Supplementary Information

DFT mechanistic insight into the base-free nickel-catalyzed Suzuki–Miyaura cross-coupling of acid fluoride: concerted versus stepwise transmetalation

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SI1: Figures S1-S5 in the main text

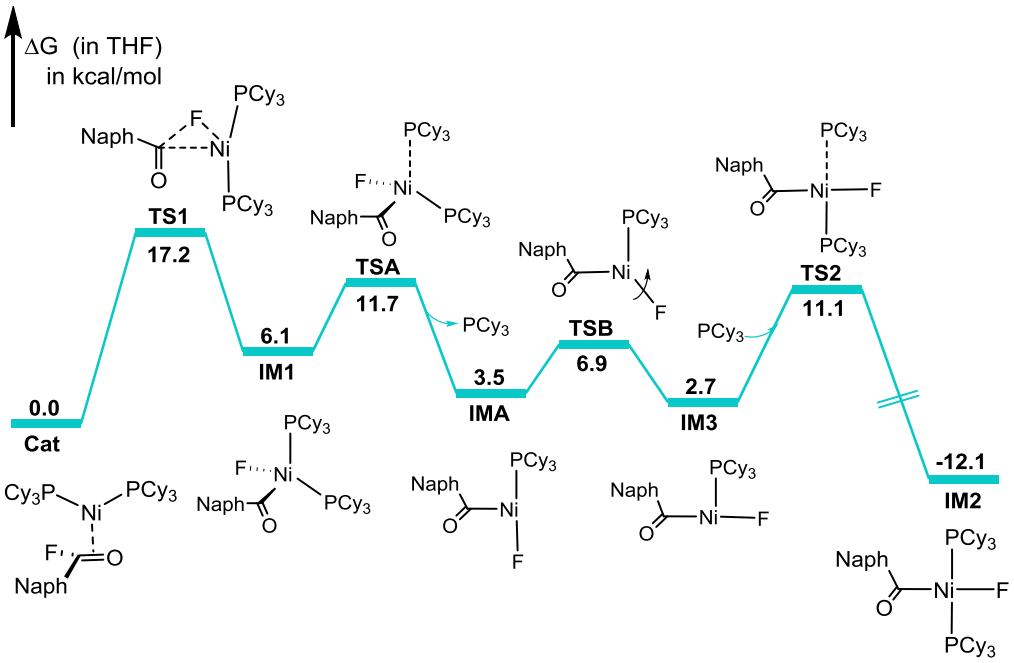


Figure S1. Free energy profile for the conversion of **IM1** to **IM2**. Free energies are relative to **Cat** and PCy_3 and mass-balanced.

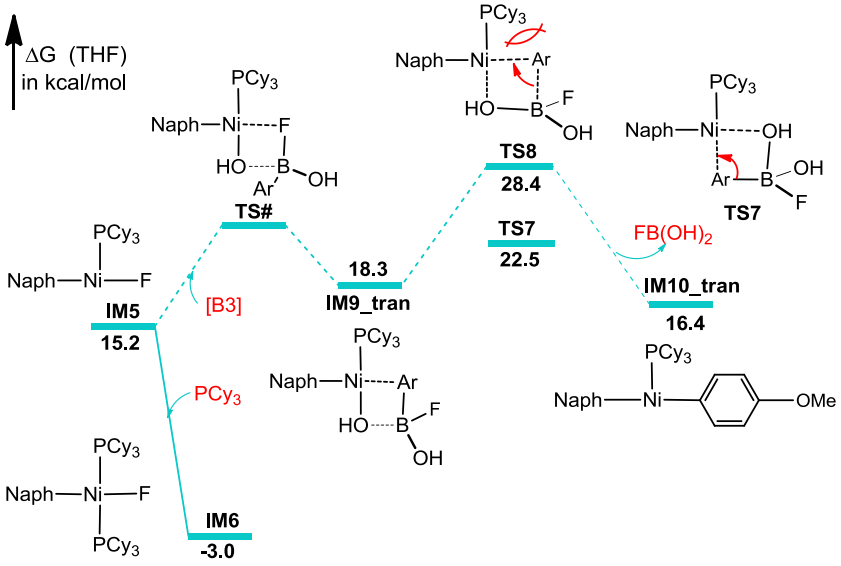


Figure S2. Energetic results for **IM5** directly to undergo stepwise transmetalation without first converting to **IM7**. As illustrated, the pathway passes through **TS8** which is 5.9 kcal/mol higher than **TS7**. Because of the much higher **TS8** than **TS7**, we exclude the pathway. We also attempted to locate **TS#**, but we could not obtain the transition state with several attempts.

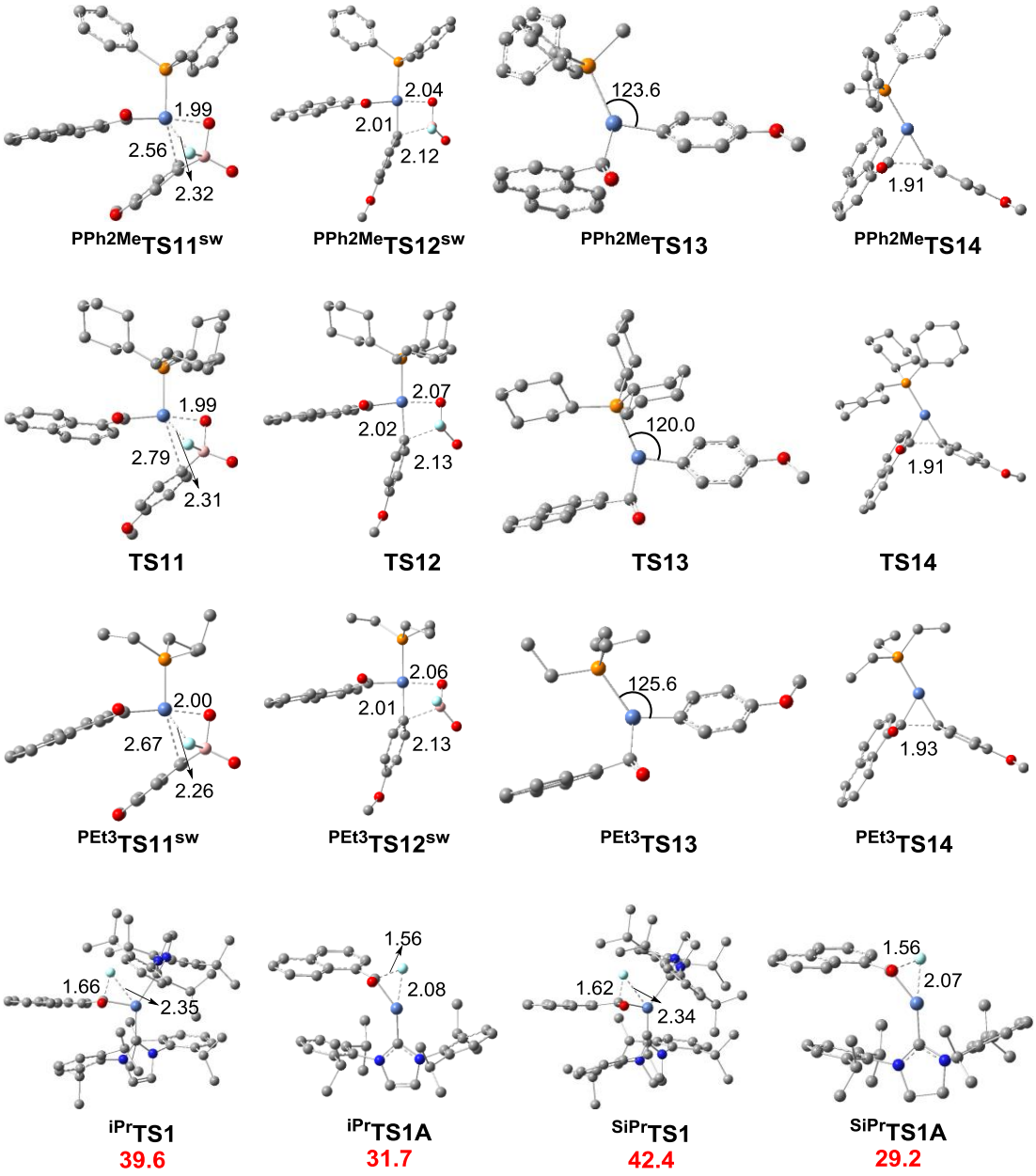
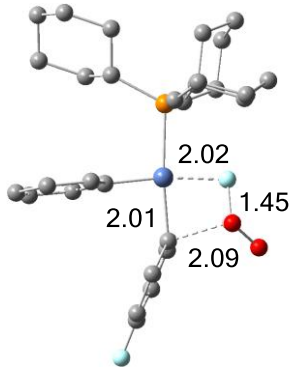
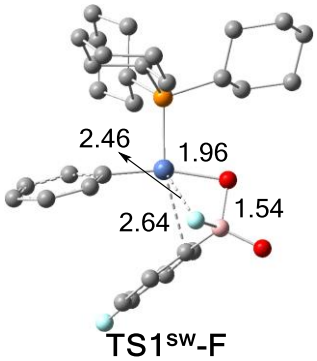


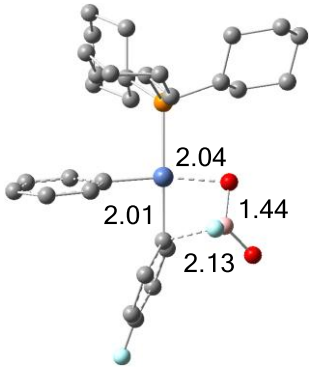
Figure S3. Optimized structures of the transition states in **Table 1**, along with the key bond lengths in angstroms and bond angles in degrees. Values in red are the barriers (in kcal/mol) of oxidative addition of **1a** to Ni(0) with one or two iPr or SiPr ligands. The lower values (31.7 and 29.2 kcal/mol) with one NHC ligand are used in **Table 1**. Trivial H atoms are omitted for clarity.



TS^{con}-F



$TS1^{sw}$-F



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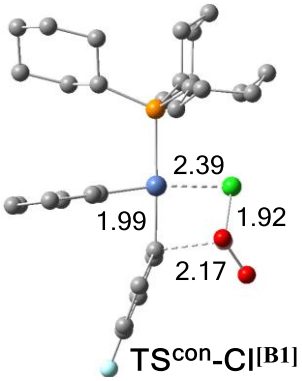
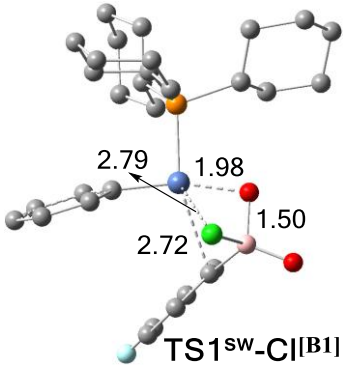
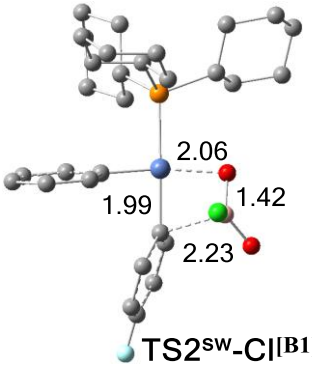


TS^{con}-Cl[B1]



$TS1^{sw}$-Cl[B1]



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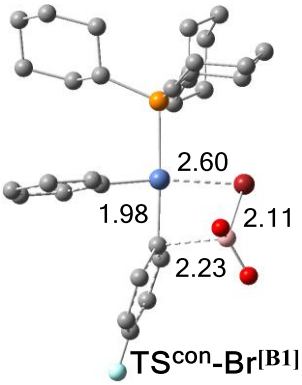

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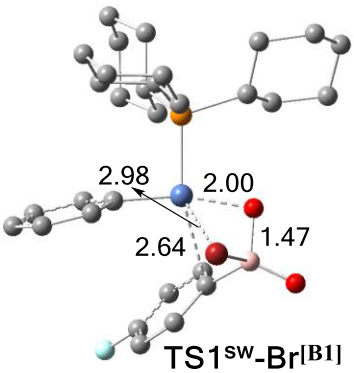

