	0.150643
C	7.175139	-1.229559	2.053094
H	5.248957	-1.725923	1.247270
C	8.200381	-0.281275	2.119760
H	8.867343	1.665281	1.473807
H	7.272993	-2.174782	2.581224
H	9.094492	-0.485561	2.703048
C	4.292702	-0.692847	-1.618361
C	5.417348	-1.452900	-1.978520
C	3.091068	-0.913526	-2.314698
C	5.333136	-2.418201	-2.984750
H	6.364543	-1.297860	-1.471729
C	3.003981	-1.883612	-3.313314
H	2.204027	-0.328066	-2.093782
C	4.127255	-2.641744	-3.650609
H	6.215734	-2.998298	-3.243812
H	2.053260	-2.034178	-3.815108
H	4.063913	-3.396959	-4.429792
C	0.728799	-2.071111	2.107514
C	0.732372	-2.899115	0.976294
C	1.277769	-2.558779	3.308459
C	1.280034	-4.183791	1.041368
H	0.314746	-2.537448	0.045132
C	1.820005	-3.841491	3.370568
H	1.270085	-1.945401	4.205812
C	1.824426	-4.657050	2.234116
H	1.275737	-4.803526	0.149121
H	2.237902	-4.205168	4.305786
H	2.250297	-5.655852	2.283745
C	-1.240031	-0.309981	3.336754
C	-1.792146	-1.475337	3.887033
C	-1.746547	0.932071	3.754330
C	-2.803061	-1.399304	4.848025
H	-1.436222	-2.448583	3.567594
C	-2.750942	1.007650	4.718435
H	-1.373057	1.851707	3.313378

C	-3.281676	-0.159786	5.271673
H	-3.216796	-2.314934	5.262136
H	-3.124620	1.979428	5.030601
H	-4.066791	-0.102341	6.020730
C	-0.703716	3.823118	0.453650
C	-0.778776	4.240758	1.791885
C	-1.462945	4.514742	-0.503637
C	-1.575832	5.325810	2.162449
H	-0.209077	3.729255	2.562167
C	-2.252782	5.604474	-0.134766
H	-1.430832	4.206409	-1.543621
C	-2.312698	6.015172	1.198670
H	-1.612118	5.635049	3.203767
H	-2.819626	6.134841	-0.895358
H	-2.925483	6.866082	1.483518
C	0.901839	2.837091	-1.731137
C	0.697767	2.008840	-2.840809
C	1.595937	4.049524	-1.898298
C	1.185502	2.382758	-4.097124
H	0.163386	1.070623	-2.744401
C	2.074354	4.421436	-3.152323
H	1.750895	4.713884	-1.051950
C	1.871445	3.585364	-4.255463
H	1.021880	1.721008	-4.942475
H	2.604874	5.362727	-3.269713
H	2.248923	3.875023	-5.232666
C	-5.014173	3.146375	-0.793371
C	-5.753100	2.933678	-1.960618
C	-5.884165	1.643660	-2.480383
C	-5.300750	0.561631	-1.822644
C	-4.558037	0.770167	-0.649444
C	-4.404019	2.072118	-0.149483
H	-4.903861	4.148370	-0.389549
H	-6.221278	3.773393	-2.468005
H	-6.438850	1.479641	-3.400025
H	-5.376703	-0.437536	-2.236645
H	-3.813795	2.227319	0.748040
O	-0.784737	-1.249700	-1.137781
S	-1.306982	-1.517569	-2.530677
O	-0.450465	-0.972933	-3.601067
O	-2.761037	-1.346912	-2.673953
C	-1.030389	-3.358862	-2.621629
F	0.267234	-3.654532	-2.408390
F	-1.378586	-3.827339	-3.824284
F	-1.753926	-4.000524	-1.687400
O	-2.794400	-0.232687	0.594170
C	-3.909812	-0.360782	0.071646
C	-4.630544	-1.655230	0.227666
C	-6.032838	-1.729850	0.248412
C	-3.875387	-2.825179	0.416017
C	-6.668028	-2.953810	0.457250
C	-4.513055	-4.047438	0.602257
C	-5.909968	-4.113787	0.628333
H	-6.624062	-0.829017	0.120214
H	-7.753234	-3.001596	0.483793
H	-6.406046	-5.069208	0.778711
H	-3.922527	-4.951662	0.721300
H	-2.794628	-2.760146	0.379097
H	-1.390508	1.299792	-1.065250

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B3LYP/BS1 SCF energy: -3742.896029 a.u.

M06/BS2 SCF energy in PhMe: -3742.09590920 a.u.

M06/BS2 Free energy in PhMe: -3741.46599520 a.u.

C	1.280396	1.183323	1.831654
C	2.287146	1.700338	2.885002
H	3.111962	2.246221	2.415560
H	1.797242	2.378369	3.594734
H	2.721090	0.869105	3.451811
C	0.107160	0.536645	2.631507
H	-0.433122	1.334802	3.155972
H	0.525694	-0.122395	3.401395
C	0.794289	2.429774	1.040820
H	1.665066	2.901189	0.575243
H	0.385622	3.153206	1.755524
C	1.945790	0.112996	0.928602
H	1.220446	-0.219044	0.179477
H	2.178900	-0.770204	1.534713
P	-1.154785	-0.431901	1.649403
P	3.476137	0.621479	-0.061788
P	-0.490803	2.228159	-0.327169
Ni	-1.571910	0.389619	-0.426712
C	4.852418	0.216540	1.115740
C	5.830029	1.198286	1.336442
C	4.964597	-1.005191	1.801896

C	6.885908	0.974666	2.224742
H	5.760797	2.145818	0.807453
C	6.015741	-1.230777	2.690404
H	4.235508	-1.792642	1.629112
C	6.978127	-0.239305	2.905401
H	7.633578	1.747569	2.382776
H	6.087814	-2.181568	3.212460
H	7.797225	-0.416365	3.597502
C	3.551471	-0.803014	-1.252592
C	4.762097	-1.457718	-1.535424
C	2.414731	-1.166059	-1.996323
C	4.824451	-2.457013	-2.509048
H	5.662935	-1.194719	-0.989387
C	2.473521	-2.172045	-2.961569
H	1.461676	-0.671524	-1.841500
C	3.680973	-2.823311	-3.220934
H	5.772018	-2.952653	-2.705888
H	1.566682	-2.435334	-3.498691
H	3.731116	-3.606048	-3.973306
C	-0.574661	-2.178410	1.776090
C	-0.199982	-2.868993	0.614918
C	-0.489906	-2.828385	3.018403
C	0.264684	-4.183871	0.699438
H	-0.277702	-2.392005	-0.355750
C	-0.026494	-4.140591	3.098684
H	-0.801710	-2.317137	3.925701
C	0.353909	-4.819840	1.937474
H	0.548368	-4.707332	-0.208931
H	0.031336	-4.634710	4.065010
H	0.711613	-5.844209	1.999764
C	-2.669712	-0.379678	2.699231
C	-2.657382	-0.091473	4.073584
C	-3.897787	-0.656376	2.072047
C	-3.846537	-0.079185	4.805611
H	-1.723368	0.122804	4.585046
C	-5.082575	-0.646557	2.809140
H	-3.922658	-0.881614	1.009490
C	-5.060535	-0.356587	4.174953
H	-3.821814	0.145458	5.868748
H	-6.024048	-0.861409	2.311259
H	-5.985309	-0.345582	4.745529
C	-1.646576	3.637703	-0.034651
C	-2.213954	3.821192	1.236719
C	-2.054860	4.472073	-1.084993
C	-3.150678	4.830619	1.457932
H	-1.939036	3.168324	2.061141
C	-2.993553	5.481024	-0.861323
H	-1.641849	4.335335	-2.078880
C	-3.540993	5.665569	0.408882
H	-3.578580	4.959603	2.448384
H	-3.297692	6.120952	-1.685079
H	-4.271754	6.451165	0.580094
C	0.444246	2.681355	-1.847803
C	0.419131	1.853127	-2.979090
C	1.200989	3.866508	-1.885243
C	1.145694	2.201089	-4.121507
H	-0.165903	0.938826	-2.973947
C	1.915514	4.214071	-3.029338
H	1.223520	4.530801	-1.025116
C	1.891679	3.378228	-4.149769
H	1.122517	1.545101	-4.986797
H	2.491292	5.135477	-3.046261
H	2.453513	3.647096	-5.040234
O	-2.581008	-1.173611	-0.963683
S	-2.456560	-1.557330	-2.448622
O	-1.046532	-1.699912	-2.862103
O	-3.372406	-0.843683	-3.339297
C	-3.118908	-3.293299	-2.336662
F	-2.338121	-4.048594	-1.550216
F	-3.149036	-3.838247	-3.558113
F	-4.358425	-3.289633	-1.832974
H	-1.900598	1.072381	-1.686862

TS8

B3LYP/BS1 SCF energy: -4152.023620 a.u.

M06/BS2 SCF energy in PhMe: -4151.05237040 a.u.

M06/BS2 Free energy in PhMe: -4150.16118240 a.u.

C	1.903600	1.112375	2.018298
C	2.927568	1.777152	2.969471
H	3.418206	2.634608	2.497490
H	2.434239	2.135746	3.881542
H	3.709015	1.067214	3.262778
C	1.207908	0.000721	2.857564
H	0.610780	0.489786	3.635027
H	1.973712	-0.584847	3.379029

C	0.888883	2.222352	1.629806
H	1.443197	3.073311	1.222226
H	0.416788	2.573420	2.555180
C	2.625515	0.465390	0.806468
H	1.867444	0.065775	0.124907
H	3.205337	-0.396728	1.157097
P	0.094722	-1.196583	1.932732
P	3.734406	1.563445	-0.260017
P	-0.537125	1.883406	0.408901
Ni	-1.045786	-0.155162	0.164043
C	5.368586	1.429984	0.616282
C	6.050948	2.619721	0.910609
C	5.957156	0.211366	0.995772
C	7.281094	2.598926	1.574440
H	5.612366	3.570275	0.616120
C	7.183295	0.186660	1.660082
H	5.462790	-0.726206	0.755019
C	7.847534	1.381830	1.952932
H	7.794379	3.531819	1.793230
H	7.624345	-0.765092	1.945760
H	8.803707	1.361320	2.469464
C	4.009470	0.426044	-1.705749
C	5.275984	0.328707	-2.308686
C	2.937893	-0.249660	-2.315018
C	5.465895	-0.435701	-3.461100
H	6.125361	0.845889	-1.872510
C	3.127871	-1.019694	-3.463794
H	1.933240	-0.182019	-1.912909
C	4.394752	-1.118221	-4.040840
H	6.457308	-0.498856	-3.903422
H	2.274658	-1.535957	-3.894214
H	4.545396	-1.716843	-4.935532
C	1.228870	-2.648505	1.710475
C	1.463305	-3.140214	0.420245
C	1.873709	-3.264636	2.798034
C	2.327196	-4.220428	0.216367
H	0.961036	-2.682613	-0.422085
C	2.736622	-4.340272	2.594597
H	1.690697	-2.913432	3.810590
C	2.966503	-4.819680	1.300654
H	2.488971	-4.589055	-0.792471
H	3.227049	-4.807728	3.444796
H	3.637986	-5.659870	1.143475
C	-1.024700	-1.820529	3.275992
C	-1.557486	-0.980614	4.267861
C	-1.468578	-3.154864	3.234211
C	-2.485567	-1.458766	5.195270
H	-1.252210	0.059492	4.331394
C	-2.397843	-3.632161	4.158409
H	-1.078955	-3.828588	2.477034
C	-2.909937	-2.787018	5.145540
H	-2.873688	-0.789700	5.959193
H	-2.719288	-4.669235	4.107284
H	-3.630329	-3.160094	5.868452
C	-1.789753	3.058564	1.135259
C	-2.301264	2.757244	2.410537
C	-2.288455	4.192409	0.477177
C	-3.254791	3.572653	3.018894
H	-1.956961	1.865888	2.929308
C	-3.249313	5.008673	1.083591
H	-1.926423	4.450487	-0.512050
C	-3.732369	4.706958	2.356307
H	-3.628467	3.319923	4.007959
H	-3.616184	5.884722	0.554751
H	-4.474898	5.345083	2.827688
C	0.102156	2.783473	-1.086125
C	0.188216	2.102882	-2.307780
C	0.562807	4.111924	-1.023205
C	0.717190	2.731548	-3.439265
H	-0.154018	1.075846	-2.383828
C	1.078101	4.742735	-2.153889
H	0.517147	4.663381	-0.087862
C	1.158476	4.051449	-3.366489
H	0.785700	2.177500	-4.371038
H	1.425150	5.770679	-2.086794
H	1.569418	4.540622	-4.245789
O	-1.103553	-1.800544	-1.067710
S	-1.327462	-1.918861	-2.557303
O	-0.453094	-1.067738	-3.380341
O	-2.765291	-1.944214	-2.920094
C	-0.743745	-3.657410	-2.876030
F	0.585884	-3.737067	-2.685725
F	-1.011740	-4.004627	-4.137752
F	-1.345683	-4.520396	-2.050075
H	-2.507250	0.363936	-0.567699
C	-4.681947	-0.502491	0.076375

C	-5.327373	0.675321	0.830661
C	-6.050739	1.663411	-0.090754
C	-5.084060	2.192889	-1.154420
C	-4.404540	1.085228	-1.981133
N	-3.826244	0.041761	-1.044706
H	-6.923010	1.189139	-0.558328
H	-6.015472	0.267456	1.581878
H	-5.601542	2.867735	-1.847995
H	-6.438367	2.501243	0.501432
H	-4.308400	2.785890	-0.656565
H	-4.541857	1.212792	1.377269
H	-3.535209	-0.749301	-1.633480
C	-3.753957	-1.282619	1.018712
H	-4.315037	-1.644282	1.887332
H	-3.307698	-2.145223	0.514495
H	-2.940617	-0.643027	1.387054
C	-5.744853	-1.500568	-0.439896
H	-5.291245	-2.236567	-1.112507
H	-6.166670	-2.043587	0.413594
H	-6.574730	-1.023952	-0.964263
C	-3.235240	1.676651	-2.782570
H	-2.723118	0.905975	-3.367080
H	-3.614952	2.433665	-3.478091
H	-2.503114	2.153791	-2.129675
C	-5.383825	0.451081	-2.996092
H	-5.594604	1.180223	-3.786825
H	-4.936639	-0.431047	-3.465320
H	-6.340670	0.164296	-2.556376

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B3LYP/BS1 SCF energy: -4152.043932 a.u.

M06/BS2 SCF energy in PhMe: -4151.07371758 a.u.

M06/BS2 Free energy in PhMe: -4150.17888258 a.u.

C	2.194759	0.092714	2.221227
C	3.281498	0.285975	3.306781
H	3.807510	1.238692	3.184241
H	2.835899	0.277711	4.309601
H	4.029688	-0.514037	3.262078
C	1.491915	-1.256778	2.565293
H	0.988199	-1.128682	3.529864
H	2.260820	-2.023279	2.719629
C	1.223359	1.301811	2.359164
H	1.816106	2.221149	2.327450
H	0.771991	1.253621	3.358230
C	2.850623	-0.015180	0.819403
H	2.053147	-0.120589	0.074072
H	3.441380	-0.938211	0.768974
P	0.229845	-1.921942	1.329266
P	3.902406	1.439578	0.231938
P	-0.217845	1.499225	1.122885
Ni	-0.604803	-0.318129	0.155288
C	5.591716	0.996416	0.867366
C	6.321609	1.999301	1.523127
C	6.175353	-0.275671	0.737612
C	7.592648	1.741755	2.044667
H	5.885644	2.990133	1.627166
C	7.442504	-0.537449	1.258772
H	5.642253	-1.064454	0.213178
C	8.153632	0.471177	1.916085
H	8.141283	2.532528	2.550092
H	7.878068	-1.527638	1.149540
H	9.141028	0.266024	2.321801
C	4.049013	1.007974	-1.569640
C	5.281607	1.035952	-2.243268
C	2.887117	0.775061	-2.327556
C	5.350896	0.812068	-3.620128
H	6.197198	1.226441	-1.691859
C	2.956849	0.543132	-3.701679
H	1.908262	0.778404	-1.858279
C	4.191342	0.557773	-4.354047
H	6.317980	0.832818	-4.117238
H	2.037750	0.354087	-4.248985
H	4.248469	0.378290	-5.424701
C	1.210771	-3.277468	0.504181
C	1.299576	-3.283569	-0.894916
C	1.862819	-4.293408	1.224258
C	2.030033	-4.273864	-1.559350
H	0.788350	-2.514736	-1.464659
C	2.591385	-5.281623	0.563088
H	1.790328	-4.322392	2.309016
C	2.678625	-5.272056	-0.832793
H	2.085614	-4.259723	-2.644735
H	3.088456	-6.061449	1.135129
H	3.246929	-6.042390	-1.348021
C	-0.893824	-2.947034	2.405773

C	-1.234245	-2.612271	3.727652
C	-1.558043	-4.042308	1.818964
C	-2.191124	-3.343692	4.437217
H	-0.750704	-1.777968	4.226610
C	-2.510689	-4.774078	2.526076
H	-1.318504	-4.328470	0.798414
C	-2.834764	-4.428010	3.841471
H	-2.424623	-3.066314	5.462502
H	-2.997859	-5.621508	2.049604
H	-3.574520	-5.000460	4.394828
C	-1.556234	2.106339	2.284335
C	-2.093354	1.187275	3.207455
C	-2.122372	3.391954	2.243157
C	-3.137056	1.541123	4.062692
H	-1.696247	0.176849	3.246765
C	-3.175166	3.746582	3.094362
H	-1.732948	4.131792	1.551977
C	-3.686828	2.826178	4.009892
H	-3.520887	0.811456	4.771959
H	-3.585612	4.752625	3.045793
H	-4.498354	3.105263	4.676845
C	0.287224	3.081978	0.264571
C	0.202452	3.130947	-1.134095
C	0.770150	4.215778	0.943419
C	0.587205	4.277963	-1.836387
H	-0.148984	2.262022	-1.683574
C	1.147537	5.362667	0.245948
H	0.846812	4.210488	2.027899
C	1.057880	5.395728	-1.149044
H	0.526617	4.286134	-2.921499
H	1.517532	6.228739	0.789426
H	1.361249	6.286417	-1.693535
O	-1.191553	-1.064867	-1.687405
S	-1.499558	-0.439272	-3.015724
O	-0.619955	0.657708	-3.441335
O	-2.967772	-0.191949	-3.186437
C	-1.147643	-1.840052	-4.186592
F	0.144793	-2.187511	-4.094571
F	-1.405831	-1.468970	-5.444001
F	-1.901286	-2.904354	-3.884600
H	-3.294086	0.785716	-0.169905
C	-4.932645	-0.512721	-0.109057
C	-5.739458	0.119108	1.040683
C	-6.514589	1.379569	0.635605
C	-5.558251	2.440092	0.074894
C	-4.743948	1.956172	-1.138463
N	-4.107173	0.599594	-0.781345
H	-7.297395	1.137471	-0.093763
H	-6.418587	-0.647484	1.432469
H	-6.109070	3.338169	-0.229254
H	-7.029542	1.785204	1.513852
H	-4.866027	2.749721	0.868714
H	-5.049717	0.374044	1.856666
H	-3.676066	0.218666	-1.658602
C	-3.914879	-1.525686	0.433266
H	-4.444173	-2.314130	0.978061
H	-3.337946	-1.987974	-0.372602
H	-3.203649	-1.060041	1.124840
C	-5.821371	-1.207777	-1.153080
H	-5.246102	-1.462540	-2.049072
H	-6.196361	-2.140051	-0.718738
H	-6.687881	-0.615331	-1.452281
C	-3.570164	2.903033	-1.429120
H	-2.977360	2.552968	-2.279833
H	-3.962848	3.896075	-1.671565
H	-2.908470	3.006051	-0.563829
C	-5.596215	1.817243	-2.410261
H	-5.859803	2.822169	-2.755799
H	-5.030982	1.324703	-3.206988
H	-6.527995	1.272625	-2.250316

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B3LYP/BS1 SCF energy: -4152.038385 a.u.

M06/BS2 SCF energy in PhMe: -4151.06352002 a.u.

M06/BS2 Free energy in PhMe: -4150.17298602 a.u.

C	-2.722948	1.794009	0.649289
C	-3.960435	2.683903	0.911340
H	-4.612646	2.246769	1.675885
H	-3.660094	3.680308	1.259891
H	-4.555299	2.809280	-0.001175
C	-1.835089	2.568145	-0.381191
H	-1.379221	3.411729	0.152413
H	-2.484948	2.997786	-1.154631
C	-2.003318	1.626265	2.021103
H	-2.714655	1.183157	2.725523

H	-1.764019	2.626887	2.402086
C	-3.160803	0.440311	0.033300
H	-2.256095	-0.153829	-0.139919
H	-3.607538	0.618681	-0.951821
P	-0.432284	1.602278	-1.203025
P	-4.301382	-0.664515	1.053360
P	-0.404336	0.595548	2.092437
Ni	0.244522	0.124246	0.145116
C	-5.979929	-0.206425	0.402483
C	-6.983430	0.091634	1.336534
C	-6.296992	-0.127909	-0.964788
C	-8.264923	0.466279	0.922248
H	-6.755159	0.030837	2.397955
C	-7.574301	0.245912	-1.381953
H	-5.544377	-0.373679	-1.709365
C	-8.561489	0.546344	-0.438288
H	-9.028073	0.694583	1.662043
H	-7.801381	0.301048	-2.443786
H	-9.556522	0.838327	-0.764440
C	-3.995786	-2.295438	0.213929
C	-5.051299	-3.159897	-0.121907
C	-2.679847	-2.756347	0.024864
C	-4.800593	-4.427555	-0.651515
H	-6.079290	-2.840956	0.021668
C	-2.429793	-4.018721	-0.515210
H	-1.830461	-2.136687	0.296644
C	-3.489901	-4.860375	-0.857860
H	-5.635903	-5.074835	-0.908407
H	-1.401218	-4.333574	-0.672423
H	-3.296512	-5.844180	-1.277902
C	-1.222863	1.144565	-2.838284
C	-1.268772	-0.209579	-3.197498
C	-1.762784	2.092203	-3.722723
C	-1.852647	-0.610028	-4.402799
H	-0.840048	-0.950632	-2.528551
C	-2.343031	1.696032	-4.927995
H	-1.717111	3.150833	-3.477304
C	-2.392289	0.341179	-5.269285
H	-1.881815	-1.665329	-4.662247
H	-2.753519	2.443496	-5.602939
H	-2.844650	0.031644	-6.208235
C	0.697050	2.962293	-1.794564
C	0.464415	4.340401	-1.669630
C	1.894778	2.545764	-2.407977
C	1.398633	5.272926	-2.134020
H	-0.453320	4.705055	-1.218851
C	2.817719	3.475164	-2.886033
H	2.092733	1.480430	-2.507331
C	2.576674	4.845781	-2.744909
H	1.195470	6.335742	-2.025141
H	3.728377	3.130798	-3.371619
H	3.298473	5.571214	-3.111554
C	0.721089	1.735395	3.049257
C	1.046820	2.989342	2.498185
C	1.367625	1.355777	4.237811
C	1.967346	3.835787	3.116040
H	0.587734	3.301674	1.564269
C	2.295664	2.199912	4.855020
H	1.143385	0.395439	4.690723
C	2.600081	3.444293	4.299879
H	2.190742	4.802645	2.670853
H	2.774366	1.883746	5.779208
H	3.315710	4.103470	4.784920
C	-0.837891	-0.660591	3.403986
C	-0.459964	-1.991136	3.172779
C	-1.517623	-0.355301	4.595856
C	-0.754420	-2.992306	4.103404
H	0.060742	-2.237500	2.250446
C	-1.813507	-1.351894	5.525603
H	-1.810747	0.670348	4.806598
C	-1.433194	-2.674757	5.279724
H	-0.459458	-4.019299	3.903153
H	-2.341900	-1.098291	6.441577
H	-1.668649	-3.452121	6.002359
O	0.890907	-1.806780	-0.403437
S	2.215791	-2.116819	-0.999803
O	3.197167	-2.736446	-0.068543
O	2.811752	-1.026388	-1.831327
C	1.818866	-3.454065	-2.228951
F	1.256406	-4.498090	-1.608034
F	2.942923	-3.866648	-2.834338
F	0.973951	-2.994355	-3.156721
H	4.770069	-1.506171	0.139371
C	5.084982	0.438370	0.867403
C	6.374323	0.239452	1.686864
C	7.646458	0.155321	0.834705

C	7.537642	-0.994510	-0.174457
C	6.326275	-0.879239	-1.118136
N	5.079266	-0.605369	-0.265553
H	7.831503	1.105900	0.319802
H	6.440555	1.061544	2.408396
H	8.440971	-1.061371	-0.791903
H	8.511970	-0.013106	1.485423
H	7.465714	-1.943576	0.375329
H	6.278928	-0.683744	2.275874
H	4.279113	-0.422483	-0.908268
C	3.848350	0.138922	1.725803
H	3.836912	0.811843	2.588183
H	2.913902	0.301179	1.175248
H	3.851418	-0.891956	2.096009
C	4.964268	1.855782	0.288788
H	4.142687	1.926809	-0.431814
H	4.730045	2.541016	1.109361
H	5.880185	2.211415	-0.188245
C	6.070127	-2.214911	-1.836505
H	5.205682	-2.151320	-2.503131
H	6.951724	-2.473311	-2.432159
H	5.887657	-3.027273	-1.125612
C	6.496818	0.229413	-2.167571
H	7.270931	-0.079376	-2.877332
H	5.570247	0.378798	-2.732196
H	6.802859	1.186571	-1.742420

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B3LYP/BS1 SCF energy: -3023.907667 a.u.

M06/BS2 SCF energy in PhMe: -3023.00607525 a.u.

M06/BS2 Free energy in PhMe: -3022.32147725 a.u.

C	1.419531	0.784979	-1.775105
C	2.267703	1.155716	-3.017253
H	3.002962	1.931520	-2.776547
H	1.628869	1.531849	-3.825455
H	2.813750	0.287916	-3.401851
C	0.477725	-0.369762	-2.222857
H	-0.091237	-0.010901	-3.088116
H	1.094003	-1.200223	-2.585450
C	0.639456	2.085563	-1.416152
H	1.359193	2.908427	-1.322753
H	0.000909	2.345322	-2.270459
C	2.346961	0.382130	-0.595363
H	1.742994	-0.033216	0.217541
P	-0.807116	-1.082966	-1.038791
P	-0.524811	2.133200	0.056307
Ni	-1.923884	0.427924	0.138920
C	0.127363	-2.407841	-0.150738
C	0.119000	-2.421397	1.251133
C	0.839019	-3.410942	-0.831320
C	0.808038	-3.409252	1.959088
H	-0.444823	-1.665689	1.788272
C	1.520834	-4.401091	-0.125258
H	0.851753	-3.429896	-1.917474
C	1.508044	-4.400583	1.272485
H	0.790648	-3.404243	3.045301
H	2.064215	-5.171214	-0.666275
H	2.043846	-5.169783	1.821871
C	-1.861017	-2.033620	-2.230615
C	-2.275412	-3.347095	-1.956295
C	-2.388849	-1.393981	-3.365853
C	-3.165095	-4.007583	-2.806397
H	-1.906778	-3.860001	-1.074590
C	-3.270942	-2.057070	-4.219096
H	-2.125155	-0.363576	-3.587774
C	-3.661174	-3.369169	-3.943897
H	-3.469958	-5.024576	-2.574151
H	-3.658547	-1.543671	-5.095282
H	-4.350723	-3.885887	-4.605988
C	-1.289325	3.797385	-0.225351
C	-2.084887	3.967214	-1.372440
C	-1.193120	4.861800	0.683375
C	-2.730155	5.177147	-1.623446
H	-2.217964	3.141774	-2.067217
C	-1.850966	6.069900	0.437597
H	-0.603969	4.754466	1.588081
C	-2.613592	6.235168	-0.718864
H	-3.335444	5.288306	-2.519243
H	-1.761641	6.883408	1.153014
H	-3.120820	7.176925	-0.910465
C	0.574144	2.398938	1.520451
C	0.313081	1.661348	2.684965
C	1.651196	3.302370	1.525505
C	1.107182	1.816749	3.824662
H	-0.516278	0.959177	2.694549

C	2.446654	3.457494	2.661298
H	1.867461	3.899404	0.643614
C	2.176329	2.713368	3.814085
H	0.887190	1.237878	4.717559
H	3.274429	4.161737	2.648585
H	2.794873	2.837112	4.699027
C	-5.270482	0.720805	-1.098576
C	-4.584842	-0.364781	-0.605572
C	-3.700626	-0.212551	0.514298
C	-3.583184	1.085067	1.135537
C	-4.383692	2.165339	0.632140
C	-5.187423	1.996130	-0.467307
H	-5.904439	0.595643	-1.973700
H	-4.694683	-1.340811	-1.066784
H	-3.227735	1.164351	2.160806
H	-4.368016	3.115622	1.160821
H	-5.790155	2.820324	-0.839578
I	-3.745404	-2.013779	1.953883
H	2.826452	1.284747	-0.200461
P	3.672555	-0.910529	-0.971398
C	4.180619	-1.408483	0.743474
C	4.918659	-2.599138	0.855499
C	3.888676	-0.695974	1.917621
C	5.367055	-3.055311	2.095193
H	5.139841	-3.175786	-0.039665
C	4.326762	-1.157737	3.161184
H	3.315281	0.224705	1.878767
C	5.069467	-2.335521	3.254345
H	5.941152	-3.976378	2.156928
H	4.086137	-0.590776	4.057057
H	5.410997	-2.691958	4.222702
C	5.124931	0.155477	-1.450494
C	5.756001	-0.112049	-2.674298
C	5.634938	1.189353	-0.648805
C	6.856889	0.638884	-3.095314
H	5.380287	-0.916163	-3.302705
C	6.733159	1.941647	-1.065546
H	5.182581	1.399265	0.317133
C	7.345951	1.669242	-2.292189
H	7.331239	0.416863	-4.047825
H	7.116536	2.736861	-0.430924
H	8.203000	2.254308	-2.615419

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B3LYP/BS1 SCF energy: -3023.902612 a.u.

M06/BS2 SCF energy in PhMe: -3022.99619491 a.u.

M06/BS2 Free energy in PhMe: -3022.31088591 a.u.

C	1.263891	0.546209	-1.876023
C	2.040421	0.808375	-3.191238
H	2.732044	1.651017	-3.082167
H	1.348451	1.040194	-4.009965
H	2.625462	-0.067591	-3.490240
C	0.383754	-0.709953	-2.143328
H	-0.244823	-0.488283	-3.013382
H	1.043112	-1.531944	-2.443945
C	0.419455	1.836121	-1.648714
H	1.093202	2.701645	-1.674638
H	-0.252900	1.954162	-2.507650
C	2.255956	0.350505	-0.695961
H	1.711416	-0.012894	0.180802
P	-0.808350	-1.383451	-0.840320
P	-0.707621	1.995377	-0.157697
Ni	-2.062025	0.240056	0.066883
C	0.274231	-2.491676	0.177513
C	0.256629	-2.373486	1.574150
C	1.102898	-3.467456	-0.405459
C	1.049211	-3.205102	2.370661
H	-0.395047	-1.642592	2.040738
C	1.889892	-4.299273	0.389560
H	1.126901	-3.592120	-1.484127
C	1.865936	-4.168391	1.781025
H	1.021543	-3.097963	3.451524
H	2.524409	-5.047513	-0.077994
H	2.484172	-4.813674	2.399122
C	-1.739996	-2.605129	-1.883473
C	-1.963734	-3.923514	-1.453899
C	-2.358356	-2.182587	-3.072606
C	-2.754508	-4.796965	-2.204191
H	-1.517203	-4.276039	-0.530206
C	-3.138013	-3.058036	-3.828224
H	-2.250954	-1.155696	-3.411061
C	-3.337527	-4.371586	-3.398282
H	-2.909906	-5.813614	-1.852303
H	-3.597384	-2.708948	-4.749444
H	-3.947437	-5.053562	-3.984697

C	-1.550280	3.595452	-0.576221
C	-2.295094	3.675570	-1.766815
C	-1.556753	4.700610	0.288048
C	-2.994806	4.835196	-2.097489
H	-2.348969	2.819458	-2.434106
C	-2.268190	5.858312	-0.038642
H	-1.005706	4.664241	1.221826
C	-2.982668	5.933677	-1.233932
H	-3.557100	4.876897	-3.026768
H	-2.258831	6.702550	0.645886
H	-3.531760	6.836090	-1.488651
C	0.408054	2.462104	1.240964
C	0.202622	1.852442	2.487291
C	1.437530	3.410916	1.112817
C	1.014355	2.175346	3.579252
H	-0.597660	1.125959	2.603736
C	2.250144	3.729542	2.200647
H	1.600277	3.914922	0.163911
C	2.040632	3.109757	3.437116
H	0.838593	1.696330	4.538625
H	3.042528	4.464721	2.086479
H	2.671981	3.361839	4.285101
C	-5.465206	-1.015466	-1.319859
C	-4.552394	-1.393289	-0.352231
C	-3.807247	-0.388657	0.307888
C	-4.114780	0.988975	0.119219
C	-5.048712	1.334849	-0.894764
C	-5.702907	0.349805	-1.610728
H	-5.992063	-1.784050	-1.880244
H	-4.359789	-2.440797	-0.147650
H	-3.849753	1.740350	0.854318
H	-5.302343	2.382175	-1.040846
H	-6.441247	0.617920	-2.361953
I	-3.229015	-0.805151	2.687453
H	2.674782	1.324740	-0.421771
P	3.676278	-0.863458	-0.977114
C	4.268844	-1.131649	0.761416
C	5.161471	-2.199010	0.959690
C	3.899026	-0.360804	1.874912
C	5.681913	-2.478180	2.223162
H	5.449371	-2.818642	0.113359
C	4.410365	-0.646696	3.143438
H	3.208469	0.469833	1.769413
C	5.304885	-1.702478	3.321881
H	6.375007	-3.305855	2.351226
H	4.106815	-0.037595	3.991217
H	5.702631	-1.922137	4.309262
C	5.018172	0.266860	-1.607207
C	5.630270	-0.056737	-2.827068
C	5.462449	1.408160	-0.919693
C	6.646945	0.743100	-3.356162
H	5.306486	-0.943355	-3.367210
C	6.477021	2.208802	-1.444280
H	5.024923	1.665995	0.041585
C	7.070474	1.879146	-2.666335
H	7.107617	0.476448	-4.303941
H	6.810508	3.087247	-0.897265
H	7.862414	2.502269	-3.073628

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B3LYP/BS1 SCF energy: -3023.950939 a.u.

M06/BS2 SCF energy in PhMe: -3023.04547985 a.u.

M06/BS2 Free energy in PhMe: -3022.35914885 a.u.

C	1.353212	0.146055	-1.931427
C	2.203785	0.179443	-3.224713
H	2.899782	1.025397	-3.215504
H	1.562368	0.276412	-4.109025
H	2.793536	-0.735912	-3.340205
C	0.481226	-1.133169	-2.015846
H	-0.045345	-1.107712	-2.975737
H	1.137710	-2.010035	-2.050484
C	0.471691	1.423925	-1.980968
H	1.115615	2.291457	-2.164958
H	-0.187674	1.347975	-2.854069
C	2.276691	0.168053	-0.682778
H	1.675839	0.003607	0.217564
P	-0.844601	-1.510251	-0.728560
P	-0.651481	1.840248	-0.535006
Ni	-1.969993	0.127394	0.245434
C	0.082572	-2.459029	0.553788
C	0.099337	-1.991419	1.876270
C	0.801927	-3.623575	0.237537
C	0.816974	-2.672062	2.862067
H	-0.458022	-1.094743	2.134066
C	1.509751	-4.308202	1.225019

H	0.802852	-4.007013	-0.778825
C	1.519748	-3.832641	2.538760
H	0.822948	-2.294369	3.880475
H	2.058079	-5.209802	0.966012
H	2.077865	-4.363004	3.305179
C	-1.813245	-2.775972	-1.666723
C	-2.164092	-4.009746	-1.100181
C	-2.291640	-2.466683	-2.950652
C	-2.947348	-4.919694	-1.811842
H	-1.841004	-4.257922	-0.095899
C	-3.071981	-3.377687	-3.661683
H	-2.074325	-1.502691	-3.403133
C	-3.398095	-4.611104	-3.095349
H	-3.210524	-5.869448	-1.354428
H	-3.429346	-3.119547	-4.654985
H	-4.007478	-5.321659	-3.647112
C	-1.718503	3.120830	-1.333229
C	-2.459329	2.764243	-2.472607
C	-1.886438	4.404795	-0.797190
C	-3.324781	3.675882	-3.075758
H	-2.376939	1.763144	-2.889128
C	-2.753855	5.316688	-1.402159
H	-1.351175	4.694251	0.100004
C	-3.471955	4.958193	-2.543060
H	-3.888772	3.380990	-3.956661
H	-2.872539	6.307235	-0.971512
H	-4.148649	5.668857	-3.009582
C	0.476722	2.778760	0.588201
C	0.582445	2.411348	1.936998
C	1.270275	3.837153	0.112321
C	1.465534	3.080942	2.788460
H	-0.046890	1.619021	2.326787
C	2.150145	4.506734	0.963052
H	1.194282	4.156144	-0.923690
C	2.251449	4.127614	2.304204
H	1.526369	2.788994	3.833384
H	2.751951	5.326322	0.579463
H	2.934164	4.651207	2.968093
C	-4.469862	-2.923024	1.903163
C	-3.387594	-2.054729	1.718848
C	-3.338801	-1.175677	0.627220
C	-4.417649	-1.194529	-0.273696
C	-5.503840	-2.054198	-0.090047
C	-5.532754	-2.928266	0.999249
H	-4.483026	-3.588150	2.764642
H	-2.588932	-2.059935	2.455316
H	-4.426169	-0.519254	-1.127876
H	-6.329063	-2.038191	-0.799264
H	-6.376337	-3.598780	1.144587
I	-3.139293	1.709839	1.940944
H	2.717946	1.166706	-0.588360
P	3.642139	-1.137608	-0.645386
C	4.149604	-1.088378	1.137954
C	4.914899	-2.173708	1.597510
C	3.834669	-0.065115	2.046476
C	5.367185	-2.229316	2.915948
H	5.155479	-2.984414	0.913638
C	4.276749	-0.125707	3.370473
H	3.240109	0.788481	1.736486
C	5.046592	-1.204223	3.808559
H	5.963065	-3.075756	3.247856
H	4.019921	0.676411	4.057914
H	5.391521	-1.247400	4.838324
C	5.069956	-0.233552	-1.428888
C	5.709591	-0.843263	-2.518250
C	5.553723	1.004942	-0.977233
C	6.793744	-0.229109	-3.150820
H	5.354316	-1.807847	-2.873169
C	6.635735	1.621053	-1.606021
H	5.094026	1.486462	-0.117902
C	7.257193	1.005813	-2.696730
H	7.275570	-0.716546	-3.994476
H	6.998852	2.578941	-1.242077
H	8.101350	1.485629	-3.185018

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B3LYP/BS1 SCF energy: -3369.513528 a.u.

M06/BS2 SCF energy in PhMe: -3368.46233253 a.u.

M06/BS2 Free energy in PhMe: -3367.67305253 a.u.

C	1.827930	-0.407968	1.868762
C	2.489814	-0.673529	3.245360
H	3.247874	0.081608	3.477125
H	1.741565	-0.649154	4.046813
H	2.977838	-1.653974	3.265050
C	0.683915	-1.457284	1.767840

H	0.007555	-1.280200	2.614782
H	1.117306	-2.454019	1.913934
C	1.280669	1.040390	1.933303
H	2.126177	1.730130	2.035039
H	0.708580	1.129981	2.863136
C	2.873987	-0.599547	0.733895
H	2.458333	-0.245075	-0.213319
H	3.071156	-1.669688	0.607746
P	-0.439794	-1.505857	0.275248
P	4.506565	0.322199	0.972133
P	0.126028	1.784973	0.645469
Ni	-1.627028	0.540652	0.107191
C	5.555102	-0.950495	1.836619
C	6.195983	-0.575831	3.026689
C	5.757724	-2.251937	1.348944
C	7.007261	-1.477710	3.720606
H	6.057437	0.431233	3.413092
C	6.565372	-3.155200	2.039848
H	5.295634	-2.559303	0.414191
C	7.190940	-2.770318	3.229347
H	7.494986	-1.169088	4.641688
H	6.713041	-4.158179	1.647305
H	7.822127	-3.474105	3.765579
C	5.237671	0.253915	-0.730351
C	6.328875	1.106224	-0.973815
C	4.788901	-0.568334	-1.775089
C	6.962163	1.127155	-2.216288
H	6.683814	1.760490	-0.180390
C	5.415176	-0.538900	-3.023736
H	3.945304	-1.235743	-1.633695
C	6.503779	0.304533	-3.248045
H	7.807554	1.790365	-2.381152
H	5.047523	-1.180585	-3.820369
H	6.989766	0.324020	-4.220001
C	0.622105	-2.292898	-1.023924
C	0.879931	-1.650526	-2.240070
C	1.177717	-3.564445	-0.795208
C	1.685028	-2.262087	-3.206459
H	0.424914	-0.691940	-2.452268
C	1.984983	-4.170331	-1.756517
H	0.964309	-4.095690	0.128488
C	2.240550	-3.518615	-2.967479
H	1.860749	-1.754529	-4.150824
H	2.402518	-5.155791	-1.567027
H	2.858722	-3.996844	-3.722850
C	-1.552062	-2.926365	0.691587
C	-2.380467	-3.413548	-0.335001
C	-1.609180	-3.536634	1.952757
C	-3.231170	-4.493177	-0.104521
H	-2.368249	-2.933696	-1.310585
C	-2.465492	-4.619203	2.180020
H	-0.987332	-3.188228	2.770503
C	-3.274974	-5.102527	1.152622
H	-3.862998	-4.856050	-0.910643
H	-2.489937	-5.085259	3.161950
H	-3.936718	-5.946444	1.329081
C	-0.180099	3.393526	1.522239
C	-0.649249	3.390795	2.846267
C	0.022666	4.627203	0.888855
C	-0.875664	4.585332	3.527683
H	-0.860782	2.453524	3.353086
C	-0.211742	5.824057	1.569614
H	0.363930	4.661159	-0.139468
C	-0.653451	5.808341	2.891772
H	-1.234357	4.559023	4.553244
H	-0.048014	6.769314	1.059171
H	-0.831710	6.740353	3.421268
C	1.187264	2.276750	-0.778607
C	0.718672	2.059558	-2.082537
C	2.429346	2.911202	-0.596053
C	1.481564	2.459527	-3.183274
H	-0.240473	1.574023	-2.245845
C	3.188532	3.305022	-1.696992
H	2.808868	3.107148	0.402029
C	2.716309	3.078488	-2.993136
H	1.101475	2.282345	-4.185591
H	4.152083	3.781756	-1.542252
H	3.312483	3.384234	-3.848690
C	-4.295457	3.574747	1.269966
C	-4.410379	4.395121	0.146276
C	-3.654412	4.102189	-0.989648
C	-2.792020	2.999731	-1.005620
C	-2.670313	2.159809	0.112122
C	-3.430789	2.475498	1.251308
H	-4.874480	3.790041	2.166064
H	-5.080232	5.251625	0.156498

H	-3.738010	4.726425	-1.876923
H	-2.240113	2.783133	-1.913892
H	-3.357892	1.856713	2.143967
O	-3.303952	-0.492332	0.696144
C	-4.416270	-0.388552	0.164482
C	-5.603137	-1.099226	0.643914
C	-6.823818	-0.879171	-0.015148
C	-5.544008	-1.980608	1.738014
C	-7.978395	-1.526998	0.419017
C	-6.698712	-2.624743	2.167493
C	-7.914706	-2.397212	1.510359
H	-6.856437	-0.202185	-0.865099
H	-8.922650	-1.357044	-0.089950
H	-8.814476	-2.903519	1.850146
H	-6.658034	-3.307923	3.011278
H	-4.589904	-2.153078	2.225026
H	-4.538828	0.256475	-0.714044
I	-2.529045	-0.233930	-2.893887

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B3LYP/BS1 SCF energy: -3369.524132 a.u.

M06/BS2 SCF energy in PhMe: -3368.46976073 a.u.

M06/BS2 Free energy in PhMe: -3367.68234173 a.u.

C	-2.228749	0.924833	-1.960682
C	-3.352609	1.335534	-2.943010
H	-4.135130	1.909512	-2.436681
H	-2.952993	1.958791	-3.752532
H	-3.822667	0.454045	-3.392116
C	-1.137322	0.258696	-2.844731
H	-0.763453	1.006942	-3.554913
H	-1.599141	-0.530757	-3.448992
C	-1.705413	2.238828	-1.323883
H	-2.532147	2.721737	-0.790346
H	-1.427848	2.916684	-2.138206
C	-2.765663	-0.081232	-0.904995
H	-2.017037	-0.220817	-0.118286
H	-2.905444	-1.058049	-1.381267
P	0.374432	-0.454954	-2.021589
P	-4.363134	0.422682	-0.026326
P	-0.253263	2.262194	-0.120357
Ni	1.431411	0.892040	-0.475744
C	-5.648242	-0.409951	-1.087561
C	-6.669721	0.383860	-1.629397
C	-5.662593	-1.789564	-1.350783
C	-7.670856	-0.178341	-2.426154
H	-6.681474	1.451613	-1.423228
C	-6.660255	-2.354259	-2.145360
H	-4.900189	-2.431567	-0.916691
C	-7.666181	-1.548666	-2.687351
H	-8.454006	0.453256	-2.837671
H	-6.658379	-3.424545	-2.336104
H	-8.445059	-1.989961	-3.303727
C	-4.353638	-0.701116	1.446748
C	-5.277332	-0.395828	2.461621
C	-3.501902	-1.801624	1.630605
C	-5.359755	-1.174298	3.615670
H	-5.933973	0.463796	2.347005
C	-3.571864	-2.572098	2.794374
H	-2.767366	-2.069675	0.877801
C	-4.502382	-2.263677	3.787102
H	-6.084396	-0.923013	4.386094
H	-2.891175	-3.408712	2.924431
H	-4.552917	-2.863186	4.692000
C	-0.098985	-2.159731	-1.535376
C	0.196873	-2.604761	-0.239644
C	-0.754127	-3.031966	-2.425353
C	-0.152819	-3.896443	0.165117
H	0.697735	-1.964226	0.481231
C	-1.105288	-4.318287	-2.019057
H	-0.980981	-2.715974	-3.440464
C	-0.805314	-4.751630	-0.722437
H	0.100143	-4.206655	1.175229
H	-1.610034	-4.983562	-2.714723
H	-1.078898	-5.755998	-0.410174
C	1.514718	-0.646117	-3.462499
C	2.078521	-1.878119	-3.821821
C	1.900620	0.504619	-4.171519
C	2.989319	-1.958911	-4.878505
H	1.810249	-2.777812	-3.278581
C	2.807000	0.422122	-5.227546
H	1.502903	1.477814	-3.892971
C	3.353312	-0.812789	-5.585818
H	3.413012	-2.923160	-5.146172
H	3.090727	1.322497	-5.765748
H	4.060459	-0.878520	-6.408099

C	0.160315	4.062777	-0.175778
C	0.381522	4.691157	-1.412047
C	0.347079	4.805886	0.998809
C	0.753121	6.034153	-1.474265
H	0.280034	4.135161	-2.340493
C	0.719192	6.149312	0.934885
H	0.213080	4.335240	1.966167
C	0.918854	6.768993	-0.299208
H	0.915739	6.503144	-2.441005
H	0.858624	6.708756	1.855711
H	1.208259	7.815235	-0.345623
C	-1.028454	1.972307	1.516714
C	-0.617249	0.886922	2.302662
C	-2.052275	2.812537	1.991856
C	-1.208232	0.645303	3.544960
H	0.167346	0.213125	1.969830
C	-2.636634	2.572421	3.233800
H	-2.385436	3.662401	1.402667
C	-2.214621	1.489331	4.011691
H	-0.860622	-0.201785	4.128603
H	-3.424232	3.229885	3.592041
H	-2.675504	1.303389	4.977743
C	4.272256	3.754996	0.571273
C	4.466608	3.591460	1.945275
C	3.691470	2.663859	2.641391
C	2.722987	1.903363	1.972253
C	2.515191	2.062230	0.594327
C	3.302812	2.999502	-0.094554
H	4.873145	4.472318	0.015968
H	5.217591	4.180447	2.466127
H	3.836701	2.519170	3.709483
H	2.153591	1.175459	2.544086
H	3.164078	3.153553	-1.163526
O	2.990434	-0.288162	-0.654963
C	3.586326	-0.891591	0.260516
C	4.760239	-1.717822	0.017196
C	5.289794	-2.444339	1.099831
C	5.368450	-1.787122	-1.251481
C	6.422953	-3.233013	0.911859
C	6.500413	-2.572702	-1.427219
C	7.026630	-3.294512	-0.346560
H	4.790208	-2.400879	2.065073
H	6.831443	-3.800224	1.742835
H	7.911846	-3.908666	-0.490856
H	6.979659	-2.627535	-2.400738
H	4.945546	-1.219509	-2.074288
H	3.218940	-0.835681	1.293308
I	1.775421	-2.217568	3.380372

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B3LYP/BS1 SCF energy: -3369.494128 a.u.

M06/BS2 SCF energy in PhMe: -3368.44281759 a.u.

M06/BS2 Free energy in PhMe: -3367.65396759 a.u.

C	-2.129685	1.682252	1.493183
C	-3.175271	2.472709	2.316864
H	-3.811351	1.800717	2.901256
H	-2.682236	3.158666	3.016822
H	-3.825642	3.062439	1.662070
C	-1.234238	2.762328	0.823926
H	-0.763887	3.356996	1.616182
H	-1.871144	3.455167	0.261980
C	-1.316608	0.839330	2.511898
H	-2.007398	0.184349	3.054497
H	-0.892912	1.524549	3.254793
C	-2.826874	0.811466	0.411713
H	-2.097843	0.125458	-0.031140
H	-3.175630	1.460372	-0.399099
P	0.149064	2.221158	-0.297724
P	-4.263414	-0.260703	1.015519
P	0.105323	-0.264856	1.960076
Ni	1.456572	0.501194	0.338990
C	-5.719120	0.848274	0.667383
C	-6.576750	1.163735	1.731547
C	-6.015571	1.363201	-0.605413
C	-7.691338	1.984248	1.537541
H	-6.370576	0.761053	2.720561
C	-7.127230	2.182173	-0.802776
H	-5.385362	1.107887	-1.453710
C	-7.966755	2.497179	0.269883
H	-8.344051	2.217827	2.374810
H	-7.343903	2.569345	-1.795241
H	-8.834433	3.133029	0.114601
C	-4.424675	-1.484608	-0.365751
C	-5.244505	-2.597565	-0.109852
C	-3.792250	-1.396308	-1.615909

C	-5.440039	-3.582804	-1.077081
H	-5.729331	-2.693957	0.859149
C	-3.973525	-2.392084	-2.579432
H	-3.143537	-0.559625	-1.855374
C	-4.800023	-3.484488	-2.314867
H	-6.081792	-4.433044	-0.860126
H	-3.459382	-2.313116	-3.533054
H	-4.937411	-4.258298	-3.065285
C	-0.606851	1.996384	-1.953692
C	-0.313593	0.846644	-2.700179
C	-1.478265	2.962325	-2.491360
C	-0.891530	0.655778	-3.958640
H	0.368067	0.087229	-2.330072
C	-2.051968	2.768835	-3.746702
H	-1.701219	3.873285	-1.941572
C	-1.761394	1.612856	-4.480442
H	-0.640007	-0.246483	-4.509215
H	-2.722578	3.521128	-4.153612
H	-2.209871	1.466235	-5.459512
C	1.173205	3.748435	-0.417441
C	1.595389	4.244225	-1.659074
C	1.622845	4.382532	0.753237
C	2.428210	5.363134	-1.726712
H	1.279374	3.755385	-2.573906
C	2.451497	5.501614	0.683153
H	1.337004	4.001495	1.730677
C	2.854825	5.996808	-0.559330
H	2.745368	5.735186	-2.696980
H	2.784626	5.983507	1.598462
H	3.501339	6.868271	-0.615079
C	0.972102	-0.481324	3.578799
C	1.421193	0.658773	4.268042
C	1.250862	-1.744684	4.117034
C	2.104479	0.539945	5.476952
H	1.245409	1.651395	3.860074
C	1.937533	-1.862102	5.328003
H	0.937694	-2.640413	3.593087
C	2.360749	-0.724082	6.013644
H	2.437817	1.433604	5.997726
H	2.140943	-2.849948	5.732293
H	2.890768	-0.819206	6.957382
C	-0.697467	-1.871834	1.592332
C	-0.519625	-2.465887	0.335593
C	-1.511586	-2.513461	2.545394
C	-1.134593	-3.683628	0.034098
H	0.096193	-2.003379	-0.431205
C	-2.118061	-3.730747	2.243600
H	-1.665371	-2.072329	3.526412
C	-1.929842	-4.317032	0.987233
H	-0.972800	-4.115604	-0.948979
H	-2.742574	-4.218260	2.987384
H	-2.409741	-5.263332	0.753476
C	4.585296	-1.038036	2.586434
C	4.511933	-2.430780	2.472787
C	3.684780	-3.015531	1.508840
C	2.919931	-2.212310	0.662164
C	2.973969	-0.806432	0.765137
C	3.833892	-0.237684	1.729908
H	5.241256	-0.583992	3.324612
H	5.115448	-3.059229	3.123161
H	3.646710	-4.096912	1.404422
H	2.321631	-2.674163	-0.120298
H	3.942335	0.844210	1.782867
O	2.587087	1.055423	-1.035782
C	3.330111	-0.023197	-1.087583
C	4.804716	0.133934	-1.183849
C	5.578997	-0.963278	-1.588219
C	5.419871	1.369931	-0.937621
C	6.959348	-0.828473	-1.728484
C	6.799303	1.500589	-1.080821
C	7.571333	0.401163	-1.470839
H	5.091797	-1.911499	-1.800186
H	7.555901	-1.679071	-2.046299
H	8.647391	0.506140	-1.583263
H	7.275343	2.460132	-0.895501
H	4.803257	2.217104	-0.653326
H	2.922229	-0.892120	-1.620773
I	1.360112	-2.778559	-3.121415

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B3LYP/BS1 SCF energy: -3369.521049 a.u.

M06/BS2 SCF energy in PhMe: -3368.46981968 a.u.

M06/BS2 Free energy in PhMe: -3367.67844368 a.u.

C	-1.978784	-2.386772	-0.048669
C	-3.035902	-3.517201	-0.038638

H	-3.797443	-3.354545	-0.807696
H	-2.568740	-4.491028	-0.230683
H	-3.545801	-3.568232	0.929308
C	-0.914454	-2.814695	0.998927
H	-0.481137	-3.767477	0.674526
H	-1.415852	-3.016580	1.952509
C	-1.362432	-2.372766	-1.471775
H	-2.159735	-2.203620	-2.203740
H	-0.953729	-3.368396	-1.680860
C	-2.621442	-1.026483	0.341301
H	-1.908226	-0.219239	0.147186
H	-2.816077	-1.016064	1.419506
P	0.513620	-1.685739	1.388783
P	-4.209866	-0.579994	-0.587099
P	0.002025	-1.156103	-1.905971
Ni	1.524265	-0.680509	-0.283553
C	-5.504460	-1.173258	0.612862
C	-6.431381	-2.128625	0.171313
C	-5.613697	-0.691398	1.927885
C	-7.431742	-2.605726	1.022862
H	-6.371100	-2.498955	-0.849525
C	-6.610906	-1.165288	2.780125
H	-4.927510	0.074021	2.281753
C	-7.521165	-2.126281	2.329859
H	-8.141858	-3.345949	0.663042
H	-6.683867	-0.779138	3.793695
H	-8.300290	-2.492078	2.993547
C	-4.314345	1.250877	-0.335420
C	-5.334362	1.906619	-1.048981
C	-3.454723	2.023690	0.460013
C	-5.498481	3.287658	-0.957240
H	-6.002908	1.328831	-1.683868
C	-3.601660	3.412285	0.532678
H	-2.649278	1.565761	1.025406
C	-4.626540	4.045280	-0.170396
H	-6.297330	3.774042	-1.511741
H	-2.893838	3.991515	1.118475
H	-4.737677	5.124820	-0.114133
C	-0.103000	-0.564289	2.695817
C	-0.009648	0.825696	2.553162
C	-0.695063	-1.102771	3.853842
C	-0.509578	1.670422	3.547917
H	0.448215	1.279910	1.680225
C	-1.187761	-0.256706	4.845504
H	-0.756675	-2.178894	3.995024
C	-1.097774	1.130954	4.691576
H	-0.422824	2.743354	3.400406
H	-1.638399	-0.681121	5.738728
H	-1.483162	1.788009	5.466623
C	1.718815	-2.812090	2.198706
C	2.412854	-2.394258	3.344408
C	2.023201	-4.063489	1.637914
C	3.369328	-3.224726	3.929713
H	2.211174	-1.419578	3.772757
C	2.979857	-4.890855	2.225494
H	1.523661	-4.403329	0.734693
C	3.652969	-4.473993	3.375851
H	3.897484	-2.887989	4.817203
H	3.198933	-5.859003	1.783484
H	4.397644	-5.118511	3.834694
C	0.763306	-2.041110	-3.339507
C	1.384084	-3.278564	-3.095765
C	0.794023	-1.516292	-4.638133
C	2.003686	-3.982191	-4.127576
H	1.394614	-3.696036	-2.091128
C	1.413433	-2.223567	-5.672011
H	0.340023	-0.554126	-4.846616
C	2.017620	-3.455912	-5.422051
H	2.476883	-4.938192	-3.920542
H	1.422863	-1.805288	-6.674872
H	2.498658	-4.002908	-6.228087
C	-0.875001	0.305252	-2.574168
C	-0.626026	1.571671	-2.026327
C	-1.829138	0.178601	-3.602825
C	-1.306556	2.696176	-2.500062
H	0.081506	1.710969	-1.214593
C	-2.496034	1.303761	-4.081784
H	-2.050567	-0.793649	-4.034630
C	-2.234913	2.563255	-3.530809
H	-1.104208	3.655886	-2.033304
H	-3.229078	1.195331	-4.876539
H	-2.768233	3.435707	-3.897693
C	3.661636	-0.274318	-3.063286
C	3.316568	0.876518	-3.765768
C	2.907009	2.025829	-3.074168
C	2.853652	2.032783	-1.684034

C	3.229934	0.885277	-0.956793
C	3.618051	-0.277318	-1.660959
H	3.978065	-1.167127	-3.594617
H	3.363717	0.883753	-4.851443
H	2.628308	2.920737	-3.623844
H	2.521753	2.918687	-1.145558
H	3.989381	-1.136904	-1.109386
O	2.715071	-0.289997	1.036315
C	3.322517	0.903766	0.578686
C	4.763958	1.012977	1.062853
C	5.359126	2.277083	1.166544
C	5.511717	-0.124167	1.387639
C	6.689585	2.399865	1.568280
C	6.841615	0.000468	1.795432
C	7.436081	1.261008	1.881200
H	4.773981	3.166061	0.941067
H	7.139453	3.386218	1.646612
H	8.471054	1.356917	2.199548
H	7.413211	-0.888816	2.050987
H	5.036525	-1.099027	1.341995
H	2.775669	1.790270	0.932623
I	0.638305	4.303148	0.722934

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B3LYP/BS1 SCF energy: -3369.512603 a.u.

M06/BS2 SCF energy in PhMe: -3368.46076081 a.u.

M06/BS2 Free energy in PhMe: -3367.67329581 a.u.

C	-1.503972	-2.587065	-0.403904
C	-2.277716	-3.905684	-0.650720
H	-2.899135	-3.836301	-1.548705
H	-1.585834	-4.746135	-0.786104
H	-2.936071	-4.137311	0.193153
C	-0.580113	-2.887735	0.811910
H	0.096965	-3.703152	0.531788
H	-1.195573	-3.271576	1.633824
C	-0.676000	-2.320187	-1.690126
H	-1.365788	-2.230348	-2.536468
H	-0.046037	-3.194627	-1.890851
C	-2.486079	-1.423698	-0.086940
H	-1.943988	-0.472995	-0.100821
H	-2.873942	-1.544150	0.930537
P	0.490917	-1.550651	1.540801
P	-3.933679	-1.251121	-1.298099
P	0.464306	-0.839572	-1.774104
Ni	1.617946	-0.374636	0.069668
C	-5.271501	-2.162003	-0.378125
C	-5.878281	-3.263132	-0.999469
C	-5.719259	-1.781234	0.897764
C	-6.893829	-3.978843	-0.359187
H	-5.556022	-3.560039	-1.994880
C	-6.732675	-2.493054	1.539117
H	-5.287043	-0.909963	1.383585
C	-7.320762	-3.596027	0.912528
H	-7.353077	-4.829501	-0.856303
H	-7.070605	-2.182740	2.524622
H	-8.113262	-4.147759	1.411368
C	-4.469594	0.501984	-1.055470
C	-5.475775	0.952347	-1.930492
C	-3.942894	1.407618	-0.122486
C	-5.951252	2.260380	-1.860935
H	-5.887328	0.271762	-2.673185
C	-4.400597	2.728036	-0.068223
H	-3.161973	1.111268	0.570679
C	-5.409351	3.153547	-0.932350
H	-6.734151	2.586287	-2.541476
H	-3.940714	3.420514	0.631527
H	-5.762728	4.180300	-0.889560
C	-0.573852	-0.617926	2.694521
C	-0.668189	0.777448	2.613250
C	-1.313057	-1.307168	3.675772
C	-1.498910	1.479922	3.491840
H	-0.109908	1.342575	1.872839
C	-2.137777	-0.603479	4.549761
H	-1.234599	-2.387169	3.770525
C	-2.232618	0.789875	4.455877
H	-1.558467	2.560328	3.387367
H	-2.704290	-1.141909	5.304916
H	-2.878866	1.335708	5.137941
C	1.675571	-2.480334	2.597279
C	2.022686	-1.981742	3.862287
C	2.318321	-3.634800	2.121966
C	2.973036	-2.641070	4.643278
H	1.553647	-1.079151	4.238355
C	3.263836	-4.293797	2.907025
H	2.097720	-4.026192	1.132913

C	3.591468	-3.799853	4.171539
H	3.229455	-2.243865	5.621281
H	3.746229	-5.190461	2.527892
H	4.328139	-4.313312	4.783166
C	1.655077	-1.346998	-3.090816
C	2.399598	-2.527055	-2.921250
C	1.895145	-0.550004	-4.220065
C	3.341050	-2.916082	-3.872780
H	2.256486	-3.144362	-2.037634
C	2.842275	-0.940961	-5.169610
H	1.340195	0.370740	-4.365060
C	3.561930	-2.124668	-5.002312
H	3.906902	-3.831735	-3.726802
H	3.012418	-0.316965	-6.042573
H	4.295056	-2.427345	-5.744772
C	-0.504098	0.543964	-2.461358
C	-0.472722	1.792982	-1.823579
C	-1.276384	0.383465	-3.628339
C	-1.196667	2.870469	-2.339959
H	0.091132	1.944779	-0.907104
C	-1.989880	1.462327	-4.144418
H	-1.316723	-0.574932	-4.138883
C	-1.948897	2.704655	-3.501645
H	-1.179395	3.812295	-1.798501
H	-2.585720	1.330852	-5.043408
H	-2.518019	3.539220	-3.901142
C	6.373694	-2.040337	0.414394
C	6.880629	-2.025868	-0.886702
C	6.316601	-1.174221	-1.840155
C	5.256566	-0.337784	-1.489674
C	4.746663	-0.347783	-0.185045
C	5.308152	-1.208521	0.764678
H	6.808498	-2.699784	1.161049
H	7.710337	-2.673786	-1.157070
H	6.700854	-1.160055	-2.856483
H	4.823877	0.326862	-2.234035
H	4.900718	-1.219612	1.769921
O	2.875773	0.116569	1.291934
C	3.599335	0.573328	0.222261
C	3.918055	2.071050	0.273228
C	2.888671	2.978395	0.552806
C	5.221839	2.550350	0.094758
C	3.149548	4.343475	0.650026
C	5.485465	3.918623	0.199773
C	4.453061	4.816036	0.473108
H	1.869518	2.636032	0.711100
H	2.323335	5.015885	0.864011
H	4.660383	5.880250	0.548665
H	6.503005	4.277643	0.067358
H	6.034869	1.863753	-0.113811
H	2.834428	0.510037	-0.734472
I	-0.848494	4.575294	1.202771

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B3LYP/BS1 SCF energy: -3369.508000 a.u.

M06/BS2 SCF energy in PhMe: -3368.45579178 a.u.

M06/BS2 Free energy in PhMe: -3367.67085278 a.u.

C	1.460170	-2.590858	0.446974
C	2.230397	-3.903631	0.732550
H	2.827044	-3.822039	1.646293
H	1.536829	-4.744123	0.859004
H	2.911827	-4.144124	-0.090315
C	0.573851	-2.907296	-0.792672
H	-0.112292	-3.719139	-0.523605
H	1.214102	-3.301019	-1.590273
C	0.595181	-2.312090	1.706394
H	1.261335	-2.206763	2.570056
H	-0.029457	-3.191649	1.900702
C	2.447803	-1.428589	0.142790
H	1.904231	-0.478616	0.136891
H	2.857966	-1.557647	-0.864898
P	-0.474241	-1.564412	-1.546670
P	3.869062	-1.240772	1.382181
P	-0.565639	-0.840928	1.763477
Ni	-1.627461	-0.334047	-0.082281
C	5.225001	-2.168499	0.505823
C	5.822233	-3.255122	1.161124
C	5.695617	-1.813953	-0.769357
C	6.850578	-3.982073	0.554865
H	5.481899	-3.532019	2.156314
C	6.721721	-2.537101	-1.376965
H	5.271082	-0.954111	-1.281526
C	7.300155	-3.625378	-0.716646
H	7.301856	-4.821256	1.078153
H	7.076914	-2.246986	-2.362567

H	8.102515	-4.185950	-1.189221
C	4.413481	0.507053	1.119774
C	5.378833	0.983748	2.025912
C	3.929446	1.384622	0.137898
C	5.856883	2.290064	1.940210
H	5.756060	0.325151	2.805704
C	4.389278	2.703303	0.065923
H	3.180939	1.065996	-0.580789
C	5.357597	3.155126	0.962485
H	6.608098	2.636755	2.645797
H	3.962542	3.374696	-0.674064
H	5.712442	4.180736	0.905977
C	0.612620	-0.695374	-2.732305
C	0.735543	0.699862	-2.687498
C	1.339905	-1.422695	-3.694408
C	1.581035	1.363136	-3.582481
H	0.189203	1.295196	-1.961323
C	2.179269	-0.758684	-4.585601
H	1.241181	-2.503332	-3.760073
C	2.301814	0.634433	-4.527691
H	1.661707	2.444490	-3.507072
H	2.736190	-1.327514	-5.325567
H	2.959682	1.149541	-5.222529
C	-1.674932	-2.506735	-2.581141
C	-1.992912	-2.066640	-3.875137
C	-2.366389	-3.609240	-2.052996
C	-2.961982	-2.730679	-4.629581
H	-1.484382	-1.205979	-4.295965
C	-3.330018	-4.274392	-2.810782
H	-2.168315	-3.954209	-1.041813
C	-3.628746	-3.838070	-4.103321
H	-3.193227	-2.378753	-5.631085
H	-3.848724	-5.130777	-2.388610
H	-4.378576	-4.356362	-4.694656
C	-1.745498	-1.360052	3.085700
C	-2.457509	-2.562097	2.938647
C	-2.008930	-0.549184	4.199307
C	-3.391066	-2.957543	3.895750
H	-2.296762	-3.192610	2.067612
C	-2.948022	-0.945722	5.154598
H	-1.479257	0.388917	4.326985
C	-3.636271	-2.150895	5.009336
H	-3.930068	-3.892082	3.767579
H	-3.135883	-0.309656	6.015216
H	-4.361903	-2.459146	5.756955
C	0.393067	0.555784	2.441186
C	0.381456	1.787445	1.769852
C	1.153129	0.418566	3.618552
C	1.116573	2.869399	2.260009
H	-0.180310	1.916092	0.849066
C	1.874624	1.503376	4.111303
H	1.178410	-0.525970	4.155228
C	1.857050	2.726771	3.432497
H	1.118650	3.795953	1.692571
H	2.460210	1.390233	5.019497
H	2.435414	3.564199	3.812224
C	-6.273259	-1.980309	-0.649316
C	-6.756856	-2.040983	0.659031
C	-6.202099	-1.217723	1.643056
C	-5.179456	-0.328489	1.316298
C	-4.694974	-0.258676	0.002255
C	-5.241341	-1.099691	-0.976956
H	-6.697125	-2.620305	-1.418384
H	-7.559174	-2.728632	0.913116
H	-6.561475	-1.270517	2.666902
H	-4.741787	0.300178	2.086987
H	-4.852389	-1.054548	-1.988636
O	-2.826409	0.307354	-1.389524
C	-3.603213	0.703460	-0.414814
C	-3.817106	2.180763	-0.230100
C	-2.815120	3.075937	-0.639068
C	-5.024965	2.691263	0.275636
C	-3.005187	4.450234	-0.530293
C	-5.217402	4.069555	0.372687
C	-4.208916	4.949601	-0.023601
H	-1.875888	2.713140	-1.043755
H	-2.198998	5.110146	-0.838381
H	-4.359305	6.022803	0.059195
H	-6.159781	4.452210	0.755692
H	-5.823889	2.020769	0.569920
H	-2.574008	0.464291	0.828967
I	0.891401	4.525288	-1.369291

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B3LYP/BS1 SCF energy: -3369.528312 a.u.

M06/BS2 SCF energy in PhMe: -3368.46900046 a.u.

M06/BS2 Free energy in PhMe: -3367.68452346 a.u.

C	1.989127	-2.249805	-0.964693
C	2.993656	-3.296754	-1.504917
H	3.758872	-3.534139	-0.759470
H	2.480981	-4.230499	-1.767504
H	3.503302	-2.924467	-2.400128
C	0.910628	-2.113946	-2.080195
H	0.423839	-3.089228	-2.202678
H	1.413529	-1.902184	-3.030680
C	1.389864	-2.848230	0.337067
H	2.207534	-3.027051	1.044277
H	0.966133	-3.830373	0.099132
C	2.696585	-0.889109	-0.709796
H	2.019687	-0.229048	-0.158390
H	2.897608	-0.398096	-1.668499
P	-0.452007	-0.856938	-1.876158
P	4.299557	-0.993923	0.292979
P	0.061039	-1.922759	1.295019
Ni	-1.352840	-0.727004	0.208116
C	5.569468	-1.014550	-1.068821
C	6.464049	-2.092950	-1.127571
C	5.689612	0.007753	-2.025053
C	7.443740	-2.160776	-2.122162
H	6.394377	-2.885043	-0.385567
C	6.666081	-0.056749	-3.018850
H	5.027529	0.869032	-1.981009
C	7.544476	-1.143379	-3.071180
H	8.128425	-3.004655	-2.151463
H	6.747643	0.744711	-3.748853
H	8.307168	-1.190876	-3.844163
C	4.499442	0.731064	0.931183
C	5.573465	0.930936	1.818327
C	3.658069	1.817322	0.649264
C	5.807095	2.180420	2.389396
H	6.228737	0.098197	2.065928
C	3.875346	3.065488	1.241043
H	2.812496	1.714315	-0.022568
C	4.953313	3.250427	2.106231
H	6.646462	2.314663	3.067511
H	3.178405	3.874327	1.039949
H	5.119974	4.220482	2.567030
C	0.225278	0.691784	-2.584674
C	0.205169	1.865106	-1.817698
C	0.784797	0.722208	-3.876187
C	0.743872	3.051033	-2.326545
H	-0.219889	1.881550	-0.817815
C	1.317835	1.906205	-4.381336
H	0.794090	-0.172435	-4.494173
C	1.299666	3.070925	-3.605112
H	0.719135	3.937623	-1.698570
H	1.746336	1.920884	-5.380172
H	1.719072	3.992027	-4.001219
C	-1.719658	-1.423261	-3.096697
C	-2.377588	-0.498643	-3.923552
C	-2.133527	-2.766489	-3.130080
C	-3.405988	-0.911441	-4.773339
H	-2.082164	0.545277	-3.909310
C	-3.157501	-3.177761	-3.984153
H	-1.659934	-3.504578	-2.487847
C	-3.796717	-2.250612	-4.809981
H	-3.899429	-0.181310	-5.409025
H	-3.455083	-4.222859	-4.003206
H	-4.594150	-2.570251	-5.475019
C	-0.753553	-3.312624	2.201279
C	-1.234413	-4.427034	1.494925
C	-0.980111	-3.241446	3.583115
C	-1.905014	-5.455638	2.156881
H	-1.095079	-4.497985	0.418984
C	-1.652592	-4.271209	4.244042
H	-0.630137	-2.382321	4.145549
C	-2.113152	-5.381744	3.535684
H	-2.263975	-6.313907	1.594938
H	-1.814328	-4.202135	5.316282
H	-2.632633	-6.183661	4.053044
C	0.958358	-0.945524	2.556106
C	0.688215	0.424223	2.694790
C	1.927615	-1.544082	3.382779
C	1.377835	1.187782	3.639991
H	-0.048616	0.917991	2.067354
C	2.603126	-0.781632	4.332962
H	2.149512	-2.604559	3.296915
C	2.330142	0.584666	4.460075
H	1.165136	2.250959	3.702333
H	3.348589	-1.252428	4.968161
H	2.869235	1.178086	5.193372

C	-5.275981	-2.778248	0.414729
C	-6.267665	-2.563186	1.376339
C	-6.508574	-1.274125	1.856609
C	-5.770441	-0.197213	1.367732
C	-4.762007	-0.407485	0.411115
C	-4.516467	-1.710382	-0.055482
H	-5.092801	-3.779562	0.035630
H	-6.851229	-3.399841	1.750805
H	-7.270582	-1.106131	2.612174
H	-5.950882	0.803045	1.747074
H	-3.752008	-1.872957	-0.808760
O	-2.703904	0.555125	-0.302385
C	-3.923969	0.718939	-0.069267
C	-4.500295	2.060133	-0.273387
C	-3.664656	3.183808	-0.126397
C	-5.853040	2.238182	-0.629754
C	-4.181428	4.462976	-0.311059
C	-6.353392	3.519587	-0.839754
C	-5.520426	4.632144	-0.673289
H	-2.626809	3.070139	0.175764
H	-3.528157	5.316999	-0.158747
H	-5.919863	5.631838	-0.823629
H	-7.391662	3.653158	-1.130562
H	-6.497739	1.375539	-0.765942
H	-1.875213	-0.729986	1.587007
I	-0.186531	4.277898	1.370677

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B3LYP/BS1 SCF energy: -3369.526082 a.u.

M06/BS2 SCF energy in PhMe: -3368.46678513 a.u.

M06/BS2 Free energy in PhMe: -3367.68007013 a.u.

C	2.218955	0.738236	1.938570
C	3.293630	1.077404	2.999758
H	4.049190	1.761802	2.601398
H	2.837721	1.556767	3.875173
H	3.810594	0.172705	3.337983
C	1.144469	-0.099982	2.691401
H	0.658975	0.546560	3.432439
H	1.649293	-0.889606	3.258715
C	1.648123	2.097319	1.454043
H	2.454367	2.636454	0.947316
H	1.382922	2.690246	2.335653
C	2.843061	-0.084920	0.777444
H	2.095961	-0.229312	-0.010568
H	3.100309	-1.086382	1.140587
P	-0.206161	-0.908343	1.682201
P	4.355929	0.689265	-0.062741
P	0.166358	2.172271	0.281581
Ni	-1.070291	0.426976	0.024404
C	5.747206	-0.010930	0.951109
C	6.718022	0.876497	1.438554
C	5.879308	-1.377234	1.253362
C	7.785045	0.419225	2.217363
H	6.635309	1.935529	1.205459
C	6.940892	-1.836759	2.032563
H	5.157465	-2.089600	0.862279
C	7.895531	-0.938162	2.518952
H	8.527124	1.122887	2.585800
H	7.027915	-2.897068	2.256402
H	8.723109	-1.297517	3.125113
C	4.470798	-0.333002	-1.605599
C	5.718739	-0.782618	-2.072664
C	3.342391	-0.549318	-2.413903
C	5.827413	-1.446490	-3.295495
H	6.612589	-0.621505	-1.477663
C	3.450422	-1.223005	-3.631721
H	2.356089	-0.204623	-2.118584
C	4.693442	-1.674601	-4.077347
H	6.802652	-1.789602	-3.632925
H	2.549301	-1.390191	-4.215287
H	4.778240	-2.197922	-5.026281
C	0.469531	-2.592120	1.356507
C	0.535173	-3.072506	0.042885
C	0.941556	-3.399540	2.408579
C	1.073808	-4.336863	-0.216237
H	0.174997	-2.466276	-0.785741
C	1.475289	-4.659441	2.145472
H	0.878927	-3.054364	3.437652
C	1.544943	-5.129277	0.829301
H	1.123051	-4.689429	-1.242657
H	1.835151	-5.275116	2.965818
H	1.964613	-6.111069	0.625427
C	-1.531736	-1.208267	2.939650
C	-2.208166	-2.437188	2.991623
C	-1.968537	-0.170395	3.779724

C	-3.272033	-2.628178	3.875559
H	-1.904673	-3.250171	2.340895
C	-3.028327	-0.363475	4.666354
H	-1.492033	0.804730	3.741241
C	-3.682864	-1.595672	4.719373
H	-3.779587	-3.588743	3.901031
H	-3.343660	0.451323	5.312903
H	-4.508771	-1.747143	5.409007
C	-0.848939	3.527679	1.043335
C	-1.075915	3.583429	2.427385
C	-1.470011	4.484845	0.226034
C	-1.884649	4.576469	2.983366
H	-0.617187	2.853163	3.087923
C	-2.274388	5.480858	0.781594
H	-1.319948	4.456433	-0.848193
C	-2.483373	5.532986	2.161552
H	-2.039444	4.604996	4.058807
H	-2.735930	6.219365	0.131510
H	-3.104368	6.313365	2.593116
C	0.870840	2.980742	-1.214941
C	0.620333	2.457315	-2.488705
C	1.657386	4.141443	-1.088956
C	1.157910	3.079919	-3.619976
H	0.023213	1.557372	-2.605640
C	2.185988	4.759472	-2.219191
H	1.848445	4.575576	-0.110950
C	1.938545	4.226560	-3.488847
H	0.962491	2.653685	-4.599798
H	2.791376	5.655407	-2.110097
H	2.356747	4.707144	-4.369500
C	-5.029075	2.825895	0.270979
C	-5.937274	3.032669	-0.771634
C	-6.172406	2.022066	-1.706504
C	-5.516007	0.797514	-1.590784
C	-4.594321	0.586035	-0.551183
C	-4.349097	1.614967	0.372646
H	-4.839249	3.611157	0.996315
H	-6.459250	3.982217	-0.856770
H	-6.866588	2.185947	-2.525838
H	-5.691857	0.014713	-2.321215
H	-3.635231	1.452428	1.173320
O	-2.670770	-0.747239	-0.072911
C	-3.862742	-0.700117	-0.430089
C	-4.548364	-1.982946	-0.719512
C	-3.774607	-3.072469	-1.160637
C	-5.931863	-2.147243	-0.525790
C	-4.383473	-4.297410	-1.418977
C	-6.529862	-3.382886	-0.765041
C	-5.757932	-4.456488	-1.217197
H	-2.714276	-2.924712	-1.337568
H	-3.785912	-5.127875	-1.784043
H	-6.228274	-5.416318	-1.414732
H	-7.596485	-3.508038	-0.600436
H	-6.531207	-1.316370	-0.167822
H	-1.645826	1.408987	-0.899138
I	-0.746654	-1.124860	-3.062606

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B3LYP/BS1 SCF energy: -2792.917090 a.u.

M06/BS2 SCF energy in PhMe: -2792.11520266 a.u.

M06/BS2 Free energy in PhMe: -2791.50696866 a.u.

C	0.845612	0.170203	-1.935406
C	1.599847	0.370038	-3.271589
H	2.360705	-0.403091	-3.422376
H	0.905412	0.323050	-4.119242
H	2.103374	1.342904	-3.298272
C	-0.288960	1.240039	-1.929923
H	-1.009245	0.982624	-2.717741
H	0.135059	2.206537	-2.226147
C	0.261649	-1.267765	-1.971730
H	1.085486	-1.978928	-2.095695
H	-0.361666	-1.357784	-2.868923
C	1.801870	0.389104	-0.732930
H	1.280060	0.130155	0.195177
H	2.048418	1.453670	-0.662350
P	-1.346519	1.484316	-0.400819
P	3.398099	-0.621640	-0.728909
P	-0.809941	-1.875484	-0.549481
Ni	-2.023660	-0.468431	0.528203
C	4.593622	0.552299	-1.540994
C	5.297050	0.093899	-2.664751
C	4.842401	1.856770	-1.083491
C	6.212724	0.917423	-3.325315
H	5.125480	-0.917871	-3.024666
C	5.756416	2.681178	-1.739618

H	4.331179	2.228122	-0.198962
C	6.442320	2.213893	-2.864614
H	6.746702	0.544477	-4.195519
H	5.939404	3.687197	-1.370258
H	7.155650	2.856560	-3.373911
C	3.903965	-0.466700	1.049346
C	4.864978	-1.383639	1.507977
C	3.403178	0.480941	1.957360
C	5.325577	-1.346167	2.824214
H	5.251647	-2.137243	0.825867
C	3.854647	0.511448	3.279070
H	2.655430	1.204887	1.648025
C	4.818738	-0.398305	3.715703
H	6.072889	-2.062609	3.155764
H	3.450043	1.251130	3.965175
H	5.169267	-0.371971	4.744123
C	-0.367781	2.629954	0.675169
C	-0.497388	2.503935	2.067782
C	0.501570	3.613459	0.170093
C	0.218456	3.339835	2.928652
H	-1.171653	1.758927	2.478161
C	1.216481	4.447598	1.031251
H	0.635660	3.737442	-0.900390
C	1.076851	4.312346	2.414595
H	0.098451	3.227692	4.002785
H	1.881630	5.202358	0.619864
H	1.633396	4.962069	3.084813
C	-2.697533	2.516930	-1.125644
C	-2.565216	3.888906	-1.384819
C	-3.895298	1.872508	-1.474291
C	-3.602012	4.597226	-1.994253
H	-1.661789	4.416419	-1.095947
C	-4.927533	2.580798	-2.091439
H	-4.032419	0.822635	-1.230995
C	-4.782336	3.944071	-2.354074
H	-3.487864	5.661605	-2.182400
H	-5.851290	2.069355	-2.347868
H	-5.589884	4.498046	-2.825294
C	-1.827147	-3.150863	-1.420735
C	-2.656151	-2.741012	-2.478522
C	-1.865780	-4.491581	-1.015409
C	-3.485731	-3.653400	-3.128679
H	-2.667653	-1.699423	-2.791131
C	-2.699952	-5.404070	-1.665951
H	-1.248385	-4.828755	-0.189638
C	-3.508199	-4.990406	-2.724748
H	-4.119687	-3.317920	-3.945062
H	-2.716533	-6.440467	-1.339476
H	-4.156621	-5.701912	-3.228591
C	0.342287	-2.821182	0.532886
C	0.287807	-2.624679	1.921536
C	1.271928	-3.737836	0.012657
C	1.147748	-3.324925	2.770223
H	-0.437321	-1.928945	2.333618
C	2.124191	-4.441648	0.862737
H	1.326973	-3.918270	-1.057003
C	2.065977	-4.233012	2.243144
H	1.096589	-3.158480	3.842461
H	2.835204	-5.149840	0.446029
H	2.734574	-4.778025	2.903979
H	-2.416535	-1.764499	1.086319
I	-3.802971	0.342844	2.179270

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B3LYP/BS1 SCF energy: -3202.037911 a.u.

M06/BS2 SCF energy in PhMe: -3201.06565952 a.u.

M06/BS2 Free energy in PhMe: -3200.19553652 a.u.