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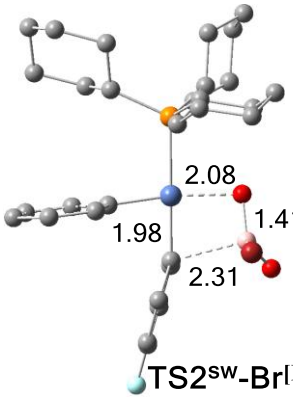
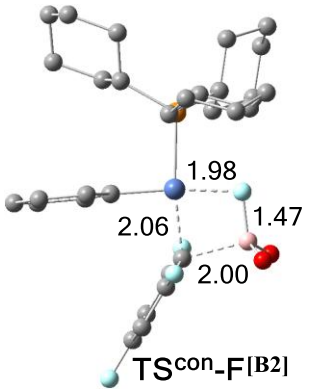
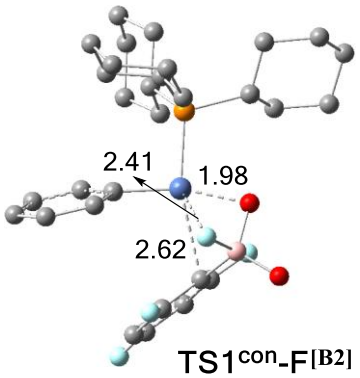
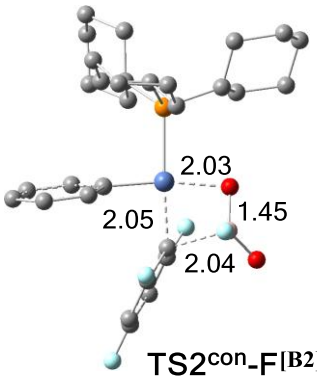


$TS2^{sw}$-Br[B1]


1.98
2.06
1.47
2.00
TS^con-F[B2]


2.41
1.98
2.62
TS1^con-F[B2]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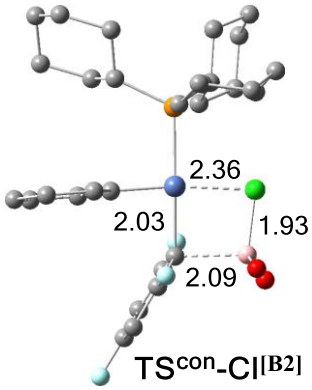
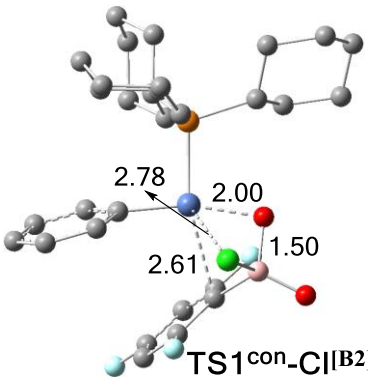
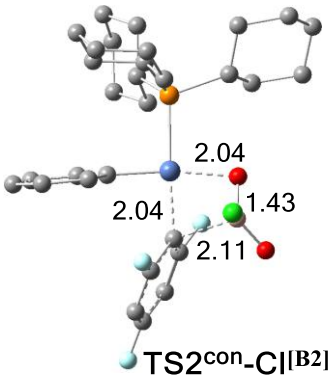
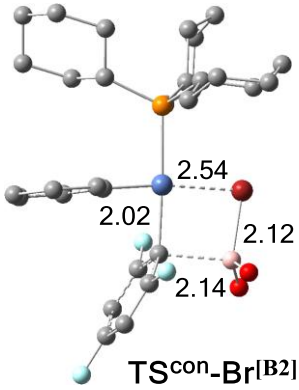
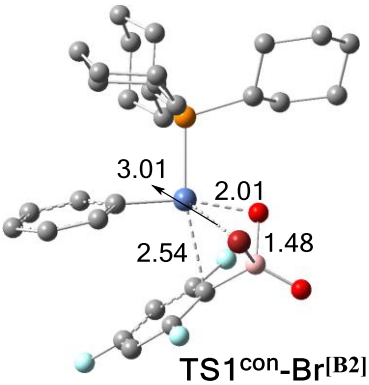
2.05
1.45
2.04
TS2^con-F[B2]

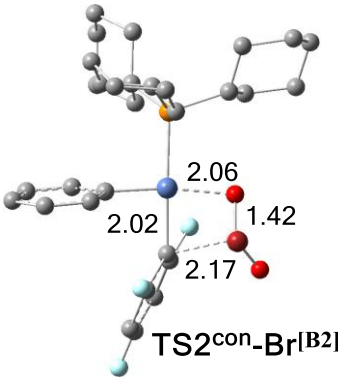

2.36
2.03
1.93
2.09
TS^con-Cl[B2]


2.78
2.00
1.50
2.61
TS1^con-Cl[B2]


2.04
2.04
1.43
2.11
TS2^con-Cl[B2]


2.54
2.02
2.12
2.14
TS^con-Br[B2]


3.01
2.01
2.54
1.48
TS1^con-Br[B2]


2.06
2.02
1.42
2.17
TS2^con-Br[B2]

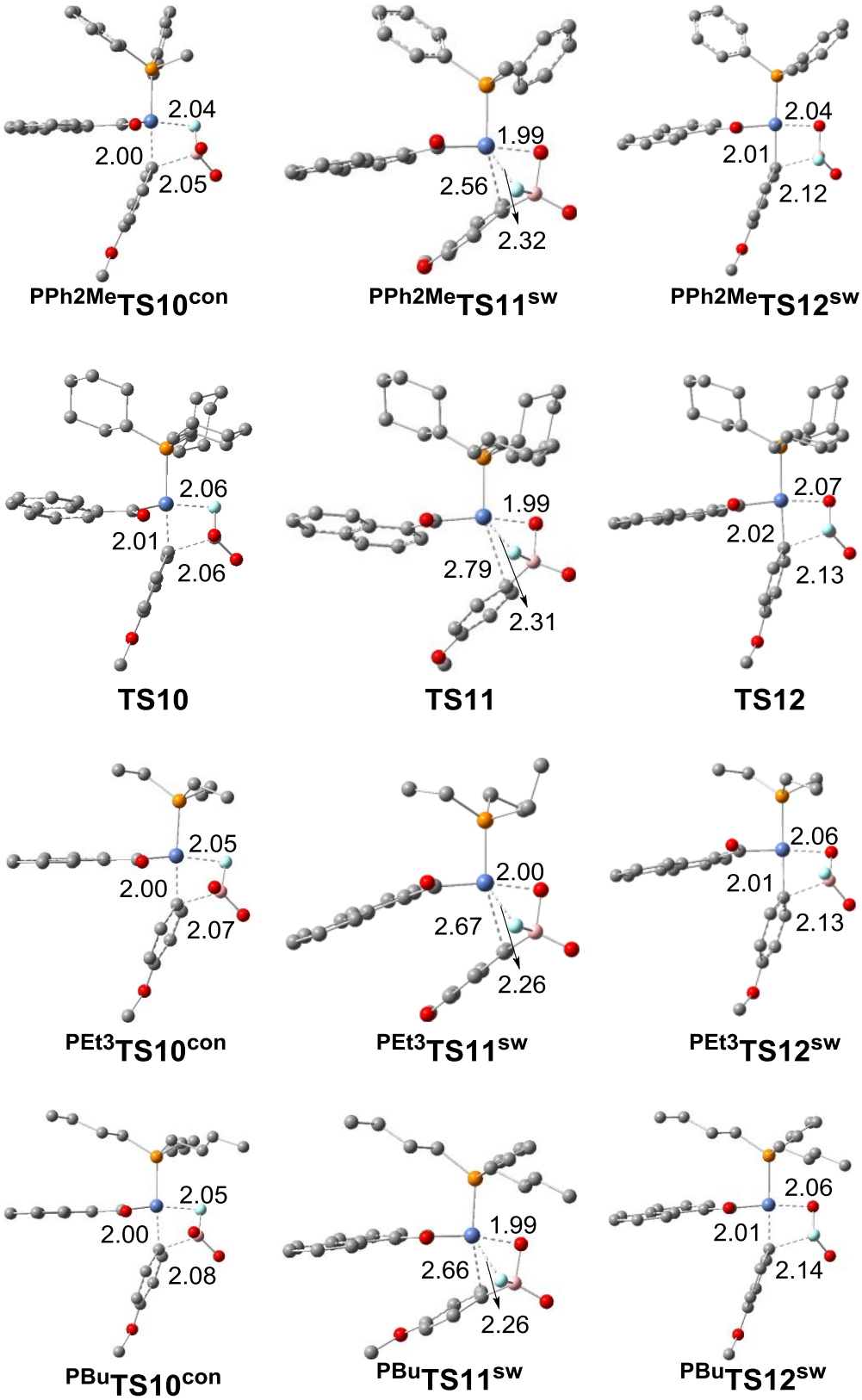


Figure. S4. Optimized structures of the transition states in **Table 2**, along with key bond lengths in angstroms. Trivial H atoms are omitted for clarity.

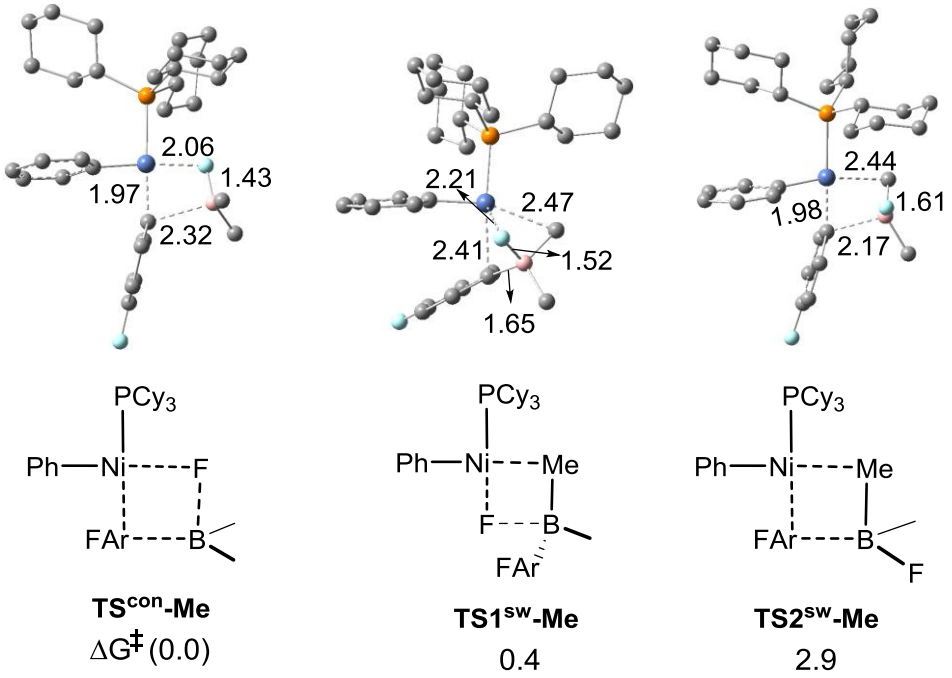


Figure S5. Comparing the barriers (in kcal/mol) of the transition states for the concerted and stepwise transmetalation pathways of **Ph[Ni]F** with $FPhBMe_2$. Key bond lengths are given in Å. Trivial H atoms are omitted for clarity.