C	1.824356	-0.064210	-1.870822
C	2.651559	-0.207610	-3.172948
H	3.128456	-1.191226	-3.240881
H	2.008668	-0.088740	-4.053801
H	3.441304	0.549865	-3.225015
C	1.110641	1.315951	-1.994316
H	0.409782	1.240288	-2.835836
H	1.857300	2.071554	-2.270755
C	0.810567	-1.241795	-1.883340
H	1.373359	-2.181926	-1.874315
H	0.299127	-1.210846	-2.852114
C	2.764880	-0.080071	-0.634395
H	2.166029	-0.147419	0.278464
H	3.297746	0.874600	-0.574893
P	0.093861	1.950100	-0.557192
P	4.023399	-1.491712	-0.534035
P	-0.603802	-1.404398	-0.622933
Ni	-1.374902	0.390431	0.195724

C	5.466308	-0.813133	-1.487847
C	6.104555	-1.671935	-2.395363
C	5.957170	0.497195	-1.352299
C	7.195424	-1.237776	-3.153647
H	5.739785	-2.689917	-2.510121
C	7.043551	0.935067	-2.110144
H	5.499198	1.178764	-0.640287
C	7.664510	0.068475	-3.014652
H	7.675138	-1.919164	-3.851560
H	7.409398	1.952001	-1.992177
H	8.511016	0.411037	-3.604113
C	4.606112	-1.279155	1.217676
C	5.969349	-1.211408	1.550520
C	3.671187	-1.320767	2.266914
C	6.380734	-1.160530	2.884182
H	6.719167	-1.191600	0.766330
C	4.082637	-1.261965	3.598517
H	2.610751	-1.410099	2.054062
C	5.440126	-1.178886	3.914430
H	7.441732	-1.102806	3.114908
H	3.336679	-1.288029	4.388787
H	5.760908	-1.135169	4.951986
C	1.376233	2.759588	0.515056
C	1.552591	2.312312	1.831301
C	2.193002	3.797967	0.037415
C	2.537407	2.875966	2.646958
H	0.906856	1.532277	2.222152
C	3.174906	4.361869	0.851722
H	2.054278	4.178906	-0.971564
C	3.351417	3.898150	2.158877
H	2.663954	2.514509	3.663747
H	3.797984	5.166531	0.469096
H	4.116133	4.337725	2.794062
C	-0.715398	3.447436	-1.301806
C	-0.629043	3.817151	-2.653162
C	-1.489119	4.247135	-0.438928
C	-1.296787	4.950145	-3.129247
H	-0.035316	3.235651	-3.350593
C	-2.147706	5.379759	-0.914346
H	-1.581473	3.972109	0.608229
C	-2.056659	5.735191	-2.263200
H	-1.213661	5.218916	-4.179534
H	-2.736578	5.983698	-0.228725
H	-2.572725	6.617039	-2.633886
C	-1.585838	-2.649691	-1.616005
C	-2.103615	-2.252435	-2.862863
C	-1.870518	-3.951099	-1.173764
C	-2.851997	-3.128039	-3.649718
H	-1.922614	-1.243697	-3.227974
C	-2.628780	-4.827604	-1.956697
H	-1.491057	-4.294087	-0.217277
C	-3.117849	-4.423804	-3.198959
H	-3.228967	-2.796881	-4.614169
H	-2.828869	-5.832186	-1.592429
H	-3.698787	-5.108923	-3.810445
C	0.132203	-2.466095	0.717804
C	-0.174925	-2.158118	2.053048
C	0.953209	-3.577675	0.458662
C	0.314253	-2.945582	3.099401
H	-0.800077	-1.295397	2.268055
C	1.443346	-4.362593	1.503555
H	1.207617	-3.847042	-0.561656
C	1.122062	-4.050365	2.827013
H	0.061340	-2.690304	4.125237
H	2.080307	-5.214763	1.282503
H	1.506002	-4.662251	3.639000
H	-2.940950	-0.404562	0.214819
C	-4.973421	0.387699	-0.810005
C	-5.405301	-0.661135	-1.852971
C	-6.200636	-1.827566	-1.259302
C	-5.380989	-2.506882	-0.158497
C	-4.944485	-1.549344	0.966291
N	-4.310391	-0.309101	0.362090
H	-7.167218	-1.482547	-0.870560
H	-5.986335	-0.147302	-2.629122
H	-5.947692	-3.328485	0.297359
H	-6.429030	-2.554777	-2.047742
H	-4.487388	-2.953459	-0.609274
H	-4.508718	-1.062659	-2.339847
H	-4.211836	0.379441	1.118797
C	-3.936011	1.339898	-1.430215
H	-4.348097	1.786842	-2.342647
H	-3.673165	2.151745	-0.745768
H	-3.012939	0.807040	-1.690585
C	-6.171982	1.246643	-0.348777
H	-5.889525	1.892567	0.490250

H	-6.484388	1.896135	-1.174462
H	-7.040384	0.656378	-0.050538
C	-3.879603	-2.230095	1.842727
H	-3.537878	-1.565007	2.641924
H	-4.309828	-3.128708	2.299588
H	-3.010205	-2.528092	1.253483
C	-6.131381	-1.173345	1.880225
H	-6.438915	-2.058254	2.449056
H	-5.838761	-0.402083	2.601768
H	-7.005522	-0.816650	1.332606
I	-2.263142	1.516489	2.478897

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B3LYP/BS1 SCF energy: -3202.055489 a.u.

M06/BS2 SCF energy in PhMe: -3201.08416450 a.u.

M06/BS2 Free energy in PhMe: -3200.21184550 a.u.

C	2.035860	0.222649	-1.869249
C	2.935112	0.267969	-3.130586
H	3.382938	-0.709165	-3.342987
H	2.349352	0.561932	-4.010587
H	3.750487	0.989909	-3.009914
C	1.375909	1.635735	-1.791836
H	0.685620	1.716930	-2.641954
H	2.160825	2.387282	-1.950901
C	0.998294	-0.907640	-2.128070
H	1.550415	-1.842977	-2.271588
H	0.514332	-0.692071	-3.087872
C	2.895984	-0.039578	-0.602568
H	2.232555	-0.243053	0.245272
H	3.446391	0.870824	-0.342788
P	0.361155	2.085718	-0.275523
P	4.107797	-1.491152	-0.693298
P	-0.424116	-1.219543	-0.896848
Ni	-0.847830	0.431046	0.330508
C	5.642602	-0.691572	-1.370682
C	6.347046	-1.386110	-2.365842
C	6.135265	0.557719	-0.955415
C	7.504599	-0.850929	-2.937341
H	5.979705	-2.354253	-2.697929
C	7.289086	1.096710	-1.525627
H	5.623016	1.111108	-0.172908
C	7.975797	0.394036	-2.520069
H	8.034027	-1.405078	-3.708263
H	7.654726	2.064714	-1.192007
H	8.873711	0.815781	-2.964451
C	4.528321	-1.675943	1.105705
C	5.841009	-1.618309	1.600322
C	3.497633	-2.016341	2.000306
C	6.110271	-1.866981	2.948578
H	6.662196	-1.373369	0.934700
C	3.766178	-2.254796	3.347772
H	2.474854	-2.107468	1.646379
C	5.075048	-2.179501	3.829646
H	7.134921	-1.811215	3.308463
H	2.948755	-2.506928	4.018573
H	5.285342	-2.368442	4.879190
C	1.652141	2.811212	0.859276
C	1.773541	2.284680	2.152773
C	2.499760	3.863545	0.477131
C	2.731862	2.784635	3.038836
H	1.106402	1.484854	2.463616
C	3.456328	4.364679	1.360429
H	2.404219	4.306417	-0.511585
C	3.576583	3.822488	2.643625
H	2.814687	2.362264	4.036834
H	4.103825	5.181755	1.050864
H	4.321458	4.213395	3.332304
C	-0.473886	3.651574	-0.844657
C	-0.303605	4.262669	-2.096902
C	-1.372514	4.241785	0.064858
C	-1.009917	5.422933	-2.431361
H	0.387020	3.846954	-2.823821
C	-2.066041	5.405535	-0.263260
H	-1.527129	3.775532	1.035339
C	-1.891145	5.999415	-1.517137
H	-0.861491	5.878902	-3.407561
H	-2.747401	5.847789	0.459676
H	-2.435752	6.903754	-1.776690
C	-1.672728	-1.881949	-2.129867
C	-2.119939	-1.038165	-3.168714
C	-2.281907	-3.146106	-2.018373
C	-3.119706	-1.439451	-4.055803
H	-1.676031	-0.051944	-3.285756
C	-3.289416	-3.547827	-2.901803
H	-1.948975	-3.835072	-1.248447

C	-3.715737	-2.698403	-3.925440
H	-3.428269	-0.770547	-4.855958
H	-3.726278	-4.538720	-2.799440
H	-4.488298	-3.016388	-4.620415
C	0.104484	-2.798432	-0.048283
C	-0.187448	-2.914370	1.320790
C	0.749137	-3.872278	-0.685608
C	0.154159	-4.068371	2.032609
H	-0.679604	-2.085063	1.824475
C	1.094147	-5.023748	0.024100
H	0.978711	-3.821748	-1.746207
C	0.797870	-5.124394	1.386029
H	-0.077522	-4.135726	3.092770
H	1.597898	-5.840877	-0.486047
H	1.072404	-6.019458	1.938385
H	-3.839679	-0.856806	-0.409009
C	-5.236672	0.693728	-0.487724
C	-6.218357	0.070869	-1.498143
C	-7.133942	-1.002923	-0.894775
C	-6.302365	-2.126693	-0.261782
C	-5.332081	-1.637823	0.829274
N	-4.527844	-0.460294	0.245914
H	-7.814803	-0.561632	-0.156640
H	-6.809134	0.884183	-1.935764
H	-6.952029	-2.889639	0.183129
H	-7.769345	-1.422120	-1.683276
H	-5.721668	-2.626741	-1.049109
H	-5.640638	-0.375020	-2.319549
H	-3.917677	-0.059688	1.005311
C	-4.133760	1.477386	-1.213295
H	-4.591522	2.302540	-1.769277
H	-3.406345	1.898053	-0.512257
H	-3.596247	0.845182	-1.926551
C	-5.924968	1.622758	0.524021
H	-5.241000	1.894207	1.334860
H	-6.208438	2.543025	0.003408
H	-6.832632	1.199832	0.957292
C	-4.296691	-2.719662	1.172033
H	-3.587840	-2.363887	1.926532
H	-4.816301	-3.597357	1.570518
H	-3.734759	-3.034161	0.287142
C	-6.048927	-1.211166	2.119588
H	-6.401713	-2.114798	2.626988
H	-5.362351	-0.693664	2.797432
H	-6.918467	-0.575302	1.946733
I	-2.235538	0.680174	2.634638

4 (M06 OPT)

M06/BS1 SCF energy: -3972.243734 a.u.

M06/BS2 SCF energy in PhMe: --3973.03719353 a.u.

M06/BS2 Free energy in PhMe: -3972.32155153 a.u.

C	1.730342	0.364038	2.060764
C	2.733467	0.536237	3.205164
H	3.421063	1.371994	3.014842
H	2.214635	0.741600	4.152650
H	3.340729	-0.371128	3.335085
C	0.735878	-0.725832	2.513980
H	0.162124	-0.348678	3.376373
H	1.299100	-1.596321	2.884444
C	1.020874	1.715507	1.876428
H	1.771067	2.492147	1.659282
H	0.565240	1.994844	2.838306
C	2.446715	-0.098300	0.784874
H	1.733850	-0.096254	-0.053424
H	2.769927	-1.142451	0.917378
P	-0.510230	-1.289789	1.268850
P	3.901136	0.931893	0.214563
P	-0.316394	1.929543	0.588962
Ni	-1.649856	0.308760	0.190035
C	5.299015	0.051154	1.051441
C	6.165291	0.811441	1.839631
C	5.531584	-1.323215	0.930774
C	7.233107	0.216237	2.506749
H	5.995081	1.885363	1.933220
C	6.596231	-1.920823	1.595154
H	4.881867	-1.933859	0.299816
C	7.447522	-1.151859	2.386403
H	7.897236	0.823118	3.120409
H	6.768095	-2.991420	1.491667
H	8.281394	-1.622607	2.904979
C	4.086716	0.275743	-1.501052
C	4.937707	0.989879	-2.351768
C	3.432119	-0.851533	-2.007860
C	5.132346	0.591540	-3.669610
H	5.446564	1.878670	-1.973102

C	3.616935	-1.246100	-3.329816
H	2.763502	-1.442141	-1.381186
C	4.465213	-0.525826	-4.164675
H	5.799922	1.160657	-4.315237
H	3.092862	-2.126481	-3.701755
H	4.608334	-0.834843	-5.198978
C	0.358978	-2.551738	0.271097
C	0.180865	-2.552464	-1.114162
C	1.207157	-3.501406	0.854331
C	0.854741	-3.481558	-1.904969
H	-0.509035	-1.848612	-1.582358
C	1.892802	-4.413239	0.061465
H	1.331443	-3.535985	1.937713
C	1.720016	-4.400466	-1.322555
H	0.691805	-3.482252	-2.981640
H	2.556689	-5.142381	0.523148
H	2.253968	-5.118634	-1.942955
C	-1.713162	-2.211130	2.288671
C	-2.121007	-3.504990	1.960152
C	-2.355017	-1.535432	3.332120
C	-3.128810	-4.125280	2.692013
H	-1.673250	-4.020981	1.111093
C	-3.356669	-2.159128	4.064570
H	-2.087639	-0.501309	3.562563
C	-3.741526	-3.459026	3.747517
H	-3.443468	-5.132659	2.425168
H	-3.848115	-1.625291	4.876275
H	-4.532317	-3.946890	4.314706
C	-1.095866	3.466361	1.201374
C	-1.591651	3.485006	2.509289
C	-1.362837	4.546944	0.359627
C	-2.321782	4.572159	2.973220
H	-1.439674	2.627355	3.168127
C	-2.102384	5.629934	0.822188
H	-1.022123	4.530854	-0.674260
C	-2.578230	5.647915	2.128727
H	-2.702756	4.572383	3.993051
H	-2.316798	6.458763	0.150025
H	-3.160009	6.495728	2.486175
C	0.612501	2.346651	-0.927110
C	0.503805	1.501772	-2.036800
C	1.470610	3.450267	-0.986065
C	1.251021	1.751178	-3.183853
H	-0.179073	0.648862	-2.007504
C	2.201698	3.707370	-2.139771
H	1.566704	4.117115	-0.128048
C	2.094970	2.855068	-3.236383
H	1.170201	1.078647	-4.035401
H	2.864318	4.570252	-2.178362
H	2.678118	3.050580	-4.134853
C	-4.884252	2.821330	0.013369
C	-4.856870	3.435715	-1.236943
C	-3.822200	3.150163	-2.118581
C	-2.805735	2.266219	-1.752400
C	-2.822519	1.651616	-0.501470
C	-3.873978	1.936878	0.375547
H	-5.700184	3.026016	0.706633
H	-5.649380	4.125092	-1.525702
H	-3.802803	3.610619	-3.106450
H	-2.010151	2.054919	-2.467541
H	-3.914558	1.451661	1.355562
O	-2.904577	-1.099255	-0.276171
S	-3.383105	-1.260890	-1.708589
O	-2.289812	-1.117896	-2.675446
O	-4.659355	-0.635684	-2.001353
C	-3.734026	-3.064991	-1.649419
F	-2.621256	-3.749161	-1.376764
F	-4.197377	-3.467212	-2.824200
F	-4.631013	-3.333520	-0.712771

TS4(M06 OPT)

M06/BS1 SCF energy: -4317.579714 a.u.

M06/BS2 SCF energy in PhMe: -4318.46866557 a.u.

M06/BS2 Free energy in PhMe: -4317.64611157 a.u.

C	-2.118481	-0.103059	-2.099972
C	-2.969157	-0.257668	-3.365981
H	-3.816109	0.442472	-3.372029
H	-2.370031	-0.058330	-4.266191
H	-3.376452	-1.275821	-3.444977
C	-0.900843	-1.032935	-2.302725
H	-0.327952	-0.651961	-3.165368
H	-1.261453	-2.034582	-2.585625
C	-1.694033	1.372419	-2.027673
H	-2.592594	2.007297	-1.976203
H	-1.202828	1.624765	-2.979696

C	-2.921977	-0.534678	-0.863636
H	-2.363873	-0.267234	0.044794
H	-3.020653	-1.630599	-0.860185
P	0.338717	-1.171071	-0.939808
P	-4.620238	0.231923	-0.667511
P	-0.527145	1.997955	-0.712226
Ni	1.253498	0.852062	-0.397255
C	-5.675218	-1.048783	-1.491744
C	-6.504178	-0.650111	-2.542383
C	-5.683893	-2.392163	-1.100786
C	-7.312483	-1.572195	-3.202453
H	-6.511352	0.397852	-2.846995
C	-6.490112	-3.314861	-1.755919
H	-5.064388	-2.715746	-0.261615
C	-7.304042	-2.906118	-2.810870
H	-7.950979	-1.247184	-4.022653
H	-6.489779	-4.357328	-1.440288
H	-7.936536	-3.629556	-3.323105
C	-4.974681	-0.184714	1.094130
C	-6.143351	0.368707	1.632370
C	-4.167631	-0.969069	1.921136
C	-6.496135	0.146714	2.957571
H	-6.780452	0.989795	0.998784
C	-4.514720	-1.184974	3.252463
H	-3.245517	-1.415122	1.549372
C	-5.676969	-0.629122	3.775225
H	-7.410809	0.583431	3.356416
H	-3.863479	-1.794660	3.879293
H	-5.945994	-0.799527	4.816648
C	-0.478866	-2.223117	0.331493
C	-0.459478	-1.864876	1.679743
C	-1.117518	-3.412287	-0.044091
C	-1.093562	-2.660788	2.631921
H	0.076002	-0.977334	2.002143
C	-1.760795	-4.198850	0.903058
H	-1.109530	-3.734287	-1.086830
C	-1.754529	-3.820384	2.245955
H	-1.054365	-2.363483	3.679640
H	-2.259986	-5.116642	0.595890
H	-2.255956	-4.439682	2.988442
C	1.560195	-2.364649	-1.613175
C	2.439729	-2.956921	-0.698333
C	1.681765	-2.674188	-2.968651
C	3.418920	-3.839881	-1.131793
H	2.352929	-2.717782	0.359820
C	2.656230	-3.572724	-3.399814
H	1.014149	-2.227694	-3.704327
C	3.525690	-4.155129	-2.484534
H	4.108022	-4.272292	-0.407026
H	2.731268	-3.816801	-4.458722
H	4.293018	-4.849016	-2.825229
C	-0.362328	3.731944	-1.290507
C	-0.004112	3.990030	-2.617409
C	-0.467425	4.801242	-0.398350
C	0.227121	5.290294	-3.048087
H	0.133293	3.168922	-3.322373
C	-0.227701	6.101600	-0.828688
H	-0.715047	4.615637	0.645956
C	0.115709	6.349728	-2.153136
H	0.504709	5.475361	-4.084594
H	-0.306801	6.924315	-0.120166
H	0.303508	7.368746	-2.487337
C	-1.532262	2.108341	0.810721
C	-1.023812	1.546375	1.983496
C	-2.794822	2.713655	0.832549
C	-1.769730	1.561371	3.157822
H	-0.031286	1.097548	1.986609
C	-3.536871	2.733258	2.007789
H	-3.202257	3.173606	-0.068618
C	-3.027962	2.153015	3.168890
H	-1.351829	1.109349	4.056751
H	-4.525311	3.190551	2.014097
H	-3.622885	2.157112	4.080833
C	3.396702	4.418845	-0.679769
C	3.428926	4.911300	0.623159
C	2.771618	4.217358	1.631399
C	2.075541	3.042124	1.343303
C	2.041979	2.535415	0.042926
C	2.708168	3.243410	-0.963920
H	3.905949	4.954356	-1.481722
H	3.966267	5.831577	0.849475
H	2.799358	4.582744	2.657560
H	1.567019	2.529799	2.160623
H	2.680137	2.879003	-1.992735
O	2.226645	-0.348065	1.185034
S	2.755726	-0.094393	2.560964

O	1.700421	0.208543	3.532033
O	3.979044	0.703480	2.599230
C	3.330416	-1.785623	2.990549
F	2.324034	-2.656767	2.929934
F	3.842432	-1.810765	4.211087
F	4.267651	-2.177823	2.124326
O	3.052564	0.272258	-1.463750
C	4.078571	0.180017	-0.793793
C	5.217826	-0.648021	-1.178165
C	6.200207	-0.902050	-0.216280
C	5.306651	-1.218293	-2.451985
C	7.267604	-1.735108	-0.526908
C	6.384922	-2.029829	-2.764647
C	7.360873	-2.290113	-1.801027
H	6.095753	-0.461697	0.776616
H	8.029870	-1.947907	0.219978
H	8.204128	-2.933785	-2.048186
H	6.466238	-2.473992	-3.755704
H	4.511943	-1.024895	-3.171257
H	4.172773	0.716321	0.169605

11(M06 OPT)

M06/BS1 SCF energy: -4317.582628 a.u.

M06/BS2 SCF energy in PhMe: -4318.47349911 a.u.

M06/BS2 Free energy in PhMe: -4317.65111711 a.u.

C	2.135176	1.563709	1.879148
C	3.315044	2.068259	2.715996
H	4.110544	2.489729	2.086485
H	2.988998	2.856258	3.410492
H	3.752121	1.251204	3.307754
C	1.036025	1.174708	2.886703
H	0.633119	2.087795	3.354706
H	1.480565	0.582163	3.699809
C	1.654800	2.735591	1.009792
H	2.496331	3.116318	0.412003
H	1.355355	3.557329	1.676678
C	2.544379	0.343830	1.033339
H	1.735597	0.092915	0.329357
H	2.669425	-0.533438	1.687725
P	-0.406173	0.244885	2.197277
P	4.102503	0.597853	0.020185
P	0.274260	2.468598	-0.216086
Ni	-1.291060	1.057914	0.274634
C	5.320202	-0.275203	1.109813
C	6.425670	0.437737	1.577590
C	5.176980	-1.615975	1.485240
C	7.361172	-0.164324	2.416191
H	6.551214	1.480519	1.281061
C	6.108669	-2.220011	2.320536
H	4.331297	-2.197389	1.111574
C	7.201530	-1.493682	2.790015
H	8.216914	0.406158	2.774549
H	5.986098	-3.264610	2.603789
H	7.931047	-1.968178	3.444750
C	3.921264	-0.652912	-1.318758
C	4.918310	-0.598593	-2.301194
C	2.894586	-1.591437	-1.458129
C	4.903809	-1.467832	-3.384267
H	5.715252	0.142924	-2.210987
C	2.865045	-2.447898	-2.557183
H	2.092217	-1.664042	-0.719714
C	3.870064	-2.391012	-3.516287
H	5.691874	-1.413891	-4.134427
H	2.037598	-3.142278	-2.673588
H	3.840030	-3.060702	-4.374278
C	0.034321	-1.511528	2.443298
C	-0.183764	-2.429584	1.412248
C	0.585570	-1.953633	3.654061
C	0.143010	-3.772598	1.597439
H	-0.594534	-2.099695	0.455504
C	0.912995	-3.291269	3.831330
H	0.748610	-1.252505	4.473992
C	0.690259	-4.201871	2.800253
H	-0.030515	-4.480267	0.790480
H	1.340246	-3.624838	4.775714
H	0.946518	-5.251198	2.938290
C	-1.712465	0.593499	3.438024
C	-2.259066	-0.373353	4.282732
C	-2.240122	1.890262	3.463840
C	-3.299000	-0.044139	5.148759
H	-1.874134	-1.392582	4.263788
C	-3.274012	2.219419	4.330375
H	-1.849165	2.647294	2.779025
C	-3.805715	1.249922	5.177207
H	-3.715243	-0.807186	5.804569

H	-3.674053	3.231989	4.337167
H	-4.621081	1.503262	5.852457
C	-0.333799	4.183994	-0.422445
C	-0.682692	4.929641	0.707158
C	-0.612211	4.702218	-1.689724
C	-1.287957	6.174193	0.575668
H	-0.499266	4.532973	1.707724
C	-1.216821	5.946732	-1.820055
H	-0.377325	4.117608	-2.578519
C	-1.556273	6.684735	-0.690359
H	-1.552803	6.744803	1.464428
H	-1.435093	6.335079	-2.813271
H	-2.032697	7.657900	-0.796819
C	1.175337	2.075862	-1.750834
C	0.915350	0.887565	-2.433865
C	2.146519	2.959853	-2.243041
C	1.592808	0.597097	-3.615865
H	0.192175	0.168145	-2.045197
C	2.835618	2.655967	-3.408132
H	2.357288	3.895586	-1.722560
C	2.551545	1.477345	-4.098654
H	1.360864	-0.333136	-4.129675
H	3.591613	3.343801	-3.783743
H	3.089917	1.244193	-5.016279
C	-4.200591	3.479307	-1.350888
C	-4.223338	3.189688	-2.713728
C	-3.313505	2.277269	-3.235579
C	-2.373516	1.662387	-2.405658
C	-2.332598	1.957459	-1.041728
C	-3.260126	2.869620	-0.524809
H	-4.913065	4.188762	-0.929251
H	-4.953696	3.668917	-3.364500
H	-3.331467	2.029574	-4.296577
H	-1.677978	0.942860	-2.836869
H	-3.252299	3.116038	0.540438
O	-1.165196	-1.412075	-1.437434
S	-1.332208	-2.202052	-2.686107
O	-0.257538	-2.019844	-3.662328
O	-2.704423	-2.218550	-3.196400
C	-1.067234	-3.910242	-2.066851
F	0.176272	-4.038337	-1.581434
F	-1.231844	-4.806883	-3.026916
F	-1.909803	-4.189793	-1.072138
O	-2.765222	-0.184398	0.658877
C	-3.396715	-0.798133	-0.212215
C	-4.101872	-2.034826	0.074390
C	-4.813554	-2.652804	-0.959283
C	-4.028669	-2.630794	1.340898
C	-5.448434	-3.865637	-0.728104
C	-4.663104	-3.840667	1.564769
C	-5.369414	-4.456618	0.529495
H	-4.816927	-2.195411	-1.946581
H	-5.991245	-4.358418	-1.531872
H	-5.858698	-5.413488	0.707079
H	-4.607066	-4.315009	2.542851
H	-3.468271	-2.129284	2.129179
H	-3.459570	-0.407050	-1.240705

TS5(M06 OPT)

M06/BS1 SCF energy: -4317.555969 a.u.

M06/BS2 SCF energy in PhMe: -4318.44639833 a.u.

M06/BS2 Free energy in PhMe: -4317.62404433 a.u.

C	-2.190105	-2.392997	0.597427
C	-3.341023	-3.385465	0.788536
H	-3.975447	-3.443682	-0.105616
H	-2.954803	-4.394872	0.993330
H	-3.983770	-3.086714	1.629188
C	-1.313591	-2.499026	1.861920
H	-0.848129	-3.497139	1.900811
H	-1.951510	-2.420649	2.755348
C	-1.398518	-2.857081	-0.637495
H	-2.087431	-2.940180	-1.491310
H	-1.019444	-3.872364	-0.443655
C	-2.719669	-0.956647	0.460150
H	-1.874508	-0.281833	0.261163
H	-3.145237	-0.627151	1.422285
P	0.032138	-1.245116	2.014804
P	-3.961574	-0.622046	-0.907068
P	0.040143	-1.838606	-1.250538
Ni	1.196717	-0.703344	0.228736
C	-5.530939	-1.043971	-0.019583
C	-6.364634	-2.016419	-0.575257
C	-5.906269	-0.450342	1.191125
C	-7.535300	-2.408235	0.070108
H	-6.085478	-2.476083	-1.525154

C	-7.072485	-0.839090	1.838809
H	-5.284252	0.337024	1.620858
C	-7.887390	-1.822892	1.280631
H	-8.174007	-3.169559	-0.375419
H	-7.352807	-0.369393	2.780771
H	-8.801390	-2.126265	1.789074
C	-4.037226	1.221320	-0.816627
C	-5.226122	1.843005	-1.222883
C	-2.944590	2.030750	-0.491690
C	-5.321317	3.227662	-1.283267
H	-6.092030	1.234052	-1.487930
C	-3.035860	3.419102	-0.558449
H	-1.980993	1.614185	-0.202606
C	-4.225708	4.020818	-0.950240
H	-6.256755	3.689508	-1.597304
H	-2.157429	4.016704	-0.316879
H	-4.297196	5.105722	-1.006793
C	-0.721795	0.158801	2.893496
C	-0.598207	1.440838	2.355427
C	-1.486119	-0.038600	4.050802
C	-1.257281	2.512226	2.951303
H	0.003841	1.622514	1.466241
C	-2.131931	1.036222	4.648227
H	-1.574068	-1.032582	4.493655
C	-2.024786	2.311132	4.092233
H	-1.159975	3.500753	2.505582
H	-2.724109	0.879295	5.548331
H	-2.542380	3.148805	4.557089
C	1.236003	-1.998849	3.161947
C	1.718436	-1.296270	4.267735
C	1.800625	-3.238039	2.840519
C	2.727961	-1.840500	5.055951
H	1.311123	-0.313911	4.502826
C	2.807005	-3.780758	3.629550
H	1.461507	-3.781399	1.955882
C	3.270432	-3.082028	4.741809
H	3.094800	-1.285583	5.917566
H	3.234916	-4.748592	3.373599
H	4.060419	-3.504891	5.359961
C	1.061156	-3.113146	-2.077006
C	1.510354	-4.211046	-1.333995
C	1.500955	-2.958885	-3.392359
C	2.370701	-5.143715	-1.898134
H	1.194257	-4.334422	-0.295439
C	2.369715	-3.890024	-3.953939
H	1.178753	-2.097803	-3.976882
C	2.802332	-4.983574	-3.212806
H	2.707532	-5.996120	-1.310420
H	2.711823	-3.754254	-4.978636
H	3.480528	-5.711008	-3.655663
C	-0.695170	-0.832538	-2.574727
C	-0.621675	0.555271	-2.472471
C	-1.394883	-1.413779	-3.641185
C	-1.244881	1.369311	-3.416379
H	-0.098061	1.024093	-1.638337
C	-2.006389	-0.602866	-4.586342
H	-1.461838	-2.498896	-3.734782
C	-1.936380	0.786698	-4.471060
H	-1.185422	2.452478	-3.299991
H	-2.550848	-1.055349	-5.413576
H	-2.429898	1.414938	-5.210723
C	4.490901	-1.833793	-1.874209
C	4.535229	-1.092616	-3.055836
C	3.666548	-0.020893	-3.248057
C	2.744493	0.317916	-2.261723
C	2.700268	-0.403649	-1.060904
C	3.589829	-1.478655	-0.881645
H	5.166118	-2.676107	-1.727653
H	5.262822	-1.345487	-3.826405
H	3.716196	0.567357	-4.163191
H	2.113069	1.197630	-2.393082
H	3.597139	-2.017801	0.071484
O	0.242335	2.597571	-0.359069
S	0.844781	3.736624	-1.097457
O	-0.070530	4.433357	-1.999624
O	2.194510	3.454511	-1.609850
C	1.138920	4.909344	0.280253
F	-0.022771	5.278997	0.827365
F	1.772495	5.997724	-0.130933
F	1.871301	4.319190	1.224311
O	2.205611	0.331865	1.418185
C	2.881312	0.920386	0.479215
C	4.347472	1.036085	0.612793
C	5.019119	1.947922	-0.203780
C	5.046755	0.283991	1.559185
C	6.396515	2.090597	-0.085706

C	6.421792	0.433008	1.673440
C	7.097589	1.330977	0.847247
H	4.444257	2.544887	-0.914203
H	6.924360	2.802187	-0.718208
H	8.176815	1.445289	0.939573
H	6.973114	-0.146712	2.412453
H	4.492895	-0.404204	2.199671
H	2.400052	1.744160	-0.066493

12(M06 OPT)

M06/BS1 SCF energy: -4317.583893 a.u.

M06/BS2 SCF energy in PhMe: -4318.47252347 a.u.

M06/BS2 Free energy in PhMe: -4317.64504147 a.u.

C	-2.118167	-2.382284	0.989536
C	-3.275536	-3.265360	1.464490
H	-4.030201	-3.398675	0.677181
H	-2.914107	-4.263116	1.753283
H	-3.777600	-2.816454	2.333461
C	-1.065857	-2.412259	2.118100
H	-0.623539	-3.420279	2.173889
H	-1.562652	-2.240916	3.085135
C	-1.538434	-3.022184	-0.281048
H	-2.341727	-3.143941	-1.023610
H	-1.182746	-4.035329	-0.037527
C	-2.596246	-0.942953	0.737122
H	-1.788766	-0.365007	0.262668
H	-2.803888	-0.448392	1.698886
P	0.321435	-1.205705	1.994123
P	-4.092203	-0.768758	-0.383140
P	-0.144687	-2.151344	-1.166045
Ni	1.298985	-0.988358	0.081046
C	-5.413394	-0.602156	0.904500
C	-6.473443	-1.510759	0.892683
C	-5.394041	0.396522	1.884701
C	-7.486933	-1.437444	1.845495
H	-6.502708	-2.285569	0.124512
C	-6.403406	0.473052	2.836353
H	-4.586670	1.132123	1.892596
C	-7.450874	-0.446355	2.819690
H	-8.307238	-2.153491	1.823594
H	-6.377842	1.257137	3.591930
H	-8.242800	-0.382947	3.564534
C	-3.924306	0.982631	-0.926537
C	-4.765857	1.372834	-1.975671
C	-3.010571	1.913645	-0.423921
C	-4.697751	2.656870	-2.503807
H	-5.469697	0.650138	-2.394182
C	-2.922986	3.192503	-0.967112
H	-2.321289	1.653482	0.379429
C	-3.766094	3.566210	-2.007656
H	-5.357675	2.941404	-3.322703
H	-2.165917	3.882037	-0.596512
H	-3.678141	4.560041	-2.443379
C	-0.328535	0.331458	2.713419
C	-0.212337	1.535257	2.018963
C	-1.030592	0.292106	3.925685
C	-0.830000	2.682630	2.509865
H	0.339021	1.598177	1.082534
C	-1.634815	1.442341	4.416395
H	-1.105576	-0.635101	4.496357
C	-1.545918	2.635726	3.700434
H	-0.747326	3.605216	1.937668
H	-2.180656	1.406509	5.357703
H	-2.032484	3.532833	4.079814
C	1.595295	-1.841132	3.128299
C	2.193343	-1.002881	4.071314
C	2.087596	-3.138168	2.951157
C	3.254454	-1.467318	4.841666
H	1.838610	0.019700	4.189769
C	3.148934	-3.598576	3.720180
H	1.649784	-3.793632	2.195997
C	3.733584	-2.761539	4.667569
H	3.716094	-0.806597	5.572985
H	3.525350	-4.609892	3.576372
H	4.568799	-3.118745	5.267380
C	0.596869	-3.569749	-2.059131
C	1.192452	-4.577814	-1.291687
C	0.658103	-3.654802	-3.450217
C	1.824007	-5.654736	-1.899514
H	1.175407	-4.512821	-0.201152
C	1.290052	-4.735972	-4.060183
H	0.225493	-2.866076	-4.064404
C	1.873956	-5.734721	-3.289720
H	2.282355	-6.430967	-1.289145
H	1.329091	-4.791871	-5.146887

H	2.369755	-6.576242	-3.770394
C	-0.979210	-1.112228	-2.403590
C	-0.710477	0.256817	-2.401717
C	-1.900180	-1.632000	-3.324899
C	-1.321095	1.103975	-3.322531
H	-0.040284	0.699304	-1.664952
C	-2.502956	-0.788763	-4.248685
H	-2.147001	-2.694922	-3.325375
C	-2.207238	0.575656	-4.252702
H	-1.115118	2.174093	-3.274872
H	-3.215266	-1.195687	-4.964737
H	-2.692002	1.232440	-4.973464
C	3.602583	-2.253802	-2.119376
C	3.228046	-1.765347	-3.365188
C	2.692361	-0.482188	-3.489370
C	2.565238	0.335256	-2.375268
C	2.965791	-0.131542	-1.110618
C	3.468596	-1.446531	-0.990483
H	4.009439	-3.259593	-2.024239
H	3.342577	-2.393944	-4.247354
H	2.383663	-0.110021	-4.465179
H	2.200617	1.361221	-2.461640
H	3.828694	-1.792959	-0.020048
O	0.234195	2.616110	-0.778524
S	0.838306	3.754048	-1.511921
O	-0.071195	4.439421	-2.430402
O	2.199750	3.489775	-2.003585
C	1.106362	4.948154	-0.146949
F	-0.069237	5.324223	0.374704
F	1.740571	6.034276	-0.561511
F	1.819924	4.379338	0.824068
O	2.349601	0.069702	1.128934
C	2.993926	0.788611	0.116010
C	4.401155	1.171404	0.499669
C	5.008973	2.231391	-0.174948
C	5.103574	0.478595	1.483923
C	6.322123	2.579485	0.118574
C	6.415538	0.836939	1.780964
C	7.028885	1.881503	1.095557
H	4.431260	2.785726	-0.918814
H	6.793575	3.407674	-0.408776
H	8.055739	2.159354	1.330052
H	6.961261	0.300027	2.556569
H	4.603765	-0.326606	2.025864
H	2.440541	1.706874	-0.148889

2 (opt with the solvent correction)

B3LYP/BS1 SCF energy in PhMe: -3092.936076 a.u.

M06/BS2 SCF energy in PhMe: -3091.96646985 a.u.

M06/BS2 Free energy in PhMe: -3091.04841885 a.u.

C	1.220993	0.373160	-1.874094
C	2.125756	0.614446	-3.106217
H	2.804391	-0.228022	-3.280480
H	1.520842	0.740593	-4.012661
H	2.734184	1.517315	-2.981069
C	0.242990	1.588487	-1.845453
H	-0.372432	1.545029	-2.753295
H	0.830342	2.511164	-1.929614
C	0.481212	-0.970835	-2.132934
H	1.225475	-1.763804	-2.268942
H	-0.041074	-0.881239	-3.092999
C	2.071102	0.343672	-0.572630
H	1.441137	0.006601	0.256727
H	2.389279	1.363087	-0.330014
P	-0.998415	1.775446	-0.445095
P	3.582025	-0.786544	-0.581713
P	-0.829230	-1.581054	-0.916901
Ni	-2.128946	-0.048688	-0.041773
C	4.937458	0.374095	-1.121253
C	5.735985	-0.003683	-2.211101
C	5.217935	1.590507	-0.476891
C	6.779125	0.814371	-2.655058
H	5.539677	-0.946143	-2.717198
C	6.258509	2.408900	-0.916708
H	4.629061	1.896572	0.384079
C	7.041422	2.022950	-2.009100
H	7.386067	0.505377	-3.502357
H	6.463076	3.345466	-0.403599
H	7.853404	2.660156	-2.350071
C	3.974874	-0.918987	1.228689
C	4.929254	-1.886261	1.591151
C	3.396319	-0.144975	2.246804
C	5.306769	-2.062989	2.922252
H	5.379688	-2.509038	0.821150
C	3.765031	-0.329149	3.582410

H	2.653683	0.610438	2.012750
C	4.722474	-1.284622	3.924659
H	6.050388	-2.813850	3.177652
H	3.302239	0.281856	4.353560
H	5.009039	-1.424881	4.963825
C	-0.033177	2.610723	0.902788
C	-0.229471	2.171910	2.221053
C	0.874199	3.660949	0.676166
C	0.459783	2.761540	3.285119
H	-0.930184	1.363604	2.410143
C	1.566202	4.248845	1.736220
H	1.037734	4.035286	-0.330710
C	1.360982	3.799606	3.044312
H	0.289915	2.409449	4.299385
H	2.262740	5.060430	1.541572
H	1.898745	4.259604	3.869208
C	-2.023440	3.161248	-1.146114
C	-2.171085	4.414632	-0.532868
C	-2.773070	2.899442	-2.308436
C	-3.024938	5.380711	-1.073962
H	-1.621093	4.646321	0.373235
C	-3.616920	3.866106	-2.854009
H	-2.708622	1.923998	-2.785474
C	-3.745413	5.114151	-2.238050
H	-3.122717	6.344637	-0.580565
H	-4.181353	3.641075	-3.755532
H	-4.406935	5.866793	-2.658823
C	-1.707009	-2.801116	-2.014946
C	-2.332802	-2.321122	-3.180468
C	-1.879638	-4.153627	-1.682524
C	-3.078660	-3.168290	-3.999263
H	-2.247892	-1.270545	-3.448574
C	-2.633237	-5.001875	-2.499084
H	-1.425036	-4.555081	-0.782863
C	-3.230423	-4.515909	-3.662221
H	-3.546603	-2.773388	-4.897682
H	-2.749499	-6.046671	-2.221606
H	-3.813393	-5.177230	-4.297779
C	0.118848	-2.665997	0.247781
C	-0.109304	-2.514825	1.624422
C	1.038742	-3.640423	-0.176510
C	0.558504	-3.315185	2.554843
H	-0.815775	-1.761577	1.963159
C	1.702900	-4.443693	0.751267
H	1.232362	-3.783871	-1.235790
C	1.464390	-4.282244	2.118979
H	0.370881	-3.180772	3.616868
H	2.410265	-5.193207	0.406084
H	1.986673	-4.905613	2.839894
C	-6.191622	0.119517	2.873327
C	-5.798543	-1.155327	2.996953
C	-3.905880	0.504769	0.664513
C	-4.413392	-1.744320	2.857862
C	-3.891402	-0.895338	0.411591
C	-4.009862	-2.063188	1.398490
H	-3.658494	-1.105841	3.325098
H	-4.387912	-2.690527	3.415001
H	-3.079578	-2.645239	1.434827
H	-4.765462	-2.755224	0.998117
C	-5.393978	1.366666	2.580685
H	-5.345443	1.976164	3.499384
H	-5.979591	1.973553	1.873209
C	-3.966821	1.212394	2.010216
H	-3.566671	2.227387	1.881444
H	-3.319278	0.735056	2.751270
H	-7.258217	0.312028	3.008106
H	-6.584124	-1.886968	3.194591
H	-4.345708	1.114993	-0.131337
H	-4.283463	-1.168658	-0.571944

4 (opt with the solvent correction)

B3LYP/BS1 SCF energy in PhMe: -3973.982587 a.u.

M06/BS2 SCF energy in PhMe: -3973.02750779 a.u.

M06/BS2 Free energy in PhMe: -3972.31802179 a.u.

C	1.789627	0.325521	1.940403
C	2.773984	0.505948	3.120329
H	3.495750	1.305850	2.924267
H	2.236326	0.765700	4.040342
H	3.336703	-0.415150	3.307099
C	0.755717	-0.730077	2.423347
H	0.241860	-0.321630	3.301248
H	1.289700	-1.621057	2.772380
C	1.114396	1.705544	1.726790
H	1.882286	2.440842	1.460950
H	0.711250	2.026917	2.692796

C	2.543200	-0.190473	0.683037
H	1.869369	-0.174878	-0.179898
H	2.821440	-1.237826	0.844942
P	-0.586831	-1.279481	1.251132
P	4.066958	0.795337	0.161583
P	-0.288845	1.974728	0.498582
Ni	-1.752633	0.379391	0.140583
C	5.440770	-0.062019	1.081873
C	6.298906	0.728802	1.860870
C	5.681414	-1.444330	1.014555
C	7.361956	0.155937	2.564880
H	6.133716	1.802272	1.916816
C	6.740684	-2.019398	1.717086
H	5.047478	-2.076508	0.397976
C	7.583100	-1.219871	2.495693
H	8.015971	0.784821	3.163573
H	6.914140	-3.090727	1.652462
H	8.409814	-1.668704	3.040227
C	4.359285	0.149516	-1.553465
C	5.258075	0.878962	-2.351399
C	3.760806	-0.995529	-2.102864
C	5.561867	0.469996	-3.649961
H	5.722430	1.777682	-1.951442
C	4.055473	-1.399356	-3.407849
H	3.058704	-1.584775	-1.521931
C	4.958473	-0.671243	-4.183874
H	6.263500	1.046747	-4.247318
H	3.577893	-2.287359	-3.814437
H	5.187844	-0.987247	-5.198219
C	0.174748	-2.663058	0.304703
C	0.084948	-2.676499	-1.094474
C	0.851447	-3.710600	0.955676
C	0.672060	-3.711227	-1.829626
H	-0.463899	-1.899067	-1.615561
C	1.437160	-4.739716	0.219697
H	0.912000	-3.735064	2.040373
C	1.351144	-4.739749	-1.176295
H	0.583785	-3.713179	-2.912546
H	1.955250	-5.544119	0.735006
H	1.805153	-5.544332	-1.748670
C	-1.784934	-2.093234	2.397498
C	-2.348764	-3.342079	2.095007
C	-2.231750	-1.411172	3.542254
C	-3.312751	-3.905401	2.933269
H	-2.049930	-3.871907	1.197560
C	-3.193977	-1.977192	4.378708
H	-1.840831	-0.427229	3.787440
C	-3.734395	-3.229178	4.078710
H	-3.738435	-4.873246	2.682798
H	-3.523457	-1.436028	5.261631
H	-4.485322	-3.669480	4.728954
C	-0.949259	3.569226	1.161545
C	-1.358850	3.626272	2.504385
C	-1.123280	4.703180	0.356214
C	-1.901059	4.795981	3.035543
H	-1.273993	2.751317	3.143731
C	-1.666937	5.873594	0.889916
H	-0.848136	4.675560	-0.691880
C	-2.051617	5.926319	2.229733
H	-2.210696	4.820748	4.076910
H	-1.794265	6.742818	0.250443
H	-2.474607	6.838324	2.642077
C	0.566928	2.381786	-1.079592
C	0.301615	1.613888	-2.224302
C	1.502112	3.427884	-1.163836
C	0.950276	1.890846	-3.429902
H	-0.419649	0.802277	-2.180216
C	2.142361	3.706837	-2.371148
H	1.726174	4.036142	-0.292325
C	1.865476	2.940641	-3.506523
H	0.733016	1.286842	-4.306184
H	2.859712	4.521277	-2.422864
H	2.368302	3.157781	-4.444861
C	-5.006285	2.948039	0.185610
C	-5.072343	3.539361	-1.078769
C	-4.099333	3.229092	-2.028201
C	-3.062203	2.340746	-1.716307
C	-2.977532	1.742918	-0.451096
C	-3.969301	2.063327	0.492933
H	-5.764004	3.172237	0.933863
H	-5.878300	4.227891	-1.321499
H	-4.145432	3.671330	-3.021466
H	-2.331294	2.112282	-2.486293
H	-3.947179	1.612537	1.484413
O	-3.026082	-1.043640	-0.362592
S	-3.522491	-1.288554	-1.785672

O	-2.447447	-1.173375	-2.790808
O	-4.823581	-0.691468	-2.096055
C	-3.882077	-3.112423	-1.659285
F	-2.767675	-3.813042	-1.384343
F	-4.374862	-3.551898	-2.825263
F	-4.779363	-3.354583	-0.696067

TS4 (opt with the solvent correction)

B3LYP/BS1 SCF energy in PhMe: -4319.555483 a.u.

M06/BS2 SCF energy in PhMe: -4318.45781596 a.u.

M06/BS2 Free energy in PhMe: -4317.64663696 a.u.

C	-2.113119	0.045453	-2.042634
C	-2.882768	0.055833	-3.386872
H	-3.674982	0.811861	-3.390532
H	-2.207358	0.282694	-4.220781
H	-3.345406	-0.917659	-3.583021
C	-0.948970	-0.963727	-2.258024
H	-0.339784	-0.575932	-3.084600
H	-1.367411	-1.918390	-2.597519
C	-1.577858	1.486185	-1.846360
H	-2.428053	2.171631	-1.754662
H	-1.063460	1.767408	-2.770883
C	-3.055240	-0.414161	-0.894299
H	-2.562124	-0.259408	0.069282
H	-3.231453	-1.490928	-0.987687
P	0.271736	-1.294787	-0.892226
P	-4.711001	0.488904	-0.788181
P	-0.368798	1.975395	-0.486353
Ni	1.352372	0.660603	-0.129325
C	-5.832881	-0.598272	-1.803477
C	-6.588807	0.004369	-2.820109
C	-5.985221	-1.977606	-1.584295
C	-7.464534	-0.749398	-3.606882
H	-6.491476	1.072862	-2.997770
C	-6.857329	-2.732944	-2.368788
H	-5.430390	-2.465104	-0.786474
C	-7.598107	-2.120209	-3.384150
H	-8.041144	-0.264397	-4.390479
H	-6.964386	-3.799037	-2.184261
H	-8.278988	-2.708947	-3.993457
C	-5.291364	0.052062	0.919052
C	-6.401850	0.769213	1.399210
C	-4.714839	-0.917683	1.753641
C	-6.929752	0.515507	2.664902
H	-6.856365	1.535191	0.774486
C	-5.234995	-1.163176	3.027513
H	-3.854819	-1.490821	1.423951
C	-6.344309	-0.451632	3.485905
H	-7.791644	1.079106	3.013171
H	-4.769056	-1.915338	3.659097
H	-6.747756	-0.645343	4.476393
C	-0.626760	-2.424962	0.265617
C	-0.691817	-2.150391	1.637144
C	-1.234723	-3.596329	-0.222739
C	-1.365681	-3.019580	2.502201
H	-0.195243	-1.276902	2.039643
C	-1.909098	-4.458886	0.639427
H	-1.169827	-3.847948	-1.278161
C	-1.978176	-4.170065	2.006653
H	-1.393739	-2.796665	3.565179
H	-2.371782	-5.360747	0.246981
H	-2.496583	-4.847229	2.680424
C	1.440773	-2.487954	-1.692960
C	2.314478	-3.204522	-0.855661
C	1.518269	-2.693979	-3.078159
C	3.235258	-4.102946	-1.391660
H	2.280405	-3.054700	0.217638
C	2.442013	-3.598001	-3.612325
H	0.861430	-2.163799	-3.759432
C	3.302926	-4.303969	-2.772951
H	3.902228	-4.644149	-0.725856
H	2.481285	-3.749068	-4.688164
H	4.020648	-5.005600	-3.189584
C	-0.000517	3.688691	-1.095635
C	0.451295	3.871056	-2.413812
C	-0.106071	4.812332	-0.263804
C	0.758744	5.143467	-2.894985
H	0.586811	3.018227	-3.073502
C	0.207678	6.085174	-0.744967
H	-0.422081	4.700986	0.767189
C	0.634397	6.257025	-2.061803
H	1.102639	5.261190	-3.919296
H	0.120187	6.942091	-0.082473
H	0.876134	7.248894	-2.434139
C	-1.412375	2.233900	1.011453

C	-1.047750	1.622793	2.219930
C	-2.562570	3.042916	0.978721
C	-1.812245	1.817156	3.373067
H	-0.160908	1.000515	2.271156
C	-3.321776	3.237709	2.132227
H	-2.863288	3.535730	0.059061
C	-2.948029	2.625009	3.331781
H	-1.508965	1.338751	4.299985
H	-4.207840	3.865193	2.092247
H	-3.542975	2.776767	4.228225
C	3.911581	4.011324	-0.042957
C	3.909290	4.419005	1.293435
C	3.100387	3.744321	2.207066
C	2.299693	2.672997	1.790462
C	2.293407	2.243436	0.454159
C	3.108607	2.943415	-0.453531
H	4.534094	4.528073	-0.771079
H	4.530734	5.251054	1.616184
H	3.093179	4.039253	3.254360
H	1.701555	2.163353	2.537971
H	3.123423	2.658661	-1.502588
O	2.211327	-0.719966	1.415494
S	2.736472	-0.630341	2.822967
O	1.726816	-0.178149	3.801380
O	4.092601	-0.064319	2.930012
C	2.988846	-2.430918	3.229403
F	1.833780	-3.114298	3.172598
F	3.496732	-2.565568	4.462382
F	3.845429	-2.997298	2.357322
O	3.121884	0.039928	-1.242737
C	4.229538	-0.079780	-0.711965
C	5.459601	-0.388439	-1.448912
C	6.661647	-0.474236	-0.727146
C	5.461081	-0.585886	-2.841056
C	7.855539	-0.752804	-1.390161
C	6.653964	-0.864483	-3.498290
C	7.850525	-0.946317	-2.773847
H	6.649190	-0.321397	0.349251
H	8.785574	-0.818233	-0.832892
H	8.780899	-1.162428	-3.292641
H	6.659790	-1.018828	-4.573780
H	4.524493	-0.522111	-3.385705
H	4.331045	0.049465	0.374165

11 (opt with the solvent correction)

B3LYP/BS1 SCF energy in PhMe: -4319.567720 a.u.

M06/BS2 SCF energy in PhMe: -4318.45893824 a.u.

M06/BS2 Free energy in PhMe: -4317.64986924 a.u.

C	2.350376	1.977085	1.218010
C	3.532235	2.768088	1.827270
H	4.315820	2.954117	1.085278
H	3.195823	3.742435	2.202872
H	3.982354	2.222259	2.663739
C	1.272967	1.924377	2.335871
H	0.932143	2.947263	2.536393
H	1.734444	1.569286	3.264126
C	1.844736	2.811525	0.012491
H	2.654296	2.909592	-0.719421
H	1.639360	3.823583	0.375161
C	2.794608	0.541709	0.818125
H	2.001814	0.069319	0.228924
H	2.916372	-0.062235	1.723715
P	-0.269543	0.919776	2.041966
P	4.374888	0.434454	-0.212823
P	0.333842	2.305697	-0.993996
Ni	-1.319043	1.227724	-0.000533
C	5.659058	0.133963	1.103419
C	6.754480	1.007759	1.169843
C	5.598309	-0.934037	2.014136
C	7.756385	0.832054	2.128849
H	6.824243	1.832356	0.464404
C	6.596608	-1.112319	2.972226
H	4.774042	-1.641406	1.966436
C	7.677822	-0.227724	3.032903
H	8.596837	1.520572	2.165843
H	6.535317	-1.945612	3.667846
H	8.456208	-0.368776	3.778368
C	4.250863	-1.254511	-0.965995
C	5.203354	-1.557396	-1.955804
C	3.281163	-2.221450	-0.658036
C	5.196951	-2.791544	-2.604751
H	5.953392	-0.816286	-2.224008
C	3.259180	-3.449949	-1.324744
H	2.524328	-2.029239	0.095481
C	4.218508	-3.739800	-2.295283

H	5.945270	-3.005959	-3.363729
H	2.477286	-4.167925	-1.095369
H	4.197757	-4.694273	-2.814551
C	0.139833	-0.762913	2.659746
C	-0.147785	-1.882706	1.865751
C	0.746023	-0.950247	3.915878
C	0.169355	-3.167334	2.319644
H	-0.604996	-1.772604	0.887481
C	1.062138	-2.232223	4.363049
H	0.962882	-0.097779	4.553941
C	0.774001	-3.343177	3.564066
H	-0.059557	-4.022438	1.692323
H	1.530955	-2.363860	5.334649
H	1.021399	-4.342195	3.912981
C	-1.419919	1.634137	3.303260
C	-2.043801	0.856165	4.289350
C	-1.744654	2.999770	3.218427
C	-2.949622	1.435784	5.182157
H	-1.826929	-0.203646	4.368223
C	-2.647206	3.576785	4.111251
H	-1.299239	3.620952	2.445096
C	-3.251573	2.795395	5.099076
H	-3.418097	0.818062	5.943751
H	-2.881567	4.634989	4.031716
H	-3.955403	3.243342	5.795149
C	-0.125331	3.945418	-1.715651
C	-0.311976	5.048499	-0.865785
C	-0.377362	4.102893	-3.086477
C	-0.717866	6.282093	-1.375481
H	-0.151669	4.955270	0.205264
C	-0.781955	5.338603	-3.594798
H	-0.267438	3.261441	-3.761135
C	-0.949782	6.431754	-2.743977
H	-0.853510	7.123861	-0.701629
H	-0.970563	5.441039	-4.659886
H	-1.265025	7.392220	-3.142462
C	1.036385	1.318801	-2.373454
C	0.614290	-0.003891	-2.566803
C	2.012515	1.859680	-3.230583
C	1.138885	-0.770919	-3.610954
H	-0.119253	-0.458959	-1.908550
C	2.533068	1.092897	-4.271644
H	2.360204	2.880319	-3.096772
C	2.092989	-0.220474	-4.465965
H	0.789695	-1.791425	-3.739567
H	3.283625	1.521222	-4.930654
H	2.501207	-0.814299	-5.279354
C	-4.295321	3.245983	-2.082993
C	-4.521124	2.504426	-3.245759
C	-3.723265	1.391190	-3.511990
C	-2.703983	1.019937	-2.624233
C	-2.462127	1.756129	-1.454822
C	-3.275445	2.875123	-1.201766
H	-4.911093	4.115283	-1.860572
H	-5.311356	2.791959	-3.935134
H	-3.890147	0.801397	-4.410830
H	-2.107342	0.143578	-2.859985
H	-3.119493	3.473398	-0.305430
O	-1.176774	-2.388732	-1.179855
S	-1.661479	-3.480516	-2.072854
O	-0.896191	-3.645742	-3.323706
O	-3.135269	-3.550259	-2.195723
C	-1.245979	-5.006401	-1.094451
F	0.077678	-5.086329	-0.841935
F	-1.608471	-6.118608	-1.749004
F	-1.880071	-4.998559	0.096091
O	-2.850101	0.235360	0.734113
C	-3.448460	-0.735870	0.231379
C	-4.628154	-1.329751	0.842796
C	-5.184337	-2.470921	0.234313
C	-5.215401	-0.783830	2.001485
C	-6.321188	-3.059097	0.786074
C	-6.350377	-1.375168	2.539993
C	-6.902257	-2.512184	1.932703
H	-4.710427	-2.888988	-0.651460
H	-6.753098	-3.941805	0.323644
H	-7.790749	-2.970843	2.359108
H	-6.812000	-0.956667	3.429978
H	-4.775408	0.097282	2.457401
H	-3.084230	-1.182746	-0.698470

TS5 (opt with the solvent correction)

B3LYP/BS1 SCF energy in PhMe: -4319.536630 a.u.

M06/BS2 SCF energy in PhMe: -4318.43174683 a.u.

M06/BS2 Free energy in PhMe: -4317.62100083 a.u.

C	-2.278461	-2.266211	0.499698
C	-3.423797	-3.292891	0.670518
H	-4.065191	-3.333477	-0.215315
H	-3.020717	-4.300463	0.832169
H	-4.055648	-3.040992	1.528909
C	-1.388754	-2.434460	1.762721
H	-0.999422	-3.458543	1.771734
H	-2.010577	-2.337109	2.659643
C	-1.506626	-2.701935	-0.774259
H	-2.190421	-2.669351	-1.628682
H	-1.226230	-3.752773	-0.647285
C	-2.842063	-0.818724	0.432636
H	-2.028903	-0.121978	0.202779
H	-3.211190	-0.534658	1.424370
P	0.068952	-1.297483	1.978788
P	-4.185081	-0.464141	-0.853894
P	0.053874	-1.816673	-1.356671
Ni	1.335932	-0.775687	0.184495
C	-5.736273	-1.004744	0.014618
C	-6.634649	-1.811411	-0.700375
C	-6.062271	-0.647867	1.334849
C	-7.820551	-2.262602	-0.113244
H	-6.401998	-2.089835	-1.725580
C	-7.242921	-1.100262	1.924835
H	-5.398445	-0.001218	1.902923
C	-8.123931	-1.911256	1.202322
H	-8.503751	-2.886380	-0.683968
H	-7.480097	-0.815521	2.946923
H	-9.043903	-2.261897	1.662920
C	-4.317669	1.385573	-0.712963
C	-5.575704	2.014199	-0.711020
C	-3.173374	2.200735	-0.757024
C	-5.681274	3.406216	-0.730278
H	-6.482440	1.417526	-0.690034
C	-3.277721	3.593041	-0.772722
H	-2.180900	1.766034	-0.792924
C	-4.534019	4.201437	-0.756397
H	-6.666044	3.867521	-0.723663
H	-2.371833	4.191235	-0.807575
H	-4.617297	5.285066	-0.771347
C	-0.589662	0.144334	2.905915
C	-0.422703	1.442048	2.402678
C	-1.290782	-0.044269	4.111028
C	-0.961184	2.534291	3.088941
H	0.120597	1.614695	1.479930
C	-1.822433	1.049209	4.792695
H	-1.414109	-1.041308	4.526325
C	-1.660090	2.340228	4.279859
H	-0.829768	3.531137	2.680351
H	-2.361674	0.893870	5.723465
H	-2.078654	3.191352	4.810462
C	1.141007	-2.197715	3.181328
C	1.782296	-1.500681	4.218101
C	1.418976	-3.565323	3.016312
C	2.662563	-2.160812	5.077342
H	1.597224	-0.441346	4.356153
C	2.297405	-4.222914	3.878254
H	0.955821	-4.132735	2.214006
C	2.921090	-3.522583	4.912811
H	3.146461	-1.605178	5.875928
H	2.493288	-5.282821	3.739495
H	3.604745	-4.034903	5.584241
C	0.967660	-3.223164	-2.139046
C	1.238840	-4.369595	-1.371895
C	1.460709	-3.160358	-3.449860
C	1.960919	-5.434635	-1.909059
H	0.889200	-4.436316	-0.344962
C	2.180935	-4.229935	-3.987694
H	1.286715	-2.279892	-4.057442
C	2.429957	-5.369749	-3.223317
H	2.155682	-6.314560	-1.301660
H	2.547907	-4.165791	-5.008437
H	2.988214	-6.200781	-3.645682
C	-0.561515	-0.784955	-2.747399
C	-0.425885	0.608049	-2.698101
C	-1.222279	-1.372230	-3.842832
C	-0.930071	1.405379	-3.730920
H	0.058578	1.091496	-1.855679
C	-1.716228	-0.575431	-4.873617
H	-1.345965	-2.450260	-3.899003
C	-1.568908	0.814675	-4.819937
H	-0.820280	2.483974	-3.662387
H	-2.221142	-1.039651	-5.716628
H	-1.959831	1.433294	-5.623405
C	4.630066	-1.901690	-2.053511
C	4.637629	-1.124605	-3.217145

C	3.795982	-0.012931	-3.324468
C	2.938658	0.317898	-2.274589
C	2.905349	-0.457455	-1.098684
C	3.784370	-1.558103	-1.000784
H	5.296719	-2.755453	-1.962674
H	5.313915	-1.373367	-4.031206
H	3.819360	0.605896	-4.217870
H	2.331060	1.214097	-2.347032
H	3.827413	-2.133991	-0.077956
O	0.707880	2.655045	-0.477468
S	1.082369	3.957298	-1.106289
O	0.085754	4.485840	-2.061663
O	2.499093	4.039105	-1.522012
C	0.966704	5.127456	0.334375
F	-0.295945	5.170805	0.813703
F	1.314644	6.373113	-0.019474
F	1.769851	4.736614	1.339095
O	2.420443	0.150184	1.406309
C	3.122417	0.802476	0.518319
C	4.586761	0.953017	0.715608
C	5.260650	1.953074	-0.001742
C	5.287513	0.165719	1.641584
C	6.626893	2.151007	0.193793
C	6.651656	0.369737	1.835974
C	7.324582	1.357848	1.108703
H	4.704873	2.578509	-0.696406
H	7.144766	2.928349	-0.361366
H	8.389255	1.514386	1.262243
H	7.192787	-0.237236	2.557365
H	4.752352	-0.589095	2.209453
H	2.638286	1.644270	0.016933

12 (opt with the solvent correction)

B3LYP/BS1 SCF energy in PhMe: -4319.566060 a.u.

M06/BS2 SCF energy in PhMe: -4318.45661234 a.u.

M06/BS2 Free energy in PhMe: -4317.64419534 a.u.

C	-2.371984	-2.243279	0.516682
C	-3.551063	-3.204345	0.801091
H	-4.290599	-3.179819	-0.005141
H	-3.196868	-4.238569	0.892612
H	-4.063162	-2.938905	1.731982
C	-1.346518	-2.515207	1.652035
H	-1.035378	-3.563094	1.579373
H	-1.848569	-2.413893	2.621215
C	-1.793538	-2.675491	-0.855941
H	-2.566893	-2.555693	-1.621989
H	-1.574425	-3.747999	-0.808362
C	-2.843788	-0.763197	0.548589
H	-2.027721	-0.118288	0.208562
H	-3.050076	-0.472052	1.584437
P	0.220722	-1.519241	1.768787
P	-4.338186	-0.326660	-0.529202
P	-0.240235	-1.888097	-1.552373
Ni	1.346783	-1.178455	-0.086398
C	-5.767026	-0.719827	0.593524
C	-6.797839	-1.525257	0.086266
C	-5.875996	-0.243806	1.911805
C	-7.903115	-1.859480	0.874612
H	-6.735240	-1.892543	-0.935463
C	-6.976127	-0.578502	2.701775
H	-5.105609	0.405190	2.320302
C	-7.991644	-1.389632	2.185174
H	-8.692138	-2.483776	0.463238
H	-7.045463	-0.201558	3.719142
H	-8.849569	-1.647103	2.800889
C	-4.333481	1.530002	-0.440446
C	-5.562867	2.214476	-0.479567
C	-3.154171	2.291548	-0.470319
C	-5.607464	3.607864	-0.525139
H	-6.495474	1.657354	-0.467186
C	-3.198287	3.687477	-0.511473
H	-2.180281	1.815883	-0.471381
C	-4.424871	4.351295	-0.535759
H	-6.570570	4.112100	-0.549101
H	-2.267688	4.247192	-0.520545
H	-4.459149	5.437125	-0.567523
C	-0.220738	0.004182	2.684434
C	0.090136	1.266601	2.163213
C	-0.887509	-0.090130	3.919872
C	-0.269168	2.421181	2.863489
H	0.609809	1.372179	1.218240
C	-1.238151	1.065291	4.616173
H	-1.119682	-1.059913	4.351709
C	-0.931176	2.322716	4.086883
H	-0.021819	3.390539	2.443949

H	-1.747973	0.982962	5.572354
H	-1.206109	3.222215	4.631013
C	1.260597	-2.517905	2.910729
C	2.028569	-1.881196	3.898265
C	1.365037	-3.911255	2.761318
C	2.863526	-2.626895	4.731200
H	1.981327	-0.804677	4.012288
C	2.201465	-4.652921	3.595954
H	0.799381	-4.433272	1.994968
C	2.951247	-4.012236	4.584674
H	3.450643	-2.119113	5.491189
H	2.265939	-5.730531	3.471878
H	3.602424	-4.589953	5.234965
C	0.370081	-3.272113	-2.617837
C	0.802863	-4.450941	-1.984752
C	0.454986	-3.185540	-4.013916
C	1.291352	-5.522779	-2.731177
H	0.766828	-4.535290	-0.900924
C	0.942793	-4.261767	-4.760364
H	0.148207	-2.279924	-4.525014
C	1.360241	-5.431141	-4.124129
H	1.620940	-6.426242	-2.225317
H	0.996956	-4.180113	-5.842559
H	1.739862	-6.265351	-4.707581
C	-0.824858	-0.565520	-2.675625
C	-0.281790	0.722779	-2.560780
C	-1.822154	-0.806771	-3.640227
C	-0.718534	1.754200	-3.397860
H	0.466999	0.952289	-1.809325
C	-2.248785	0.221085	-4.478922
H	-2.264483	-1.793830	-3.742964
C	-1.696158	1.500694	-4.359237
H	-0.297816	2.748280	-3.271928
H	-3.019027	0.025042	-5.219922
H	-2.039194	2.301455	-5.008832
C	3.474228	-1.843060	-2.802436
C	3.504379	-0.887860	-3.810962
C	3.468587	0.476317	-3.481008
C	3.401753	0.882479	-2.152821
C	3.389285	-0.073233	-1.119467
C	3.416217	-1.443436	-1.454718
H	3.516079	-2.900224	-3.046593
H	3.560144	-1.194284	-4.852008
H	3.491349	1.224983	-4.268543
H	3.375080	1.938886	-1.901151
H	3.519274	-2.191169	-0.671142
O	1.018131	2.862520	-0.453047
S	1.569988	4.116242	-1.036404
O	0.851530	4.611901	-2.230686
O	3.048730	4.162366	-1.106696
C	1.157224	5.376581	0.266778
F	-0.174318	5.426835	0.486874
F	1.562546	6.603687	-0.091370
F	1.743937	5.068720	1.439997
O	2.616851	-0.579521	1.082872
C	3.394777	0.352061	0.356154
C	4.812213	0.440886	0.916287
C	5.513081	1.651240	0.828764
C	5.437944	-0.669912	1.494609
C	6.825524	1.743622	1.295448
C	6.748210	-0.574971	1.967815
C	7.447696	0.630156	1.865660
H	5.025518	2.522008	0.395507
H	7.357839	2.688601	1.220892
H	8.468097	0.703070	2.233757
H	7.222959	-1.442744	2.420085
H	4.885078	-1.599289	1.590306
H	2.953283	1.356629	0.403668

4-I (opt with the solvent correction)

B3LYP/BS1 SCF energy in PhMe: -3023.950939 a.u.

M06/BS2 SCF energy in PhMe: -3023.04303482 a.u.

M06/BS2 Free energy in PhMe: -3022.35504582 a.u.

C	-1.378918	0.129270	1.903387
C	-2.214188	0.150956	3.206481
H	-2.901775	1.003788	3.220102
H	-1.562892	0.228898	4.085608
H	-2.809722	-0.761481	3.317712
C	-0.516797	-1.157564	1.964876
H	0.003847	-1.154938	2.928121
H	-1.176911	-2.032297	1.978849
C	-0.484276	1.396748	1.967788
H	-1.117086	2.271299	2.156469
H	0.169833	1.303556	2.842913
C	-2.316564	0.179339	0.665386

H	-1.729688	0.017693	-0.244407
P	0.817919	-1.533507	0.689512
P	0.651105	1.819367	0.537943
Ni	1.989619	0.106190	-0.238010
C	-0.085711	-2.451206	-0.630204
C	-0.031300	-1.987279	-1.953282
C	-0.845584	-3.598583	-0.344001
C	-0.712369	-2.658909	-2.971054
H	0.553346	-1.101982	-2.188489
C	-1.517638	-4.273226	-1.363340
H	-0.904630	-3.978402	0.672035
C	-1.451169	-3.805430	-2.678447
H	-0.660136	-2.286173	-3.990098
H	-2.096551	-5.162232	-1.128414
H	-1.978705	-4.330488	-3.469948
C	1.759476	-2.819301	1.631606
C	2.043357	-4.083814	1.096537
C	2.267760	-2.497841	2.901794
C	2.791765	-5.010850	1.825215
H	1.690229	-4.349338	0.106719
C	3.013276	-3.425312	3.628872
H	2.099449	-1.513330	3.330269
C	3.273547	-4.688526	3.093898
H	3.000746	-5.985486	1.392598
H	3.394323	-3.156989	4.610609
H	3.854691	-5.412288	3.658902
C	1.733930	3.073932	1.359508
C	2.464202	2.687483	2.496600
C	1.919926	4.365745	0.847884
C	3.337810	3.577800	3.120299
H	2.363198	1.681415	2.896628
C	2.794878	5.256210	1.474341
H	1.391462	4.680552	-0.044877
C	3.503188	4.868108	2.611976
H	3.893137	3.260941	3.999100
H	2.925354	6.253748	1.063554
H	4.185275	5.562367	3.095193
C	-0.448711	2.780698	-0.591702
C	-0.541972	2.426591	-1.945169
C	-1.231892	3.847546	-0.116014
C	-1.399694	3.119899	-2.803895
H	0.070580	1.620362	-2.333440
C	-2.086301	4.540335	-0.974178
H	-1.169472	4.152603	0.925040
C	-2.172968	4.176601	-2.320909
H	-1.452774	2.836532	-3.851560
H	-2.680844	5.365742	-0.591681
H	-2.836524	4.718219	-2.989794
C	4.573266	-2.912699	-1.836161
C	3.465287	-2.073314	-1.668431
C	3.378129	-1.187854	-0.583007
C	4.447467	-1.176245	0.331067
C	5.559782	-2.006417	0.164431
C	5.626745	-2.883460	-0.921198
H	4.612976	-3.583899	-2.692302
H	2.673083	-2.109810	-2.411456
H	4.428608	-0.498224	1.183313
H	6.374756	-1.965866	0.884749
H	6.489989	-3.531452	-1.053617
I	3.223042	1.720846	-1.913841
H	-2.746625	1.183991	0.588572
P	-3.700891	-1.105362	0.629149
C	-4.238628	-1.039788	-1.145530
C	-5.050675	-2.097814	-1.590141
C	-3.903679	-0.028748	-2.060492
C	-5.526261	-2.138082	-2.901118
H	-5.309775	-2.899709	-0.902258
C	-4.369914	-0.074272	-3.377067
H	-3.275987	0.803885	-1.759603
C	-5.184216	-1.125720	-3.800687
H	-6.156663	-2.963633	-3.221890
H	-4.096372	0.717765	-4.069816
H	-5.546718	-1.158172	-4.824840
C	-5.114168	-0.202885	1.441511
C	-5.760820	-0.830604	2.517007
C	-5.583875	1.051334	1.018207
C	-6.839068	-0.218698	3.162507
H	-5.417364	-1.806577	2.852065
C	-6.659834	1.664836	1.660295
H	-5.117272	1.548461	0.171632
C	-7.289173	1.031267	2.736145
H	-7.326690	-0.719778	3.994883
H	-7.011771	2.634831	1.317817
H	-8.129031	1.508739	3.234249

TS4-I (opt with the solvent correction)

B3LYP/BS1 SCF energy in PhMe: -3369.570411 a.u.

M06/BS2 SCF energy in PhMe: -3368.46119829 a.u.

M06/BS2 Free energy in PhMe: -3367.67186529 a.u.

C	-1.729382	-0.514723	-1.829772
C	-2.305338	-0.874170	-3.222635
H	-3.046306	-0.138710	-3.553604
H	-1.510182	-0.900445	-3.977426
H	-2.788512	-1.857183	-3.208061
C	-0.603569	-1.560162	-1.588623
H	0.123186	-1.433481	-2.400969
H	-1.028181	-2.564570	-1.701420
C	-1.158116	0.919277	-1.965600
H	-1.983075	1.612684	-2.165311
H	-0.532051	0.932974	-2.864091
C	-2.846492	-0.620436	-0.751615
H	-2.494408	-0.191342	0.190330
H	-3.052512	-1.678212	-0.556387
P	0.428154	-1.529493	-0.032859
P	-4.459832	0.272833	-1.165360
P	-0.069433	1.740186	-0.667324
Ni	1.610496	0.526642	0.126483
C	-5.470155	-1.067302	-1.972641
C	-6.068120	-0.786740	-3.210431
C	-5.689261	-2.328711	-1.394595
C	-6.854238	-1.742046	-3.861215
H	-5.917182	0.187713	-3.669192
C	-6.471602	-3.284956	-2.042386
H	-5.258492	-2.564362	-0.424729
C	-7.055305	-2.994083	-3.279177
H	-7.309343	-1.506059	-4.819771
H	-6.631798	-4.255328	-1.579025
H	-7.666986	-3.738860	-3.781698
C	-5.298256	0.370825	0.486239
C	-6.392367	1.250107	0.574695
C	-4.928966	-0.348803	1.632939
C	-7.103372	1.396669	1.765820
H	-6.686927	1.828654	-0.298309
C	-5.633921	-0.194440	2.829690
H	-4.086773	-1.032184	1.609453
C	-6.723894	0.674360	2.899775
H	-7.947613	2.080158	1.810404
H	-5.328406	-0.758632	3.707242
H	-7.270597	0.792299	3.831771
C	-0.709273	-2.222678	1.256274
C	-0.999222	-1.512734	2.427115
C	-1.287465	-3.491897	1.072335
C	-1.853868	-2.053827	3.393107
H	-0.539013	-0.548848	2.601381
C	-2.143387	-4.028890	2.033001
H	-1.058257	-4.073730	0.183454
C	-2.428320	-3.309922	3.198584
H	-2.057372	-1.491723	4.300513
H	-2.578932	-5.012616	1.877788
H	-3.086550	-3.733598	3.952623
C	1.541429	-2.988100	-0.310015
C	2.202618	-3.534148	0.804106
C	1.765474	-3.563366	-1.570160
C	3.056128	-4.627331	0.660054
H	2.056467	-3.098232	1.786942
C	2.619887	-4.661134	-1.710795
H	1.278264	-3.172521	-2.456659
C	3.266330	-5.197706	-0.597788
H	3.555111	-5.033509	1.535876
H	2.773453	-5.096535	-2.695045
H	3.929143	-6.051829	-0.708462
C	0.354032	3.262288	-1.644569
C	0.910449	3.133506	-2.928594
C	0.162282	4.551308	-1.126676
C	1.233741	4.259605	-3.684741
H	1.113317	2.151317	-3.346119
C	0.493057	5.678640	-1.882370
H	-0.244575	4.685128	-0.130722
C	1.021505	5.538207	-3.165228
H	1.658269	4.135803	-4.677631
H	0.336111	6.668047	-1.461120
H	1.273957	6.416647	-3.753088
C	-1.218160	2.369433	0.631463
C	-0.887689	2.189639	1.982329
C	-2.400307	3.058980	0.306454
C	-1.723633	2.679300	2.989451
H	0.025816	1.666472	2.249155
C	-3.232041	3.547382	1.313583
H	-2.672015	3.228029	-0.730945
C	-2.896368	3.356525	2.657167
H	-1.450118	2.530625	4.030480

H	-4.144553	4.073805	1.048715
H	-3.549100	3.735460	3.438906
C	4.394855	3.546840	-0.843823
C	4.366891	4.420606	0.244013
C	3.474381	4.172421	1.288450
C	2.628050	3.058707	1.250115
C	2.653574	2.155143	0.174218
C	3.543291	2.436837	-0.877741
H	5.074769	3.728634	-1.674224
H	5.026481	5.284691	0.275203
H	3.437205	4.841986	2.145614
H	1.961051	2.890646	2.089059
H	3.581030	1.786455	-1.747945
O	3.277336	-0.527998	-0.725237
C	4.405720	-0.618062	-0.232302
C	5.558909	-1.194991	-0.928323
C	6.782823	-1.263312	-0.242200
C	5.468751	-1.666530	-2.250213
C	7.905138	-1.802768	-0.867619
C	6.591319	-2.201629	-2.871404
C	7.808411	-2.270084	-2.180797
H	6.843745	-0.894934	0.778808
H	8.850971	-1.857727	-0.336558
H	8.683142	-2.689968	-2.670503
H	6.526407	-2.566620	-3.892695
H	4.517049	-1.609947	-2.768630
H	4.578944	-0.254058	0.790758
I	2.534685	-0.193073	2.962977

11-I (opt with the solvent correction)

B3LYP/BS1 SCF energy in PhMe: -3369.588412 a.u.

M06/BS2 SCF energy in PhMe: -3368.46471037 a.u.

M06/BS2 Free energy in PhMe: -3367.67815837 a.u.

C	2.359190	1.319017	1.597606
C	3.490705	1.969854	2.428685
H	4.276020	2.381526	1.786155
H	3.100394	2.793062	3.039676
H	3.954857	1.241644	3.102558
C	1.272058	0.919760	2.632514
H	0.919125	1.830287	3.133060
H	1.728491	0.303541	3.415811
C	1.839531	2.427569	0.644800
H	2.656676	2.743769	-0.013270
H	1.594757	3.298178	1.262268
C	2.883837	0.060531	0.852218
H	2.119588	-0.294118	0.153428
H	3.040415	-0.743489	1.579650
P	-0.281097	0.067907	2.055087
P	4.455795	0.293714	-0.168235
P	0.353219	2.192691	-0.483799
Ni	-1.375376	1.055415	0.271137
C	5.793444	-0.134643	1.054550
C	6.817802	0.802230	1.258360
C	5.847684	-1.349239	1.758459
C	7.860729	0.543726	2.152303
H	6.797996	1.742451	0.712255
C	6.887034	-1.610288	2.651910
H	5.082472	-2.104818	1.598609
C	7.895577	-0.662651	2.852291
H	8.644833	1.282524	2.297063
H	6.915400	-2.556497	3.186521
H	8.706775	-0.868390	3.545840
C	4.455544	-1.232201	-1.222259
C	5.369007	-1.248637	-2.291139
C	3.613920	-2.342154	-1.049482
C	5.447264	-2.342407	-3.153002
H	6.020461	-0.392585	-2.453213
C	3.681176	-3.432280	-1.921542
H	2.890699	-2.369325	-0.241214
C	4.597403	-3.436786	-2.973877
H	6.162606	-2.334813	-3.971636
H	3.010176	-4.274852	-1.776674
H	4.644694	-4.283927	-3.652971
C	0.118024	-1.721463	1.949290
C	-0.326797	-2.455856	0.839399
C	0.852756	-2.381874	2.951835
C	-0.044853	-3.820479	0.729186
H	-0.891353	-1.977120	0.044896
C	1.134116	-3.743066	2.839833
H	1.200316	-1.841428	3.827911
C	0.685882	-4.464176	1.728200
H	-0.402325	-4.362641	-0.141263
H	1.701315	-4.241035	3.621799
H	0.906322	-5.524882	1.644090
C	-1.349102	0.258329	3.552842

C	-1.815341	-0.827340	4.306403
C	-1.748585	1.556328	3.917566
C	-2.644740	-0.617252	5.411768
H	-1.537777	-1.840168	4.035506
C	-2.574845	1.764011	5.021244
H	-1.422420	2.413560	3.332563
C	-3.023151	0.675568	5.774628
H	-2.994146	-1.470334	5.987231
H	-2.871589	2.774453	5.289462
H	-3.666743	0.836094	6.635252
C	0.014478	3.961214	-0.905846
C	-0.146182	4.900535	0.126785
C	-0.165270	4.381404	-2.231818
C	-0.453593	6.230490	-0.160831
H	-0.045254	4.602129	1.167124
C	-0.472716	5.712864	-2.517079
H	-0.075768	3.671356	-3.046120
C	-0.613384	6.641741	-1.485439
H	-0.570070	6.943281	0.651232
H	-0.606822	6.019390	-3.550828
H	-0.852177	7.677515	-1.710877
C	1.036986	1.428253	-2.006537
C	0.513879	0.213384	-2.473353
C	2.087402	2.036767	-2.716637
C	1.016326	-0.377793	-3.634741
H	-0.291708	-0.279669	-1.937829
C	2.583829	1.447976	-3.878578
H	2.512766	2.975515	-2.373793
C	2.046983	0.242495	-4.340548
H	0.590737	-1.315811	-3.978312
H	3.392944	1.930244	-4.420278
H	2.437621	-0.214060	-5.245723
C	-4.194175	3.679764	-1.329538
C	-4.440519	3.215527	-2.624501
C	-3.708608	2.133140	-3.113038
C	-2.733490	1.517799	-2.315876
C	-2.472527	1.974127	-1.014870
C	-3.219496	3.065419	-0.537442
H	-4.759704	4.521230	-0.934134
H	-5.195875	3.692634	-3.244207
H	-3.891893	1.756755	-4.117054
H	-2.189443	0.674313	-2.731608
H	-3.048171	3.451128	0.466611
O	-2.993219	0.085157	0.830615
C	-3.680881	-0.719009	0.172527
C	-4.904851	-1.313519	0.684812
C	-5.559434	-2.270932	-0.112506
C	-5.439742	-0.946091	1.935977
C	-6.739054	-2.857280	0.340919
C	-6.618185	-1.532896	2.377339
C	-7.266114	-2.488067	1.580990
H	-5.129570	-2.554178	-1.070117
H	-7.244495	-3.599495	-0.269491
H	-8.187683	-2.944353	1.932952
H	-7.039167	-1.251531	3.338405
H	-4.927439	-0.202528	2.537640
H	-3.369581	-1.014621	-0.837315
I	-2.346063	-3.278417	-2.897712

TS5-I (opt with the solvent correction)

B3LYP/BS1 SCF energy in PhMe: -3369.559109 a.u.

M06/BS2 SCF energy in PhMe: -3368.43834034 a.u.

M06/BS2 Free energy in PhMe: -3367.64713534 a.u.