SI2: IRC results to verify the stepwise and concerted mechanisms

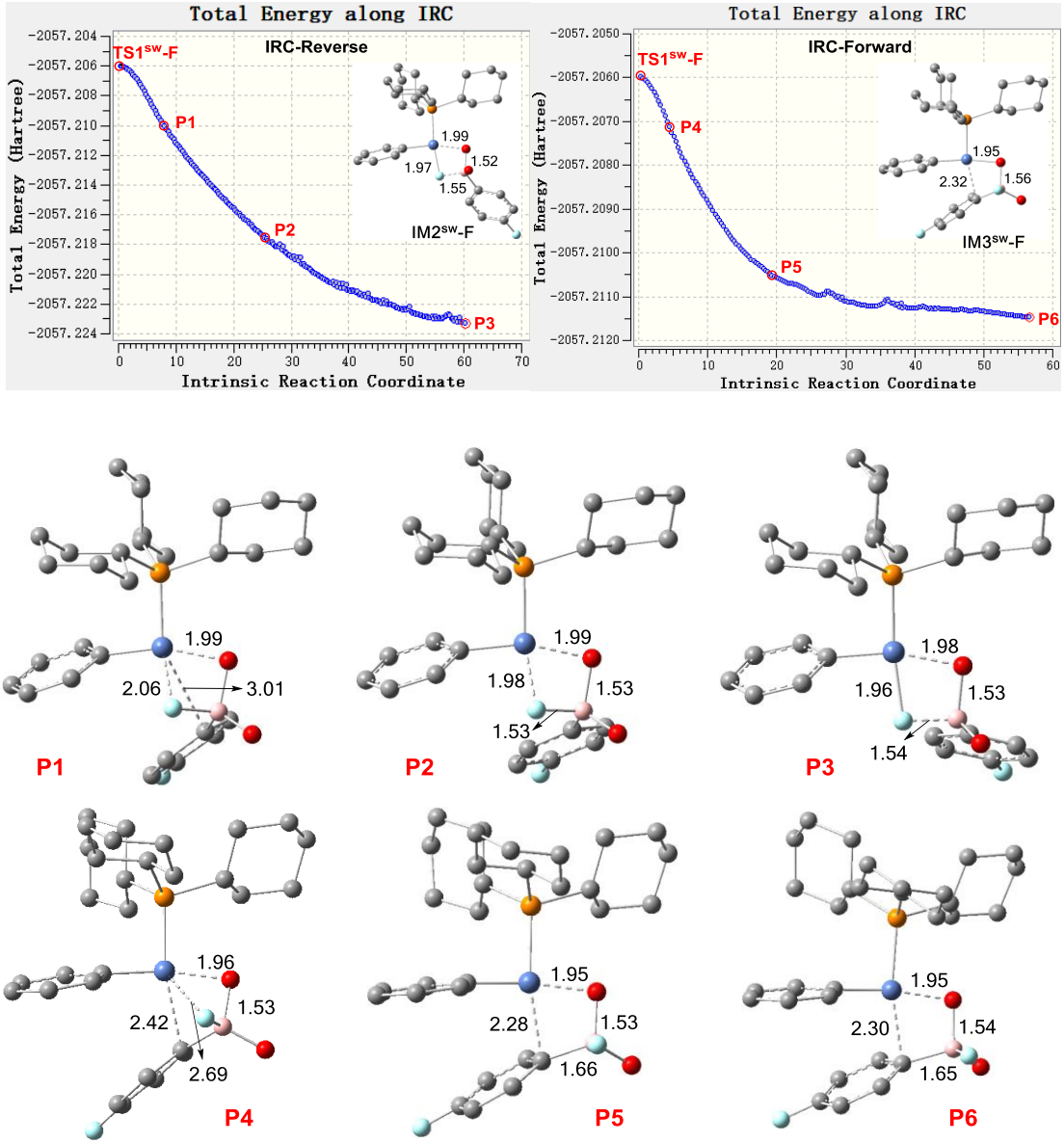


Figure S6. IRC results to show that **TS1^{sw}-F** connects to **IM2^{sw}-F** and **IM3^{sw}-F** correctly. Values are key bond lengths in angstroms. Trivial H atoms are omitted for clarity.

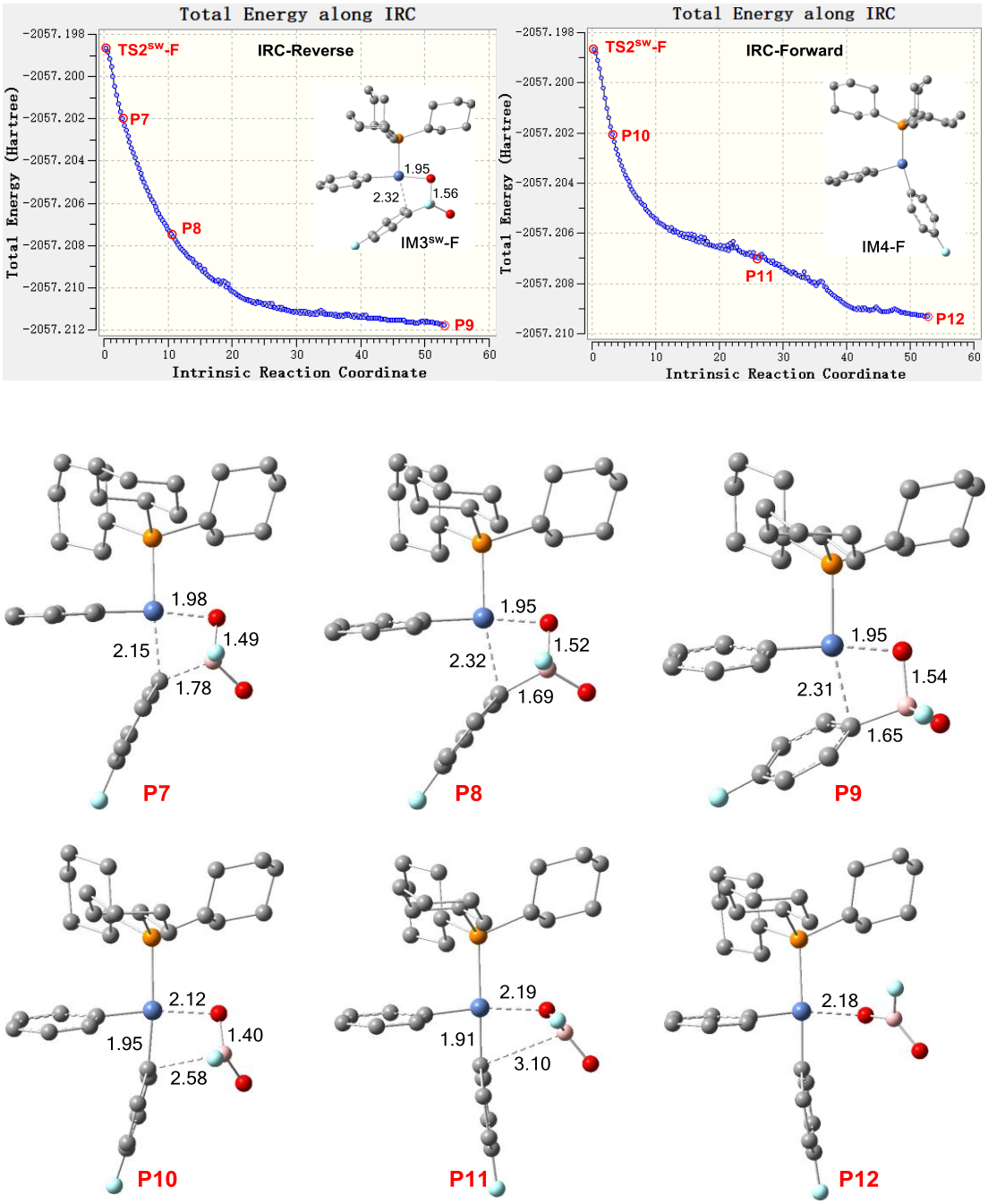


Figure S7. IRC results to show that **TS2^{sw}-F** connects to **IM3^{sw}-F** and **IM4-F** + $FB(OH)_2$ correctly. Values are key bond lengths in angstroms. Trivial H atoms are omitted for clarity.

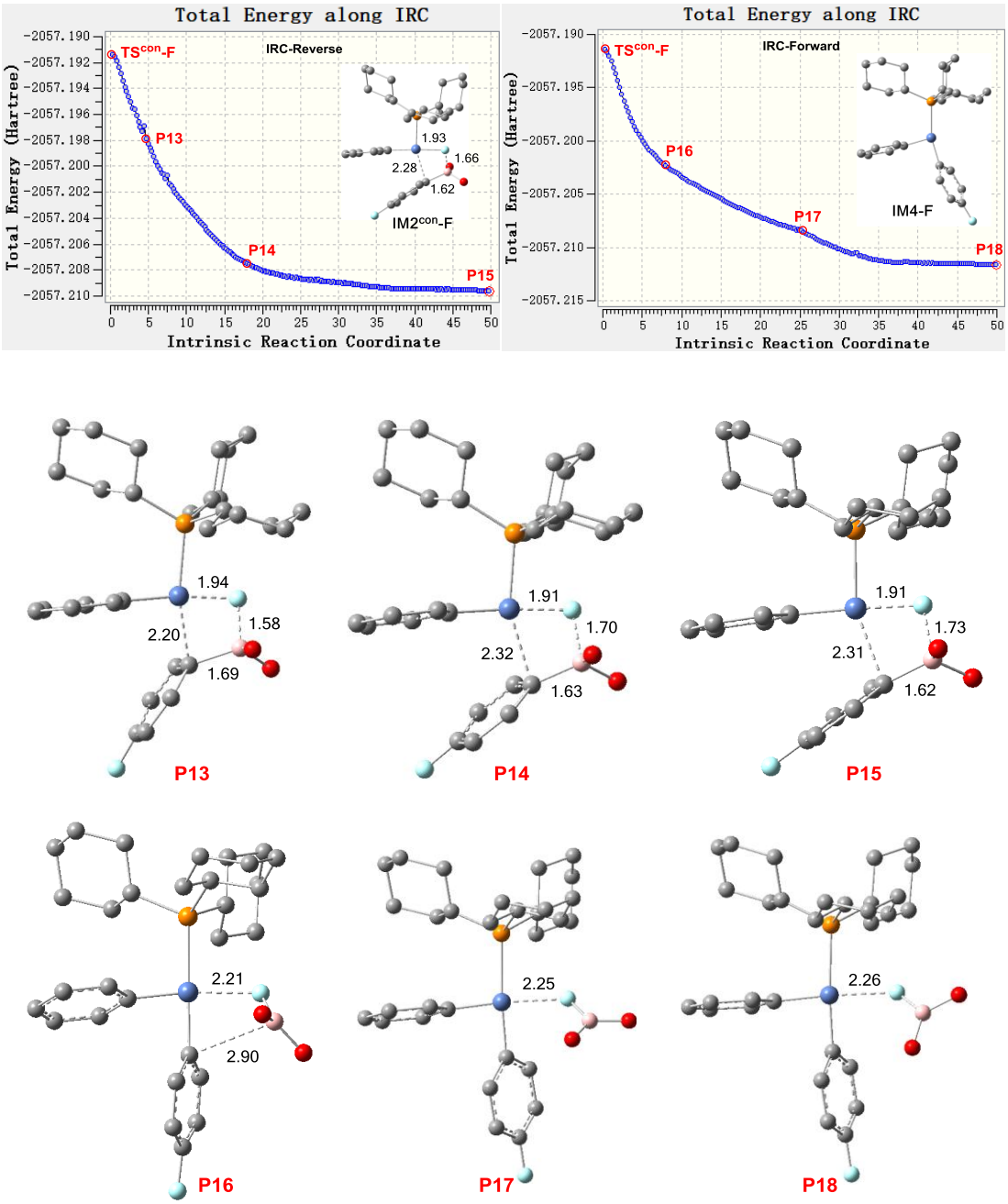
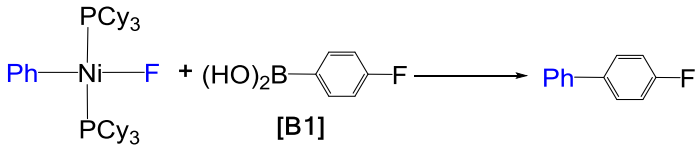


Figure S8. IRC results to show that **TS^{con}-F** connects to **IM2^{con}-F** and **IM4-F** + $FB(OH)_2$ correctly. Values are key bond lengths in angstroms, Trivial H atoms are omitted for clarity.

SI3: Table S1. Comparing barriers (in kcal/mol) of the concerted and stepwise transmetalation mechanism at various DFT levels.



Method	$\Delta G^{\neq}$(**TS^{con}-F**)	$\Delta G^{\neq}$(**TS1^{sw}-F**)	$\Delta G^{\neq}$(**TS2^{sw}-F**)	**$\Delta\Delta G^{\neq}$**	ref
M06(SMD)/BSII// B3LYP(gas)/BSI	32.4	25.2	26.8	**5.6**	(1)
M06L(SMD)/BSII// B3LYP(gas)/BSI	34.2	23.9	29.9	**4.3**	(2)
B3LYP-D3(SMD)/BSII// B3LYP(gas)/BSI	38.9	25.7	33.8	**5.1**	(3) (4)
wB97XD(SMD)/BSII// B3LYP(gas)/BSI	38.6	26.0	33.4	**5.2**	(5)
TPSS-D3(SMD)/BSII// B3LYP(gas)/BSI	33.3	22.8	28.2	**5.1**	(6) (4)
BP86-D3(SMD)/BSII// B3LYP(gas)/BSI	36.2	26.3	31.0	**5.2**	(7) (4)

SMD calculations used tetrahydrofuran as solvent.