C	-2.234905	2.160817	0.279506
C	-3.302986	3.257296	0.510406
H	-3.948131	3.015344	1.361141
H	-2.830224	4.224631	0.719484
H	-3.941581	3.377355	-0.371466
C	-1.334620	2.706095	-0.863108
H	-0.889921	3.649395	-0.524346
H	-1.961054	2.960159	-1.725575
C	-1.435119	2.053615	1.604527
H	-2.120197	1.779479	2.414456
H	-1.062502	3.054721	1.848354
C	-2.908629	0.825890	-0.145387
H	-2.166638	0.020733	-0.141892
H	-3.260650	0.920811	-1.178673
P	0.089725	1.679297	-1.479641
P	-4.330988	0.233385	0.947962
P	0.049391	0.913446	1.788980
Ni	1.433209	0.678734	0.033478
C	-5.813547	0.991476	0.111771
C	-6.705574	1.733146	0.900799
C	-6.101945	0.831387	-1.253762
C	-7.849025	2.311152	0.341720

H	-6.504176	1.858579	1.962145
C	-7.240946	1.408945	-1.815375
H	-5.442536	0.237663	-1.881851
C	-8.116924	2.152266	-1.018262
H	-8.528770	2.881984	0.969288
H	-7.450646	1.272796	-2.873442
H	-9.005996	2.598840	-1.456014
C	-4.513458	-1.533306	0.415205
C	-5.342682	-2.339446	1.215063
C	-3.891308	-2.117339	-0.699271
C	-5.554834	-3.682334	0.904267
H	-5.823870	-1.910622	2.091537
C	-4.091202	-3.466899	-1.002485
H	-3.240109	-1.532664	-1.340924
C	-4.925125	-4.251806	-0.205261
H	-6.202504	-4.286572	1.534598
H	-3.590257	-3.902179	-1.862957
H	-5.077393	-5.301273	-0.442815
C	-0.606697	0.545530	-2.744663
C	-0.249377	-0.810958	-2.740178
C	-1.494474	1.017159	-3.729430
C	-0.778828	-1.684808	-3.693945
H	0.449961	-1.196507	-2.006822
C	-2.019446	0.142874	-4.680179
H	-1.770951	2.067365	-3.766524
C	-1.664661	-1.210123	-4.661521
H	-0.486460	-2.730428	-3.668957
H	-2.703198	0.518386	-5.436820
H	-2.075145	-1.889258	-5.403920
C	1.087217	2.917627	-2.416620
C	1.502863	2.676888	-3.734243
C	1.517219	4.092383	-1.774837
C	2.311498	3.600840	-4.400379
H	1.201874	1.768099	-4.243580
C	2.322048	5.014212	-2.443497
H	1.232006	4.295947	-0.745749
C	2.720107	4.771336	-3.760566
H	2.622490	3.398890	-5.421646
H	2.639714	5.920056	-1.934152
H	3.347922	5.488914	-4.281651
C	0.828307	1.679790	3.280779
C	1.220395	3.028848	3.214757
C	1.070753	0.966303	4.462328
C	1.810745	3.655114	4.311217
H	1.070767	3.599979	2.301521
C	1.664701	1.595682	5.559838
H	0.796817	-0.079899	4.535982
C	2.030519	2.939620	5.490933
H	2.100564	4.700314	4.242745
H	1.839737	1.028035	6.469751
H	2.488099	3.426806	6.347636
C	-0.661283	-0.686998	2.333589
C	-0.343959	-1.858116	1.630066
C	-1.528292	-0.767458	3.438959
C	-0.864309	-3.090823	2.030401
H	0.310897	-1.822620	0.764470
C	-2.043174	-1.999656	3.839025
H	-1.795505	0.125684	3.996388
C	-1.710334	-3.162064	3.136569
H	-0.597885	-3.981520	1.469501
H	-2.709900	-2.050182	4.695566
H	-2.115419	-4.120323	3.449693
C	4.598993	1.026214	2.685727
C	4.620772	-0.139446	3.458853
C	3.846131	-1.243256	3.087952
C	3.042005	-1.181487	1.949609
C	2.998955	-0.014487	1.159274
C	3.807243	1.078349	1.540632
H	5.213466	1.878432	2.964608
H	5.255849	-0.193909	4.339418
H	3.879056	-2.156058	3.677231
H	2.475437	-2.060034	1.653479
H	3.843126	1.966457	0.911904
O	2.569746	0.325515	-1.413926
C	3.355780	-0.524113	-0.808695
C	4.824473	-0.405370	-0.996698
C	5.645681	-1.492311	-0.661683
C	5.390577	0.748515	-1.559849
C	7.021638	-1.419131	-0.873072
C	6.765652	0.816326	-1.771857
C	7.583541	-0.264331	-1.424136
H	5.200771	-2.392733	-0.246511
H	7.653194	-2.264998	-0.616058
H	8.656068	-0.209529	-1.592011
H	7.202459	1.707906	-2.214384
H	4.742727	1.573146	-1.840359

H	2.997916	-1.552739	-0.685912
I	1.749246	-4.416626	-1.082835

12-I (opt with the solvent correction)

B3LYP/BS1 SCF energy in PhMe: -3369.588671 a.u.

M06/BS2 SCF energy in PhMe: -3368.46319099 a.u.

M06/BS2 Free energy in PhMe: -3367.67290699 a.u.

C	2.103876	-2.358626	0.132781
C	3.146508	-3.501339	0.172089
H	3.903950	-3.325828	0.943005
H	2.665296	-4.461496	0.395666
H	3.662701	-3.597771	-0.789028
C	1.048054	-2.813487	-0.911494
H	0.624452	-3.765575	-0.571078
H	1.552812	-3.032983	-1.859591
C	1.478960	-2.293090	1.550470
H	2.268027	-2.080481	2.279693
H	1.093369	-3.287857	1.801534
C	2.767110	-1.021846	-0.302642
H	2.065221	-0.196615	-0.146672
H	2.969049	-1.058614	-1.378591
P	-0.418279	-1.746653	-1.325743
P	4.349067	-0.545612	0.614246
P	0.070053	-1.117766	1.936312
Ni	-1.534264	-0.848365	0.343004
C	5.665534	-1.273830	-0.483979
C	6.611951	-2.130481	0.098148
C	5.775466	-0.986954	-1.854936
C	7.634006	-2.697869	-0.668337
H	6.549776	-2.354822	1.160544
C	6.793713	-1.552513	-2.622672
H	5.072125	-0.304008	-2.324892
C	7.724821	-2.411657	-2.030870
H	8.358328	-3.359321	-0.199819
H	6.866179	-1.317033	-3.681565
H	8.519806	-2.849163	-2.629133
C	4.510185	1.252862	0.196875
C	5.474111	1.971908	0.926136
C	3.749378	1.941792	-0.760662
C	5.681194	3.331706	0.696338
H	6.065681	1.461730	1.683488
C	3.945480	3.308076	-0.980648
H	2.990382	1.428704	-1.342249
C	4.912908	4.005551	-0.256328
H	6.434036	3.867303	1.269288
H	3.335188	3.824945	-1.716188
H	5.060632	5.068363	-0.427626
C	0.157303	-0.501322	-2.538209
C	-0.146497	0.855408	-2.356592
C	0.910576	-0.892523	-3.660725
C	0.301831	1.811049	-3.272017
H	-0.736201	1.178338	-1.505451
C	1.353524	0.062999	-4.574424
H	1.142587	-1.939474	-3.835643
C	1.052580	1.414923	-4.379519
H	0.057439	2.856327	-3.104252
H	1.931786	-0.249173	-5.439907
H	1.400360	2.157127	-5.092718
C	-1.497667	-2.918500	-2.242862
C	-2.060252	-2.563307	-3.477415
C	-1.820155	-4.164748	-1.679769
C	-2.905491	-3.449615	-4.146778
H	-1.845900	-1.595124	-3.915370
C	-2.666339	-5.047068	-2.350933
H	-1.423324	-4.454547	-0.710464
C	-3.207873	-4.692471	-3.588782
H	-3.332646	-3.160917	-5.102922
H	-2.903615	-6.008967	-1.904786
H	-3.867107	-5.379919	-4.111684
C	-0.602969	-1.924720	3.456991
C	-1.201411	-3.190056	3.321813
C	-0.578367	-1.319824	4.720902
C	-1.752165	-3.838716	4.426715
H	-1.247482	-3.674033	2.348658
C	-1.128726	-1.972874	5.827153
H	-0.138565	-0.336929	4.847668
C	-1.716078	-3.230610	5.684510
H	-2.211864	-4.815667	4.304445
H	-1.099004	-1.491755	6.800972
H	-2.145725	-3.734092	6.546052
C	0.848756	0.454729	2.458298
C	0.401334	1.655645	1.887637
C	1.885901	0.493846	3.409584
C	0.968344	2.876444	2.260560
H	-0.391375	1.648549	1.146634

C	2.445040	1.714347	3.785138
H	2.256599	-0.420040	3.864585
C	1.987561	2.905078	3.211710
H	0.611772	3.790603	1.794736
H	3.244873	1.733852	4.520320
H	2.433219	3.852801	3.500390
C	-3.416797	-0.022622	3.169910
C	-3.222970	1.282358	3.610291
C	-3.099379	2.323564	2.678494
C	-3.180402	2.064254	1.313550
C	-3.408890	0.754693	0.854259
C	-3.504734	-0.295187	1.793350
H	-3.523871	-0.832420	3.884677
H	-3.168842	1.496584	4.674124
H	-2.936437	3.342602	3.018114
H	-3.069512	2.876977	0.600271
H	-3.786589	-1.292456	1.461393
O	-2.815642	-0.685329	-0.946319
C	-3.597540	0.446927	-0.634958
C	-5.067288	0.216356	-0.989769
C	-5.934307	1.311261	-1.111293
C	-5.571850	-1.074562	-1.180348
C	-7.284353	1.117647	-1.404451
C	-6.923189	-1.268116	-1.479350
C	-7.784234	-0.174804	-1.588255
H	-5.550563	2.320654	-0.979702
H	-7.943954	1.976665	-1.497384
H	-8.834903	-0.325798	-1.822783
H	-7.301803	-2.276186	-1.631776
H	-4.894515	-1.919427	-1.112966
H	-3.250560	1.326991	-1.198685
I	-1.139544	5.078041	-0.903910

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B3LYP/BS1 SCF energy: -3092.880032 a.u.

M06/BS2 SCF energy in PhMe: -3091.96804736 a.u.

M06/BS2 Free energy in PhMe: -3091.18776636 a.u.

C	-0.059687	0.386571	-2.807195
C	-0.104077	0.522047	-4.349064
H	0.330235	1.476038	-4.672704
H	0.460789	-0.285634	-4.830730
H	-1.136249	0.478424	-4.717993
C	-0.542523	-1.061996	-2.478630
H	0.291695	-1.742294	-2.684240
H	-1.345034	-1.328094	-3.176926
C	1.420462	0.634760	-2.382106
H	1.592511	1.716411	-2.406571
H	2.090440	0.188780	-3.126155
C	-1.012055	1.480641	-2.237830
H	-2.042554	1.139214	-2.387763
H	-0.891097	2.395659	-2.830282
P	-1.120510	-1.416911	-0.713179
P	-0.826170	1.871638	-0.404236
P	1.884688	0.016892	-0.668014
Ni	0.061986	0.066994	0.588308
C	0.185962	3.444394	-0.411688
C	1.217842	3.579740	0.526066
C	-0.085524	4.524564	-1.268529
C	1.966333	4.758208	0.603898
H	1.441629	2.748958	1.188793
C	0.665267	5.697224	-1.200374
H	-0.904024	4.464086	-1.981289
C	1.694719	5.816980	-0.261398
H	2.766795	4.839269	1.334254
H	0.441303	6.522086	-1.872421
H	2.277330	6.732998	-0.205551
C	-2.473790	2.661710	-0.019066
C	-2.763026	2.922353	1.331655
C	-3.425255	3.035597	-0.980703
C	-3.960091	3.530947	1.708955
H	-2.044556	2.642045	2.095806
C	-4.627674	3.640056	-0.604697
H	-3.242532	2.859455	-2.035842
C	-4.900763	3.889464	0.740368
H	-4.158872	3.721998	2.760518
H	-5.350372	3.916763	-1.368393
H	-5.836112	4.359981	1.031816
C	-2.980808	-1.309321	-0.923398
C	-3.727221	-0.509682	-0.048849
C	-3.668691	-2.034610	-1.912322
C	-5.118578	-0.421653	-0.163499
H	-3.217218	0.055614	0.722359
C	-5.054802	-1.948686	-2.030880
H	-3.122440	-2.690644	-2.584867
C	-5.785044	-1.138470	-1.155451

H	-5.673061	0.214281	0.521286
H	-5.567285	-2.519778	-2.801271
H	-6.866262	-1.072764	-1.246834
C	-1.000746	-3.282321	-0.657764
C	-1.191412	-3.886596	0.596968
C	-0.743533	-4.115941	-1.757107
C	-1.133267	-5.271579	0.749684
H	-1.384104	-3.260650	1.464379
C	-0.675730	-5.503838	-1.606140
H	-0.590873	-3.693531	-2.745252
C	-0.870693	-6.087298	-0.353993
H	-1.287967	-5.713207	1.730974
H	-0.471035	-6.128234	-2.472419
H	-0.818018	-7.166631	-0.237900
C	2.752583	-1.588624	-1.079522
C	2.378522	-2.769414	-0.427755
C	3.806010	-1.642463	-2.009529
C	3.026370	-3.978200	-0.703913
H	1.570528	-2.743349	0.293908
C	4.451929	-2.845354	-2.288919
H	4.140723	-0.734558	-2.505090
C	4.061437	-4.019301	-1.636180
H	2.711649	-4.883696	-0.192305
H	5.265304	-2.866947	-3.010075
H	4.566464	-4.957161	-1.853022
C	3.407994	1.010934	-0.263675
C	4.028404	0.744139	0.970721
C	3.979788	1.989085	-1.090260
C	5.174835	1.432007	1.365207
H	3.612768	-0.016659	1.624812
C	5.127445	2.682298	-0.694780
H	3.540869	2.224614	-2.053806
C	5.728367	2.409063	0.533448
H	5.636249	1.204867	2.322954
H	5.550430	3.436658	-1.353543
H	6.620725	2.948580	0.839704
C	-0.501551	0.169947	2.613010
C	0.821621	-0.273754	2.502969
C	-0.573557	-1.077708	5.415078
C	1.322622	-1.636933	2.935309
C	0.764109	-1.116733	5.456508
C	1.735453	-1.667206	4.432765
H	0.583033	-2.412211	2.717710
H	2.213721	-1.914007	2.357089
H	2.011589	-2.700088	4.703739
H	2.666836	-1.091167	4.531267
C	-1.701238	-0.629520	3.121784
H	-2.165116	-1.216451	2.321755
H	-2.466325	0.095351	3.430107
C	-1.453403	-1.607102	4.311059
H	-2.433904	-1.873887	4.727632
H	-1.034007	-2.542140	3.926918
H	-0.607032	1.239868	2.779227
H	1.583945	0.503195	2.592664
H	-1.087748	-0.610179	6.255684
H	1.242576	-0.700008	6.344190

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B3LYP/BS1 SCF energy: -3092.885950 a.u.

M06/BS2 SCF energy in PhMe: -3091.96664923 a.u.

M06/BS2 Free energy in PhMe: -3091.18555123 a.u.

C	-0.820554	-0.032756	-1.818143
C	-1.517526	-0.109532	-3.196753
H	-0.774720	-0.178863	-4.000934
H	-2.173277	-0.985608	-3.261650
H	-2.129239	0.779108	-3.387249
C	-1.877947	-0.136559	-0.683270
H	-1.364472	-0.030215	0.280042
H	-2.323649	-1.138063	-0.703050
C	0.165559	-1.241630	-1.760957
H	1.006166	-0.998360	-2.420381
H	-0.324549	-2.123548	-2.188666
C	-0.056422	1.321128	-1.775511
H	-0.772849	2.118804	-1.562155
H	0.339161	1.526624	-2.776335
P	-3.225524	1.180604	-0.671083
P	1.404335	1.505742	-0.579247
P	0.885985	-1.721799	-0.084205
Ni	1.497598	0.059783	1.100773
C	2.799076	1.501736	-1.824893
C	3.766704	0.490163	-1.767949
C	2.886426	2.447724	-2.862912
C	4.793200	0.419829	-2.715669
H	3.707360	-0.255390	-0.981986
C	3.911255	2.383762	-3.806318

H	2.154030	3.248035	-2.928890
C	4.869628	1.367820	-3.734859
H	5.528462	-0.378122	-2.652011
H	3.962651	3.126999	-4.598109
H	5.668222	1.318685	-4.470625
C	1.282605	3.316002	-0.173255
C	2.424618	4.134171	-0.119093
C	0.055572	3.871191	0.231580
C	2.340856	5.460241	0.309350
H	3.388756	3.738117	-0.422815
C	-0.028511	5.197643	0.658427
H	-0.850797	3.271740	0.216970
C	1.113608	5.999124	0.699280
H	3.238907	6.072449	0.335163
H	-0.991384	5.602455	0.959412
H	1.048009	7.031765	1.031423
C	-4.571218	0.430377	-1.712200
C	-5.070389	1.193395	-2.778304
C	-5.123029	-0.840466	-1.483218
C	-6.084307	0.698982	-3.603067
H	-4.658952	2.182943	-2.962675
C	-6.135274	-1.337038	-2.304458
H	-4.770447	-1.443910	-0.650830
C	-6.617243	-0.568577	-3.368214
H	-6.457108	1.304591	-4.425169
H	-6.551990	-2.322638	-2.112510
H	-7.407108	-0.956118	-4.006411
C	-3.927015	0.966426	1.033747
C	-4.648237	2.053085	1.557069
C	-3.784609	-0.181636	1.831104
C	-5.222278	1.992704	2.827532
H	-4.755566	2.957480	0.962551
C	-4.349105	-0.238784	3.107723
H	-3.230980	-1.041280	1.466064
C	-5.071411	0.845505	3.608768
H	-5.777835	2.844842	3.210630
H	-4.225318	-1.135366	3.710232
H	-5.508943	0.798723	4.602496
C	-0.354513	-3.044074	0.413401
C	-1.066012	-2.943050	1.615107
C	-0.592090	-4.164304	-0.402965
C	-1.991633	-3.922353	1.991965
H	-0.892609	-2.092526	2.260733
C	-1.517368	-5.140329	-0.034539
H	-0.036529	-4.287077	-1.328927
C	-2.222257	-5.022194	1.166781
H	-2.526513	-3.823935	2.933448
H	-1.683051	-5.997972	-0.681778
H	-2.939814	-5.785112	1.457235
C	2.259990	-2.885903	-0.583707
C	2.768041	-3.742816	0.411897
C	2.862201	-2.927792	-1.850381
C	3.830502	-4.606249	0.151784
H	2.315940	-3.742685	1.400503
C	3.929906	-3.792740	-2.113003
H	2.508496	-2.290841	-2.653214
C	4.419533	-4.633995	-1.115342
H	4.197768	-5.259419	0.939288
H	4.372494	-3.807881	-3.106004
H	5.248397	-5.306042	-1.320916
C	2.034182	2.005969	3.386597
C	3.379494	1.838541	2.635560
C	3.493358	0.546652	1.850088
C	0.853356	1.327092	2.702041
C	3.153695	-0.708847	2.316438
C	0.440463	0.026508	2.956190
C	2.672465	-0.985594	3.734598
C	1.130740	-0.947400	3.894306
H	3.035755	-1.971698	4.051307
H	0.874958	-0.727855	4.945329
H	2.126590	1.627341	4.411525
H	3.489324	2.668298	1.930278
H	4.215490	1.934510	3.348999
H	3.134659	-0.267767	4.421948
H	0.735997	-1.951091	3.696596
H	1.819021	3.076650	3.483826
H	3.525158	-1.564720	1.758176
H	-0.601387	-0.198209	2.733971
H	0.120087	1.999778	2.263964
H	4.134007	0.603316	0.973463

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B3LYP/BS1 SCF energy: -2780.839247 a.u.

M06/BS2 SCF energy in PhMe: -2780.06958319 a.u.

M06/BS2 Free energy in PhMe: -2779.46282019 a.u.

C	0.008093	0.009906	2.143268
C	0.009520	0.014680	3.694567
H	0.696711	-0.743531	4.089632
H	0.324127	0.990189	4.085227
H	-0.990961	-0.199412	4.090054
C	-0.866673	1.232037	1.710617
H	-0.264602	2.137183	1.851332
H	-1.721280	1.310311	2.394225
C	1.505039	0.153753	1.713394
H	1.989083	-0.818185	1.864493
H	1.996525	0.862843	2.391137
C	-0.614198	-1.360257	1.719452
H	-1.697391	-1.296055	1.875098
H	-0.242355	-2.137883	2.397807
P	-1.494202	1.276371	-0.076384
P	-0.351930	-1.928182	-0.069372
P	1.863816	0.665312	-0.076085
Ni	0.010743	0.005363	-0.926824
C	0.957399	-3.249426	0.118192
C	2.063123	-3.222516	-0.741488
C	0.870652	-4.285780	1.063267
C	3.065143	-4.193510	-0.653852
H	2.143467	-2.425870	-1.474849
C	1.869806	-5.253796	1.156574
H	0.008569	-4.352696	1.722230
C	2.972457	-5.208355	0.297791
H	3.919533	-4.145781	-1.323713
H	1.785953	-6.048114	1.894368
H	3.751296	-5.963219	0.370779
C	-1.817397	-3.043257	-0.359327
C	-2.100036	-3.375225	-1.695205
C	-2.642659	-3.574302	0.643612
C	-3.166028	-4.214491	-2.019476
H	-1.479969	-2.961530	-2.487862
C	-3.717745	-4.406482	0.321192
H	-2.458644	-3.342625	1.688658
C	-3.982448	-4.730850	-1.009961
H	-3.363508	-4.459355	-3.060156
H	-4.347627	-4.802338	1.114075
H	-4.818494	-5.378981	-1.259470
C	-3.286080	0.777559	0.105196
C	-3.802648	-0.180377	-0.776917
C	-4.148708	1.339257	1.061724
C	-5.140331	-0.579215	-0.701913
H	-3.144908	-0.625883	-1.517104
C	-5.482279	0.940279	1.143445
H	-3.786149	2.108291	1.739219
C	-5.981508	-0.022615	0.260817
H	-5.516229	-1.332134	-1.389446
H	-6.134834	1.385132	1.890841
H	-7.021378	-0.332969	0.324706
C	-1.751154	3.100268	-0.363938
C	-1.897640	3.512852	-1.699176
C	-1.813846	4.076990	0.641628
C	-2.106548	4.854154	-2.020522
H	-1.837924	2.771661	-2.493561
C	-2.012560	5.422548	0.322213
H	-1.704441	3.800302	1.686107
C	-2.161161	5.815918	-1.008416
H	-2.219698	5.149135	-3.060767
H	-2.052312	6.163426	1.116981
H	-2.316523	6.862893	-1.255389
C	2.343710	2.462440	0.110694
C	1.743030	3.406264	-0.731958
C	3.298003	2.907959	1.041014
C	2.072891	4.761953	-0.642826
H	1.001788	3.074993	-1.452763
C	3.626988	4.259521	1.135916
H	3.803780	2.194443	1.686721
C	3.012664	5.191462	0.293457
H	1.586183	5.477757	-1.299862
H	4.367373	4.586153	1.862184
H	3.269752	6.245102	0.367500
C	3.563763	-0.043307	-0.362823
C	3.991558	-0.128712	-1.698633
C	4.437344	-0.486304	0.642117
C	5.251560	-0.632713	-2.021287
H	3.322107	0.196565	-2.492324
C	5.695923	-1.001391	0.321267
H	4.144575	-0.437951	1.686984
C	6.108170	-1.074898	-1.009899
H	5.561609	-0.686678	-3.061911
H	6.354959	-1.343960	1.115279
H	7.087833	-1.474975	-1.257896

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B3LYP/BS1 SCF energy: -3092.859192 a.u.

M06/BS2 SCF energy in PhMe: -3091.92941944 a.u.

M06/BS2 Free energy in PhMe: -3091.15771144 a.u.

C	-1.021985	0.289026	-1.075184
C	-2.166579	0.600045	-2.063097
H	-2.422387	-0.287274	-2.653540
H	-3.071985	0.928478	-1.543821
H	-1.879174	1.395587	-2.760374
C	-0.739379	1.495751	-0.134091
H	0.223691	1.321986	0.359281
H	-1.489801	1.535198	0.662502
C	-1.378950	-0.956789	-0.215045
H	-0.585101	-1.097904	0.528593
H	-1.382282	-1.848151	-0.853881
C	0.241209	-0.001820	-1.941214
H	0.567168	0.959373	-2.354586
H	-0.046150	-0.630372	-2.793321
P	-0.565343	3.178186	-0.960710
P	1.776175	-0.776318	-1.149924
P	-2.990386	-0.850703	0.757610
Ni	2.536231	-0.482954	0.886791
C	1.459430	-2.597807	-1.392979
C	1.453466	-3.447176	-0.275735
C	1.248101	-3.160786	-2.661158
C	1.230579	-4.819484	-0.418856
H	1.624345	-3.023394	0.711393
C	1.019781	-4.529929	-2.806608
H	1.278874	-2.529933	-3.545667
C	1.008889	-5.363208	-1.685319
H	1.234937	-5.462016	0.458168
H	0.857481	-4.947395	-3.797120
H	0.835515	-6.430048	-1.799624
C	3.015626	-0.495433	-2.526640
C	4.316776	-0.981670	-2.302852
C	2.762921	0.166607	-3.738050
C	5.323782	-0.822279	-3.252788
H	4.537122	-1.491241	-1.368151
C	3.775873	0.340465	-4.687337
H	1.775523	0.554131	-3.962932
C	5.057535	-0.153425	-4.450839
H	6.318633	-1.213432	-3.054950
H	3.554509	0.861748	-5.615400
H	5.842825	-0.018104	-5.189855
C	-2.260414	3.931370	-0.874028
C	-2.471162	5.063975	-1.680381
C	-3.329971	3.470139	-0.089353
C	-3.698885	5.725979	-1.690041
H	-1.662372	5.427429	-2.310423
C	-4.564031	4.126307	-0.105735
H	-3.218535	2.590594	0.537570
C	-4.751928	5.256859	-0.901863
H	-3.835563	6.601932	-2.319052
H	-5.378714	3.751140	0.508817
H	-5.712550	5.765169	-0.912608
C	0.312740	4.095928	0.396325
C	1.651988	4.453222	0.173771
C	-0.279453	4.445720	1.620877
C	2.386520	5.128884	1.152230
H	2.119208	4.205886	-0.776492
C	0.451197	5.122509	2.598505
H	-1.321284	4.200285	1.807451
C	1.786987	5.464105	2.367499
H	3.421170	5.401376	0.960175
H	-0.023291	5.387854	3.539993
H	2.352939	5.997046	3.127196
C	-4.217988	-1.640770	-0.396226
C	-5.365542	-0.906575	-0.730595
C	-4.066217	-2.927253	-0.938529
C	-6.330823	-1.434153	-1.592255
H	-5.500888	0.089129	-0.315211
C	-5.028062	-3.457310	-1.798459
H	-3.197612	-3.527324	-0.679846
C	-6.162688	-2.710628	-2.129069
H	-7.211587	-0.848074	-1.841935
H	-4.894880	-4.455391	-2.208408
H	-6.911916	-3.124910	-2.798724
C	-2.758821	-2.202284	2.008490
C	-3.595317	-2.165171	3.137301
C	-1.816885	-3.240365	1.914343
C	-3.507659	-3.139529	4.131993
H	-4.319500	-1.359969	3.237851
C	-1.720821	-4.210565	2.915405
H	-1.150383	-3.303880	1.059883
C	-2.566451	-4.165497	4.024830
H	-4.167208	-3.091810	4.994717

H	-0.985444	-5.006245	2.823142
H	-2.490234	-4.921458	4.801962
C	3.031618	1.440400	3.088603
C	4.144323	1.604675	2.009035
C	4.441882	0.358356	1.200453
C	1.891302	0.532074	2.661483
C	4.487654	-0.931808	1.689476
C	1.822108	-0.831867	2.861115
C	4.336247	-1.342209	3.142729
C	2.872150	-1.702233	3.522646
H	4.969048	-2.216459	3.340234
H	2.764794	-1.680077	4.619557
H	3.469636	1.076126	4.023547
H	3.833211	2.388685	1.308699
H	5.057126	1.982552	2.498087
H	4.709103	-0.550426	3.799798
H	2.678179	-2.742251	3.228443
H	2.628356	2.435349	3.308735
H	4.856687	-1.707830	1.017411
H	0.849905	-1.307568	2.725198
H	0.975655	1.037761	2.362462
H	4.818026	0.537099	0.193585

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B3LYP/BS1 SCF energy: -3092.857813 a.u.

M06/BS2 SCF energy in PhMe: -3091.92709113 a.u.

M06/BS2 Free energy in PhMe: -3091.15910913 a.u.

C	1.097341	0.644823	1.114400
C	2.213061	1.451398	1.811627
H	1.805149	2.333669	2.316819
H	2.724481	0.839247	2.563620
H	2.965069	1.799024	1.096787
C	1.674149	-0.693011	0.565711
H	0.862254	-1.243945	0.058967
H	1.997218	-1.315726	1.411151
C	0.035379	0.318964	2.206588
H	-0.325816	1.258213	2.638494
H	0.526065	-0.232974	3.015895
C	0.473865	1.446069	-0.061586
H	-0.371541	0.867641	-0.460401
H	1.211118	1.521780	-0.868446
P	3.065161	-0.566786	-0.701162
P	-0.204787	3.154059	0.354954
P	-1.492810	-0.677498	1.692119
Ni	-1.390107	-1.753181	-0.193716
C	1.247235	4.256432	-0.025055
C	1.680052	5.133607	0.980378
C	1.918637	4.271101	-1.258378
C	2.760466	5.994240	0.767996
H	1.165019	5.140937	1.938098
C	2.996932	5.128930	-1.474503
H	1.590977	3.617654	-2.062595
C	3.421864	5.992094	-0.460177
H	3.081840	6.665501	1.560343
H	3.503891	5.127688	-2.436245
H	4.261318	6.661361	-0.630144
C	-1.285800	3.477917	-1.119543
C	-2.247367	4.493185	-0.981012
C	-1.220983	2.788977	-2.342023
C	-3.103607	4.823489	-2.031897
H	-2.327916	5.024568	-0.035711
C	-2.085096	3.110397	-3.392018
H	-0.496534	1.993362	-2.487272
C	-3.026354	4.130187	-3.241656
H	-3.836675	5.615828	-1.902842
H	-2.018513	2.563606	-4.329313
H	-3.697049	4.379786	-4.059669
C	4.589986	-0.606524	0.365797
C	5.482126	0.472015	0.270513
C	4.902788	-1.658128	1.242168
C	6.647880	0.509213	1.040096
H	5.259391	1.289841	-0.410613
C	6.066107	-1.624635	2.010991
H	4.242659	-2.518964	1.313442
C	6.940951	-0.538646	1.913131
H	7.325719	1.354615	0.954455
H	6.294146	-2.448384	2.682896
H	7.848275	-0.514111	2.511064
C	3.084825	-2.288828	-1.393265
C	3.796418	-2.471419	-2.591798
C	2.448629	-3.404119	-0.823519
C	3.886825	-3.727139	-3.192450
H	4.281339	-1.617560	-3.059731
C	2.529543	-4.661008	-1.429584
H	1.875827	-3.302546	0.093153

C	3.251097	-4.827256	-2.612628
H	4.445532	-3.844451	-4.117450
H	2.027317	-5.510216	-0.972929
H	3.312685	-5.805349	-3.082310
C	-1.729001	-1.806928	3.145283
C	-0.652496	-2.588020	3.599925
C	-2.988557	-2.004764	3.732201
C	-0.823444	-3.518098	4.624964
H	0.329645	-2.477934	3.146960
C	-3.160380	-2.939762	4.755552
H	-3.840863	-1.423764	3.394484
C	-2.079616	-3.696787	5.208921
H	0.025576	-4.105646	4.964985
H	-4.143893	-3.073177	5.198876
H	-2.214264	-4.421838	6.007015
C	-2.849814	0.564805	1.892916
C	-3.686090	0.835896	0.801204
C	-3.055014	1.268082	3.092647
C	-4.701699	1.790925	0.900614
H	-3.529412	0.298901	-0.130554
C	-4.071966	2.215803	3.194896
H	-2.423503	1.068347	3.954569
C	-4.896802	2.480111	2.097074
H	-5.334398	1.995978	0.041436
H	-4.220125	2.750608	4.129501
H	-5.687091	3.222039	2.177013
C	-2.958565	-2.877261	-4.716898
C	-4.074578	-2.647064	-4.012836
C	-1.306627	-2.694673	-1.938934
C	-4.268522	-1.888133	-2.716623
C	-2.460972	-3.062079	-1.222862
C	-3.924822	-2.720077	-1.462304
H	-3.708595	-0.948846	-2.703289
H	-5.326734	-1.605323	-2.645899
H	-4.326503	-2.205286	-0.576952
H	-4.482319	-3.667727	-1.524497
C	-1.533314	-2.437797	-4.490996
H	-1.250887	-1.751377	-5.306822
H	-0.885697	-3.317681	-4.626527
C	-1.178619	-1.775365	-3.143465
H	-0.128885	-1.457627	-3.205298
H	-1.757722	-0.856101	-3.021586
H	-3.078729	-3.479224	-5.620027
H	-4.986088	-3.103445	-4.401767
H	-0.460806	-3.382360	-1.842193
H	-2.348694	-3.963009	-0.611086

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B3LYP/BS1 SCF energy: -2780.820703 a.u.

M06/BS2 SCF energy in PhMe: -2780.04231044 a.u.

M06/BS2 Free energy in PhMe: -2779.43976144 a.u.

C	-0.166647	-0.193861	1.547818
C	0.261720	-0.447305	3.016540
H	1.030515	0.262651	3.339357
H	-0.594501	-0.337817	3.693566
H	0.667561	-1.457381	3.142465
C	-1.331778	-1.207504	1.295993
H	-2.180292	-0.905342	1.923514
H	-1.001134	-2.187361	1.665665
C	-0.620175	1.298451	1.496194
H	0.194599	1.914287	1.894477
H	-1.459971	1.415564	2.191092
C	1.012791	-0.493040	0.583334
H	0.727225	-0.173147	-0.425346
H	1.169851	-1.576959	0.537728
P	-2.062163	-1.436275	-0.431180
P	2.647266	0.364393	0.974758
P	-1.214644	2.089844	-0.124053
Ni	-2.100155	0.510771	-1.187591
C	3.525668	-0.919117	2.000994
C	4.021870	-0.523460	3.251972
C	3.736828	-2.244989	1.588917
C	4.700007	-1.425759	4.076014
H	3.874291	0.502082	3.582259
C	4.413760	-3.148629	2.408076
H	3.383528	-2.573729	0.614929
C	4.895798	-2.741327	3.655546
H	5.075519	-1.099571	5.042625
H	4.570423	-4.170540	2.071542
H	5.424626	-3.445837	4.292332
C	3.545655	0.183146	-0.639690
C	4.654414	1.023407	-0.837108
C	3.203845	-0.716201	-1.663120
C	5.410341	0.956847	-2.007806
H	4.922379	1.741495	-0.065747

C	3.953401	-0.776078	-2.840530
H	2.349140	-1.377253	-1.556449
C	5.060047	0.056187	-3.015651
H	6.266627	1.614155	-2.136612
H	3.670990	-1.479247	-3.620352
H	5.642529	0.006304	-3.932035
C	-0.990288	-2.767301	-1.174687
C	-0.363757	-2.508134	-2.402645
C	-0.794351	-4.021111	-0.574534
C	0.446427	-3.470882	-3.011391
H	-0.516620	-1.542755	-2.879636
C	0.016281	-4.983249	-1.178015
H	-1.290005	-4.258867	0.363136
C	0.640522	-4.709721	-2.398127
H	0.919341	-3.253809	-3.965963
H	0.155057	-5.949654	-0.699817
H	1.268298	-5.461090	-2.869964
C	-3.604456	-2.403404	-0.034373
C	-4.609879	-2.420977	-1.015587
C	-3.834366	-3.098264	1.164428
C	-5.799108	-3.122040	-0.815343
H	-4.455685	-1.869657	-1.940513
C	-5.029192	-3.792426	1.371094
H	-3.085945	-3.102722	1.951121
C	-6.013148	-3.809231	0.381607
H	-6.562311	-3.122936	-1.589321
H	-5.188880	-4.321368	2.307482
H	-6.942420	-4.348819	0.544367
C	-2.259879	3.467003	0.566821
C	-3.410324	3.119727	1.299288
C	-2.024490	4.825590	0.308564
C	-4.279037	4.097918	1.780278
H	-3.637751	2.071818	1.482462
C	-2.900100	5.805855	0.783653
H	-1.154033	5.126531	-0.264817
C	-4.026226	5.448399	1.524735
H	-5.158821	3.804656	2.347618
H	-2.695825	6.852805	0.573176
H	-4.704846	6.212301	1.894913
C	0.278479	2.981661	-0.767061
C	0.545132	2.901017	-2.142429
C	1.141171	3.743943	0.038216
C	1.641873	3.560975	-2.701212
H	-0.116057	2.312461	-2.774141
C	2.236430	4.405706	-0.517620
H	0.955006	3.834729	1.104583
C	2.490052	4.313589	-1.888642
H	1.833963	3.483154	-3.768003
H	2.893065	4.991376	0.120587
H	3.346151	4.826001	-2.319664

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B3LYP/BS1 SCF energy: -3189.973717 a.u.

M06/BS2 SCF energy in PhMe: -3189.01807532 a.u.

M06/BS2 Free energy in PhMe: -3188.15928832 a.u.

C	-1.092052	0.214526	-1.564469
C	-1.776452	0.530820	-2.911703
H	-2.228431	1.528175	-2.911715
H	-1.059557	0.500439	-3.739667
H	-2.566816	-0.199291	-3.121055
C	-0.341719	-1.140719	-1.757921
H	0.503630	-0.955035	-2.427686
H	-1.002269	-1.839682	-2.285015
C	-0.103968	1.342156	-1.135100
H	0.619609	0.937588	-0.413012
H	-0.677229	2.105066	-0.596109
C	-2.171381	0.057059	-0.452294
H	-1.657116	-0.081194	0.505842
H	-2.755354	-0.851850	-0.636550
P	0.372572	-2.045208	-0.252786
P	-3.327494	1.526923	-0.210093
P	0.745820	2.372262	-2.468898
Ni	1.442238	-1.069509	1.223144
C	-4.794045	1.064099	-1.258731
C	-5.224863	1.984187	-2.225860
C	-5.497908	-0.143709	-1.124286
C	-6.320621	1.703589	-3.046541
H	-4.694989	2.927041	-2.337705
C	-6.592294	-0.426681	-1.941371
H	-5.198602	-0.865007	-0.368304
C	-7.005418	0.496447	-2.906529
H	-6.637725	2.428222	-3.792184
H	-7.126610	-1.366120	-1.822911
H	-7.859008	0.275489	-3.542192
C	-3.997074	1.196943	1.489969

C	-4.610691	2.279052	2.144356
C	-3.930515	-0.034296	2.162730
C	-5.156322	2.134767	3.420280
H	-4.656311	3.245611	1.647611
C	-4.467163	-0.177089	3.444825
H	-3.458953	-0.893675	1.696802
C	-5.084158	0.903957	4.076241
H	-5.629348	2.985000	3.905200
H	-4.404552	-1.139543	3.946921
H	-5.501777	0.789991	5.073295
C	-1.104059	-3.036301	0.327939
C	-1.424135	-3.037932	1.693186
C	-1.898350	-3.802022	-0.541890
C	-2.512794	-3.770073	2.177340
H	-0.804028	-2.456968	2.371773
C	-2.989893	-4.528527	-0.064364
H	-1.656996	-3.847360	-1.600647
C	-3.302332	-4.512441	1.297961
H	-2.740401	-3.761282	3.240672
H	-3.593167	-5.113012	-0.754587
H	-4.150760	-5.080953	1.670141
C	1.335920	-3.403270	-1.108457
C	1.399037	-4.679109	-0.519358
C	2.106883	-3.173434	-2.259386
C	2.190493	-5.688626	-1.067037
H	0.819813	-4.887642	0.375323
C	2.898111	-4.184727	-2.810137
H	2.112207	-2.198975	-2.734980
C	2.943236	-5.447318	-2.218666
H	2.216421	-6.666892	-0.593001
H	3.479816	-3.979076	-3.705480
H	3.557814	-6.234129	-2.648351
C	1.484247	3.677840	-1.369676
C	0.601140	4.552149	-0.707906
C	2.862365	3.910940	-1.241528
C	1.079153	5.598747	0.079625
H	-0.473473	4.418707	-0.812377
C	3.341589	4.969474	-0.463854
H	3.570371	3.265774	-1.751375
C	2.454197	5.812970	0.205382
H	0.375812	6.254447	0.586895
H	4.413847	5.133234	-0.385027
H	2.828015	6.634957	0.810250
C	2.240728	1.408665	-2.990266
C	2.656374	1.564359	-4.323318
C	2.992600	0.568403	-2.151400
C	3.794749	0.913142	-4.804329
H	2.079985	2.203563	-4.987883
C	4.128479	-0.087590	-2.631432
H	2.687414	0.410710	-1.119112
C	4.534094	0.085854	-3.957652
H	4.099850	1.049349	-5.838679
H	4.692472	-0.739521	-1.969343
H	5.419042	-0.424992	-4.328497
C	4.012314	-0.434890	2.616460
C	4.414096	0.839900	1.848472
C	3.901925	2.132650	2.495258
C	2.383146	2.073823	2.698605
C	1.921210	0.840241	3.498536
N	2.511149	-0.392394	2.837139
H	4.411770	2.312634	3.450767
H	5.507517	0.862194	1.753920
H	2.029229	2.977932	3.209590
H	4.145671	2.985796	1.851789
H	1.894930	2.053673	1.716462
H	4.006564	0.768420	0.832364
H	2.281325	-1.190233	3.439976
C	4.310538	-1.675517	1.756098
H	5.378193	-1.706546	1.504944
H	4.063619	-2.600255	2.292127
H	3.721649	-1.665358	0.830787
C	4.830008	-0.586811	3.920570
H	4.412081	-1.376208	4.557509
H	5.855199	-0.880375	3.668892
H	4.894701	0.327208	4.512613
C	0.391122	0.711368	3.417387
H	0.031890	-0.136783	4.014060
H	-0.083567	1.620081	3.806409
H	0.067045	0.553347	2.382235
C	2.282743	0.974085	4.996687
H	1.623267	1.715855	5.460749
H	2.129939	0.025008	5.525565
H	3.308420	1.299010	5.175920

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B3LYP/BS1 SCF energy: -3973.867836 a.u.

M06/BS2 SCF energy in PhMe: -3972.95033523 a.u.

M06/BS2 Free energy in PhMe: -3972.24869723 a.u.

C	-2.020575	0.383083	1.857258
C	-3.070563	0.532780	2.985668
H	-3.795138	1.320547	2.750315
H	-2.584985	0.791216	3.934740
H	-3.627521	-0.397888	3.140565
C	-1.104452	-0.806958	2.274869
H	-0.621683	-0.539903	3.223420
H	-1.740203	-1.673269	2.491147
C	-1.259462	1.745264	1.823524
H	-2.003172	2.552488	1.810524
H	-0.717976	1.851187	2.771472
C	-2.722953	0.144106	0.492618
H	-1.959598	-0.109328	-0.251722
P	0.314363	-1.349521	1.139890
P	0.020606	2.075302	0.470686
Ni	1.076712	0.302600	0.069178
C	-0.393590	-2.791205	0.203327
C	-0.040918	-2.908051	-1.150701
C	-1.236684	-3.767843	0.759614
C	-0.513400	-3.968011	-1.927826
H	0.608131	-2.155715	-1.592296
C	-1.708190	-4.829404	-0.014206
H	-1.525780	-3.710321	1.804969
C	-1.349077	-4.930486	-1.360525
H	-0.232838	-4.036602	-2.975590
H	-2.360528	-5.574698	0.433824
H	-1.722849	-5.753883	-1.963641
C	1.395684	-2.180753	2.413577
C	1.661700	-3.558814	2.454088
C	2.061750	-1.353304	3.338481
C	2.548374	-4.091026	3.396001
H	1.171150	-4.225425	1.752402
C	2.939540	-1.883981	4.282863
H	1.898288	-0.277923	3.306182
C	3.187655	-3.259263	4.316003
H	2.730054	-5.163286	3.413735
H	3.436002	-1.222919	4.989030
H	3.874013	-3.675320	5.048684
C	0.858510	3.564746	1.216248
C	1.469211	3.442970	2.478541
C	1.038526	4.768588	0.515090
C	2.206701	4.490077	3.029733
H	1.380613	2.513302	3.035847
C	1.782182	5.816416	1.063556
H	0.592562	4.894760	-0.466397
C	2.366058	5.685411	2.324214
H	2.660882	4.370522	4.010441
H	1.900355	6.739946	0.501749
H	2.941293	6.502493	2.751463
C	-1.016679	2.841664	-0.873940
C	-0.836307	2.376133	-2.185184
C	-1.972678	3.846741	-0.649224
C	-1.592412	2.891899	-3.242147
H	-0.097479	1.599754	-2.370259
C	-2.729206	4.364415	-1.701646
H	-2.120254	4.242777	0.352176
C	-2.542868	3.885210	-3.001481
H	-1.435888	2.518297	-4.251008
H	-3.462317	5.143582	-1.508070
H	-3.132799	4.287980	-3.820753
C	4.776830	-3.641178	-0.022039
C	4.553215	-2.263427	0.019155
C	5.173499	-1.469257	-0.938877
C	5.998921	-1.990330	-1.930911
C	6.207325	-3.370483	-1.958874
C	5.599435	-4.193310	-1.007112
H	4.300445	-4.274101	0.720021
H	3.911961	-1.815280	0.770689
H	6.463307	-1.328390	-2.653663
H	6.848126	-3.799106	-2.723944
H	5.767895	-5.266131	-1.033363
O	5.007603	-0.060099	-0.854172
S	3.875102	0.614862	-1.826169
O	2.547627	0.072875	-1.516102
O	4.330802	0.673185	-3.207492
C	4.046975	2.324801	-1.061423
F	3.121943	3.097905	-1.624227
F	5.259514	2.798189	-1.335337
F	3.867050	2.265936	0.249631
H	-3.186933	1.080565	0.161555
P	-4.004254	-1.238597	0.437390
C	-5.586360	-0.309988	0.770045
C	-6.401037	-0.761829	1.818650

C	-6.014910	0.799206	0.022969
C	-7.603957	-0.119339	2.124044
H	-6.087743	-1.624960	2.401388
C	-7.215041	1.443161	0.324233
H	-5.414745	1.156757	-0.809886
C	-8.012307	0.986182	1.377695
H	-8.220232	-0.484038	2.941995
H	-7.532053	2.299510	-0.265983
H	-8.948187	1.487561	1.610746
C	-4.158561	-1.514332	-1.392487
C	-4.798340	-2.698866	-1.795682
C	-3.688618	-0.642355	-2.388183
C	-4.981806	-2.995858	-3.146169
H	-5.152342	-3.396816	-1.040503
C	-3.862171	-0.943826	-3.741415
H	-3.181311	0.279622	-2.121687
C	-4.511658	-2.117926	-4.125126
H	-5.483623	-3.916355	-3.434003
H	-3.489468	-0.254637	-4.495286
H	-4.646404	-2.349591	-5.178580

^{os}TS9

B3LYP/BS1 SCF energy: -3973.808893 a.u.

M06/BS2 SCF energy in PhMe: -3972.94419642 a.u.

M06/BS2 Free energy in PhMe: -3972.24478942 a.u.

C	-1.939123	-0.086970	1.934221
C	-2.962175	-0.141988	3.095397
H	-3.637304	0.720514	3.068474
H	-2.448094	-0.141209	4.064258
H	-3.575681	-1.047891	3.046737
C	-1.105905	-1.395362	2.027048
H	-0.672120	-1.448118	3.033745
H	-1.786050	-2.251378	1.948015
C	-1.074223	1.178775	2.213823
H	-1.746685	2.025698	2.395786
H	-0.530060	1.021204	3.153606
C	-2.670529	0.058016	0.570702
H	-1.945900	-0.071520	-0.240070
P	0.360301	-1.703611	0.881026
P	0.233484	1.712398	0.981708
Ni	1.549993	0.012167	0.405450
C	-0.344659	-2.504066	-0.626229
C	0.206468	-2.145782	-1.868643
C	-1.384671	-3.448948	-0.596859
C	-0.263128	-2.726095	-3.048641
H	0.998796	-1.402795	-1.915283
C	-1.849430	-4.030395	-1.777600
H	-1.843862	-3.735167	0.344131
C	-1.288422	-3.671372	-3.004986
H	0.173633	-2.433557	-3.999383
H	-2.656577	-4.756629	-1.737301
H	-1.656907	-4.120514	-3.923276
C	1.146861	-3.083818	1.847270
C	0.981216	-4.448142	1.567072
C	1.979148	-2.715356	2.919419
C	1.627224	-5.415978	2.341763
H	0.361068	-4.762863	0.734742
C	2.613146	-3.680927	3.699653
H	2.150857	-1.661037	3.127028
C	2.440920	-5.037451	3.410541
H	1.491120	-6.468523	2.106399
H	3.254364	-3.374498	4.521888
H	2.942576	-5.792080	4.010316
C	1.142103	2.970500	1.987787
C	1.818692	2.533054	3.141408
C	1.273114	4.314000	1.605889
C	2.576006	3.418285	3.905995
H	1.767107	1.487779	3.437351
C	2.037714	5.198701	2.370095
H	0.781186	4.675081	0.709439
C	2.686681	4.757504	3.523201
H	3.088089	3.060008	4.795207
H	2.125560	6.236193	2.058132
H	3.281424	5.447779	4.115253
C	-0.695675	2.713913	-0.264308
C	-0.405807	2.526471	-1.624528
C	-1.679123	3.652022	0.097259
C	-1.094134	3.254200	-2.600760
H	0.365155	1.822141	-1.923455
C	-2.365786	4.374568	-0.878350
H	-1.905474	3.832336	1.144892
C	-2.076398	4.173508	-2.231567
H	-0.853090	3.101701	-3.649353
H	-3.122581	5.096873	-0.583261
H	-2.611110	4.737539	-2.991342

C	4.368199	-3.435916	-0.019727
C	4.091283	-2.105117	-0.400236
C	5.039537	-1.530364	-1.152285
C	6.229746	-2.016579	-1.615349
C	6.485201	-3.343526	-1.223641
C	5.559388	-4.038146	-0.435340
H	3.658014	-3.981136	0.596232
H	3.143800	-1.597056	-0.068390
H	6.919959	-1.445233	-2.227962
H	7.407682	-3.825604	-1.541049
H	5.770154	-5.062686	-0.140780
O	4.873551	0.550432	-2.000076
S	3.563337	1.135524	-1.598136
O	3.257566	0.881413	-0.141485
O	2.426981	0.907425	-2.508195
C	3.857289	2.974771	-1.615476
F	2.724361	3.612862	-1.280394
F	4.224291	3.369847	-2.838744
F	4.811624	3.303211	-0.743345
H	-3.061141	1.077601	0.481667
P	-4.064394	-1.169229	0.234831
C	-5.553188	-0.243538	0.863753
C	-6.370178	-0.878584	1.810557
C	-5.913253	1.041335	0.424975
C	-7.507886	-0.245722	2.318719
H	-6.112065	-1.878174	2.152306
C	-7.047913	1.676063	0.930040
H	-5.313093	1.545383	-0.328481
C	-7.847436	1.034332	1.880576
H	-8.127526	-0.753853	3.053173
H	-7.313321	2.669764	0.577734
H	-8.732682	1.529011	2.271661
C	-4.301426	-0.969154	-1.594639
C	-5.134711	-1.913259	-2.220260
C	-3.716311	0.029036	-2.389321
C	-5.390381	-1.853669	-3.589562
H	-5.587289	-2.704057	-1.625835
C	-3.962213	0.082131	-3.764113
H	-3.062007	0.775750	-1.951505
C	-4.801119	-0.854586	-4.368040
H	-6.042657	-2.591375	-4.050166
H	-3.495351	0.862366	-4.359863
H	-4.991650	-0.809905	-5.437145

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B3LYP/BS1 SCF energy: -3742.323444 a.u.

M06/BS2 SCF energy in PhMe: -3741.51991789 a.u.

M06/BS2 Free energy in PhMe: -3740.90170589 a.u.

C	-1.408177	-0.225710	-2.035486
C	-2.422733	-0.479147	-3.177030
H	-2.867211	-1.477049	-3.094290
H	-1.933353	-0.403148	-4.155718
H	-3.238274	0.250753	-3.155388
C	-0.916707	1.240235	-2.210784
H	-0.457931	1.332064	-3.202572
H	-1.789656	1.902000	-2.211972
C	-0.262821	-1.260159	-2.273181
H	-0.725454	-2.240841	-2.437702
H	0.247040	-0.996588	-3.209337
C	-2.073126	-0.468007	-0.653798
H	-1.383394	-0.153576	0.137299
P	0.340959	1.950918	-1.006623
P	1.101001	-1.460310	-1.007189
Ni	1.866579	0.494217	-0.195097
C	-0.640071	2.858898	0.255219
C	-0.304924	2.688853	1.608398
C	-1.690363	3.729772	-0.084637
C	-1.006679	3.379519	2.599905
H	0.499843	2.017719	1.897466
C	-2.386082	4.418246	0.907807
H	-1.963401	3.881590	-1.125315
C	-2.044856	4.242935	2.252223
H	-0.737322	3.235428	3.642094
H	-3.195661	5.088728	0.632191
H	-2.590224	4.778528	3.024647
C	1.137726	3.259909	-2.041203
C	1.143739	4.617001	-1.690338
C	1.855014	2.854751	-3.181258
C	1.831993	5.547727	-2.473116
H	0.615208	4.953096	-0.804743
C	2.535173	3.785603	-3.964230
H	1.896189	1.802314	-3.453746
C	2.524058	5.137742	-3.612311
H	1.825913	6.595850	-2.186172
H	3.082466	3.453406	-4.842308

H	3.059097	5.863762	-4.218224
C	2.366843	-2.435348	-1.936176
C	3.690812	-2.378172	-1.468077
C	2.082174	-3.221470	-3.064184
C	4.700884	-3.097299	-2.108253
H	3.932422	-1.770708	-0.600649
C	3.096168	-3.933960	-3.707152
H	1.070777	-3.283384	-3.454399
C	4.406737	-3.874664	-3.229969
H	5.718924	-3.041749	-1.732838
H	2.859999	-4.535636	-4.580996
H	5.195008	-4.428851	-3.732316
C	0.434637	-2.670894	0.220085
C	0.506095	-2.349800	1.584333
C	-0.114565	-3.905140	-0.164502
C	0.024075	-3.246342	2.543400
H	0.943960	-1.407634	1.903851
C	-0.598967	-4.793959	0.794138
H	-0.154028	-4.185380	-1.214159
C	-0.532049	-4.464274	2.151374
H	0.093422	-2.988874	3.596807
H	-1.020749	-5.746382	0.483877
H	-0.905017	-5.160052	2.898318
O	4.290391	1.815641	2.913431
S	3.520847	0.738377	2.294880
O	3.560098	0.760891	0.765749
O	2.159955	0.462177	2.805168
C	4.476534	-0.823364	2.631531
F	3.863267	-1.876351	2.053787
F	4.548894	-1.047116	3.947058
F	5.714447	-0.736080	2.134555
H	-2.232292	-1.543917	-0.518756
P	-3.692334	0.456247	-0.341107
C	-4.957467	-0.807418	-0.861779
C	-5.901683	-0.426248	-1.826610
C	-5.031095	-2.105784	-0.331204
C	-6.884195	-1.318907	-2.263526
H	-5.866295	0.579758	-2.238190
C	-6.010608	-2.999340	-0.764574
H	-4.329668	-2.418456	0.438130
C	-6.938625	-2.608412	-1.734318
H	-7.606375	-1.005089	-3.012863
H	-6.054790	-3.999752	-0.341340
H	-7.702823	-3.304831	-2.069416
C	-3.823621	0.344038	1.505016
C	-4.733423	1.221290	2.119493
C	-3.091889	-0.534377	2.320598
C	-4.921328	1.210666	3.501636
H	-5.295575	1.922352	1.507049
C	-3.269769	-0.536390	3.706180
H	-2.372404	-1.223394	1.889535
C	-4.186480	0.331854	4.300322
H	-5.633800	1.894786	3.955512
H	-2.688532	-1.220158	4.319430
H	-4.323348	0.327890	5.378466

TS1a

B3LYP/BS1 SCF energy: -4728.622377 a.u.

M06/BS2 SCF energy in PhMe: -4727.39304824 a.u.

M06/BS2 Free energy in PhMe: -4726.32259624 a.u.

C	3.255722	-1.825656	-0.951846
C	4.534112	-2.514398	-1.488921
H	5.360774	-2.438813	-0.775984
H	4.351097	-3.579978	-1.675087
H	4.862720	-2.055929	-2.427735
C	2.146596	-2.159963	-1.988447
H	2.018064	-3.248788	-2.002361
H	2.495714	-1.881073	-2.989206
C	2.944699	-2.496376	0.410032
H	3.784240	-2.319172	1.091117
H	2.907255	-3.577871	0.242364
C	3.464169	-0.289469	-0.848199
H	2.595761	0.156981	-0.354919
H	3.496383	0.139813	-1.855893
P	0.441198	-1.428531	-1.770865
P	4.975119	0.296498	0.129157
P	1.396244	-2.076940	1.408543
Ni	-0.479422	-1.491076	0.354739
C	6.302674	0.279895	-1.174873
C	7.500862	-0.389871	-0.886998
C	6.175243	0.914964	-2.422099
C	8.540538	-0.438712	-1.820353
H	7.619295	-0.876590	0.078375
C	7.208869	0.865359	-3.357181

H	5.269097	1.467359	-2.657703
C	8.394123	0.185779	-3.058913
H	9.462025	-0.961798	-1.577792
H	7.094041	1.362677	-4.317143
H	9.200087	0.150481	-3.787331
C	4.655277	2.123345	0.242535
C	5.762781	2.990342	0.299836
C	3.375520	2.676201	0.406980
C	5.593169	4.360446	0.494104
H	6.767742	2.593699	0.183793
C	3.204865	4.049578	0.600431
H	2.485487	2.058537	0.398444
C	4.311815	4.896715	0.641918
H	6.465337	5.008907	0.529035
H	2.200598	4.442883	0.720931
H	4.178529	5.964703	0.793611
C	0.593211	0.219633	-2.574432
C	0.272725	1.373750	-1.848797
C	1.092176	0.348424	-3.884214
C	0.464642	2.638297	-2.415460
H	-0.120128	1.311328	-0.839836
C	1.273204	1.609358	-4.448989
H	1.331515	-0.535125	-4.470607
C	0.963445	2.757428	-3.711745
H	0.216154	3.516852	-1.829797
H	1.657551	1.696399	-5.462030
H	1.113417	3.740549	-4.150239
C	-0.528335	-2.437134	-2.980220
C	-1.414637	-1.831722	-3.884003
C	-0.453726	-3.839809	-2.954440
C	-2.185941	-2.607058	-4.751736
H	-1.499986	-0.750705	-3.916522
C	-1.220565	-4.612997	-3.825266
H	0.199058	-4.343070	-2.246101
C	-2.088317	-3.998309	-4.729747
H	-2.864520	-2.118618	-5.445903
H	-1.142675	-5.696464	-3.792836
H	-2.687155	-4.600207	-5.407627
C	1.255540	-3.655898	2.366054
C	1.161408	-4.870865	1.666448
C	1.158546	-3.680316	3.764224
C	1.002611	-6.078876	2.345732
H	1.201794	-4.883178	0.579791
C	1.006763	-4.890315	4.444373
H	1.193213	-2.754564	4.326943
C	0.931231	-6.092222	3.740288
H	0.934664	-7.007486	1.785134
H	0.938313	-4.887555	5.528753
H	0.811429	-7.032169	4.272102
C	2.010005	-0.819154	2.600295
C	1.426417	0.453909	2.628720
C	3.082982	-1.097437	3.467589
C	1.880043	1.426324	3.524431
H	0.619007	0.710634	1.954745
C	3.534896	-0.127375	4.359689
H	3.561032	-2.073208	3.458598
C	2.929016	1.132939	4.394002
H	1.396896	2.398843	3.531341
H	4.361804	-0.355201	5.027060
H	3.282091	1.885194	5.094270
C	-2.567981	-2.821675	3.834932
C	-2.906992	-1.624752	4.465332
C	-2.508556	-0.415600	3.889823
C	-1.779336	-0.408181	2.696725
C	-1.397216	-1.604160	2.063897
C	-1.813290	-2.807953	2.654924
H	-2.877385	-3.773246	4.262880
H	-3.477909	-1.632254	5.390898
H	-2.765586	0.530058	4.361953
H	-1.529470	0.549806	2.251680
H	-1.546236	-3.762143	2.207451
O	-0.231963	2.738912	0.933572
S	-1.225621	3.561568	1.669457
O	-0.893997	3.871974	3.067429
O	-2.642403	3.158759	1.423207
C	-1.131017	5.199108	0.791481
F	0.082265	5.759311	0.931327
F	-2.047603	6.056896	1.256505
F	-1.356235	5.038291	-0.535694
O	-2.061482	-0.608706	-0.331307
C	-3.253675	-0.751498	-0.718644
C	-3.795876	-2.130758	-0.957419

C	-5.043094	-2.219122	-1.598189
C	-3.164916	-3.320405	-0.558150
C	-5.645217	-3.453024	-1.839700
C	-3.768924	-4.555578	-0.780122
C	-5.009689	-4.624691	-1.422168
H	-5.531586	-1.300605	-1.912347
H	-6.607670	-3.503512	-2.342358
H	-5.479881	-5.589883	-1.593767
H	-3.277225	-5.468563	-0.452764
H	-2.202314	-3.263489	-0.059387
H	-4.078591	0.702276	-0.579410
C	-4.623029	2.556998	-1.606000
C	-5.859832	2.019500	-2.352214
C	-7.124715	1.980972	-1.485548
C	-6.885161	1.147872	-0.219328
C	-5.679853	1.621491	0.617208
N	-4.477029	1.769964	-0.310618
H	-7.437995	2.998607	-1.222192
H	-6.019499	2.638191	-3.243936
H	-7.772877	1.160003	0.424787
H	-7.952366	1.547206	-2.060097
H	-6.723244	0.100704	-0.506242
H	-5.639719	1.004209	-2.710633
H	-3.709151	2.195185	0.242195
C	-3.345753	2.286235	-2.419205
H	-3.419345	2.786299	-3.391340
H	-2.464852	2.679145	-1.903338
H	-3.195425	1.216369	-2.586694
C	-4.714849	4.075708	-1.363902
H	-3.921449	4.414273	-0.692989
H	-4.583564	4.587905	-2.324090
H	-5.674136	4.396158	-0.954841
C	-5.299882	0.552098	1.654186
H	-4.424548	0.858168	2.233101
H	-6.134812	0.409095	2.348916
H	-5.079704	-0.411545	1.187446
C	-5.980254	2.930080	1.373916
H	-6.659347	2.704565	2.203824
H	-5.063081	3.355514	1.791363
H	-6.466930	3.686633	0.755682

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B3LYP/BS1 SCF energy: -4728.622455 a.u.

M06/BS2 SCF energy in PhMe: -4727.39381990 a.u.

M06/BS2 Free energy in PhMe: -4726.32293890 a.u.

C	3.287614	-1.804653	-0.928752
C	4.579189	-2.476319	-1.455442
H	5.400903	-2.383005	-0.738816
H	4.414002	-3.545865	-1.635352
H	4.905117	-2.018833	-2.395673
C	2.188228	-2.163794	-1.967524
H	2.077686	-3.254720	-1.975374
H	2.537224	-1.885650	-2.968532
C	2.981554	-2.469847	0.437051
H	3.816545	-2.277097	1.119502
H	2.958800	-3.552984	0.276941
C	3.470478	-0.264581	-0.835696
H	2.594386	0.170061	-0.345642
H	3.496209	0.158174	-1.846285
P	0.468540	-1.461051	-1.762391
P	4.970747	0.353504	0.137916
P	1.422723	-2.063539	1.424696
Ni	-0.459037	-1.517369	0.357876
C	6.298321	0.352778	-1.166378
C	7.507347	-0.296040	-0.875842
C	6.160520	0.980619	-2.416172
C	8.547662	-0.331670	-1.809069
H	7.633777	-0.776768	0.091514
C	7.194866	0.944219	-3.351058
H	5.245362	1.516939	-2.654086
C	8.391082	0.285354	-3.050120
H	9.477586	-0.838627	-1.564452
H	7.071894	1.435658	-4.313042
H	9.197534	0.260315	-3.778426
C	4.620421	2.175442	0.240565
C	5.714635	3.058745	0.305024
C	3.331366	2.710580	0.389850
C	5.523568	4.426949	0.492001
H	6.726335	2.676162	0.200497
C	3.139160	4.082091	0.576495
H	2.450692	2.079795	0.374517

C	4.233250	4.945295	0.625546
H	6.385937	5.088046	0.532772
H	2.128376	4.461704	0.686086
H	4.083138	6.011772	0.772024
C	0.596592	0.184444	-2.576556
C	0.251022	1.337158	-1.859862
C	1.104424	0.314928	-3.882686
C	0.428363	2.601710	-2.431098
H	-0.151575	1.271938	-0.855102
C	1.270064	1.575750	-4.452601
H	1.363085	-0.567675	-4.462234
C	0.936522	2.722373	-3.723674
H	0.163022	3.479440	-1.851532
H	1.661480	1.663844	-5.462851
H	1.075464	3.705604	-4.165587
C	-0.472709	-2.498717	-2.969406
C	-1.347422	-1.921429	-3.902095
C	-0.384750	-3.899795	-2.912893
C	-2.093336	-2.722590	-4.768717
H	-1.444706	-0.842385	-3.957558
C	-1.126162	-4.698740	-3.782179
H	0.258429	-4.381241	-2.180878
C	-1.981814	-4.111889	-4.716331
H	-2.763468	-2.255628	-5.485523
H	-1.038661	-5.780463	-3.725161
H	-2.561108	-4.733889	-5.393061
C	1.303974	-3.632543	2.401134
C	1.228352	-4.856764	1.715434
C	1.204573	-3.642420	3.799284
C	1.085405	-6.059015	2.408235
H	1.270378	-4.880863	0.629008
C	1.068229	-4.846568	4.493025
H	1.225426	-2.709959	4.351558
C	1.011229	-6.057435	3.802728
H	1.031572	-6.994837	1.858172
H	0.997377	-4.832314	5.577176
H	0.903470	-6.992828	4.345064
C	2.011301	-0.781965	2.604353
C	1.403081	0.479905	2.619359
C	3.087693	-1.030628	3.476350
C	1.836650	1.469913	3.505736
H	0.590981	0.712778	1.942200
C	3.519503	-0.043223	4.359357
H	3.584318	-1.997115	3.478001
C	2.889722	1.205568	4.379727
H	1.335459	2.433294	3.502739
H	4.349442	-0.248464	5.030294
H	3.227182	1.971644	5.072675
C	-2.542652	-2.854264	3.840665
C	-2.904857	-1.658671	4.460603
C	-2.526010	-0.447460	3.876232
C	-1.794037	-0.436754	2.684796
C	-1.388252	-1.630495	2.061944
C	-1.784977	-2.836311	2.662697
H	-2.836256	-3.807798	4.275399
H	-3.477842	-1.668851	5.384899
H	-2.800242	0.497016	4.341257
H	-1.559070	0.522142	2.233014
H	-1.500167	-3.789409	2.223719
O	-0.315248	2.738701	0.908251
S	-1.292373	3.574473	1.649553
O	-0.942606	3.899378	3.039301
O	-2.716655	3.177458	1.428573
C	-1.203824	5.201768	0.751600
F	0.005085	5.770612	0.889617
F	-2.128016	6.059615	1.201977
F	-1.422897	5.023407	-0.574423
O	-2.037144	-0.647657	-0.344853
C	-3.221140	-0.794728	-0.759008
C	-3.750080	-2.183556	-0.992577
C	-4.980798	-2.284001	-1.662293
C	-3.130118	-3.365707	-0.556135
C	-5.576799	-3.522059	-1.897954
C	-3.728940	-4.605022	-0.770545
C	-4.952771	-4.686085	-1.442885
H	-5.460082	-1.369603	-2.002870
H	-6.525985	-3.582005	-2.424481
H	-5.418962	-5.654305	-1.608615
H	-3.246537	-5.511943	-0.413448
H	-2.180239	-3.299620	-0.034429
H	-4.109808	0.775489	-0.571853
C	-4.653908	2.578021	-1.594079

C	-5.863663	2.005194	-2.357527
C	-7.136661	1.915907	-1.505885
C	-6.886313	1.079576	-0.243692
C	-5.711489	1.586907	0.615612
N	-4.501209	1.783989	-0.299074
H	-7.488679	2.919662	-1.238379
H	-6.033991	2.626577	-3.245285
H	-7.782897	1.054904	0.387514
H	-7.941157	1.458730	-2.094725
H	-6.682635	0.041534	-0.537292
H	-5.604210	1.001408	-2.721271
H	-3.745393	2.220839	0.266412
C	-3.356477	2.348912	-2.386327
H	-3.436600	2.837168	-3.363882
H	-2.499007	2.780467	-1.862278
H	-3.165567	1.283344	-2.539322
C	-4.797272	4.088570	-1.334566
H	-4.031143	4.443615	-0.640953
H	-4.657977	4.614940	-2.285620
H	-5.776156	4.374534	-0.946727
C	-5.302978	0.522587	1.645703
H	-4.455894	0.861450	2.247848
H	-6.145406	0.330279	2.319033
H	-5.025631	-0.421123	1.169069
C	-6.058541	2.880707	1.375041
H	-6.736230	2.627480	2.197767
H	-5.158880	3.332180	1.803295
H	-6.564717	3.624940	0.757632

2a

B3LYP/BS1 SCF energy: -3357.455815 a.u.

M06/BS2 SCF energy in PhMe: -3356.43304867 a.u.

M06/BS2 Free energy in PhMe: -3355.65334267 a.u.

C	-1.577140	-0.055775	-1.947535
C	-2.482265	-0.151337	-3.199446
H	-3.212950	0.664010	-3.225055
H	-1.883413	-0.089934	-4.116488
H	-3.035988	-1.096717	-3.217311
C	-0.505083	-1.170655	-2.122374
H	0.127779	-0.901297	-2.976654
H	-1.010368	-2.102183	-2.401785
C	-0.929207	1.355020	-1.978931
H	-1.717326	2.113256	-1.909846
H	-0.466196	1.481601	-2.963682
C	-2.411581	-0.303517	-0.660595
H	-1.788747	-0.109113	0.219059
H	-2.692820	-1.361901	-0.619093
P	0.679944	-1.578518	-0.719353
P	-3.952962	0.770235	-0.461209
P	0.404671	1.784115	-0.722413
Ni	1.735349	0.180259	0.195888
C	-5.274329	-0.313341	-1.203431
C	-6.087501	0.240903	-2.203055
C	-5.516420	-1.638056	-0.804497
C	-7.106322	-0.507352	-2.799134
H	-5.920389	1.268683	-2.516737
C	-6.532009	-2.388191	-1.397343
H	-4.919054	-2.084980	-0.013904
C	-7.328956	-1.824730	-2.398273
H	-7.724745	-0.059940	-3.573062
H	-6.706854	-3.411535	-1.074499
H	-8.121506	-2.409546	-2.857854
C	-4.317091	0.558549	1.345581
C	-5.201857	1.489193	1.916211
C	-3.781100	-0.442059	2.172022
C	-5.556030	1.414077	3.263333
H	-5.612986	2.283610	1.297605
C	-4.125888	-0.511147	3.524090
H	-3.086573	-1.175732	1.774717
C	-5.015979	0.412863	4.073257
H	-6.246126	2.142193	3.682151
H	-3.696614	-1.291923	4.147034
H	-5.283345	0.356235	5.125228
C	-0.279814	-2.818126	0.264750
C	-0.416885	-2.639374	1.649797
C	-0.905819	-3.922123	-0.342115
C	-1.169283	-3.543723	2.406762
H	0.074558	-1.804878	2.138838
C	-1.656063	-4.820715	0.415343
H	-0.797765	-4.093271	-1.409880
C	-1.792182	-4.630756	1.793819
H	-1.259724	-3.395629	3.479648
H	-2.131516	-5.669608	-0.069029
H	-2.376034	-5.331643	2.384672

C	1.915123	-2.602777	-1.647833
C	2.275028	-3.898539	-1.251315
C	2.595706	-2.021490	-2.732634
C	3.270256	-4.601633	-1.934567
H	1.784632	-4.363516	-0.402913
C	3.585695	-2.725482	-3.416813
H	2.366627	-1.003895	-3.039449
C	3.924597	-4.021768	-3.020972
H	3.534552	-5.604489	-1.609972
H	4.096385	-2.258632	-4.255000
H	4.697344	-4.570954	-3.552005
C	1.208306	3.219582	-1.568452
C	1.642576	3.096132	-2.898755
C	1.509667	4.401997	-0.876476
C	2.327026	4.134901	-3.529383
H	1.459923	2.180380	-3.455505
C	2.198737	5.439529	-1.506398
H	1.216766	4.511912	0.161616
C	2.603915	5.313974	-2.835314
H	2.647068	4.019453	-4.561769
H	2.423290	6.345894	-0.950617
H	3.138655	6.123784	-3.324364
C	-0.554086	2.544053	0.660704
C	-0.409307	2.033830	1.960603
C	-1.436517	3.616659	0.445327
C	-1.134823	2.586740	3.019635
H	0.270466	1.206678	2.151973
C	-2.151993	4.170865	1.505799
H	-1.558032	4.032588	-0.551150
C	-2.003355	3.654392	2.795971
H	-1.016188	2.178277	4.019292
H	-2.827703	5.002392	1.323808
H	-2.566060	4.082327	3.621254
C	5.056578	2.741907	-0.168437
C	5.125575	3.453700	1.031718
C	4.193824	3.182599	2.034541
C	3.208735	2.207669	1.839839
C	3.107333	1.487648	0.636811
C	4.062436	1.778354	-0.358613
H	5.775699	2.939355	-0.961489
H	2.517689	1.995882	2.652383
H	4.028835	1.254733	-1.313560
C	2.523818	-0.750892	1.641159
C	3.783060	-1.570758	1.673764
C	4.125460	-2.265647	2.845573
C	4.615575	-1.669290	0.552648
C	5.279274	-3.043574	2.892239
C	5.773947	-2.445436	0.598563
C	6.106518	-3.134038	1.767372
H	3.471409	-2.173852	3.707372
H	5.539655	-3.577825	3.802861
H	7.009451	-3.738893	1.804028
H	6.416220	-2.513265	-0.275602
H	4.350639	-1.126234	-0.348183
O	1.856524	-0.636292	2.675358
H	5.897385	4.204770	1.183396
H	4.237970	3.721956	2.979179

TS2a

B3LYP/BS1 SCF energy: -3357.445425 a.u.

M06/BS2 SCF energy in PhMe: -3356.42397076 a.u.

M06/BS2 Free energy in PhMe: -3355.64316776 a.u.

C	-1.556459	-0.056103	-1.977959
C	-2.478564	-0.161479	-3.216845
H	-3.226839	0.638324	-3.225384
H	-1.895113	-0.081144	-4.142312
H	-3.012419	-1.118299	-3.233676
C	-0.474089	-1.160003	-2.169611
H	0.144375	-0.884604	-3.033009
H	-0.976280	-2.094070	-2.447323
C	-0.933698	1.367605	-2.015950
H	-1.740115	2.108879	-1.988851
H	-0.437263	1.488818	-2.985672
C	-2.366001	-0.322153	-0.679145
H	-1.731556	-0.117276	0.189865
H	-2.622073	-1.386693	-0.634819
P	0.745368	-1.556932	-0.787708
P	-3.929119	0.711518	-0.448492
P	0.343949	1.838894	-0.715280
Ni	1.627687	0.213843	0.157845
C	-5.236848	-0.410821	-1.157811
C	-6.084346	0.114890	-2.144208
C	-5.435384	-1.738861	-0.746224
C	-7.094730	-0.664099	-2.714815

H	-5.950879	1.144606	-2.467549
C	-6.442430	-2.519621	-1.313453
H	-4.809988	-2.164247	0.034455
C	-7.274277	-1.984152	-2.301298
H	-7.740288	-0.238439	-3.478843
H	-6.583352	-3.545100	-0.980854
H	-8.060192	-2.592745	-2.741044
C	-4.245244	0.492784	1.367097
C	-5.140119	1.400976	1.957777
C	-3.664686	-0.492998	2.181614
C	-5.460953	1.318237	3.312805
H	-5.584743	2.184462	1.348537
C	-3.975834	-0.569206	3.541457
H	-2.960145	-1.208824	1.769812
C	-4.876636	0.332195	4.110496
H	-6.159546	2.028931	3.747274
H	-3.511382	-1.337714	4.154228
H	-5.117879	0.269983	5.168499
C	-0.170468	-2.800820	0.234258
C	-0.167122	-2.653312	1.630397
C	-0.883012	-3.872664	-0.332631
C	-0.866760	-3.557066	2.437151
H	0.382782	-1.836124	2.087894
C	-1.581287	-4.770446	0.474507
H	-0.884906	-4.019862	-1.409337
C	-1.576531	-4.612180	1.863639
H	-0.850102	-3.432353	3.516683
H	-2.125743	-5.594393	0.020382
H	-2.120262	-5.312235	2.492688
C	1.946353	-2.585187	-1.763303
C	2.246686	-3.919874	-1.457085
C	2.659210	-1.963423	-2.804913
C	3.216372	-4.617803	-2.182786
H	1.730144	-4.420294	-0.645268
C	3.622488	-2.660787	-3.532162
H	2.474355	-0.917577	-3.039334
C	3.903682	-3.994885	-3.223996
H	3.433576	-5.651673	-1.927235
H	4.158100	-2.160908	-4.335190
H	4.656247	-4.539432	-3.787879
C	1.222043	3.213292	-1.594377
C	1.810285	2.956056	-2.845164
C	1.423328	4.473618	-1.012952
C	2.544315	3.937281	-3.509798
H	1.703507	1.977222	-3.307100
C	2.163707	5.454988	-1.676041
H	1.001766	4.694442	-0.038494
C	2.720745	5.194652	-2.927804
H	2.982405	3.717473	-4.480093
H	2.303590	6.426048	-1.208144
H	3.293282	5.960864	-3.443625
C	-0.662432	2.690821	0.579176
C	-0.542951	2.272223	1.914037
C	-1.546994	3.738902	0.271063
C	-1.293242	2.893266	2.916905
H	0.135411	1.461056	2.170717
C	-2.289206	4.359479	1.274903
H	-1.650227	4.082783	-0.754534
C	-2.163930	3.935623	2.600989
H	-1.196383	2.554500	3.944666
H	-2.967746	5.169882	1.021538
H	-2.747059	4.415683	3.382469
C	5.139911	2.367936	-0.147718
C	5.051412	3.388894	0.801768
C	4.064666	3.326386	1.789359
C	3.169209	2.257457	1.816554
C	3.219354	1.234004	0.853249
C	4.247302	1.295027	-0.110855
H	5.912586	2.401265	-0.912667
H	2.429915	2.187927	2.609531
H	4.350415	0.504587	-0.848872
C	2.592303	-0.397458	1.644374
C	3.708796	-1.391670	1.827043
C	4.027819	-1.803900	3.130649
C	4.413569	-1.945657	0.750538
C	5.037131	-2.738737	3.352187
C	5.418803	-2.887460	0.969977
C	5.736930	-3.283137	2.271503
H	3.468824	-1.374671	3.956196
H	5.279319	-3.044822	4.367132
H	6.523888	-4.013571	2.442681
H	5.950316	-3.314867	0.123635

H	4.160268	-1.651379	-0.261835
O	1.814601	-0.182311	2.604150
H	5.757791	4.215154	0.783742
H	4.001482	4.105334	2.546239

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B3LYP/BS1 SCF energy: -3357.495306 a.u.

M06/BS2 SCF energy in PhMe: -3356.46097180 a.u.

M06/BS2 Free energy in PhMe: -3355.67955180 a.u.

C	-1.432866	0.351138	-2.091256
C	-2.300333	0.389777	-3.372211
H	-3.096639	1.137685	-3.292968
H	-1.689219	0.645699	-4.246255
H	-2.771775	-0.581249	-3.560045
C	-0.279249	-0.649378	-2.402599
H	0.369028	-0.196854	-3.163225
H	-0.709282	-1.543994	-2.867241
C	-0.881822	1.790533	-1.886991
H	-1.721858	2.491042	-1.846808
H	-0.309526	2.059920	-2.782904
C	-2.267135	-0.145961	-0.879185
H	-1.684559	0.001116	0.037792
H	-2.431246	-1.224852	-0.975488
P	0.882687	-1.216960	-1.035483
P	-3.926552	0.709297	-0.595963
P	0.294561	2.115526	-0.457742
Ni	1.521714	0.394453	0.283111
C	-5.097122	-0.413019	-1.510918
C	-5.934434	0.162245	-2.478024
C	-5.201502	-1.793211	-1.272379
C	-6.842714	-0.617822	-3.198882
H	-5.873763	1.231309	-2.667810
C	-6.107176	-2.574789	-1.989688
H	-4.582388	-2.261020	-0.511132
C	-6.929147	-1.988858	-2.956854
H	-7.481907	-0.153557	-3.945504
H	-6.176735	-3.641307	-1.790430
H	-7.635818	-2.598709	-3.513668
C	-4.288094	0.229825	1.159114
C	-5.297038	0.959366	1.810894
C	-3.636155	-0.787552	1.874746
C	-5.657087	0.672843	3.127515
H	-5.802045	1.763410	1.280253
C	-3.987698	-1.067160	3.197755
H	-2.846848	-1.372749	1.413280
C	-5.000041	-0.341758	3.826933
H	-6.442702	1.248463	3.610296
H	-3.466840	-1.856365	3.734047
H	-5.271531	-0.561079	4.856201
C	-0.007916	-2.670879	-0.311146
C	-0.079368	-2.788426	1.084437
C	-0.630849	-3.653171	-1.102226
C	-0.759782	-3.857075	1.676479
H	0.398070	-2.045091	1.713365
C	-1.311481	-4.718013	-0.511685
H	-0.577362	-3.599481	-2.186185
C	-1.379576	-4.820759	0.881087
H	-0.793272	-3.930343	2.759902
H	-1.785888	-5.468780	-1.138394
H	-1.909504	-5.651319	1.340054
C	2.210300	-1.977320	-2.084480
C	2.533443	-3.341488	-2.064585
C	2.974867	-1.119523	-2.894669
C	3.578943	-3.836750	-2.849321
H	1.973354	-4.025019	-1.435328
C	4.011437	-1.615084	-3.683289
H	2.771292	-0.051290	-2.896785
C	4.316085	-2.978491	-3.664983
H	3.812759	-4.898000	-2.821276
H	4.589110	-0.934136	-4.302543
H	5.126683	-3.365800	-4.276407
C	1.317663	3.485338	-1.169790
C	2.707140	3.320612	-1.265475
C	0.739857	4.676899	-1.637753
C	3.500381	4.321830	-1.833305
H	3.168475	2.417483	-0.876540
C	1.532653	5.674303	-2.204145
H	-0.331944	4.834545	-1.548984
C	2.915552	5.496556	-2.306232
H	4.576247	4.181905	-1.897561
H	1.072634	6.592037	-2.561620

H	3.532970	6.275649	-2.745824
C	-0.682646	2.990637	0.848435
C	-0.065940	3.110273	2.108130
C	-1.947485	3.566590	0.659063
C	-0.699886	3.797986	3.143060
H	0.908722	2.658213	2.270317
C	-2.582532	4.245425	1.702586
H	-2.464628	3.483219	-0.290389
C	-1.960375	4.366221	2.944763
H	-0.207908	3.884115	4.108438
H	-3.566524	4.676923	1.538833
H	-2.456117	4.895181	3.754560
C	5.991374	-1.534442	-0.223414
C	6.871276	-0.449960	-0.227819
C	6.471204	0.755975	0.352833
C	5.210642	0.872565	0.938237
C	4.318122	-0.214846	0.961223
C	4.730026	-1.417040	0.361174
H	6.277995	-2.472620	-0.691594
H	4.897713	1.808169	1.390737
H	4.044160	-2.256813	0.318347
C	2.970925	-0.026054	1.606154
C	2.555544	-0.903575	2.755420
C	1.467133	-0.501687	3.558329
C	3.211352	-2.098719	3.103985
C	1.032613	-1.277971	4.630457
C	2.773851	-2.875930	4.177972
C	1.677645	-2.478530	4.944755
H	0.969778	0.433841	3.328435
H	0.190458	-0.938293	5.229223
H	1.341706	-3.083350	5.783183
H	3.303653	-3.794289	4.420283
H	4.082827	-2.420950	2.546376
O	2.509442	1.220988	1.620354
H	7.854215	-0.542028	-0.682940
H	7.146538	1.608688	0.356432

TS11

B3LYP/BS1 SCF energy: -4191.295247 a.u.

M06/BS2 SCF energy in PhMe: -4190.31283573 a.u.

M06/BS2 Free energy in PhMe: -4189.39361373 a.u.