(1) (a) Zhao, Y.; Truhlar, D. G., The M06 Suite of Density Functionals for Main Group Thermochemistry, Thermochemical Kinetics, Noncovalent Interactions, Excited States, and Transition Elements: Two New Functionals and Systematic Testing of Four M06-Class Functionals and 12 other Functionals. *Theor. Chem. Acc.* **2008**, *120*, 215-241. (b) Zhao, Y.; Truhlar, D. G., Density Functionals with Broad Applicability in Chemistry. *Acc. Chem. Res.* **2008**, *41*, 157-167. (c) Zhao, Y.; Truhlar, D. G., Benchmark Energetic Data in a Model System for Grubbs II Metathesis Catalysis and Their Use for the Development, Assessment, and Validation of Electronic Structure Methods. *J. Chem. Theory Comput* **2009**, *5*, 324-333.

(2) (a) Zhao, Y.; Truhlar, D. G. The M06 suite of density functionals for main group thermochemistry, thermochemical kinetics, noncovalent interactions, excited states, and transition elements: two new functionals and systematic testing of four M06class functionals and 12 other functionals. *Theor. Chem. Acc.* **2008**, *120*, 215−241. (b) Zhao, Y.; Truhlar, D. G. Density functionals with broad applicability in chemistry. *Acc. Chem. Res.* **2008**, *41*, 157−167.

(3) (a) Stephens, P. J.; Devlin, F. J.; Chabalowski, C. F. Frisch, M. J., Ab initio calculation of vibrational absorption and circular dichroism spectra using density functional force fields. *J. Phys. Chem.* **1994**, *98*, 11623-11627;

(4) (a) Grimme, S.; Ehrlich, S.; Goerigk. L., Effect of the damping function in dispersion corrected density functional theory. *J. Comput. Chem.* **2011**, *32*, 1456. (b) (b) Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H. A consistent and accurate ab initio parametrization of

density functional dispersion correction (DFT-D) for the 94 elements H-Pu. *J. Chem. Phys.* **2010**, *132*, 154104−154119.
(5) Chai, J. D.; Head-Gordon, M., Long-range corrected hybrid density functionals with damped atom-atom dispersion corrections. *Phys. Chem. Chem. Phys.* **2008**, *10* (44), 6615-20.
(6) Tao, J.; Perdew, J. P.; Staroverov, V. N.; Scuseria, G. E., Climbing the density functional ladder: nonempirical meta-generalized gradient approximation designed for molecules and solids. *Phys. Rev. Let.t* **2003**, *91* (14), 146401.
(7) (a) Becke, A. D. A new mixing of Hartree−Fock and local density−functional theories. *J. Chem. Phys.* **1993**, *98*, 1372−1377. (b) Becke, A. D. Density−functional thermochemistry. III. The role of exact exchange. *J. Chem. Phys.* **1993**, *98*, 5648−5652. (c) Perdew, J. P.; Chevary, J. A.; Vosko, S. H.; Jackson, K. A.; Pederson, M. R.; Singh, D. J.; Fiolhais, C. Atoms, molecules, solids, and surfaces: applications of the generalized gradient approximation for exchange and correlation. *Phys. Rev. B: Condens. Matter Mater. Phys.* **1992**, *46*, 6671−6687.

SI 4: Cartesian Coordinates in Å, SCF Energies and Free Energies (in a.u.) at 298.15 K and 1 atm for the Optimized Structures [BSI= 6-31G(d,p), BSII=6-311++G(d,p)]

$Ni(COD)_2$

B3LYP/BSI SCF energy: -795.077215a.u.

M06/BSII SCF energy in solution: -794.754008a.u.

M06/BSII free energy in solution: -794.432186a.u.

C	-1.369941	1.527440	-0.613325
C	1.370308	-1.527394	-0.613472
C	2.241652	-1.839890	0.586658
C	2.622370	-0.591215	1.415857
C	1.510736	0.450539	1.472898
C	1.370078	1.527291	0.613494
C	2.241466	1.839935	-0.586549
C	2.622367	0.591300	-1.415746
C	-1.510900	0.450664	-1.472726
C	-2.622745	-0.590832	-1.415540
C	-2.242081	-1.839680	-0.586547
C	-1.370369	-1.527407	0.613367
C	-1.510611	-0.450649	1.472861
C	-2.622003	0.591359	1.416018
C	-2.241057	1.840048	0.586921
C	1.510835	-0.450543	-1.472873
H	-0.760300	2.358514	-0.962943
H	-0.980154	0.511855	-2.419074
H	-0.760799	-2.358686	0.962631
H	-0.979498	-0.512043	2.418977
H	0.979711	0.511704	2.419076
H	0.760344	2.358357	0.962974
H	0.980032	-0.511886	-2.419177
H	0.760818	-2.358619	-0.963012
H	-2.869688	-0.904421	-2.436326
H	-3.536630	-0.137548	-1.019374
H	-1.686840	-2.533915	-1.229287
H	-3.152444	-2.380259	-0.281030
H	-2.868495	0.905049	2.436881
H	-3.536197	0.138463	1.020126
H	-1.685270	2.534002	1.229501
H	-3.151295	2.381070	0.281800
H	3.151990	-2.380658	0.281386
H	1.686086	-2.534034	1.229219
H	3.536427	-0.138060	1.019965
H	2.868995	-0.904943	2.436675
H	3.151711	2.380785	-0.281155
H	1.685881	2.534043	-1.229127
H	3.536454	0.138244	-1.019802
H	2.869058	0.905081	-2.436535
Ni	-0.000019	-0.000282	-0.000362

COD

B3LYP/BSI SCF energy: -312.04183a.u.

M06/BSII SCF energy in solution: -311.861739a.u.

M06/BSII free energy in solution: -311.712692a.u.

C	1.220335	1.230513	-0.496132
C	-0.001083	1.703590	-0.220182
C	-1.076667	1.111107	0.665525
C	-1.922765	0.018040	-0.021970
C	-1.220335	-1.230513	-0.496132
C	0.001083	-1.703590	-0.220182
C	1.076668	-1.111107	0.665523
C	1.922765	-0.018039	-0.021969
H	1.828574	1.832647	-1.172649
H	-0.281010	2.633453	-0.715385
H	-1.828576	-1.832648	-1.172647
H	0.281008	-2.633455	-0.715384
H	-1.759957	1.915946	0.961492
H	-0.658426	0.726670	1.598397
H	-2.425703	0.464292	-0.891867
H	-2.739415	-0.274759	0.656569
H	1.759959	-1.915946	0.961489
H	0.658427	-0.726673	1.598397
H	2.425706	-0.464291	-0.891866
H	2.739414	0.274760	0.656571

$Ni(PCy_3)_2$

B3LYP/BSI SCF energy: -2265.387789a.u.

M06/BSII SCF energy in solution: -2264.60791a.u.

M06/BSII free energy in solution: -2263.718744a.u.

C	2.959807	0.720406	1.493153
C	0.857945	-4.125555	3.043636
C	2.906378	-4.026139	1.568933
C	1.655086	-4.832530	1.939813
C	0.434456	0.575490	3.303764
C	1.118795	0.387888	4.673863
C	-0.019866	2.039935	3.126464
C	0.189163	0.826093	5.820957
C	-0.945252	2.481696	4.272518
C	-0.286392	2.275380	5.644277
C	2.844551	2.139006	0.893698
C	3.981837	0.710182	2.647711
C	4.214780	2.654416	0.422039
C	5.356098	1.217796	2.173859
C	5.256259	2.617776	1.550581
C	1.757482	-1.854582	2.280335
C	0.506093	-2.680075	2.653137
C	2.557944	-2.579981	1.176634
Ni	0.000000	0.000000	0.000000
P	1.270614	-0.103827	1.741243
P	-1.270614	0.103827	-1.741243
C	-2.959807	-0.720406	-1.493153
C	-0.434456	-0.575490	-3.303764
C	-1.757482	1.854582	-2.280335
C	-2.844551	-2.139006	-0.893698
C	-3.981837	-0.710182	-2.647711
C	-1.118795	-0.387888	-4.673863
C	0.019866	-2.039935	-3.126464
C	-0.506093	2.680075	-2.653137
C	-2.557944	2.579981	-1.176634
C	-4.214780	-2.654416	-0.422039
C	-5.356098	-1.217796	-2.173859
C	-0.189163	-0.826093	-5.820957
C	0.945252	-2.481696	-4.272518
C	-0.857945	4.125555	-3.043636
C	-2.906378	4.026139	-1.568933
C	-5.256259	-2.617776	-1.550581
C	0.286392	-2.275380	-5.644277
C	-1.655086	4.832530	-1.939813
H	3.370874	0.089986	0.690484
H	1.450901	-4.118269	3.969846
H	-0.061021	-4.680994	3.268410
H	3.594624	-4.013745	2.426544
H	3.445091	-4.511933	0.745998
H	1.932107	-5.845633	2.255985
H	1.019697	-4.944135	1.049699
H	-0.485590	-0.028012	3.316119
H	2.036279	0.986281	4.717565
H	1.419449	-0.654565	4.824677
H	0.857726	2.699405	3.105216
H	-0.524742	2.154003	2.160131
H	0.703724	0.708217	6.782727
H	-0.684587	0.159276	5.851758
H	-1.229005	3.533105	4.140377
H	-1.876185	1.898596	4.226433
H	-0.981161	2.548801	6.447755
H	0.576481	2.951072	5.735071
H	2.444272	2.830923	1.646140
H	2.130258	2.129849	0.062564
H	3.628982	1.360386	3.457724
H	4.086136	-0.293433	3.074478
H	4.116323	3.673895	0.029097
H	4.563643	2.030650	-0.413639
H	6.062222	1.223470	3.013505
H	5.762107	0.517205	1.430093
H	4.967950	3.337837	2.330129
H	6.236295	2.939335	1.177495
H	2.396311	-1.783240	3.172146
H	-0.038921	-2.205978	3.476755
H	-0.176787	-2.688454	1.792442
H	3.482222	-2.037731	0.948942
H	1.961978	-2.581091	0.253301
H	-3.370874	-0.089986	-0.690484
H	0.485590	0.028012	-3.316119
H	-2.396311	1.783240	-3.172146
H	-2.130258	-2.129849	-0.062564
H	-2.444272	-2.830923	-1.646140
H	-4.086136	0.293433	-3.074478
H	-3.628982	-1.360386	-3.457724
H	-1.419449	0.654565	-4.824677
H	-2.036279	-0.986281	-4.717565
H	0.524742	-2.154003	-2.160131
H	-0.857726	-2.699405	-3.105216
H	0.176787	2.688454	-1.792442
H	0.038921	2.205978	-3.476755
H	-1.961978	2.581091	-0.253301

H	-3.482222	2.037731	-0.948942
H	-4.563643	-2.030650	0.413639
H	-4.116323	-3.673895	-0.029097
H	-5.762107	-0.517205	-1.430093
H	-6.062222	-1.223470	-3.013505
H	0.684587	-0.159276	-5.851758
H	-0.703724	-0.708217	-6.782727
H	1.876185	-1.898596	-4.226433
H	1.229005	-3.533105	-4.140377
H	0.061021	4.680994	-3.268410
H	-1.450901	4.118269	-3.969846
H	-3.445091	4.511933	-0.745998
H	-3.594624	4.013745	-2.426544
H	-6.236295	-2.939335	-1.177495
H	-4.967950	-3.337837	-2.330129
H	-0.576481	-2.951072	-5.735071
H	0.981161	-2.548801	-6.447755
H	-1.019697	4.944135	-1.049699
H	-1.932107	5.845633	-2.255985

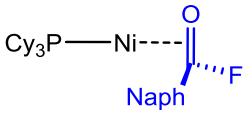
PCy_3

B3LYP/BSI SCF energy: -1047.202489a.u.

M06/BSII SCF energy in solution: -1046.79376a.u.

M06/BSII free energy in solution: -1046.35825a.u.