C	1.590205	-0.555243	2.241963
C	2.463095	-0.718944	3.511960
H	3.007099	0.201898	3.744415
H	1.840013	-0.964851	4.380631
H	3.199405	-1.520721	3.385514
C	0.919562	-1.950667	2.047384
H	0.597586	-2.319766	3.027553
H	1.691724	-2.648387	1.707515
C	0.556529	0.561659	2.558141
H	1.088257	1.415638	2.991017
H	-0.116333	0.195689	3.342660
C	2.483451	-0.222485	1.008555
H	1.847753	0.107285	0.179980
H	2.980739	-1.139741	0.671246
P	-0.527596	-2.164278	0.858739
P	3.799395	1.110904	1.293982
P	-0.575702	1.271603	1.200447
Ni	-1.084044	-0.162354	-0.297912
C	5.285938	0.063916	1.710746
C	5.945307	0.300941	2.925516
C	5.795001	-0.928774	0.857515
C	7.072741	-0.441039	3.288790
H	5.571988	1.075074	3.592006
C	6.919300	-1.672076	1.216399
H	5.320441	-1.109875	-0.103755
C	7.560102	-1.431109	2.435358
H	7.569623	-0.242964	4.235254
H	7.300647	-2.435035	0.542241
H	8.437973	-2.008707	2.713391
C	4.248948	1.627650	-0.427723
C	5.107609	2.735833	-0.539720
C	3.787317	1.024033	-1.605230
C	5.504352	3.211955	-1.788422
H	5.465218	3.230874	0.360555
C	4.167601	1.511366	-2.858789
H	3.119876	0.173128	-1.566169
C	5.030529	2.602656	-2.954030
H	6.174276	4.066055	-1.852476
H	3.775148	1.033478	-3.751422
H	5.328287	2.981152	-3.928571
C	-0.089156	-3.780903	0.056363
C	-0.201122	-3.906667	-1.334056

C	0.336402	-4.892015	0.807152
C	0.118180	-5.113938	-1.964860
H	-0.526794	-3.054765	-1.919010
C	0.653592	-6.093919	0.177630
H	0.410076	-4.823145	1.889490
C	0.545639	-6.206554	-1.212655
H	0.039804	-5.188504	-3.045783
H	0.981565	-6.944371	0.770123
H	0.795655	-7.143817	-1.703153
C	-1.889259	-2.759356	1.981833
C	-2.006165	-2.387710	3.330779
C	-2.895304	-3.580929	1.439186
C	-3.083750	-2.820378	4.110089
H	-1.251017	-1.762451	3.796788
C	-3.969930	-4.013166	2.214607
H	-2.824749	-3.903856	0.404661
C	-4.071253	-3.633515	3.555833
H	-3.141188	-2.524522	5.154658
H	-4.725543	-4.657321	1.771962
H	-4.906214	-3.974611	4.161786
C	-1.840514	2.034191	2.343848
C	-2.690427	1.158018	3.042062
C	-2.028555	3.413664	2.518838
C	-3.674699	1.639920	3.904549
H	-2.594034	0.086119	2.898351
C	-3.020305	3.898203	3.377355
H	-1.407337	4.120727	1.981349
C	-3.843191	3.016437	4.077565
H	-4.312781	0.938122	4.435861
H	-3.145302	4.971572	3.496390
H	-4.610755	3.395680	4.746947
C	0.419113	2.732879	0.625805
C	0.619944	2.906916	-0.750262
C	0.997865	3.660753	1.512090
C	1.360981	3.989536	-1.232408
H	0.225364	2.180925	-1.453521
C	1.727091	4.746857	1.030271
H	0.876547	3.546287	2.585485
C	1.908272	4.915010	-0.345761
H	1.521970	4.086810	-2.301918
H	2.163614	5.454683	1.730248
H	2.487239	5.755394	-0.719571
O	-0.728781	-0.832774	-2.219015
S	-0.063427	-0.310920	-3.475718
O	0.576935	1.005609	-3.316033
O	-0.872808	-0.532256	-4.683013
C	1.360695	-1.500242	-3.670411
F	2.019604	-1.667485	-2.506409
F	2.229996	-1.037110	-4.579296
F	0.923606	-2.701713	-4.074762
H	-2.462477	0.815976	-0.887514
C	-4.586660	-0.087823	-1.358430
C	-5.130842	0.024329	0.081318
C	-5.754968	1.377373	0.410411
C	-4.712395	2.468439	0.181441
C	-4.140676	2.499616	-1.249233
N	-3.636625	1.091847	-1.631516
H	-6.657207	1.552020	-0.189674
H	-5.852011	-0.788620	0.228731
H	-5.129355	3.460123	0.393583
H	-6.073940	1.391798	1.459264
H	-3.891723	2.317233	0.884955
H	-4.302715	-0.159266	0.777340
C	-3.796305	-1.405672	-1.443958
H	-4.450082	-2.219697	-1.113353
H	-3.445800	-1.642582	-2.450288
H	-2.925543	-1.385198	-0.776681
C	-5.743289	-0.181580	-2.378440
H	-5.378165	-0.219279	-3.408433
H	-6.285281	-1.115687	-2.194728
H	-6.466429	0.631039	-2.300239
C	-2.940750	3.465975	-1.276137
H	-2.625290	3.716182	-2.293285
H	-3.233542	4.400991	-0.786716
H	-2.081439	3.059145	-0.742616
C	-5.208463	3.073427	-2.211596
H	-5.370554	4.120499	-1.932524
H	-4.887089	3.070753	-3.255757
H	-6.174644	2.571551	-2.146639
C	-3.110397	1.074324	-3.020280
H	-2.238744	1.724350	-3.082346
H	-2.785598	0.074953	-3.282021
H	-3.858815	1.403924	-3.742695

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B3LYP/BS1 SCF energy: -4191.331070 a.u.

M06/BS2 SCF energy in PhMe: -4190.34314586 a.u.

M06/BS2 Free energy in PhMe: -4189.42043286 a.u.

C	2.109872	0.708622	-2.045377
C	3.164801	1.152630	-3.088060
H	3.902992	0.364521	-3.273680
H	2.684739	1.388216	-4.046217
H	3.705039	2.044679	-2.751680
C	1.057871	1.857261	-2.001848
H	0.508788	1.858646	-2.950881
H	1.594241	2.813337	-1.964028
C	1.531658	-0.642409	-2.562040
H	2.326713	-1.390183	-2.472213
H	1.329364	-0.545918	-3.635306
C	2.767817	0.540201	-0.645885
H	2.038396	0.062979	0.020861
H	2.983834	1.529434	-0.226218
P	-0.255433	1.840187	-0.638209
P	4.320132	-0.528603	-0.582396
P	-0.008663	-1.401440	-1.744112
Ni	-0.785903	-0.161985	-0.199107
C	5.674028	0.734714	-0.801380
C	6.620130	0.518154	-1.814017
C	5.808454	1.877689	0.003456
C	7.664786	1.421631	-2.028037
H	6.536060	-0.366482	-2.440855
C	6.849087	2.782228	-0.207414
H	5.103558	2.057957	0.811016
C	7.779866	2.557084	-1.225900
H	8.387160	1.236273	-2.819078
H	6.938034	3.661075	0.426591
H	8.591924	3.261235	-1.388391
C	4.477052	-0.860436	1.236519
C	5.363367	-1.886414	1.608077
C	3.785228	-0.181222	2.251861
C	5.569404	-2.210431	2.948845
H	5.891779	-2.440282	0.835375
C	3.979684	-0.514575	3.594847
H	3.080763	0.607758	2.008505
C	4.874874	-1.524974	3.948051
H	6.261585	-3.006180	3.212358
H	3.422587	0.015044	4.363258
H	5.023566	-1.783113	4.993376
C	0.564617	2.894796	0.672326
C	0.493192	2.449220	1.999918
C	1.254811	4.090574	0.407813
C	1.100386	3.168078	3.034547
H	-0.033801	1.525908	2.216951
C	1.860388	4.811966	1.437627
H	1.309321	4.474790	-0.607453
C	1.787392	4.349957	2.755164
H	1.037967	2.798960	4.055182
H	2.388869	5.735180	1.212434
H	2.263279	4.909699	3.556362
C	-1.441044	3.079780	-1.389636
C	-2.039668	2.791881	-2.631040
C	-1.844765	4.253143	-0.728851
C	-2.971013	3.657540	-3.205450
H	-1.788575	1.872815	-3.152275
C	-2.787078	5.115240	-1.296924
H	-1.413046	4.507201	0.233641
C	-3.349278	4.828301	-2.541848
H	-3.405496	3.413167	-4.171974
H	-3.072148	6.020685	-0.766053
H	-4.073849	5.504365	-2.988222
C	-1.183676	-1.560729	-3.186637
C	-1.268700	-0.611519	-4.218472
C	-2.101138	-2.628351	-3.206351
C	-2.232287	-0.717604	-5.225995
H	-0.569608	0.218678	-4.253579
C	-3.063297	-2.737102	-4.210417
H	-2.047248	-3.393032	-2.436480
C	-3.137447	-1.778789	-5.225802
H	-2.265307	0.027937	-6.017140
H	-3.748634	-3.581729	-4.207575
H	-3.882820	-1.866132	-6.011987
C	0.540805	-3.188437	-1.644187
C	0.269679	-3.917658	-0.479465
C	1.196844	-3.836474	-2.705988
C	0.654997	-5.258607	-0.372027
H	-0.250091	-3.442971	0.345825
C	1.584101	-5.171193	-2.598890
H	1.399228	-3.298665	-3.628891
C	1.315390	-5.886162	-1.427213
H	0.436648	-5.805888	0.541490
H	2.092397	-5.655665	-3.429260

H	1.618453	-6.926908	-1.342537
O	-1.718744	-0.593411	1.694870
S	-1.502835	-1.712560	2.708940
O	-1.700937	-3.060003	2.150355
O	-2.179506	-1.408631	3.983880
C	0.313876	-1.605658	3.110670
F	1.056900	-1.794678	2.015194
F	0.622264	-2.541187	4.011265
F	0.605472	-0.399702	3.627510
H	-3.592788	-0.381865	1.611309
C	-4.904734	1.129974	2.143498
C	-4.372980	2.096963	1.067522
C	-4.893522	1.819954	-0.342101
C	-4.502249	0.403937	-0.760351
C	-5.047542	-0.700708	0.164695
N	-4.634999	-0.330031	1.636528
H	-5.980579	1.964390	-0.397047
H	-4.630387	3.113333	1.387388
H	-4.854686	0.181705	-1.773990
H	-4.449851	2.537848	-1.036712
H	-3.404382	0.330056	-0.791373
H	-3.276670	2.039912	1.054658
C	-4.089034	1.335398	3.433870
H	-4.066806	2.409433	3.646054
H	-4.534379	0.840244	4.301066
H	-3.059750	0.986021	3.328086
C	-6.388900	1.378406	2.448163
H	-6.800145	0.651357	3.154167
H	-6.463640	2.360954	2.925489
H	-7.022623	1.400030	1.561341
C	-4.355882	-2.029958	-0.193526
H	-4.850383	-2.899279	0.250524
H	-4.400118	-2.147194	-1.280490
H	-3.299664	-2.039200	0.090154
C	-6.566131	-0.872107	0.013659
H	-6.748979	-1.299051	-0.977827
H	-6.985254	-1.571203	0.743100
H	-7.122023	0.064802	0.068162
C	-5.052703	-1.374262	2.631735
H	-4.725663	-2.347834	2.273669
H	-4.545464	-1.185859	3.574345
H	-6.133890	-1.362184	2.754733

TS12

B3LYP/BS1 SCF energy: -4113.890212 a.u.

M06/BS2 SCF energy in PhMe: -4112.93507470 a.u.

M06/BS2 Free energy in PhMe: -4112.05220470 a.u.

C	-1.829048	-0.946907	1.991794
C	-2.810191	-1.518483	3.043624
H	-3.339100	-2.399086	2.664642
H	-2.272414	-1.818483	3.951821
H	-3.562107	-0.772511	3.324169
C	-1.046518	0.188035	2.722412
H	-0.383177	-0.289138	3.455004
H	-1.755476	0.803846	3.289067
C	-0.884106	-2.115574	1.604965
H	-1.493876	-2.929347	1.199522
H	-0.442699	-2.495361	2.532888
C	-2.607158	-0.367301	0.780902
H	-1.885808	-0.057589	0.018834
H	-3.133918	0.541801	1.091571
P	0.013672	1.301049	1.658279
P	-3.825701	-1.521330	-0.089899
P	0.578878	-1.894225	0.399910
Ni	1.273651	0.100669	0.087753
C	-5.393905	-1.194313	0.854890
C	-6.094854	-2.294889	1.369361
C	-5.910640	0.092929	1.081819
C	-7.272400	-2.119316	2.102001
H	-5.712011	-3.297758	1.194864
C	-7.084078	0.271998	1.813973
H	-5.400363	0.960075	0.670679
C	-7.766761	-0.834790	2.328265
H	-7.801044	-2.984776	2.493407
H	-7.469493	1.274813	1.980545
H	-8.681624	-0.694132	2.898157
C	-4.151477	-0.567379	-1.651263
C	-5.436964	-0.585303	-2.222077
C	-3.121584	0.066080	-2.366406
C	-5.685512	0.026566	-3.451106
H	-6.254818	-1.073001	-1.699243
C	-3.371709	0.685221	-3.592995
H	-2.105723	0.092282	-1.989703
C	-4.654891	0.669353	-4.140563
H	-6.689908	0.003560	-3.867255

H	-2.550782	1.179233	-4.105267
H	-4.850922	1.150787	-5.095234
C	-1.148868	2.698856	1.274551
C	-1.520059	2.946267	-0.053738
C	-1.679858	3.510341	2.291922
C	-2.416310	3.975759	-0.356427
H	-1.113436	2.342276	-0.857702
C	-2.572242	4.537356	1.987924
H	-1.385796	3.349059	3.326194
C	-2.944488	4.770563	0.660388
H	-2.694264	4.151898	-1.391889
H	-2.973469	5.158295	2.785110
H	-3.638793	5.572530	0.422693
C	1.131902	2.130731	2.880043
C	1.147846	1.891912	4.262178
C	2.046316	3.061958	2.351113
C	2.055282	2.559230	5.091703
H	0.448824	1.192930	4.710730
C	2.943164	3.733055	3.180035
H	2.049972	3.256398	1.281439
C	2.954048	3.480426	4.555303
H	2.049904	2.361424	6.160768
H	3.636482	4.452235	2.751500
H	3.655982	4.000283	5.201885
C	1.673186	-3.209344	1.156999
C	2.115153	-3.030446	2.480786
C	2.131921	-4.338481	0.460299
C	2.975117	-3.946249	3.087337
H	1.792485	-2.160127	3.046787
C	2.997130	-5.255629	1.064676
H	1.807579	-4.512296	-0.560392
C	3.421967	-5.065119	2.379744
H	3.296254	-3.784739	4.113309
H	3.331777	-6.124730	0.503935
H	4.090528	-5.780777	2.850475
C	-0.084560	-2.722310	-1.125349
C	-0.013063	-2.041303	-2.348258
C	-0.689697	-3.992291	-1.098952
C	-0.521473	-2.614160	-3.517461
H	0.426253	-1.050080	-2.383534
C	-1.189262	-4.568161	-2.265990
H	-0.766930	-4.543259	-0.165563
C	-1.105196	-3.879495	-3.479671
H	-0.466231	-2.061091	-4.450699
H	-1.651190	-5.551232	-2.226563
H	-1.502454	-4.325923	-4.387429
O	1.738934	1.722413	-1.023407
S	1.373656	1.865585	-2.487753
O	-0.050209	1.604667	-2.773579
O	2.351932	1.270059	-3.414892
C	1.588470	3.703461	-2.686797
F	0.781595	4.368909	-1.849114
F	1.297697	4.065090	-3.941168
F	2.856811	4.052828	-2.421186
H	2.816497	-0.501323	-0.467028
N	4.178132	-0.742771	-0.635269
C	4.109109	-1.999609	-1.492340
C	4.701216	-1.040626	0.755721
C	3.593891	-1.715282	-2.907071
H	4.376856	-1.307511	-3.555453
H	3.262403	-2.662493	-3.346249
H	2.755037	-1.020124	-2.918909
C	5.402100	-2.825603	-1.569335
H	5.221120	-3.672857	-2.240274
H	6.236366	-2.253756	-1.990879
H	5.705876	-3.237754	-0.604102
C	6.231562	-0.961425	0.915858
H	6.780167	-1.530265	0.164244
H	6.592989	0.069654	0.892189
H	6.492402	-1.373115	1.897603
C	4.019918	-0.184755	1.832315
H	2.930020	-0.181481	1.698920
H	4.242384	-0.613039	2.816243
H	4.363752	0.851177	1.833754
C	4.835831	0.392902	-1.355563
H	5.845579	0.076414	-1.649388
H	4.254350	0.548820	-2.263048
C	4.906107	1.735523	-0.626936
H	5.613689	1.749958	0.205340
H	5.240242	2.483378	-1.354916
H	3.921211	2.043163	-0.275433
H	3.358730	-2.606073	-0.979695
H	4.395406	-2.074596	0.937662

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B3LYP/BS1 SCF energy: -4113.919035 a.u.

M06/BS2 SCF energy in PhMe: -4112.96038861 a.u.

M06/BS2 Free energy in PhMe: -4112.07656961 a.u.

C	2.141756	0.912543	1.998386
C	3.223916	1.308000	3.032067
H	3.981458	1.963056	2.587359
H	2.777082	1.844432	3.878809
H	3.738063	0.423000	3.424970
C	1.079104	0.085425	2.789433
H	0.540230	0.765259	3.461752
H	1.606564	-0.625576	3.437195
C	1.571084	2.246292	1.436300
H	2.396616	2.783212	0.958147
H	1.252440	2.863753	2.284103
C	2.765356	0.028366	0.885009
H	1.994133	-0.178398	0.134064
H	3.049619	-0.941537	1.308942
P	-0.234557	-0.841670	1.795536
P	4.233187	0.756270	-0.057502
P	0.136346	2.202905	0.183118
Ni	-0.687914	0.265229	0.035371
C	5.681204	0.066187	0.878923
C	6.710390	0.952412	1.230820
C	5.803219	-1.281557	1.259577
C	7.826510	0.512715	1.948347
H	6.632681	1.997497	0.940673
C	6.914851	-1.723762	1.976887
H	5.031242	-1.994688	0.982445
C	7.929141	-0.826457	2.324693
H	8.612256	1.216106	2.212028
H	6.992440	-2.770011	2.262401
H	8.794726	-1.172350	2.883951
C	4.208921	-0.312432	-1.576395
C	5.370322	-0.922428	-2.078447
C	3.029633	-0.409062	-2.336960
C	5.346517	-1.624875	-3.285412
H	6.301049	-0.856332	-1.523563
C	3.003522	-1.119108	-3.537621
H	2.117881	0.077749	-2.003467
C	4.162890	-1.732783	-4.016524
H	6.258027	-2.092519	-3.650247
H	2.071403	-1.192225	-4.090725
H	4.144290	-2.285074	-4.952566
C	0.545760	-2.528312	1.611718
C	0.480548	-3.138632	0.349911
C	1.204814	-3.208722	2.650521
C	1.063643	-4.389874	0.128793
H	-0.022796	-2.622240	-0.462078
C	1.786253	-4.458430	2.432151
H	1.255917	-2.770006	3.643912
C	1.719216	-5.050966	1.167702
H	1.009432	-4.840963	-0.858633
H	2.291539	-4.969789	3.248014
H	2.176802	-6.022009	0.996109
C	-1.490814	-1.161428	3.140388
C	-2.126104	-0.066476	3.759342
C	-1.935676	-2.450357	3.485324
C	-3.138689	-0.250983	4.701190
H	-1.834317	0.946055	3.494115
C	-2.957820	-2.636625	4.421390
H	-1.471743	-3.319672	3.030963
C	-3.561572	-1.540186	5.039417
H	-3.596843	0.614724	5.173966
H	-3.270056	-3.646581	4.677517
H	-4.347585	-1.686088	5.775672
C	-0.995423	3.511952	0.885591
C	-1.314527	3.549500	2.254215
C	-1.650683	4.424918	0.038691
C	-2.244834	4.460471	2.760008
H	-0.824288	2.865796	2.940977
C	-2.583274	5.335130	0.540637
H	-1.416650	4.434103	-1.021795
C	-2.887618	5.357892	1.904478
H	-2.460169	4.473223	3.825988
H	-3.064972	6.036565	-0.136515
H	-3.606824	6.072361	2.296239
C	0.889191	3.171248	-1.226842
C	0.724534	2.690187	-2.532603
C	1.601863	4.368505	-1.035242
C	1.267444	3.382276	-3.621018
H	0.164316	1.775369	-2.704382
C	2.144522	5.057433	-2.118518
H	1.726108	4.773225	-0.033773
C	1.979983	4.562726	-3.416473
H	1.131362	2.990603	-4.625673
H	2.694940	5.980406	-1.952361

H	2.405911	5.098637	-4.261108
O	-1.427940	-0.952401	-1.481508
S	-1.931474	-0.793405	-2.886910
O	-1.269444	0.214011	-3.719478
O	-3.428327	-0.800195	-2.928034
C	-1.463643	-2.431744	-3.632021
F	-0.133281	-2.590037	-3.586737
F	-1.865878	-2.502340	-4.903905
F	-2.031136	-3.436583	-2.943931
H	-4.190594	-0.616961	-1.329679
N	-4.776849	-0.367272	-0.500143
C	-4.231745	1.023884	-0.095936
C	-4.484348	-1.433938	0.582053
C	-4.327925	2.013640	-1.259430
H	-5.333174	2.436840	-1.367477
H	-3.647506	2.841882	-1.042935
H	-4.020298	1.564807	-2.207835
C	-4.866862	1.574632	1.178205
H	-4.421214	2.554886	1.374662
H	-5.948830	1.718332	1.073520
H	-4.668980	0.950033	2.052953
C	-5.666004	-1.693281	1.518916
H	-6.090084	-0.779048	1.941018
H	-6.466866	-2.259776	1.032461
H	-5.294453	-2.292466	2.355618
C	-3.953128	-2.725859	-0.044141
H	-3.068403	-2.537480	-0.654103
H	-3.658500	-3.395862	0.770344
H	-4.703897	-3.241773	-0.649124
C	-6.192822	-0.331736	-1.023818
H	-6.864671	-0.189476	-0.176357
H	-6.255607	0.555219	-1.653376
C	-6.576109	-1.554038	-1.856035
H	-6.684499	-2.460404	-1.255613
H	-7.542067	-1.355769	-2.332815
H	-5.839194	-1.735558	-2.643833
H	-3.167354	0.820847	0.090614
H	-3.668166	-0.995321	1.159854

2'

B3LYP/BS1 SCF energy: -2210.241020 a.u.

M06/BS2 SCF energy in PhMe: -2209.58746343 a.u.

M06/BS2 Free energy in PhMe: -2209.01795543 a.u.

C	-0.018314	-1.422692	2.575291
C	1.296003	-0.644548	2.389862
H	2.128560	-1.213688	2.817942
H	1.231577	0.294141	2.952459
C	-1.288480	-0.571833	2.394530
H	-1.151166	0.382593	2.916413
H	-2.144950	-1.073489	2.858944
P	1.695205	-0.208743	0.604779
P	-1.695817	-0.191488	0.599995
Ni	0.008123	0.717178	-0.484243
C	-2.440495	-1.838175	0.126629
C	-1.868631	-2.583619	-0.911510
C	-3.546190	-2.382656	0.804777
C	-2.376633	-3.837384	-1.265476
H	-1.015243	-2.175477	-1.440226
C	-4.056778	-3.631789	0.455027
H	-4.022906	-1.820895	1.603662
C	-3.471703	-4.364161	-0.582662
H	-1.915328	-4.398380	-2.074212
H	-4.912840	-4.034384	0.990727
H	-3.870598	-5.337774	-0.855388
C	-3.245716	0.818490	0.802235
C	-4.292725	0.706952	-0.129883
C	-3.361282	1.796393	1.804633
C	-5.414620	1.533162	-0.056906
H	-4.237995	-0.042465	-0.914184
C	-4.485206	2.622438	1.880999
H	-2.570304	1.924470	2.537749
C	-5.517079	2.494966	0.950523
H	-6.211491	1.421911	-0.787993
H	-4.551383	3.366088	2.671256
H	-6.391372	3.137647	1.009283
C	3.260167	0.769865	0.845739
C	3.349151	1.764183	1.835080
C	4.343227	0.625400	-0.039413
C	4.483702	2.570137	1.948475
H	2.527981	1.921019	2.528411
C	5.476585	1.432282	0.070784
H	4.305288	-0.129700	-0.818949
C	5.553586	2.407455	1.067191

H	4.528726	3.326653	2.727929
H	6.301548	1.296135	-0.624079
H	6.436647	3.034709	1.154628
C	2.412302	-1.840718	0.042508
C	1.910805	-2.452169	-1.113286
C	3.441707	-2.492829	0.744297
C	2.410165	-3.680628	-1.556537
H	1.123041	-1.954360	-1.667760
C	3.941091	-3.719671	0.308894
H	3.871660	-2.032094	1.629716
C	3.424307	-4.318781	-0.843895
H	2.006468	-4.134952	-2.457832
H	4.736616	-4.207516	0.866577
H	3.814660	-5.274554	-1.183775
H	-0.043793	-2.296700	1.910797
H	-0.026367	-1.824942	3.597325
C	-1.417951	3.011515	-1.911288
C	-1.669982	1.720635	-2.732295
C	-0.624146	0.639427	-2.527490
C	-0.728592	2.764821	-0.575412
C	0.749021	0.840569	-2.518752
C	0.640778	2.784310	-0.386496
C	1.419865	2.187339	-2.762827
C	1.677626	3.003267	-1.470876
H	2.378906	2.021388	-3.269500
H	1.756824	4.075135	-1.720126
H	-0.827403	3.721710	-2.501614
H	-2.640906	1.306368	-2.438798
H	-1.762014	1.976857	-3.801869
H	0.815109	2.774030	-3.464341
H	2.651750	2.717203	-1.062608
H	-2.380505	3.504318	-1.729287
H	1.383550	-0.029011	-2.671265
H	1.006948	2.926956	0.629361
H	-1.357761	2.873766	0.303996
H	-0.983218	-0.371974	-2.711014

3'

B3LYP/BS1 SCF energy: -3091.238381 a.u.

M06/BS2 SCF energy in PhMe: -3090.59740524 a.u.

M06/BS2 Free energy in PhMe: -3090.10574924 a.u.

C	-1.659581	3.234001	-0.994940
C	-0.366745	2.937729	-1.780522
H	-0.632082	2.594391	-2.788248
H	0.217597	3.858660	-1.893692
C	-2.768127	2.172216	-1.138308
H	-3.729007	2.573611	-0.793103
H	-2.906258	1.933935	-2.200968
P	0.710060	1.622528	-0.993096
P	-2.452070	0.517885	-0.317818
Ni	-0.402625	-0.242377	-0.592614
C	1.327388	2.519798	0.503151
C	0.913603	2.091947	1.773198
C	2.174630	3.636314	0.407527
C	1.330660	2.768242	2.922724
H	0.263867	1.225393	1.859457
C	2.593012	4.309431	1.554746
H	2.520960	3.972539	-0.566221
C	2.170771	3.876568	2.815179
H	1.002391	2.422856	3.899363
H	3.252169	5.169160	1.466256
H	2.500913	4.399865	3.708745
C	2.196947	1.607649	-2.093574
C	3.390332	1.042939	-1.606036
C	2.166370	2.059903	-3.422040
C	4.517359	0.944977	-2.420789
H	3.438820	0.669057	-0.588452
C	3.296499	1.957802	-4.238129
H	1.264057	2.497741	-3.836490
C	4.474924	1.402403	-3.740828
H	5.426942	0.504301	-2.021864
H	3.251326	2.316780	-5.263194
H	5.353235	1.323462	-4.375870
C	-3.908292	-0.417586	-0.972538
C	-3.715774	-1.232954	-2.099026
C	-5.196179	-0.307811	-0.425263
C	-4.792025	-1.912280	-2.673949
H	-2.718202	-1.350743	-2.512336
C	-6.268728	-0.994442	-0.995980
H	-5.361551	0.311364	0.451943
C	-6.069392	-1.795387	-2.123138

H	-4.628579	-2.541324	-3.545086
H	-7.260536	-0.903206	-0.560539
H	-6.905548	-2.330073	-2.566113
C	-2.898093	0.786992	1.457874
C	-2.769949	-0.309887	2.329708
C	-3.319754	2.014474	1.990153
C	-3.064628	-0.185567	3.686273
H	-2.440780	-1.268346	1.937666
C	-3.605561	2.142279	3.352776
H	-3.428927	2.884240	1.350767
C	-3.480825	1.044383	4.203535
H	-2.964644	-1.047652	4.340404
H	-3.927640	3.103265	3.745335
H	-3.704262	1.144751	5.262193
C	0.574856	-2.881366	-2.759594
C	1.350072	-2.058549	-1.981859
C	0.913956	-1.688610	-0.663629
C	-0.327346	-2.226417	-0.154745
C	-1.038767	-3.169220	-0.971477
C	-0.621052	-3.466088	-2.244547
H	0.900807	-3.126965	-3.767133
H	2.297404	-1.667655	-2.341664
H	-0.478892	-2.260306	0.922434
H	-1.911983	-3.663400	-0.551965
H	-1.175185	-4.175775	-2.852963
O	1.970173	-1.329339	0.282417
S	2.975676	-2.467347	0.885712
O	4.338907	-1.964531	0.779871
O	2.606679	-3.812461	0.470136
C	2.495767	-2.289466	2.682870
F	3.263308	-3.100547	3.412532
F	1.213318	-2.629100	2.853736
F	2.672224	-1.030282	3.083000
H	-1.422247	3.408476	0.061942
H	-2.065039	4.183048	-1.370697

TS1'

B3LYP/BS1 SCF energy: -3091.223133 a.u.

M06/BS2 SCF energy in PhMe: -3090.58120033 a.u.

M06/BS2 Free energy in PhMe: -3090.08760133 a.u.

C	-1.538158	2.745417	-2.129332
C	-0.200862	2.198217	-2.668717
H	-0.402049	1.517316	-3.505344
H	0.396249	3.021583	-3.076191
C	-2.656006	1.698400	-1.973171
H	-3.624427	2.194304	-1.841281
H	-2.741325	1.101222	-2.890249
P	0.827941	1.240691	-1.438523
P	-2.382839	0.468015	-0.595985
Ni	-0.344499	-0.472277	-0.673121
C	1.351103	2.513027	-0.207564
C	1.610773	2.097520	1.106768
C	1.539058	3.864056	-0.542904
C	2.047077	3.013270	2.066344
H	1.502515	1.052445	1.371958
C	1.963724	4.779029	0.420411
H	1.366076	4.212914	-1.556859
C	2.217922	4.355590	1.727567
H	2.254615	2.666880	3.074592
H	2.102412	5.821931	0.147515
H	2.553578	5.069761	2.474787
C	2.384071	0.899131	-2.376774
C	3.489980	0.393127	-1.670479
C	2.496571	1.091114	-3.762355
C	4.680157	0.102704	-2.336848
H	3.414717	0.200531	-0.605018
C	3.689453	0.793048	-4.426308
H	1.663010	1.475005	-4.341052
C	4.784445	0.301835	-3.716099
H	5.523645	-0.287450	-1.774079
H	3.758508	0.948822	-5.499815
H	5.712028	0.071375	-4.233183
C	-3.847120	-0.636622	-0.799832
C	-3.727421	-1.708920	-1.699894
C	-5.061945	-0.449337	-0.124203
C	-4.807119	-2.560367	-1.935693
H	-2.779580	-1.889888	-2.200398
C	-6.137130	-1.310547	-0.353072
H	-5.170156	0.362372	0.588380
C	-6.014366	-2.363139	-1.261647
H	-4.699604	-3.385634	-2.634361
H	-7.070790	-1.157917	0.181831
H	-6.852364	-3.032338	-1.436964

C	-2.695371	1.424112	0.948366
C	-2.003445	1.042495	2.110035
C	-3.584089	2.509911	1.021355
C	-2.203524	1.719652	3.313775
H	-1.295513	0.219976	2.076606
C	-3.779285	3.190296	2.224387
H	-4.132151	2.833745	0.141372
C	-3.090969	2.795089	3.373339
H	-1.657404	1.408759	4.199836
H	-4.468350	4.029783	2.262301
H	-3.242473	3.326833	4.308714
C	0.897092	-3.804966	-2.006675
C	1.467435	-2.632649	-1.546579
C	0.785593	-1.910372	-0.543573
C	-0.376088	-2.429807	0.088085
C	-0.901658	-3.666440	-0.386958
C	-0.288623	-4.327109	-1.430853
H	1.367905	-4.334259	-2.832027
H	2.381779	-2.238607	-1.977525
H	-0.676705	-2.086161	1.074311
H	-1.746336	-4.114251	0.130596
H	-0.682369	-5.275536	-1.785500
O	2.107850	-1.253801	0.772955
S	2.629570	-2.132817	1.923792
O	4.041605	-1.871102	2.210835
O	2.145788	-3.513650	1.871955
C	1.717057	-1.375703	3.364871
F	1.974018	-2.041681	4.492075
F	0.378386	-1.401931	3.158887
F	2.070143	-0.088633	3.540527
H	-1.379583	3.275005	-1.181892
H	-1.894402	3.501977	-2.840728

4'

B3LYP/BS1 SCF energy: -3091.281795 a.u.

M06/BS2 SCF energy in PhMe: -3090.63958379 a.u.

M06/BS2 Free energy in PhMe: -3090.14561679 a.u.

C	0.620490	2.721646	-2.374106
C	1.897906	1.888452	-2.198489
H	2.023769	1.217084	-3.057070
H	2.775289	2.544873	-2.195588
C	-0.641413	1.891828	-2.662158
H	-1.438327	2.525465	-3.066054
H	-0.431006	1.141137	-3.435019
P	2.013750	0.802005	-0.677896
P	-1.285611	0.939620	-1.194648
Ni	0.315313	-0.535589	-0.297235
C	2.141586	1.990022	0.721633
C	1.430268	1.725377	1.903401
C	2.923002	3.156440	0.643209
C	1.505815	2.607117	2.984181
H	0.809946	0.836406	1.984651
C	2.992983	4.035440	1.723316
H	3.491189	3.379169	-0.255594
C	2.284462	3.760950	2.896372
H	0.949744	2.387519	3.890898
H	3.601059	4.932988	1.649099
H	2.340444	4.446685	3.737488
C	3.713624	0.136304	-0.940741
C	4.780986	0.421711	-0.079870
C	3.945624	-0.672693	-2.065059
C	6.057793	-0.077219	-0.348268
H	4.621482	1.028310	0.804903
C	5.221218	-1.165249	-2.333389
H	3.125243	-0.938748	-2.726382
C	6.282636	-0.865815	-1.476073
H	6.874915	0.150430	0.330905
H	5.383224	-1.791663	-3.206267
H	7.276335	-1.253687	-1.682657
C	-2.735846	0.087707	-1.946513
C	-2.553649	-1.193274	-2.490501
C	-3.996315	0.695512	-2.040323
C	-3.607381	-1.844576	-3.131923
H	-1.596801	-1.695485	-2.386575
C	-5.050513	0.038305	-2.676486
H	-4.162410	1.677229	-1.607310
C	-4.857550	-1.230374	-3.226117
H	-3.454654	-2.839525	-3.540869
H	-6.024199	0.517309	-2.736476
H	-5.680983	-1.742922	-3.716162
C	-1.989890	2.238805	-0.091487
C	-2.175446	1.927168	1.266383
C	-2.354500	3.517112	-0.548314

C	-2.724004	2.870461	2.137064
H	-1.896083	0.951406	1.650948
C	-2.894671	4.459442	0.328474
H	-2.225270	3.791732	-1.590462
C	-3.082604	4.137021	1.673582
H	-2.865887	2.609285	3.182135
H	-3.169009	5.443536	-0.042378
H	-3.504639	4.870320	2.355694
C	2.506867	-4.060318	-0.329154
C	1.699765	-2.964884	-0.647984
C	1.563564	-1.885437	0.238109
C	2.255171	-1.933179	1.454593
C	3.059333	-3.031884	1.779069
C	3.192158	-4.095846	0.887308
H	2.590473	-4.890843	-1.027260
H	1.154715	-2.972377	-1.591266
H	2.161757	-1.124527	2.175331
H	3.576183	-3.054488	2.736098
H	3.815952	-4.949492	1.140408
O	-1.153126	-1.717592	0.210144
S	-1.418986	-2.059440	1.680341
O	-1.084176	-0.933293	2.577996
O	-1.018984	-3.407876	2.075149
C	-3.280994	-2.098198	1.625590
F	-3.763830	-2.381537	2.841162
F	-3.707560	-3.025441	0.762415
F	-3.767724	-0.903481	1.244204
H	0.464949	3.361940	-1.497309
H	0.784994	3.401071	-3.220905

TS4'

B3LYP/BS1 SCF energy: -3436.852829 a.u.

M06/BS2 SCF energy in PhMe: -3436.07169343 a.u.

M06/BS2 Free energy in PhMe: -3435.47288243 a.u.

C	1.958735	1.520896	-3.177433
C	0.435525	1.335823	-3.296619
H	0.224873	0.382149	-3.795580
H	0.003295	2.126294	-3.918939
C	2.703606	0.257290	-2.725387
H	3.779290	0.379124	-2.891623
H	2.389921	-0.583439	-3.354342
P	-0.401363	1.311709	-1.633714
P	2.475278	-0.299267	-0.948659
Ni	0.409901	-0.408904	-0.238447
C	-0.250829	3.079602	-1.119666
C	0.217661	3.414454	0.157021
C	-0.617089	4.112613	-2.001648
C	0.338836	4.754359	0.536802
H	0.459552	2.635075	0.866961
C	-0.494129	5.447223	-1.621684
H	-1.016995	3.878550	-2.984653
C	-0.009915	5.770901	-0.350385
H	0.696169	4.994319	1.534113
H	-0.781531	6.234187	-2.314081
H	0.083230	6.812092	-0.052880
C	-2.191856	1.168172	-2.046319
C	-3.138412	1.654417	-1.129402
C	-2.643109	0.540633	-3.216955
C	-4.502603	1.520244	-1.385059
H	-2.810327	2.135633	-0.215368
C	-4.010367	0.413302	-3.472250
H	-1.936667	0.146044	-3.940386
C	-4.943584	0.901844	-2.557232
H	-5.220211	1.899087	-0.662513
H	-4.343073	-0.067057	-4.388915
H	-6.007287	0.800619	-2.755231
C	3.521875	-1.824843	-0.986786
C	3.342279	-2.778920	-2.001325
C	4.476761	-2.074286	0.009006
C	4.113766	-3.940301	-2.032035
H	2.586707	-2.633625	-2.768356
C	5.243986	-3.239766	-0.019732
H	4.618396	-1.363017	0.815296
C	5.069811	-4.173181	-1.041825
H	3.962251	-4.665180	-2.827520
H	5.976768	-3.416894	0.762781
H	5.669320	-5.079199	-1.063648
C	3.496331	0.905789	0.008081
C	2.999954	1.435677	1.207401
C	4.777530	1.291328	-0.425120
C	3.764555	2.334769	1.955732
H	2.018841	1.152284	1.572134
C	5.535315	2.194324	0.318634
H	5.199775	0.875072	-1.335441

C	5.029121	2.718910	1.511739
H	3.359902	2.727191	2.884210
H	6.522865	2.484258	-0.030445
H	5.622878	3.420294	2.091980
C	1.166432	-4.294899	1.171607
C	1.602732	-4.119027	2.486994
C	1.741584	-2.826346	2.989641
C	1.449874	-1.716232	2.187039
C	0.998950	-1.874640	0.868242
C	0.876602	-3.185140	0.373666
H	1.056073	-5.296844	0.761351
H	1.830793	-4.980155	3.110552
H	2.068650	-2.669967	4.015198
H	1.551403	-0.729434	2.625782
H	0.548207	-3.352416	-0.649676
O	-0.976767	0.510110	1.168420
S	-1.022169	0.653949	2.671842
O	0.164151	1.341726	3.220584
O	-1.515391	-0.542138	3.370422
C	-2.404730	1.888791	2.858104
F	-2.123113	3.032902	2.206186
F	-2.603840	2.176338	4.148673
F	-3.547654	1.397234	2.348105
O	-1.417832	-1.568904	-0.780243
C	-2.156855	-1.969307	0.121819
C	-3.368259	-2.767097	-0.108884
C	-4.121210	-3.169216	1.005510
C	-3.777881	-3.130562	-1.402871
C	-5.273505	-3.933579	0.829199
C	-4.927504	-3.893189	-1.574718
C	-5.673894	-4.295580	-0.459370
H	-3.795898	-2.874942	2.000554
H	-5.857076	-4.246118	1.690335
H	-6.571621	-4.892484	-0.598254
H	-5.249103	-4.177565	-2.572933
H	-3.187367	-2.799763	-2.251178
H	-1.922506	-1.730643	1.168155
H	2.193789	2.366138	-2.518830
H	2.347111	1.793704	-4.167312

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B3LYP/BS1 SCF energy: -3436.860186 a.u.

M06/BS2 SCF energy in PhMe: -3436.07247284 a.u.

M06/BS2 Free energy in PhMe: -3435.47481084 a.u.

C	2.292497	-1.457010	-3.228425
C	1.240100	-2.533413	-2.915663
H	1.730360	-3.426305	-2.508719
H	0.730760	-2.846283	-3.832837
C	3.311979	-1.248296	-2.097556
H	4.196456	-0.729627	-2.481875
H	3.655073	-2.223993	-1.735238
P	-0.038835	-1.982889	-1.676059
P	2.714696	-0.254318	-0.626239
Ni	0.770312	-0.860588	0.202806
C	-1.289192	-1.111049	-2.698545
C	-1.786946	0.121238	-2.251800
C	-1.761736	-1.639551	-3.914543
C	-2.735638	0.817947	-3.006016
H	-1.450832	0.563903	-1.320815
C	-2.707174	-0.942646	-4.664475
H	-1.405509	-2.601365	-4.274248
C	-3.193961	0.288593	-4.211381
H	-3.102227	1.769566	-2.634263
H	-3.064943	-1.360079	-5.602014
H	-3.929946	0.829572	-4.800245
C	-0.809872	-3.582367	-1.174761
C	-2.166586	-3.869383	-1.376685
C	-0.012072	-4.522756	-0.500455
C	-2.707923	-5.078009	-0.930604
H	-2.805211	-3.151471	-1.880445
C	-0.552421	-5.730029	-0.060126
H	1.036329	-4.308453	-0.304442
C	-1.904189	-6.011566	-0.275899
H	-3.761503	-5.285870	-1.096718
H	0.079502	-6.446850	0.457269
H	-2.327062	-6.951268	0.068716
C	4.196279	-0.333227	0.469645
C	4.852140	-1.553925	0.693774
C	4.651923	0.812344	1.139339
C	5.949679	-1.624146	1.552648
H	4.509913	-2.464128	0.209285
C	5.748218	0.739035	1.998625
H	4.144602	1.760644	0.999663

C	6.402459	-0.476602	2.205046
H	6.447872	-2.576771	1.711696
H	6.086452	1.635403	2.510791
H	7.256568	-0.530670	2.874501
C	2.695931	1.453437	-1.299502
C	1.524745	2.219418	-1.230394
C	3.840375	2.001393	-1.908961
C	1.492303	3.511627	-1.763464
H	0.628556	1.842743	-0.749768
C	3.803663	3.288395	-2.440577
H	4.767174	1.435339	-1.953017
C	2.628391	4.044792	-2.369390
H	0.575817	4.087179	-1.683256
H	4.693766	3.703978	-2.905551
H	2.606132	5.050658	-2.780215
C	2.163588	-0.545227	4.122791
C	1.889177	0.774693	4.491216
C	1.346231	1.651259	3.551477
C	1.079950	1.216770	2.246068
C	1.350536	-0.105980	1.868039
C	1.900094	-0.979141	2.820075
H	2.584241	-1.239108	4.847852
H	2.094198	1.113803	5.503771
H	1.112172	2.678225	3.821023
H	0.634146	1.921840	1.552255
H	2.128381	-2.010563	2.554830
O	-1.391577	2.200584	0.041484
S	-1.962547	3.308799	0.871688
O	-0.955215	4.185975	1.490137
O	-3.091873	2.879831	1.724386
C	-2.757619	4.375877	-0.428855
F	-1.837623	4.820239	-1.309958
F	-3.362968	5.438697	0.112838
F	-3.682029	3.679931	-1.125749
O	-0.913186	-1.349408	1.087050
C	-1.790971	-0.588513	1.541801
C	-2.981368	-1.083636	2.216789
C	-3.926935	-0.138589	2.658314
C	-3.191589	-2.460389	2.432136
C	-5.076031	-0.576730	3.315676
C	-4.339037	-2.883359	3.089311
C	-5.279770	-1.941383	3.531183
H	-3.753143	0.920427	2.474282
H	-5.810194	0.146059	3.659083
H	-6.175737	-2.278760	4.046223
H	-4.508884	-3.942302	3.263179
H	-2.450679	-3.171521	2.080863
H	-1.688832	0.495093	1.419303
H	1.808704	-0.508090	-3.492966
H	2.844631	-1.772198	-4.122960

TS5'

B3LYP/BS1 SCF energy: -3436.828803 a.u.

M06/BS2 SCF energy in PhMe: -3436.04354166 a.u.

M06/BS2 Free energy in PhMe: -3435.44548366 a.u.

C	1.933445	0.230223	-3.753493
C	2.457318	-1.092962	-3.171681
H	3.521725	-0.989771	-2.930673
H	2.380564	-1.892322	-3.915940
C	2.301556	1.458955	-2.905481
H	2.221804	2.368431	-3.509554
H	3.348242	1.388829	-2.586664
P	1.568455	-1.639940	-1.629534
P	1.254740	1.730926	-1.378669
Ni	1.009567	-0.084455	-0.070700
C	0.105264	-2.550070	-2.257084
C	-1.155847	-2.285169	-1.705858
C	0.222387	-3.516392	-3.273540
C	-2.287015	-2.962662	-2.169624
H	-1.281227	-1.564019	-0.908155
C	-0.907093	-4.191282	-3.732034
H	1.193005	-3.758757	-3.698557
C	-2.163728	-3.912516	-3.182509
H	-3.250130	-2.735794	-1.722675
H	-0.807118	-4.936854	-4.516427
H	-3.041547	-4.441273	-3.544460
C	2.692174	-2.909460	-0.915720
C	2.201602	-4.151378	-0.488037
C	4.049327	-2.608690	-0.712262
C	3.056158	-5.079418	0.110084
H	1.152491	-4.393463	-0.617944
C	4.901289	-3.538658	-0.117578

H	4.450612	-1.643295	-1.011044
C	4.406113	-4.778539	0.293579
H	2.661203	-6.037719	0.435773
H	5.950124	-3.293552	0.026666
H	5.069231	-5.503179	0.758049
C	2.143617	3.158975	-0.620966
C	3.511722	3.031495	-0.324638
C	1.495406	4.362450	-0.311977
C	4.219757	4.091121	0.239876
H	4.033075	2.099261	-0.528070
C	2.206051	5.421611	0.257844
H	0.436501	4.477034	-0.515957
C	3.567951	5.292348	0.529103
H	5.278720	3.977352	0.455748
H	1.689062	6.349072	0.488330
H	4.118973	6.119877	0.967546
C	-0.299598	2.405885	-2.081602
C	-1.528550	1.836033	-1.722620
C	-0.278878	3.480717	-2.991891
C	-2.721122	2.333728	-2.257855
H	-1.589219	1.011411	-1.019655
C	-1.468196	3.968746	-3.527348
H	0.660191	3.951733	-3.270410
C	-2.691002	3.395001	-3.160151
H	-3.659443	1.887998	-1.945284
H	-1.442361	4.799970	-4.227098
H	-3.617137	3.783699	-3.575166
C	1.887390	2.413427	3.097040
C	0.800270	3.284147	3.227771
C	-0.399451	3.016978	2.560765
C	-0.514763	1.885711	1.752989
C	0.569799	0.995234	1.608767
C	1.764063	1.272338	2.307719
H	2.814499	2.613740	3.628073
H	0.883824	4.161484	3.864338
H	-1.252877	3.679623	2.677070
H	-1.462216	1.683048	1.264265
H	2.590652	0.565265	2.261462
O	-2.659982	-0.388240	0.241924
S	-3.818920	0.107116	1.050663
O	-3.997515	1.572273	0.985852
O	-3.937160	-0.521166	2.380062
C	-5.257621	-0.559671	0.076918
F	-5.298998	0.003742	-1.148914
F	-6.421396	-0.311762	0.689061
F	-5.148347	-1.892777	-0.095202
O	0.733411	-1.542623	1.053950
C	-0.028584	-0.924744	1.929066
C	0.178331	-1.188353	3.375514
C	-0.877594	-0.919741	4.260050
C	1.367359	-1.757810	3.854819
C	-0.730122	-1.198256	5.618971
C	1.507436	-2.034566	5.212152
C	0.461573	-1.748384	6.097072
H	-1.814993	-0.522474	3.876386
H	-1.550157	-0.994518	6.301918
H	0.573025	-1.965891	7.156338
H	2.427197	-2.479367	5.583563
H	2.161684	-1.991566	3.152332
H	-1.067860	-0.742842	1.643758
H	0.848606	0.181591	-3.913165
H	2.377680	0.360172	-4.748402

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B3LYP/BS1 SCF energy: -3436.853649 a.u.

M06/BS2 SCF energy in PhMe: -3436.06806731 a.u.

M06/BS2 Free energy in PhMe: -3435.46720531 a.u.

C	2.561589	0.775805	-3.274435
C	2.579116	-0.749502	-3.091807
H	3.577457	-1.065902	-2.769927
H	2.384421	-1.248347	-4.046783
C	3.167112	1.538374	-2.086011
H	3.431860	2.557288	-2.386282
H	4.099125	1.055953	-1.767643
P	1.339827	-1.397182	-1.861816
P	2.061929	1.676911	-0.585835
Ni	1.132493	-0.307885	0.057054
C	-0.221440	-1.492028	-2.811512
C	-1.400919	-0.953701	-2.281909
C	-0.250096	-2.109661	-4.076375
C	-2.592635	-1.013546	-3.009778
H	-1.425819	-0.496659	-1.301158
C	-1.441288	-2.172351	-4.795743
H	0.645969	-2.560287	-4.495386

C	-2.612553	-1.620104	-4.264720
H	-3.489115	-0.584784	-2.573208
H	-1.456538	-2.654731	-5.769433
H	-3.538772	-1.670762	-4.830926
C	1.886148	-3.122428	-1.564405
C	0.942486	-4.158045	-1.497604
C	3.239489	-3.414183	-1.328364
C	1.351206	-5.463752	-1.224493
H	-0.108656	-3.941097	-1.648763
C	3.644048	-4.720773	-1.055989
H	3.988232	-2.626725	-1.347295
C	2.700006	-5.748880	-1.006296
H	0.610238	-6.256418	-1.174063
H	4.695094	-4.933813	-0.880959
H	3.014880	-6.766735	-0.793256
C	3.209888	2.514441	0.589092
C	4.399049	1.859166	0.951528
C	2.934600	3.772523	1.141802
C	5.301476	2.457412	1.829570
H	4.623040	0.871333	0.555561
C	3.839254	4.369205	2.024052
H	2.015993	4.289500	0.886272
C	5.023582	3.716882	2.367566
H	6.219353	1.939962	2.095190
H	3.613478	5.346556	2.441769
H	5.726352	4.184452	3.051617
C	0.829563	2.931795	-1.101198
C	-0.535080	2.676198	-0.907024
C	1.221618	4.137543	-1.715744
C	-1.495798	3.603253	-1.322529
H	-0.886872	1.765508	-0.435163
C	0.262018	5.061291	-2.122886
H	2.273334	4.367106	-1.865343
C	-1.098047	4.793368	-1.928753
H	-2.544008	3.373416	-1.163144
H	0.574746	5.990028	-2.592744
H	-1.842955	5.515985	-2.251007
C	2.182909	0.628960	3.355768
C	1.523405	1.818938	3.657179
C	0.214627	2.029975	3.205010
C	-0.448871	1.048275	2.473355
C	0.190806	-0.179592	2.192042
C	1.526049	-0.365921	2.623364
H	3.198032	0.462875	3.704377
H	2.028166	2.585691	4.237965
H	-0.300593	2.958420	3.435036
H	-1.470895	1.218388	2.149556
H	2.004334	-1.327360	2.463151
O	-2.775650	0.678822	-0.058427
S	-3.926598	0.851220	0.881978
O	-3.749730	1.972466	1.827841
O	-4.454331	-0.408898	1.438293
C	-5.261231	1.435768	-0.274856
F	-4.915615	2.606148	-0.854592
F	-6.421858	1.620339	0.365329
F	-5.465990	0.540342	-1.263029
O	0.267345	-1.837711	0.508910
C	-0.566001	-1.367460	1.557289
C	-0.874530	-2.473056	2.558165
C	-2.106888	-2.465360	3.225597
C	0.047739	-3.491272	2.828831
C	-2.393909	-3.446322	4.176809
C	-0.245431	-4.474317	3.775374
C	-1.463670	-4.449358	4.458474
H	-2.849699	-1.708993	2.981083
H	-3.353187	-3.432236	4.687656
H	-1.692120	-5.215211	5.195595
H	0.475025	-5.264235	3.975132
H	0.979388	-3.526323	2.272183
H	-1.515354	-0.986365	1.164145
H	1.545024	1.131358	-3.484593
H	3.154185	1.014212	-4.166542

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B3LYP/BS1 SCF energy: -3436.877867 a.u.

M06/BS2 SCF energy in PhMe: -3436.08678398 a.u.

M06/BS2 Free energy in PhMe: -3435.48632998 a.u.

C	-2.180340	1.433179	-3.049305
C	-2.449598	1.945994	-1.625029
H	-3.247639	1.354812	-1.159043
H	-2.800737	2.982548	-1.674900

C	-1.921923	-0.079114	-3.160710
H	-1.942650	-0.391761	-4.211278
H	-2.733600	-0.623438	-2.662149
P	-0.976865	1.856884	-0.495376
P	-0.367406	-0.773971	-2.391568
Ni	-0.216403	-0.208890	-0.158837
C	0.283586	2.928904	-1.303067
C	1.615746	2.495301	-1.375947
C	-0.057899	4.196939	-1.805922
C	2.587467	3.317985	-1.953819
H	1.906331	1.528205	-0.974891
C	0.914214	5.009032	-2.386188
H	-1.079199	4.561647	-1.732072
C	2.239554	4.568510	-2.462357
H	3.615660	2.971419	-2.002666
H	0.640305	5.987386	-2.772017
H	2.997135	5.204642	-2.912400
C	-1.462999	2.819634	0.987215
C	-0.465485	3.122671	1.928193
C	-2.770819	3.274103	1.205954
C	-0.769394	3.885838	3.052502
H	0.543134	2.749199	1.785964
C	-3.073338	4.034139	2.339606
H	-3.564985	3.045341	0.502394
C	-2.073089	4.345669	3.260036
H	0.010053	4.109939	3.774857
H	-4.090554	4.382701	2.496484
H	-2.307758	4.939741	4.139129
C	-0.709869	-2.573675	-2.571518
C	-1.425957	-3.227493	-1.556744
C	-0.347872	-3.285802	-3.724563
C	-1.778774	-4.569254	-1.698883
H	-1.700096	-2.702869	-0.646583
C	-0.696676	-4.630574	-3.858036
H	0.214716	-2.798485	-4.514523
C	-1.412991	-5.273851	-2.847266
H	-2.329864	-5.060443	-0.902168
H	-0.404338	-5.174544	-4.752211
H	-1.680160	-6.322008	-2.952116
C	0.982112	-0.426859	-3.594171
C	2.233611	-1.039135	-3.398879
C	0.814341	0.434056	-4.690183
C	3.286526	-0.784775	-4.276953
H	2.394892	-1.728543	-2.577304
C	1.873837	0.689120	-5.563233
H	-0.140792	0.909590	-4.881854
C	3.113132	0.083348	-5.357015
H	4.244505	-1.268459	-4.109205
H	1.724689	1.359365	-6.405521
H	3.937612	0.282371	-6.036367
C	-4.539565	-1.375390	1.230777
C	-4.754653	-2.748932	1.368145
C	-3.721014	-3.559946	1.842918
C	-2.484241	-2.999879	2.171782
C	-2.254678	-1.624012	2.033901
C	-3.300341	-0.820401	1.558933
H	-5.342934	-0.733881	0.874445
H	-5.718120	-3.182009	1.111920
H	-3.877409	-4.629925	1.958569
H	-1.683020	-3.637957	2.538392
H	-3.132863	0.247780	1.460157
O	2.809964	-0.329399	-0.085936
S	2.355852	-1.699175	0.210200
O	3.012399	-2.810529	-0.486298
O	0.830839	-1.835451	0.177982
C	2.757927	-1.958652	2.012849
F	4.079393	-2.100841	2.154467
F	2.152502	-3.066006	2.473383
F	2.354722	-0.914907	2.742083
O	-0.551614	0.096245	1.631640
C	-0.890160	-1.027335	2.410034
C	-0.869286	-0.632637	3.890451
C	-0.115489	-1.375280	4.806465
C	-1.608863	0.461257	4.360133
C	-0.106858	-1.042994	6.163645
C	-1.597872	0.798680	5.712820
C	-0.849499	0.045203	6.622084
H	0.481111	-2.211568	4.452196
H	0.485934	-1.631955	6.859344
H	-0.843682	0.307491	7.677157
H	-2.176493	1.651761	6.059653
H	-2.188914	1.054334	3.660782
H	-0.158424	-1.833979	2.286607
H	-1.358230	2.007048	-3.490069
H	-3.068088	1.659135	-3.654558

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B3LYP/BS1 SCF energy: -3436.840658 a.u.

M06/BS2 SCF energy in PhMe: -3436.05934968 a.u.

M06/BS2 Free energy in PhMe: -3435.46339768 a.u.

C	-1.083723	-2.324441	2.964861
C	-1.235434	-0.822071	3.265688
H	-0.328436	-0.454793	3.761888
H	-2.071626	-0.674743	3.958260
C	0.254629	-2.724300	2.320103
H	0.392492	-3.810057	2.375133
H	1.086382	-2.282061	2.882086
P	-1.529728	0.223681	1.747907
P	0.507469	-2.193886	0.550136
Ni	0.278059	-0.014669	0.363424
C	-3.252267	-0.255556	1.303684
C	-3.537348	-0.866210	0.077484
C	-4.301375	-0.008099	2.207073
C	-4.847142	-1.236810	-0.237653
H	-2.755633	-1.036409	-0.650308
C	-5.605662	-0.381822	1.891722
H	-4.104462	0.497553	3.149033
C	-5.880011	-0.999908	0.667341
H	-5.049312	-1.691667	-1.202596
H	-6.409471	-0.181273	2.595301
H	-6.899683	-1.282092	0.418295
C	-1.705795	1.933481	2.399316
C	-2.028453	2.947607	1.479720
C	-1.523943	2.262739	3.750934
C	-2.176557	4.262299	1.919507
H	-2.158540	2.707137	0.427342
C	-1.667701	3.584628	4.181288
H	-1.276710	1.499233	4.482031
C	-1.995723	4.585444	3.267048
H	-2.430126	5.037808	1.201858
H	-1.527083	3.826600	5.231655
H	-2.109585	5.613014	3.602548
C	2.189976	-2.887902	0.226801
C	3.291230	-2.335195	0.902168
C	2.401494	-3.952701	-0.659335
C	4.573197	-2.846119	0.703571
H	3.154639	-1.493446	1.574855
C	3.689175	-4.456310	-0.862883
H	1.566000	-4.387548	-1.197138
C	4.775737	-3.908538	-0.181406
H	5.412557	-2.405223	1.234229
H	3.838386	-5.278097	-1.558043
H	5.775746	-4.302592	-0.341217
C	-0.619313	-3.243389	-0.448711
C	-1.003869	-2.777096	-1.715365
C	-1.079265	-4.497258	-0.008945
C	-1.842000	-3.547466	-2.524264
H	-0.684032	-1.798377	-2.057015
C	-1.912066	-5.264484	-0.823432
H	-0.793655	-4.887163	0.963381
C	-2.295233	-4.790367	-2.081485
H	-2.151056	-3.148695	-3.485369
H	-2.265200	-6.230486	-0.472291
H	-2.951929	-5.387676	-2.708593
C	3.460791	1.184323	3.733616
C	4.827932	1.030131	3.480111
C	5.290703	1.051629	2.164176
C	4.395554	1.211643	1.103819
C	3.019668	1.337078	1.347033
C	2.566491	1.339315	2.677815
H	3.095226	1.196813	4.757183
H	5.526697	0.911705	4.303938
H	6.353510	0.957421	1.957838
H	4.774181	1.251045	0.089604
H	1.509188	1.491746	2.864930
O	-2.404138	1.817543	-1.569355
S	-1.638629	0.890672	-2.426923
O	-2.410082	-0.177468	-3.095239
O	-0.357692	0.398412	-1.813576
C	-1.038863	1.961860	-3.826613
F	-2.068767	2.323278	-4.605631
F	-0.145925	1.305688	-4.582795
F	-0.458613	3.078629	-3.357099
O	0.808569	1.861531	0.594874
C	1.999607	1.546149	0.245883
C	2.480210	1.940731	-1.125519
C	3.301577	1.126905	-1.919153
C	2.103750	3.204321	-1.596170
C	3.752792	1.579582	-3.157198
C	2.569528	3.660493	-2.829446
C	3.395571	2.852432	-3.610684

H	3.556222	0.125058	-1.583302
H	4.372488	0.934111	-3.773646
H	3.747232	3.204261	-4.576755
H	2.268801	4.641002	-3.187276
H	1.438575	3.816088	-0.995947
H	1.668158	-0.155883	-0.185833
H	-1.923298	-2.674011	2.351757
H	-1.161051	-2.864219	3.917539

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B3LYP/BS1 SCF energy: -2860.246012 a.u.

M06/BS2 SCF energy in PhMe: -2859.70752993 a.u.

M06/BS2 Free energy in PhMe: -2859.29028193 a.u.

C	0.503006	-3.204889	1.266550
C	-0.833588	-2.632833	1.778099
H	-0.710783	-2.323221	2.823224
H	-1.602683	-3.413169	1.760407
C	1.728353	-2.346450	1.630951
H	2.646876	-2.939007	1.557460
H	1.660562	-2.025119	2.678141
P	-1.440090	-1.156267	0.819332
P	1.932383	-0.779737	0.639756
Ni	0.178217	0.402697	0.345639
C	-2.147294	-1.919053	-0.702357
C	-1.686280	-1.509842	-1.962055
C	-3.151288	-2.899360	-0.624870
C	-2.212341	-2.082751	-3.123624
H	-0.936723	-0.728794	-2.045821
C	-3.670359	-3.470907	-1.784512
H	-3.543255	-3.204486	0.342412
C	-3.198701	-3.064237	-3.036870
H	-1.853541	-1.749117	-4.093070
H	-4.448228	-4.226555	-1.713251
H	-3.608922	-3.506363	-3.940916
C	-2.920892	-0.589593	1.757889
C	-3.668065	0.479222	1.228458
C	-3.329650	-1.169138	2.969751
C	-4.798019	0.946060	1.898445
H	-3.357521	0.956786	0.305798
C	-4.460421	-0.693138	3.637775
H	-2.779869	-1.997255	3.404970
C	-5.197333	0.363729	3.103690
H	-5.362208	1.773113	1.476704
H	-4.763429	-1.153782	4.574441
H	-6.077010	0.732983	3.624081
C	3.322197	0.020936	1.545240
C	3.062627	1.161643	2.318609
C	4.619557	-0.513330	1.528078
C	4.080422	1.750593	3.071109
H	2.067216	1.597146	2.314305
C	5.637076	0.082227	2.273801
H	4.846048	-1.381621	0.915877
C	5.368053	1.212340	3.049596
H	3.867739	2.635955	3.663860
H	6.640679	-0.333461	2.244411
H	6.162248	1.676159	3.628331
C	2.597015	-1.323364	-0.990778
C	2.340817	-0.521717	-2.117613
C	3.340206	-2.505094	-1.153196
C	2.834629	-0.890523	-3.370124
H	1.742697	0.379824	-2.023110
C	3.830006	-2.869273	-2.408125
H	3.540288	-3.156425	-0.307930
C	3.580491	-2.060752	-3.518649
H	2.624965	-0.260583	-4.229897
H	4.402835	-3.786395	-2.516387
H	3.960246	-2.346563	-4.495899
O	-2.499733	2.822959	-1.875303
S	-1.138627	2.442438	-1.491818
O	-0.279078	1.783296	-2.489813
O	-1.136701	1.728752	-0.135565
C	-0.285784	4.050038	-1.085560
F	-0.347569	4.871172	-2.140524
F	1.004632	3.848452	-0.779222
F	-0.882997	4.638942	-0.042316
H	1.278731	1.325224	0.037446
H	0.459011	-3.376008	0.183080
H	0.638474	-4.194139	1.721965

TS8'

B3LYP/BS1 SCF energy: -3269.377670 a.u.

M06/BS2 SCF energy in PhMe: -3268.66922264 a.u.

M06/BS2 Free energy in PhMe: -3267.99224964 a.u.

C	0.527643	3.429856	1.838107

C	1.483692	2.404518	2.477644
H	1.015890	2.005107	3.386114
H	2.417625	2.892509	2.780271
C	-0.947252	2.990775	1.830275
H	-1.593776	3.865255	1.698334
H	-1.205004	2.565042	2.807952
P	1.852972	0.975231	1.337046
P	-1.431719	1.704348	0.537672
Ni	-0.048436	0.130832	0.297920
C	3.183415	1.702364	0.272887
C	2.977106	1.812421	-1.109238
C	4.395647	2.158853	0.818121
C	3.957365	2.382947	-1.927229
H	2.062521	1.435708	-1.554726
C	5.371606	2.727179	0.001730
H	4.584192	2.056693	1.884118
C	5.151769	2.843186	-1.374601
H	3.784672	2.454676	-2.997577
H	6.305491	3.074561	0.436539
H	5.914604	3.283443	-2.011667
C	2.815539	-0.191350	2.402423
C	2.966163	-0.045683	3.790246
C	3.387643	-1.317672	1.780330
C	3.667999	-0.997042	4.536533
H	2.546309	0.812648	4.304858
C	4.092735	-2.260491	2.525966
H	3.278460	-1.453104	0.708984
C	4.233551	-2.105834	3.908166
H	3.775281	-0.863747	5.610204
H	4.530581	-3.120466	2.025837
H	4.780753	-2.843799	4.488789
C	-3.206037	1.508131	1.071222
C	-3.458023	0.958671	2.341293
C	-4.305170	1.858820	0.272608
C	-4.761837	0.783100	2.805199
H	-2.626043	0.659451	2.975013
C	-5.612618	1.675490	0.732864
H	-4.145637	2.282270	-0.713406
C	-5.846694	1.142184	2.000399
H	-4.930563	0.364252	3.794063
H	-6.448310	1.955520	0.096523
H	-6.863299	1.005677	2.359141
C	-1.541468	2.750422	-0.993283
C	-0.972942	2.264401	-2.181108
C	-2.143628	4.021081	-1.008078
C	-1.006123	3.027176	-3.351707
H	-0.497042	1.288116	-2.195785
C	-2.178841	4.781121	-2.177335
H	-2.603770	4.420807	-0.108639
C	-1.608154	4.285408	-3.352876
H	-0.556601	2.630169	-4.257672
H	-2.650978	5.760280	-2.169916
H	-1.633580	4.879462	-4.262796
O	1.077721	-1.261406	-0.708078
S	1.059959	-1.582597	-2.184696
O	1.066263	-0.406587	-3.068411
O	0.101332	-2.663942	-2.516034
C	2.736554	-2.364730	-2.378930
F	3.694643	-1.500757	-2.011536
F	2.937964	-2.718788	-3.651254
F	2.832362	-3.454953	-1.603793
H	-1.371006	-0.911210	-0.081673
C	-1.795603	-3.042871	0.926781
C	-3.079196	-2.827705	1.751910
C	-4.367731	-2.978435	0.936848
C	-4.349385	-2.012063	-0.251436
C	-3.125987	-2.193785	-1.168743
N	-1.863124	-2.198759	-0.327163
H	-4.492018	-4.014175	0.596181
H	-3.065626	-3.529767	2.595146
H	-5.253534	-2.129865	-0.861699
H	-5.232886	-2.759399	1.574349
H	-4.357984	-0.985118	0.129997
H	-3.053526	-1.817015	2.178059
H	-1.102209	-2.490629	-0.952160
C	-0.576010	-2.576761	1.743537
H	-0.554668	-3.106696	2.702962
H	0.360807	-2.777138	1.217428
H	-0.621944	-1.497383	1.947571
C	-1.579891	-4.535800	0.591826
H	-0.764172	-4.657389	-0.129206
H	-1.301276	-5.072981	1.505770
H	-2.469059	-5.020456	0.184939
C	-3.014357	-1.008074	-2.143456
H	-2.152644	-1.125066	-2.807951
H	-3.918254	-0.960893	-2.761341

H	-2.914521	-0.060290	-1.610692
C	-3.241546	-3.479594	-2.018460
H	-4.039336	-3.344578	-2.758250
H	-2.310060	-3.667930	-2.561173
H	-3.489380	-4.366793	-1.432511
H	0.594695	4.360693	2.416553
H	0.859922	3.684096	0.822711

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B3LYP/BS1 SCF energy: -3269.392675 a.u.

M06/BS2 SCF energy in PhMe: -3268.68350473 a.u.

M06/BS2 Free energy in PhMe: -3268.00208773 a.u.

C	1.610534	3.395405	1.560258
C	2.415889	2.226893	2.164615
H	1.979595	1.960785	3.136048
H	3.451041	2.541597	2.348201
C	0.081821	3.270258	1.707762
H	-0.384979	4.256495	1.599963
H	-0.158140	2.927325	2.722297
P	2.391450	0.691159	1.091068
P	-0.738358	2.044396	0.520724
Ni	0.401047	0.310081	0.318970
C	3.713882	1.115009	-0.146232
C	3.362015	1.229250	-1.499036
C	5.051704	1.331647	0.222992
C	4.321304	1.565313	-2.458769
H	2.334879	1.043655	-1.801344
C	6.009972	1.664240	-0.733854
H	5.350300	1.225757	1.263215
C	5.645259	1.784674	-2.078228
H	4.031325	1.647477	-3.503081
H	7.042229	1.825383	-0.432447
H	6.392996	2.041823	-2.824306
C	3.281216	-0.552594	2.146241
C	3.679832	-0.332310	3.474251
C	3.510948	-1.823579	1.585055
C	4.290426	-1.347315	4.217741
H	3.523831	0.634709	3.941994
C	4.129704	-2.830806	2.322812
H	3.201734	-2.022448	0.562653
C	4.519370	-2.598012	3.645437
H	4.591661	-1.153772	5.244626
H	4.303334	-3.802230	1.866481
H	4.996054	-3.385852	4.223055
C	-2.473815	2.204898	1.219843
C	-2.708484	1.702983	2.515543
C	-3.569658	2.736902	0.519308
C	-3.976333	1.751690	3.095688
H	-1.883107	1.271806	3.079332
C	-4.845042	2.774986	1.093405
H	-3.426661	3.140716	-0.478193
C	-5.055357	2.287921	2.384345
H	-4.122463	1.376377	4.106087
H	-5.673023	3.200384	0.530839
H	-6.043651	2.329882	2.834574
C	-0.836634	3.053640	-1.042982
C	-0.574703	2.399303	-2.258404
C	-1.130977	4.427447	-1.076217
C	-0.605955	3.096653	-3.468941
H	-0.338676	1.337953	-2.255641
C	-1.163638	5.125244	-2.284919
H	-1.348461	4.962473	-0.155903
C	-0.899038	4.461024	-3.485230
H	-0.395509	2.569800	-4.396062
H	-1.393952	6.187908	-2.288635
H	-0.920229	5.005714	-4.425820
O	0.398206	-1.608946	-0.500061
S	0.199074	-2.076223	-1.909999
O	0.348369	-1.055784	-2.954993
O	-1.012921	-2.949837	-2.016873
C	1.618796	-3.253898	-2.140927
F	2.778551	-2.597394	-1.994063
F	1.580218	-3.798755	-3.360188
F	1.563661	-4.231319	-1.226457
H	-2.297022	-0.952556	0.132898
C	-2.904852	-2.659471	1.185871
C	-4.112536	-2.107591	1.966572
C	-5.382544	-1.943990	1.122393
C	-5.113244	-1.026234	-0.076917
C	-3.981944	-1.525034	-0.991075
N	-2.757015	-1.848243	-0.113190
H	-5.758671	-2.919641	0.790529
H	-4.293014	-2.776626	2.816482
H	-6.014766	-0.916401	-0.691482
H	-6.172681	-1.505573	1.742415

H	-4.861265	-0.023589	0.290958
H	-3.843264	-1.129319	2.385700
H	-2.060342	-2.324370	-0.731613
C	-1.606035	-2.442702	1.978610
H	-1.690990	-2.954932	2.943112
H	-0.736601	-2.836906	1.446293
H	-1.421050	-1.379391	2.169488
C	-3.042190	-4.153333	0.850829
H	-2.273541	-4.466037	0.136398
H	-2.899697	-4.728878	1.771102
H	-4.020790	-4.418998	0.446892
C	-3.525651	-0.418742	-1.955062
H	-2.713568	-0.763044	-2.602708
H	-4.370072	-0.129480	-2.589563
H	-3.189354	0.472511	-1.416337
C	-4.383219	-2.762795	-1.810108
H	-5.106917	-2.448448	-2.569226
H	-3.517209	-3.187690	-2.325844
H	-4.858240	-3.543021	-1.212563
H	1.920730	4.315452	2.074233
H	1.880388	3.536793	0.504958

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B3LYP/BS1 SCF energy: -3269.386313 a.u.

M06/BS2 SCF energy in PhMe: -3268.67200805 a.u.

M06/BS2 Free energy in PhMe: -3267.99271905 a.u.

C	-3.880007	0.952563	1.748315
C	-2.657668	1.665021	2.370986
H	-2.282236	1.067724	3.212388
H	-2.962986	2.638547	2.775472
C	-3.798340	-0.587221	1.704727
H	-4.784232	-0.988387	1.442848
H	-3.567543	-0.960921	2.709344
P	-1.246376	1.880835	1.144404
P	-2.516790	-1.301705	0.498326
Ni	-1.101242	0.158042	-0.058911
C	-1.806084	3.440757	0.284042
C	-2.057056	3.384997	-1.094858
C	-1.996066	4.660727	0.952514
C	-2.499409	4.515922	-1.786957
H	-1.892234	2.448926	-1.622934
C	-2.431734	5.792485	0.262842
H	-1.788492	4.732519	2.017605
C	-2.688176	5.721162	-1.109506
H	-2.690679	4.454268	-2.855454
H	-2.568663	6.731225	0.794517
H	-3.027876	6.603099	-1.646952
C	0.111417	2.559432	2.226338
C	0.005863	2.783695	3.608059
C	1.347038	2.823111	1.603330
C	1.096377	3.257302	4.345543
H	-0.931500	2.597409	4.123308
C	2.428399	3.312548	2.335764
H	1.455163	2.632732	0.538032
C	2.309406	3.527632	3.713170
H	0.990558	3.423505	5.415175
H	3.367709	3.529000	1.831022
H	3.153904	3.903753	4.285261
C	-1.912943	-2.781557	1.455418
C	-1.466776	-2.631803	2.781987
C	-1.741446	-4.037260	0.846379
C	-0.896810	-3.697974	3.479544
H	-1.556140	-1.668143	3.277269
C	-1.165900	-5.103373	1.540482
H	-2.066964	-4.185938	-0.178713
C	-0.743642	-4.942468	2.862098
H	-0.575319	-3.556079	4.509069
H	-1.054721	-6.065926	1.046571
H	-0.304837	-5.775648	3.405202
C	-3.628112	-2.107585	-0.766175
C	-3.364250	-1.853469	-2.120088
C	-4.712303	-2.940225	-0.438912
C	-4.167070	-2.408691	-3.121549
H	-2.520497	-1.220121	-2.382545
C	-5.513276	-3.496627	-1.436097
H	-4.926151	-3.168330	0.602684
C	-5.243190	-3.228649	-2.781716
H	-3.949228	-2.198888	-4.165828
H	-6.346728	-4.140536	-1.165278
H	-5.868885	-3.660298	-3.559024
O	-0.195205	0.092122	-1.977120
S	1.268227	0.112702	-2.228341
O	1.893415	-1.224161	-2.429243
O	2.062668	0.991634	-1.315915
C	1.410774	0.950400	-3.881374

F	0.758050	0.250197	-4.813047
F	2.704247	1.038454	-4.234018
F	0.897624	2.182149	-3.821071
H	3.234086	-1.521711	-1.019747
C	3.229964	-1.751711	1.067387
C	4.142872	-2.982892	1.225498
C	5.637703	-2.673766	1.076788
C	5.917995	-2.038416	-0.290705
C	5.123645	-0.743905	-0.547214
N	3.649738	-1.014714	-0.217175
H	5.980292	-2.017101	1.885735
H	3.932141	-3.431490	2.202872
H	6.983734	-1.808529	-0.405438
H	6.213748	-3.601216	1.171619
H	5.669571	-2.764742	-1.077413
H	3.857801	-3.731475	0.472898
H	3.125590	-0.117317	-0.295675
C	1.773248	-2.187548	0.852689
H	1.444329	-2.784169	1.708675
H	1.092714	-1.330738	0.771087
H	1.659434	-2.797125	-0.049263
C	3.301836	-0.802751	2.272697
H	2.783776	0.141057	2.071572
H	2.791742	-1.280436	3.115055
H	4.322109	-0.579577	2.591514
C	5.167556	-0.367257	-2.037614
H	4.599119	0.545263	-2.237274
H	6.209144	-0.200657	-2.331385
H	4.757105	-1.162839	-2.667538
C	5.640001	0.439957	0.284606
H	6.616758	0.741758	-0.106931
H	4.968202	1.301012	0.200161
H	5.767642	0.203965	1.342284
H	-4.073932	1.348801	0.742772
H	-4.763396	1.212103	2.348441

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B3LYP/BS1 SCF energy: -3973.930731 a.u.

M06/BS2 SCF energy in PhMe: -3973.00870140 a.u.

M06/BS2 Free energy in PhMe: -3972.30912340 a.u.

C	-1.466723	1.157354	1.592055
C	-2.277500	1.936982	2.659971
H	-2.963793	1.276950	3.199817
H	-1.607452	2.394249	3.397716
H	-2.873470	2.732891	2.201176
C	-0.499350	2.223829	0.989130
H	0.123419	2.616626	1.801996
H	-1.116595	3.060662	0.640753
C	-0.735123	0.025266	2.374330
H	-1.491625	-0.577690	2.889219
H	-0.134583	0.493658	3.163098
C	-2.414194	0.614380	0.483921
H	-1.873371	-0.103540	-0.140382
H	-2.701055	1.442973	-0.172850
P	0.716080	1.805265	-0.363583
P	-3.975531	-0.272070	1.072364
P	0.467541	-1.158101	1.551832
Ni	2.105503	0.013844	0.289891
C	-5.202902	1.124812	1.169094
C	-5.893369	1.311004	2.375712
C	-5.492396	1.980173	0.093327
C	-6.837332	2.332308	2.512848
H	-5.689317	0.650183	3.214924
C	-6.433351	3.001068	0.227031
H	-4.993065	1.838239	-0.862032
C	-7.106821	3.180882	1.438919
H	-7.361697	2.461717	3.456074
H	-6.647545	3.652952	-0.616178
H	-7.841608	3.975092	1.541245
C	-4.543628	-1.097503	-0.488360
C	-5.592767	-2.023857	-0.352246
C	-4.011937	-0.879584	-1.768640
C	-6.105619	-2.699043	-1.459082
H	-6.011785	-2.216463	0.633091
C	-4.517120	-1.565440	-2.876600
H	-3.199825	-0.176825	-1.922618
C	-5.565444	-2.473510	-2.727592
H	-6.921046	-3.406249	-1.330440
H	-4.086920	-1.382769	-3.857973
H	-5.957402	-3.003803	-3.591472
C	-0.266357	1.678102	-1.919093
C	-0.120380	0.541696	-2.725895
C	-1.113763	2.715522	-2.344114
C	-0.820457	0.436940	-3.931696
H	0.552495	-0.254274	-2.428053

C	-1.818740	2.604475	-3.541205
H	-1.209761	3.621579	-1.751140
C	-1.673594	1.462896	-4.337437
H	-0.681129	-0.442582	-4.553603
H	-2.470584	3.413032	-3.861267
H	-2.214205	1.384701	-5.276921
C	1.657455	3.369674	-0.600716
C	2.817123	3.295711	-1.392571
C	1.279700	4.604352	-0.052711
C	3.574656	4.441722	-1.633029
H	3.132698	2.347201	-1.820999
C	2.046242	5.746715	-0.293434
H	0.394109	4.691022	0.568972
C	3.193245	5.667894	-1.083880
H	4.469493	4.369984	-2.244697
H	1.744897	6.696734	0.140088
H	3.789879	6.557417	-1.267402
C	1.169977	-2.029351	3.023327
C	1.841111	-1.286959	4.010886
C	1.102752	-3.424964	3.156132
C	2.401885	-1.924874	5.116638
H	1.958321	-0.213322	3.907753
C	1.673633	-4.059611	4.261194
H	0.606100	-4.022681	2.400118
C	2.318326	-3.312637	5.246965
H	2.917430	-1.334143	5.868729
H	1.611924	-5.141153	4.347052
H	2.761414	-3.808434	6.106427
C	-0.531709	-2.458900	0.715061
C	-0.064408	-2.988794	-0.499142
C	-1.701265	-2.991167	1.285815
C	-0.762851	-4.019484	-1.133557
H	0.850984	-2.611198	-0.942014
C	-2.397106	-4.015745	0.644975
H	-2.073684	-2.614694	2.233163
C	-1.930577	-4.530065	-0.567752
H	-0.385305	-4.420064	-2.070368
H	-3.305510	-4.409072	1.092016
H	-2.476688	-5.326580	-1.065677
C	4.054881	2.317013	3.436761
C	5.302251	1.689037	3.474014
C	5.560315	0.628768	2.604098
C	4.573095	0.196175	1.710722
C	3.302659	0.808968	1.650536
C	3.079305	1.879572	2.535644
H	3.844393	3.150630	4.104382
H	6.065895	2.027027	4.170552
H	6.530029	0.135784	2.616868
H	4.813628	-0.632777	1.045196
H	2.123390	2.402590	2.530064
O	2.577544	-1.307180	-1.170707
S	3.690695	-1.091042	-2.202588
O	4.967643	-1.680277	-1.799925
O	3.678761	0.274446	-2.750273
C	3.040421	-2.181137	-3.566224
F	2.821045	-3.421403	-3.108450
F	3.917413	-2.236475	-4.570465
F	1.875645	-1.699109	-4.040713

4'-Td

B3LYP/BS1 SCF energy: -3091.287383 a.u.

M06/BS2 SCF energy in PhMe: -3090.62502948 a.u.

M06/BS2 Free energy in PhMe: -3090.13698148 a.u.

C	0.290055	1.730245	2.923822
C	-1.101698	1.110322	2.684145
H	-1.148992	0.116568	3.144005
H	-1.859727	1.735857	3.169667
C	1.493279	0.786798	2.714581
H	2.387459	1.216018	3.181605
H	1.305334	-0.163035	3.226393
P	-1.579372	0.890530	0.896580
P	1.883313	0.334380	0.947638
Ni	-0.092152	-0.680333	-0.082841
C	-1.675414	2.615505	0.254258
C	-0.892359	2.982263	-0.849711
C	-2.519589	3.573118	0.843151
C	-0.945560	4.286386	-1.350313
H	-0.247919	2.250775	-1.327162
C	-2.568315	4.872899	0.343808
H	-3.153016	3.299012	1.683077
C	-1.779032	5.231544	-0.753962
H	-0.335851	4.555574	-2.208000
H	-3.225921	5.604855	0.805340
H	-1.821772	6.244667	-1.144934
C	-3.338201	0.360704	0.958593

C	-4.065626	0.348651	-0.244206
C	-3.967028	-0.064419	2.137910
C	-5.396996	-0.062517	-0.259019
H	-3.587434	0.646206	-1.171936
C	-5.301111	-0.477782	2.117680
H	-3.426471	-0.085503	3.078189
C	-6.019247	-0.474896	0.922101
H	-5.945542	-0.067193	-1.196802
H	-5.774705	-0.804860	3.039464
H	-7.056629	-0.798226	0.908296
C	3.357093	-0.763287	1.107269
C	3.278999	-2.088027	0.652992
C	4.563261	-0.299561	1.658166
C	4.384036	-2.936445	0.758502
H	2.352789	-2.462060	0.227139
C	5.663033	-1.149064	1.765579
H	4.651672	0.732447	1.987433
C	5.574482	-2.469760	1.315772
H	4.310005	-3.960449	0.403267
H	6.591162	-0.779319	2.193307
H	6.434074	-3.129751	1.396127
C	2.598078	1.874884	0.221513
C	2.815879	1.906064	-1.167681
C	2.955475	2.997745	0.985360
C	3.384261	3.028774	-1.769516
H	2.521625	1.060045	-1.779818
C	3.518178	4.122473	0.377744
H	2.800019	3.010742	2.059338
C	3.735835	4.140175	-1.000102
H	3.545751	3.034970	-2.844043
H	3.785998	4.983158	0.984954
H	4.173974	5.015546	-1.471971
C	-0.242975	-3.801869	2.966150
C	0.164639	-2.693233	2.215001
C	-0.560376	-2.224553	1.100816
C	-1.734702	-2.942621	0.782965
C	-2.152366	-4.053045	1.523593
C	-1.408610	-4.487206	2.622978
H	0.354523	-4.130843	3.814694
H	1.094392	-2.208974	2.508088
H	-2.337764	-2.633368	-0.066906
H	-3.061599	-4.579568	1.239733
H	-1.731473	-5.349709	3.201571
O	0.607920	-0.181474	-2.045020
S	-0.567979	-0.697547	-2.858146
O	-0.972276	0.132102	-3.989608
O	-1.617136	-1.140417	-1.893626
C	0.105262	-2.275358	-3.582175
F	-0.859994	-2.927333	-4.233783
F	0.576439	-3.062455	-2.602412
F	1.102332	-2.001966	-4.429423
H	0.402348	2.641448	2.324656
H	0.319606	2.056069	3.971857