C	0.551756	1.566550	-0.465954
H	-0.073744	2.297566	-1.002375
C	1.978382	1.727026	-1.034585
H	2.653332	1.024584	-0.527775
H	1.994032	1.464034	-2.098963
C	2.512432	3.154877	-0.834029
H	1.905797	3.852686	-1.428607
H	3.537729	3.229151	-1.217021
C	2.463058	3.571117	0.643091
H	3.165357	2.948751	1.216326
H	2.800268	4.608239	0.759766
C	1.051477	3.400675	1.223213
H	0.369887	4.108192	0.729317
H	1.044677	3.656696	2.290049
C	0.522163	1.967338	1.024859
H	-0.493653	1.893515	1.427840
H	1.139289	1.277895	1.611898
C	-1.834422	-0.123940	-0.041714
H	-1.610900	-0.071388	1.033805
C	-2.731664	1.079622	-0.410326
H	-2.228212	2.023719	-0.175498
H	-2.896623	1.078874	-1.497397
C	-4.091861	1.035258	0.306882
H	-3.934607	1.146260	1.389432
H	-4.703940	1.889973	-0.006698
C	-4.831740	-0.280924	0.036130
H	-5.777762	-0.309519	0.590362
H	-5.091733	-0.336752	-1.030597
C	-3.957001	-1.485528	0.406424
H	-4.472948	-2.422610	0.163269
H	-3.793880	-1.493399	1.493724
C	-2.595968	-1.441781	-0.308831
H	-2.751509	-1.551372	-1.391644
H	-1.999379	-2.304502	0.007115
C	0.757939	-1.508130	-0.308865
H	0.037353	-2.333616	-0.412503
C	1.191472	-1.468878	1.169518
H	0.342308	-1.226959	1.819417
H	1.932532	-0.671746	1.310102
C	1.822485	-2.804742	1.604551
H	2.144125	-2.744131	2.651770
H	1.060934	-3.596409	1.557906
C	3.006239	-3.186351	0.703932
H	3.814012	-2.453245	0.842652
H	3.414920	-4.159146	1.003280
C	2.596673	-3.211282	-0.775980
H	1.877230	-4.026963	-0.937807
H	3.465452	-3.433706	-1.407840
C	1.955747	-1.882555	-1.211963
H	2.715057	-1.090899	-1.170085
H	1.630111	-1.944029	-2.256502
P	-0.227900	-0.065324	-1.046323



B3LYP/BSI SCF energy: -1816.661219a.u.

M06/BSII SCF energy in solution: -1816.05184a.u.

M06/BSII free energy in solution: -1815.479945a.u.

C	-0.409379	-0.615962	1.437373
H	0.338965	0.181752	1.552867
C	0.379809	-1.921004	1.191925

H	-0.322083	-2.755183	1.057259	H	-2.487212	-4.090525	-2.829099
H	0.963740	-1.841272	0.268414	C	-1.913722	-2.403269	-1.591210
C	1.309284	-2.237880	2.375579	H	-1.200290	-3.008939	-1.018819
H	2.084400	-1.462234	2.437678	H	-1.332821	-1.909954	-2.380775
H	1.830877	-3.184648	2.191548	F	1.137623	3.006309	-1.329546
C	0.537817	-2.300628	3.701536	Ni	0.056317	0.521452	-1.693778
H	-0.153099	-3.155965	3.679282	P	-1.319480	-0.038162	-0.111489
H	1.226773	-2.479255	4.535724	O	1.447352	1.236535	-2.717931
C	-0.263729	-1.013061	3.939949	C	1.564434	1.683464	-1.521506
H	0.431980	-0.173584	4.079610	C	5.224888	-2.056794	-0.866012
H	-0.847823	-1.091116	4.865028	C	5.261317	-1.254157	0.250191
C	-1.201787	-0.699776	2.760041	C	4.408551	-0.123145	0.369596
H	-1.734764	0.235838	2.957992	C	3.486617	0.183507	-0.690737
H	-1.963452	-1.484824	2.694174	C	3.488436	-0.661556	-1.836983
C	-2.390715	1.392150	0.484017	C	4.331728	-1.749956	-1.917651
H	-3.059567	1.013912	1.270416	H	5.178720	0.459265	2.306718
C	-1.511035	2.514670	1.082583	H	5.883205	-2.917320	-0.945056
H	-0.922907	2.137334	1.926021	H	5.950607	-1.469187	1.062981
H	-0.791702	2.845387	0.322930	C	4.470372	0.707474	1.520363
C	-2.354179	3.713818	1.547874	C	2.628381	1.333770	-0.538244
H	-3.000013	3.403701	2.382324	H	2.824475	-0.423660	-2.656214
H	-1.693274	4.495996	1.940098	H	4.313597	-2.374781	-2.806342
C	-3.224057	4.268625	0.412486	C	2.741782	2.119807	0.602045
H	-3.848874	5.092742	0.776964	C	3.658874	1.812568	1.627790
H	-2.574965	4.687393	-0.369045	H	2.108723	2.992921	0.696909
C	-4.099315	3.164713	-0.194607	H	3.718467	2.456682	2.500440
H	-4.678160	3.555389	-1.039982				
H	-4.829974	2.827326	0.554716	**Cat**			
C	-3.260491	1.961785	-0.659451	B3LYP/BSI SCF energy: -2863.890676a.u.			
H	-2.604170	2.270641	-1.485063	M06/BSII SCF energy in solution: -2862.89845a.u.			
H	-3.930336	1.193451	-1.061122	M06/BSII free energy in solution: -2861.863047a.u.			
C	-2.562609	-1.342363	-0.673044				
H	-3.234607	-0.753092	-1.313636	C	2.848794	-0.406826	-1.648388
C	-3.431840	-2.014012	0.407727	H	2.630217	0.638898	-1.912211
H	-3.916044	-1.261970	1.040816	C	1.972845	-1.277688	-2.577776
H	-2.793020	-2.615755	1.065505	H	2.140730	-2.337714	-2.359948
C	-4.495313	-2.930063	-0.223698	H	0.912002	-1.088615	-2.378998
H	-5.080929	-3.416851	0.565443	C	2.302179	-1.021342	-4.058113
H	-5.201148	-2.318032	-0.803059	H	2.028448	0.010446	-4.319788
C	-3.859186	-3.981574	-1.144052	H	1.692145	-1.675657	-4.692655
H	-3.247177	-4.666516	-0.539940	C	3.794851	-1.235770	-4.350421
H	-4.636712	-4.593586	-1.616155	H	4.041681	-2.297855	-4.208991
C	-2.975533	-3.324909	-2.214801	H	4.015630	-1.002152	-5.398821
H	-3.607907	-2.736200	-2.894544	C	4.672924	-0.387847	-3.419007

H	4.514615	0.677407	-3.640903	C	-4.038991	-0.686852	-2.440781
H	5.734625	-0.589949	-3.606029	H	-4.511814	-1.179517	-1.581412
C	4.344241	-0.649422	-1.938026	H	-3.920217	-1.457387	-3.211794
H	4.973511	-0.018181	-1.300841	C	-4.947640	0.443116	-2.945352
H	4.599680	-1.689228	-1.698771	H	-4.531196	0.859197	-3.874612
C	3.387466	0.797664	1.003189	H	-5.940425	0.051473	-3.198029
H	4.422836	0.450880	0.886359	C	-5.068151	1.562908	-1.902505
C	3.314625	2.212314	0.395293	H	-5.592540	1.177768	-1.016669
H	3.569227	2.195508	-0.670378	H	-5.677886	2.387317	-2.292713
H	2.286106	2.584614	0.470199	C	-3.686848	2.093287	-1.477368
C	4.253402	3.189668	1.125479	H	-3.811388	2.875078	-0.720018
H	5.294920	2.874717	0.967865	H	-3.210577	2.570144	-2.343830
H	4.161588	4.189527	0.683694	C	-1.691370	2.660618	1.186471
C	3.960697	3.240073	2.631445	H	-2.093959	3.544956	0.677027
H	4.673506	3.903421	3.135861	C	-2.800713	2.121470	2.112039
H	2.963268	3.673863	2.790734	H	-3.690307	1.849020	1.535129
C	4.004014	1.836524	3.250219	H	-2.443933	1.214788	2.606057
H	3.732076	1.878946	4.311668	C	-3.193267	3.162813	3.176014
H	5.034035	1.453618	3.208082	H	-3.637636	4.040406	2.683586
C	3.069898	0.860812	2.515033	H	-3.970712	2.745340	3.827390
H	2.028173	1.180087	2.646197	C	-1.984028	3.608878	4.008489
H	3.141170	-0.130734	2.973280	H	-2.279662	4.377623	4.732775
C	2.888668	-2.091769	0.936292	H	-1.610935	2.754261	4.589469
H	2.302209	-2.098468	1.863822	C	-0.860990	4.132250	3.103883
C	4.380795	-2.220031	1.316927	H	0.022121	4.393146	3.700343
H	5.001299	-2.248325	0.412326	H	-1.191241	5.060320	2.614675
H	4.721596	-1.361057	1.901761	C	-0.475312	3.100551	2.029874
C	4.628210	-3.500736	2.137207	H	-0.052151	2.210444	2.512655
H	5.694909	-3.581699	2.380753	H	0.313198	3.516239	1.391073
H	4.094907	-3.417320	3.094687	C	-0.240676	2.627656	-1.376185
C	4.149673	-4.759648	1.401804	H	0.773013	2.634486	-0.955960
H	4.285274	-5.644414	2.035501	C	-0.700453	4.102139	-1.454936
H	4.774109	-4.916228	0.509962	H	-0.735395	4.557022	-0.461351
C	2.682179	-4.624854	0.973665	H	-1.717770	4.157860	-1.860930
H	2.037703	-4.594588	1.862175	C	0.243189	4.938078	-2.340418
H	2.372602	-5.501767	0.392005	H	-0.125076	5.969681	-2.397327
C	2.453037	-3.347195	0.149652	H	1.231827	4.987728	-1.861926
H	1.400461	-3.273984	-0.132214	C	0.394920	4.345590	-3.746932
H	3.037043	-3.419853	-0.777594	H	-0.568074	4.408183	-4.273569
C	-2.787302	0.953414	-0.956525	H	1.110137	4.933674	-4.334455
H	-3.295173	0.487557	-0.100890	C	0.835391	2.877699	-3.676314
C	-2.655877	-0.160129	-2.019932	H	1.851842	2.823587	-3.260511
H	-2.140700	0.222441	-2.908150	H	0.886970	2.445042	-4.683106
H	-2.049326	-0.981814	-1.628241	C	-0.119520	2.047421	-2.801797

H	-1.106867	2.043425	-3.278715
H	0.214147	1.006321	-2.765693
F	-1.284780	-0.589110	3.038256
Ni	-0.010660	-0.308621	0.603632
P	2.277515	-0.473479	0.150447
P	-1.145504	1.452726	-0.167847
O	-0.066216	-1.887080	1.632885
C	-1.201383	-1.296908	1.797069
C	-3.167483	-4.913408	-1.505613
C	-4.208459	-4.486204	-0.714979
C	-4.013882	-3.503012	0.293865
C	-2.703424	-2.945392	0.495997
C	-1.652350	-3.418728	-0.339168
C	-1.877246	-4.369631	-1.311585
H	-6.082836	-3.508840	0.933778
H	-3.332205	-5.665769	-2.271877
H	-5.206724	-4.895784	-0.849114
C	-5.100830	-3.073578	1.100622
C	-2.523855	-1.947469	1.523180
H	-0.660043	-3.021883	-0.185788
H	-1.051177	-4.709844	-1.930392
C	-3.621896	-1.575577	2.287894
C	-4.902522	-2.130864	2.080165
H	-3.483651	-0.851110	3.078894
H	-5.728079	-1.809788	2.709480

1a

B3LYP/BSI SCF energy: -598.474391a.u.

M06/BSII SCF energy in solution: -598.247764a.u.

M06/BSII free energy in solution: -598.133195a.u.

C	-0.389971	2.537100	-0.000041
C	0.939678	2.182787	-0.000001
C	1.336254	0.819971	0.000006
C	0.339688	-0.215797	-0.000026
C	-1.044578	0.187486	-0.000064
C	-1.378969	1.535615	-0.000076
H	3.450802	1.268930	0.000073
H	-0.683973	3.581891	-0.000047
H	1.712438	2.947433	0.000024
C	2.713484	0.470443	0.000046
C	0.783282	-1.567075	-0.000019
H	-2.424433	1.816739	-0.000110
C	2.129107	-1.867744	0.000018
C	3.106830	-0.847049	0.000052
H	0.048776	-2.360077	-0.000041
H	2.441452	-2.908161	0.000022
H	4.161629	-1.105363	0.000084
C	-2.141345	-0.803698	-0.000108
O	-2.092614	-2.001148	-0.000105
F	-3.369615	-0.202715	0.000235

[B1]

B3LYP/BSI SCF energy: -507.504036a.u.

M06/BSII SCF energy in solution: -507.36919a.u.

M06/BSII free energy in solution: -507.286288a.u.

C	-0.108536	-1.205055	-0.000054
C	-1.502157	-1.217709	-0.000050
C	-2.174489	-0.000003	-0.000002
C	-1.502153	1.217707	0.000046
C	-0.108536	1.205054	0.000044
C	0.617613	-0.000004	-0.000006
H	0.431113	-2.147398	-0.000094
H	-2.069695	-2.142335	-0.000085
H	-2.069700	2.142327	0.000084
H	0.431119	2.147393	0.000087
F	-3.524477	0.000004	0.000002
B	2.178102	0.000000	-0.000001
O	2.825110	-1.212545	0.000122
H	3.787390	-1.165094	-0.000005
O	2.825104	1.212549	-0.000056
H	3.787384	1.165099	-0.000384

[B2]

B3LYP/BSI SCF energy: -705.962058a.u.

M06/BSII SCF energy in solution: -705.845141a.u.

M06/BSII free energy in solution: -705.781622a.u.

C	0.222906	1.174274	0.094941
C	1.612837	1.213976	0.102385
C	2.281194	0.000000	0.000000
C	1.612836	-1.213977	-0.102385
C	0.222905	-1.174274	-0.094941
C	-0.533371	0.000000	0.000000
H	2.148230	2.150759	0.188954
H	2.148230	-2.150759	-0.188954
F	3.625935	0.000000	0.000000

B	-2.106309	0.000000	0.000000
O	-2.741922	0.951817	-0.748716
H	-3.703870	0.947289	-0.682889
O	-2.741921	-0.951817	0.748716
H	-3.703870	-0.947289	0.682889
F	-0.424206	-2.349323	-0.214102
F	-0.424205	2.349323	0.214102

[B3]

B3LYP/BSI SCF energy: -522.796291a.u.

M06/BSII SCF energy in solution: -522.622725a.u.

M06/BSII free energy in solution: -522.501376a.u.

C	0.464781	1.289972	-0.000068
C	-0.915920	1.424720	-0.000009
C	-1.730690	0.281169	0.000116
C	-1.143821	-0.991021	0.000117
C	0.247650	-1.101504	0.000049
C	1.085771	0.023876	0.000003
H	1.084870	2.181889	-0.000180
H	-1.393867	2.399284	-0.000066
H	-1.753165	-1.887345	0.000117
H	0.694477	-2.091817	0.000057
B	2.635453	-0.120420	-0.000033
O	3.396301	1.026415	-0.000028
H	4.349181	0.884497	-0.000153
O	3.173649	-1.387443	0.000013
H	4.136423	-1.421358	-0.000094
O	-3.075092	0.513860	0.000267
C	-3.951299	-0.601504	-0.000266
H	-4.962405	-0.190981	-0.000293
H	-3.815040	-1.224195	-0.893876
H	-3.815437	-1.224791	0.892982

TS1

B3LYP/BSI SCF energy: -2863.863531a.u.

M06/BSII SCF energy in solution: -2862.86778a.u.

M06/BSII free energy in solution: -2861.835593a.u.

C	-3.512629	-0.322201	-1.136189
H	-3.368021	-1.357868	-0.794738
C	-2.951124	-0.260379	-2.575566
H	-3.073996	0.750012	-2.979032
H	-1.873818	-0.457744	-2.572755
C	-3.677666	-1.254208	-3.497698
H	-3.470568	-2.280523	-3.162048
H	-3.280900	-1.173751	-4.516994
C	-5.195447	-1.019193	-3.496513
H	-5.408260	-0.040602	-3.950038
H	-5.698588	-1.767419	-4.120782
C	-5.763779	-1.046562	-2.070338
H	-5.665113	-2.061570	-1.659030
H	-6.836999	-0.820212	-2.083234
C	-5.032236	-0.055436	-1.146743
H	-5.449105	-0.117407	-0.135228
H	-5.219770	0.965576	-1.501262
C	-3.269963	0.236402	1.761676
H	-4.300205	0.614763	1.726977
C	-3.346294	-1.274798	2.060303
H	-3.897803	-1.803403	1.274997
H	-2.330882	-1.692281	2.070854
C	-4.012925	-1.549134	3.420145
H	-5.061295	-1.220767	3.379453
H	-4.033067	-2.629260	3.610782
C	-3.296194	-0.816095	4.562141
H	-3.816280	-0.989357	5.511988
H	-2.284871	-1.231628	4.678787
C	-3.192346	0.687176	4.271860
H	-2.626790	1.191176	5.064828
H	-4.199768	1.127975	4.279883
C	-2.529980	0.958705	2.910795
H	-1.487826	0.614640	2.932233
H	-2.485967	2.036937	2.729973
C	-2.823767	2.496710	-0.077550
H	-2.028805	2.915876	0.552590
C	-4.171926	3.044007	0.439747
H	-4.996887	2.666162	-0.176966
H	-4.370643	2.713893	1.464090
C	-4.182535	4.584536	0.403850
H	-5.154136	4.954991	0.754378
H	-3.430455	4.960755	1.111636
C	-3.873665	5.130454	-0.997361
H	-3.835885	6.226501	-0.977093
H	-4.693903	4.859451	-1.678397
C	-2.557786	4.555070	-1.537877
H	-1.717017	4.922044	-0.934298
H	-2.381781	4.904357	-2.562673
C	-2.557205	3.017812	-1.507424

H	-1.598273	2.642595	-1.872865
H	-3.344236	2.656294	-2.182839
C	2.185658	-1.542661	-1.439948
H	2.964943	-0.795496	-1.232542
C	1.481250	-1.067084	-2.731684
H	0.659643	-1.746753	-2.986581
H	1.034623	-0.081534	-2.565458
C	2.464403	-1.014609	-3.913754
H	3.220100	-0.242284	-3.716852
H	1.932689	-0.709285	-4.823347
C	3.167104	-2.361991	-4.132052
H	2.425283	-3.114447	-4.437493
H	3.890462	-2.287402	-4.953072
C	3.866244	-2.834339	-2.849600
H	4.683964	-2.141168	-2.606712
H	4.326894	-3.817989	-3.003907
C	2.888748	-2.898005	-1.662150
H	3.424533	-3.212999	-0.759519
H	2.138345	-3.672248	-1.865725
C	2.305504	-1.734708	1.510220
H	2.520682	-2.808952	1.469547
C	3.664343	-1.011852	1.415377
H	4.180198	-1.280085	0.488051
H	3.513317	0.069872	1.392442
C	4.568994	-1.368658	2.608822
H	4.826517	-2.437196	2.565281
H	5.512639	-0.816242	2.527273
C	3.890293	-1.068055	3.951700
H	4.540964	-1.364212	4.783602
H	3.737832	0.016189	4.041837
C	2.534957	-1.780641	4.055051
H	2.032904	-1.517112	4.994102
H	2.699193	-2.867710	4.084108
C	1.624810	-1.435254	2.864273
H	1.362612	-0.369915	2.898526
H	0.679742	-1.986144	2.949604
C	-0.040555	-2.913787	0.200782
H	-0.779526	-2.579656	0.941348
C	0.545199	-4.244547	0.726811
H	1.029923	-4.103828	1.696720
H	1.315895	-4.616891	0.040749
C	-0.550525	-5.315364	0.888535
H	-0.097874	-6.252896	1.233912
H	-1.245651	-4.997025	1.678698
C	-1.336070	-5.545084	-0.408262
H	-0.667667	-5.976620	-1.167064
H	-2.136663	-6.276637	-0.245508
C	-1.911986	-4.224883	-0.936552
H	-2.669002	-3.851882	-0.231928
H	-2.426880	-4.387272	-1.891559
C	-0.812060	-3.164582	-1.111699
H	-0.116776	-3.513467	-1.885169
H	-1.242108	-2.228569	-1.477080
F	0.095113	2.330372	1.176229
Ni	-0.075127	0.486805	0.122842
P	-2.462344	0.642428	0.102893
P	1.096585	-1.377414	0.095307
O	0.630420	2.264068	-1.147279
C	1.123025	1.927192	-0.062298
C	5.865026	2.593905	-2.171209
C	6.013796	2.764143	-0.815075
C	4.899935	2.670782	0.064034
C	3.597458	2.381118	-0.473141
C	3.481791	2.218985	-1.883822
C	4.583428	2.324691	-2.705869
H	6.048044	3.109781	1.844489
H	6.723502	2.673996	-2.832023
H	6.990194	2.982604	-0.389659
C	5.057806	2.881015	1.458689
C	2.487283	2.283019	0.439057
H	2.502718	2.036272	-2.305719
H	4.462746	2.209263	-3.779459
C	2.692628	2.509596	1.791775
C	3.972291	2.814161	2.301294
H	1.842512	2.454332	2.457703
H	4.091146	2.997518	3.365446

IM1

B3LYP/BSI SCF energy: -2863.886817a.u.

M06/BSII SCF energy in solution: -2862.88727a.u.

M06/BSII free energy in solution: -2861.853304a.u.

C	3.628209	0.213024	-0.689740
H	3.338255	1.180963	-0.259643
C	3.488367	0.340630	-2.223744
H	3.769604	-0.610688	-2.689763
H	2.443468	0.521560	-2.502275
C	4.392147	1.443951	-2.799575

H	4.062290	2.422989	-2.426278	H	2.202616	-2.010384	-2.962891
H	4.284714	1.475252	-3.890697	C	-1.678116	2.241332	-1.313543
C	5.860769	1.223270	-2.412807	H	-2.562805	1.590193	-1.312110
H	6.227462	0.304894	-2.893193	C	-0.983216	1.995193	-2.673732
H	6.483845	2.042732	-2.790948	H	-0.078702	2.607864	-2.753988
C	6.013896	1.093486	-0.892042	H	-0.684791	0.946821	-2.746575
H	5.756930	2.053069	-0.420608	C	-1.925019	2.353020	-3.836283
H	7.058923	0.889560	-0.628173	H	-2.778334	1.660708	-3.831876
C	5.110255	-0.010570	-0.311702	H	-1.406623	2.199740	-4.790446
H	5.235197	-0.029106	0.775150	C	-2.438585	3.796358	-3.733958
H	5.449713	-0.984734	-0.681781	H	-1.595045	4.491331	-3.856666
C	3.029939	-1.339170	1.750873	H	-3.140114	4.012498	-4.548712
H	4.096044	-1.567102	1.622450	C	-3.108420	4.052643	-2.376448
C	2.916515	-0.081454	2.641655	H	-4.021292	3.444839	-2.303008
H	3.413683	0.775771	2.170823	H	-3.424275	5.100026	-2.295552
H	1.854821	0.185252	2.737267	C	-2.174776	3.699288	-1.204299
C	3.504867	-0.308540	4.043986	H	-2.696818	3.869221	-0.256343
H	4.588377	-0.475338	3.959624	H	-1.318872	4.385756	-1.214694
H	3.375691	0.595559	4.651933	C	-1.930385	1.821892	1.607030
C	2.857834	-1.517930	4.731510	H	-1.936816	2.900150	1.803169
H	3.317967	-1.691145	5.711946	C	-3.394710	1.416621	1.337766
H	1.795807	-1.302117	4.916456	H	-3.798198	1.961248	0.478605
C	2.973323	-2.771538	3.854074	H	-3.451277	0.353115	1.095496
H	2.470993	-3.619915	4.334541	C	-4.278018	1.694845	2.567739
H	4.034017	-3.049307	3.764771	H	-4.312425	2.778141	2.756026
C	2.380663	-2.552218	2.451676	H	-5.306847	1.382428	2.353585
H	1.297921	-2.406563	2.505499	C	-3.752205	0.978551	3.818816
H	2.529201	-3.456343	1.852950	H	-4.378349	1.216806	4.687162
C	2.450550	-2.618385	-0.875662	H	-3.823117	-0.107071	3.666466
H	1.856476	-3.246079	-0.203436	C	-2.291474	1.359175	4.095096
C	3.842188	-3.260922	-1.041164	H	-1.904444	0.799287	4.955126
H	4.452711	-2.670757	-1.737242	H	-2.239879	2.423590	4.367268
H	4.383470	-3.281626	-0.088006	C	-1.399246	1.104280	2.868718
C	3.716694	-4.694235	-1.592791	H	-1.351921	0.027160	2.663482
H	4.715112	-5.128533	-1.729411	H	-0.372415	1.420434	3.090219
H	3.202353	-5.318675	-0.848861	C	0.681520	2.765465	0.613190
C	2.931293	-4.729302	-2.912194	H	1.359138	2.122979	1.192171
H	2.818131	-5.764256	-3.257550	C	0.321635	3.973427	1.510561
H	3.507693	-4.203520	-3.687698	H	-0.163042	3.643657	2.432724
C	1.558635	-4.058270	-2.761715	H	-0.394265	4.623575	0.991689
H	0.936206	-4.646481	-2.073650	C	1.567794	4.795561	1.887198
H	1.033527	-4.045267	-3.724478	H	1.266355	5.652815	2.501143
C	1.682486	-2.625396	-2.218245	H	2.226355	4.179140	2.515750
H	0.686044	-2.195359	-2.087246	C	2.344789	5.263679	0.651889

H	1.727518	5.970239	0.078921
H	3.247990	5.808605	0.950830
C	2.708165	4.070111	-0.239028
H	3.419573	3.425607	0.295937
H	3.220200	4.411416	-1.146861
C	1.462094	3.254882	-0.626183
H	0.813462	3.895538	-1.234601
H	1.745487	2.409519	-1.259160
F	0.004302	-2.387343	0.622307
Ni	-0.142682	-0.634265	0.066747
P	2.324005	-0.970829	0.035455
P	-0.730909	1.555499	0.165398
O	-1.722315	-1.033504	-1.948477
C	-1.788757	-1.153290	-0.729334
C	-6.910692	-1.992009	-1.743659
C	-6.655123	-2.517349	-0.498910
C	-5.349635	-2.473253	0.061708
C	-4.275219	-1.869255	-0.680500
C	-4.579725	-1.340569	-1.967431
C	-5.858576	-1.399935	-2.479238
H	-5.921272	-3.494053	1.880087
H	-7.911928	-2.033231	-2.163074
H	-7.450943	-2.979626	0.080065
C	-5.097392	-3.029000	1.343868
C	-2.968228	-1.817683	-0.067365
H	-3.779965	-0.909631	-2.553570
H	-6.058495	-0.991340	-3.466132
C	-2.780435	-2.370059	1.191276
C	-3.836837	-2.988650	1.892608
H	-1.776404	-2.358275	1.597796
H	-3.646264	-3.432266	2.865765

TSA

B3LYP/BSI SCF energy: -2863.883404a.u.

M06/BSII SCF energy in solution: -2862.87393a.u.

M06/BSII free energy in solution: -2861.844354a.u.

C	4.274287	0.166469	-0.660323
H	4.232650	1.105106	-0.085340
C	3.993731	0.547210	-2.130582
H	4.047617	-0.353367	-2.754777
H	2.974702	0.937431	-2.239027
C	5.014272	1.571379	-2.654697
H	4.901585	2.512132	-2.096203
H	4.805161	1.806003	-3.705840
C	6.453381	1.059016	-2.498570
H	6.597624	0.189058	-3.155247
H	7.169211	1.821032	-2.830458
C	6.743623	0.648490	-1.047789
H	6.721339	1.542716	-0.408111
H	7.755886	0.233516	-0.964869
C	5.714867	-0.370993	-0.523766
H	5.946128	-0.612547	0.519082
H	5.815844	-1.304300	-1.089401
C	3.536910	-1.270237	1.794720
H	4.530270	-1.716401	1.644291
C	3.714702	-0.002255	2.659129
H	4.372669	0.718586	2.159495
H	2.736924	0.489444	2.767280
C	4.272291	-0.319423	4.056794
H	5.294571	-0.712106	3.958277
H	4.350260	0.603989	4.644583
C	3.402785	-1.350974	4.787187
H	3.838958	-1.595477	5.763593
H	2.413669	-0.913527	4.986418
C	3.232890	-2.618674	3.940192
H	2.575282	-3.333099	4.450518
H	4.209654	-3.113969	3.837753
C	2.670056	-2.307006	2.542850
H	1.640655	-1.939912	2.622579
H	2.606898	-3.235148	1.966713
C	2.649452	-2.472174	-0.753574
H	1.921105	-2.941024	-0.080227
C	3.878618	-3.395193	-0.862290
H	4.600726	-2.972614	-1.573347
H	4.397499	-3.478383	0.099736
C	3.470592	-4.795647	-1.355502
H	4.358074	-5.434819	-1.447221
H	2.821813	-5.265908	-0.603139
C	2.724062	-4.723504	-2.695635
H	2.399453	-5.724838	-3.004639
H	3.416853	-4.367615	-3.472597
C	1.520792	-3.771395	-2.617284
H	0.770606	-4.185494	-1.930033
H	1.036216	-3.690169	-3.598160
C	1.928480	-2.374997	-2.116599
H	1.038983	-1.742554	-2.027115
H	2.583801	-1.907116	-2.863419

C	-1.512765	2.304447	-1.573031	H	2.955536	5.422347	2.010828
H	-2.424056	1.738723	-1.809680	C	2.584278	3.637253	0.823178
C	-0.472866	1.876910	-2.634455	H	2.945796	2.970901	1.618443
H	0.484393	2.377689	-2.451752	H	3.428298	3.795302	0.140784
H	-0.300534	0.800253	-2.562032	C	1.435894	2.947982	0.068520
C	-0.961892	2.235985	-4.047437	H	1.149372	3.579020	-0.781617
H	-1.853928	1.638003	-4.279938	H	1.775611	1.990144	-0.335808
H	-0.199316	1.954522	-4.783335	F	0.007444	-2.121623	0.813428
C	-1.299486	3.728518	-4.173139	Ni	-0.555937	-0.504333	0.274500
H	-0.379947	4.319645	-4.052690	P	2.820868	-0.800461	0.102972
H	-1.683043	3.951341	-5.175990	P	-1.124481	1.659134	0.148156
C	-2.318379	4.160603	-3.109004	O	-1.992792	-0.955252	-1.884790
H	-3.277646	3.659180	-3.300809	C	-2.014494	-1.161379	-0.682435
H	-2.511484	5.238163	-3.177012	C	-7.033384	-2.523894	-1.607898
C	-1.842857	3.807071	-1.688149	C	-6.705212	-3.013216	-0.365209
H	-2.609456	4.099228	-0.961080	C	-5.402909	-2.831294	0.173277
H	-0.948046	4.398145	-1.454602	C	-4.408941	-2.124807	-0.589401
C	-2.666962	2.057121	1.156634	C	-4.785768	-1.637001	-1.872208
H	-2.695426	3.148485	1.265161	C	-6.060129	-1.830940	-2.362563
C	-3.994071	1.634478	0.491207	H	-5.839836	-3.889925	2.007057
H	-4.111283	2.120809	-0.482701	H	-8.031565	-2.670402	-2.010370
H	-3.995124	0.555201	0.308757	H	-7.439805	-3.551125	0.228961
C	-5.199715	1.989639	1.380169	C	-5.075191	-3.348655	1.454968
H	-5.274135	3.083104	1.471031	C	-3.103983	-1.938400	0.004827
H	-6.121980	1.652862	0.892713	H	-4.046691	-1.121995	-2.469731
C	-5.077698	1.372804	2.779843	H	-6.316861	-1.449244	-3.346919
H	-5.929888	1.670551	3.402447	C	-2.839077	-2.462599	1.262107
H	-5.114974	0.277933	2.697263	C	-3.817315	-3.179342	1.983446
C	-3.759085	1.784938	3.448310	H	-1.836004	-2.351333	1.658871
H	-3.655359	1.298176	4.425427	H	-3.567993	-3.592668	2.956298
H	-3.770292	2.868001	3.638824				
C	-2.548533	1.434757	2.566956	**IMA**			
H	-2.474525	0.344555	2.465352	B3LYP/BSI SCF energy: -1816.677847a.u.			
H	-1.625717	1.763338	3.059664	M06/BSII SCF energy in solution: -1816.06742a.u.			
C	0.207245	2.731258	0.978024	M06/BSII free energy in solution: -1815.499162a.u.			
H	0.534459	2.090303	1.810374				
C	-0.247047	4.077427	1.587685	C	-2.864687	1.078891	0.446598
H	-1.076955	3.934126	2.285064	H	-2.505246	1.902207	1.080604
H	-0.612609	4.740673	0.793873	C	-3.380889	1.727999	-0.859807
C	0.908027	4.770504	2.333841	H	-3.724924	0.948569	-1.550829
H	0.560737	5.732442	2.729852	H	-2.570845	2.260928	-1.374307
H	1.188781	4.159334	3.203494	C	-4.535624	2.703837	-0.574901
C	2.137322	4.969297	1.438592	H	-4.151038	3.552219	0.008545
H	1.889792	5.676074	0.633451	H	-4.907397	3.118949	-1.518678

C	-5.675893	2.029602	0.201153
H	-6.140771	1.261103	-0.432667
H	-6.461022	2.758831	0.432665
C	-5.161246	1.374254	1.490834
H	-4.801157	2.153032	2.177926
H	-5.976298	0.854423	2.008462
C	-4.017324	0.385939	1.201171
H	-3.661851	-0.060090	2.137076
H	-4.408918	-0.434819	0.588655
C	-0.547385	-0.075787	1.887825
H	-1.337577	-0.469367	2.544095
C	-0.103685	1.300197	2.435085
H	-0.943681	2.002659	2.459813
H	0.643246	1.728853	1.753668
C	0.497276	1.182025	3.846405
H	-0.284994	0.854174	4.546021
H	0.825288	2.171041	4.187462
C	1.663839	0.186149	3.886058
H	2.042483	0.084172	4.909933
H	2.494074	0.575638	3.280990
C	1.237855	-1.180720	3.334933
H	2.092201	-1.867064	3.312292
H	0.491835	-1.629215	4.006849
C	0.643378	-1.060397	1.921394
H	1.424850	-0.708117	1.238285
H	0.342792	-2.050562	1.565639
C	-1.677527	-1.675823	-0.370905
H	-0.666997	-2.056019	-0.572942
C	-2.351452	-2.621447	0.646344
H	-1.821359	-2.616302	1.604591
H	-3.373356	-2.285553	0.854121
C	-2.403341	-4.057296	0.092941
H	-2.901107	-4.714040	0.816670
H	-1.377974	-4.436546	-0.020097
C	-3.119335	-4.116021	-1.264373
H	-4.178210	-3.854220	-1.124418
H	-3.102243	-5.139323	-1.657675
C	-2.486512	-3.146749	-2.273448
H	-1.467687	-3.479186	-2.513516
H	-3.048168	-3.156446	-3.215025
C	-2.421464	-1.711429	-1.724396
H	-3.443696	-1.329856	-1.596960
H	-1.919964	-1.058623	-2.446879
F	0.192399	2.484848	-2.537715
Ni	-0.167334	1.219925	-1.350494
P	-1.290388	0.078092	0.168379
C	5.928633	-1.673690	0.285816
C	6.037308	-0.307097	0.172551
C	4.952512	0.477209	-0.303651
C	3.719473	-0.164339	-0.670627
C	3.647493	-1.580005	-0.546621
C	4.720877	-2.309753	-0.080031
H	6.027482	2.347780	-0.162019
H	6.765380	-2.263248	0.649124
H	6.960578	0.198363	0.444492
C	5.080598	1.886345	-0.431942
H	2.738242	-2.083756	-0.844563
H	4.637838	-3.390093	0.000439
C	2.806384	2.043962	-1.226465
C	4.036643	2.651028	-0.895331
H	1.986998	2.642224	-1.614209
H	4.147511	3.725460	-1.006781
C	2.631366	0.670648	-1.125326
C	1.291558	0.093015	-1.486164
O	1.121537	-1.051797	-1.864997

TSB

B3LYP/BSI SCF energy: -1816.671131a.u.

M06/BSII SCF energy in solution: -1816.06248a.u.

M06/BSII free energy in solution: -1815.493792a.u.

C	2.590745	1.105998	-0.790763
H	2.844634	0.603186	-1.734634
C	1.915417	2.438585	-1.187908
H	1.606463	2.985934	-0.288404
H	1.009023	2.234889	-1.768643
C	2.875643	3.314785	-2.010454
H	3.077325	2.817704	-2.969345
H	2.390415	4.268013	-2.250744
C	4.201343	3.559123	-1.275225
H	4.012636	4.163714	-0.376379
H	4.883309	4.142833	-1.904611
C	4.862284	2.236161	-0.862262
H	5.163235	1.681971	-1.762281
H	5.779459	2.427459	-0.292346
C	3.906738	1.363969	-0.028316
H	4.398208	0.421361	0.238067
H	3.686815	1.883659	0.912582

C	2.306318	-1.769583	-0.080867	C	-5.733292	-1.790963	0.697198
H	3.246350	-1.630985	0.472746	H	-5.833563	2.696248	-1.114408
C	2.656759	-2.175105	-1.531536	H	-7.831142	-1.238991	0.618901
H	3.283832	-1.414559	-2.008577	H	-7.382477	1.007933	-0.322569
H	1.734108	-2.232819	-2.123942	C	-4.986468	2.045622	-0.911845
C	3.385267	-3.528826	-1.581125	C	-2.803146	0.341482	-0.372962
H	4.363968	-3.432901	-1.088686	H	-3.614125	-2.078039	0.681531
H	3.586853	-3.793971	-2.625533	H	-5.932351	-2.777744	1.105618
C	2.577860	-4.635557	-0.891319	C	-2.620032	1.602218	-0.921893
H	3.136557	-5.578934	-0.903377	C	-3.705351	2.463920	-1.183736
H	1.650467	-4.811881	-1.453837	H	-1.611379	1.932867	-1.155550
C	2.228495	-4.239314	0.548774	H	-3.521991	3.447463	-1.605074
H	1.608853	-5.011516	1.019733				
H	3.152573	-4.176802	1.142120	**IM3**			
C	1.492560	-2.890577	0.606697	B3LYP/BSI SCF energy: -1816.679089a.u.			
H	0.516732	-2.977921	0.115719	M06/BSII SCF energy in solution: -1816.06994a.u.			
H	1.281207	-2.634423	1.649590	M06/BSII free energy in solution: -1815.500524a.u.			
C	1.108013	0.212620	1.797653				
H	0.313491	-0.511620	2.020636	C	-1.754801	-0.613360	-1.711256
C	2.281042	-0.068130	2.763606	H	-1.772216	0.319005	-2.289354
H	2.691464	-1.070216	2.604399	C	-0.651039	-1.482511	-2.354892
H	3.098309	0.639433	2.582108	H	-0.527767	-2.418730	-1.797621
C	1.819076	0.068443	4.226031	H	0.303672	-0.948845	-2.311619
H	2.666361	-0.113354	4.898062	C	-1.002444	-1.808236	-3.816542
H	1.075699	-0.711579	4.441792	H	-0.995068	-0.877723	-4.400667
C	1.204303	1.447708	4.502011	H	-0.226858	-2.452698	-4.247151
H	1.984075	2.216741	4.403676	C	-2.379994	-2.475708	-3.938877
H	0.842667	1.502217	5.535541	H	-2.351463	-3.459808	-3.448980
C	0.063739	1.756415	3.521521	H	-2.622562	-2.659733	-4.992269
H	-0.771161	1.065647	3.701733	C	-3.473675	-1.618703	-3.285530
H	-0.324026	2.767610	3.692726	H	-3.583458	-0.680559	-3.847265
C	0.520088	1.616878	2.059127	H	-4.443191	-2.128948	-3.336383
H	1.280084	2.381092	1.848624	C	-3.136274	-1.290206	-1.819746
H	-0.322284	1.812026	1.386758	H	-3.919206	-0.652100	-1.393169
F	-0.420708	-0.117250	-3.154114	H	-3.138654	-2.221639	-1.238534
Ni	-0.301501	-0.168395	-1.374436	C	-2.528858	1.395414	0.363106
P	1.393204	-0.126463	-0.023666	H	-3.500659	0.908857	0.525017
O	-1.533538	-1.371932	0.744850	C	-2.683158	2.405233	-0.796635
C	-1.571748	-0.487386	-0.095750	H	-3.063776	1.898714	-1.690027
C	-6.811880	-0.920002	0.421197	H	-1.696688	2.799826	-1.065456
C	-6.563669	0.328193	-0.100790	C	-3.650921	3.542334	-0.425262
C	-5.235854	0.757099	-0.367433	H	-4.664877	3.132718	-0.306517
C	-4.136654	-0.123543	-0.081271	H	-3.700764	4.259591	-1.252982
C	-4.431268	-1.406738	0.455588	C	-3.243972	4.251241	0.873126

H	-3.972807	5.029962	1.127689
H	-2.280420	4.757977	0.722873
C	-3.110669	3.245982	2.024578
H	-2.776300	3.749046	2.939747
H	-4.096748	2.813849	2.248224
C	-2.126661	2.120308	1.668528
H	-1.125214	2.550578	1.533617
H	-2.051464	1.411763	2.501538
C	-1.529670	-1.249671	1.327160
H	-0.965142	-0.805522	2.157812
C	-2.973391	-1.508921	1.808948
H	-3.467806	-0.573221	2.087818
H	-3.569411	-1.951687	1.001090
C	-2.980852	-2.456575	3.022535
H	-4.015563	-2.652482	3.329123
H	-2.493440	-1.953729	3.869438
C	-2.250035	-3.773604	2.728776
H	-2.808724	-4.334783	1.965645
H	-2.229702	-4.403818	3.625858
C	-0.823348	-3.515386	2.223645
H	-0.224863	-3.054915	3.020530
H	-0.333093	-4.462303	1.966966
C	-0.819019	-2.582071	1.002093
H	-1.330056	-3.082726	0.169416
H	0.209834	-2.390818	0.682505
F	0.335067	1.831581	-1.663569
Ni	0.699682	0.887728	-0.148190
P	-1.291015	0.035292	-0.016746
O	1.361412	-0.451017	2.321471
C	1.507026	0.226307	1.323038
C	6.152285	-1.559681	-0.314538
C	6.099824	-0.230794	-0.676659
C	4.983715	0.572849	-0.329220
C	3.906558	-0.015995	0.406461
C	3.989712	-1.383927	0.769884
C	5.089734	-2.138156	0.415358
H	5.737788	2.379128	-1.257290
H	7.011948	-2.165050	-0.586923
H	6.915304	0.221176	-1.235392
C	4.914524	1.950800	-0.691364
C	2.787720	0.816526	0.773003
H	3.183730	-1.823044	1.346739
H	5.142480	-3.183986	0.703687
C	2.771117	2.160035	0.404643
C	3.842413	2.727643	-0.332108
H	1.952644	2.801019	0.726184
H	3.802681	3.776794	-0.606563

IM3-dim

B3LYP/BSI SCF energy: -3633.420696a.u.

M06/BSII SCF energy in solution: -3632.18628a.u.

M06/BSII free energy in solution: -3631.023063a.u.

C	-2.116974	3.137443	-0.881208
H	-1.145441	3.315136	-0.401804
C	-1.801263	2.769195	-2.348892
H	-2.723809	2.530937	-2.889805
H	-1.179452	1.868270	-2.378583
C	-1.086994	3.931625	-3.059544
H	-0.102357	4.085641	-2.597136
H	-0.903273	3.664378	-4.107443
C	-1.896311	5.234128	-2.977195
H	-2.833257	5.115715	-3.540641
H	-1.347931	6.055207	-3.454443
C	-2.224964	5.593018	-1.521137
H	-1.293791	5.826411	-0.985980
H	-2.844463	6.497254	-1.479106
C	-2.942484	4.437835	-0.799272
H	-3.131880	4.717112	0.243649
H	-3.923589	4.281925	-1.266074
C	-2.713019	2.299941	1.906830
H	-3.504335	3.057148	1.984694
C	-1.384018	2.970832	2.319755
H	-1.177371	3.835316	1.680615
H	-0.555968	2.271185	2.167322
C	-1.430221	3.435799	3.786011
H	-2.180286	4.233424	3.892127
H	-0.464506	3.878471	4.056841
C	-1.779396	2.289133	4.744149
H	-1.841038	2.657605	5.775203
H	-0.972096	1.543592	4.723915
C	-3.096951	1.616516	4.336507
H	-3.313446	0.764317	4.992081
H	-3.925537	2.327783	4.466171
C	-3.052814	1.144207	2.874466
H	-2.283888	0.368482	2.770536
H	-4.005212	0.672972	2.605072
C	-4.578708	1.362934	-0.210811

H	-4.710027	0.349038	0.193910	H	1.831765	-5.601718	2.359045
C	-5.596966	2.275453	0.510893	H	0.132373	-5.165656	2.494140
H	-5.410742	2.300549	1.588432	C	1.446494	-4.098738	3.861798
H	-5.495564	3.306521	0.148900	H	1.366070	-4.837301	4.668672
C	-7.039704	1.792972	0.271107	H	0.690767	-3.326693	4.065884
H	-7.740021	2.472808	0.771605	C	2.837780	-3.452005	3.862854
H	-7.168944	0.809286	0.744411	H	3.024235	-2.942749	4.815951
C	-7.373162	1.681770	-1.222130	H	3.602515	-4.237521	3.774102
H	-7.369723	2.686218	-1.670023	C	2.996041	-2.451490	2.706269
H	-8.386751	1.285063	-1.355536	H	2.301824	-1.614278	2.847871
C	-6.350037	0.800758	-1.950429	H	3.999545	-2.014438	2.729068
H	-6.436205	-0.236082	-1.597234	C	4.814951	-1.528150	-0.024544
H	-6.561037	0.780742	-3.026473	H	4.881469	-0.826604	0.817107
C	-4.911819	1.294453	-1.720378	C	5.766064	-2.706945	0.280685
H	-4.813926	2.296769	-2.156631	H	5.463444	-3.229542	1.193075
H	-4.207329	0.642313	-2.241420	H	5.731556	-3.443654	-0.531172
F	0.200187	1.149525	0.300098	C	7.214444	-2.209986	0.445899
Ni	-1.327992	0.003068	-0.163794	H	7.875708	-3.063783	0.637686
P	-2.744841	1.682689	0.126346	H	7.271647	-1.564769	1.333674
O	-2.756858	-1.214818	-2.035794	C	7.696122	-1.425219	-0.781951
C	-2.567329	-1.224228	-0.823853	H	7.754044	-2.103981	-1.645174
C	2.473745	-2.822052	-1.609728	H	8.711156	-1.045219	-0.615661
H	1.461766	-3.150126	-1.340941	C	6.739226	-0.270996	-1.111222
C	2.301172	-1.914604	-2.849201	H	6.768793	0.472260	-0.302856
H	3.269331	-1.500680	-3.157146	H	7.062204	0.245449	-2.023079
H	1.652716	-1.069590	-2.596827	C	5.294338	-0.769030	-1.282191
C	1.692859	-2.702876	-4.022466	H	5.251973	-1.437336	-2.152283
H	0.669149	-3.000856	-3.758247	H	4.633392	0.076261	-1.497101
H	1.610376	-2.051496	-4.900798	F	0.063451	-1.306265	-0.268807
C	2.518008	-3.952394	-4.360270	Ni	1.595345	-0.153650	0.157323
H	3.505671	-3.646215	-4.734968	P	2.966019	-1.880289	-0.060931
H	2.039974	-4.517297	-5.169427	O	3.440753	0.904488	1.804588
C	2.702950	-4.847205	-3.126312	C	2.885088	1.073448	0.723025
H	1.727337	-5.250640	-2.820962	C	5.025551	5.910476	1.219358
H	3.335795	-5.709703	-3.368903	C	4.589615	5.791410	-0.079808
C	3.315983	-4.067534	-1.948830	C	3.953888	4.603525	-0.531515
H	3.409510	-4.725684	-1.077251	C	3.766710	3.506377	0.379808
H	4.333393	-3.758997	-2.220978	C	4.228311	3.668443	1.716403
C	2.709697	-3.114626	1.339091	C	4.837765	4.837717	2.120475
H	3.444976	-3.916888	1.185725	H	3.664609	5.329858	-2.548359
C	1.307671	-3.762823	1.339383	H	5.509413	6.823574	1.554447
H	1.126819	-4.292591	0.398644	H	4.722420	6.608578	-0.784638
H	0.543289	-2.981412	1.399241	C	3.503893	4.491696	-1.874485
C	1.148249	-4.752775	2.506378	C	3.111995	2.316432	-0.108071

H	4.096344	2.848731	2.408576
H	5.178784	4.935025	3.147595
C	2.676284	2.275132	-1.423232
C	2.876049	3.350171	-2.315452
H	2.167760	1.379401	-1.769289
H	2.532031	3.270267	-3.342409
C	-6.500968	-4.791175	-0.926401
C	-5.920263	-4.863694	0.318354
C	-4.818139	-4.034384	0.660782
C	-4.301460	-3.103870	-0.306719
C	-4.923714	-3.063188	-1.586660
C	-5.993503	-3.881931	-1.882630
H	-4.621389	-4.839113	2.658741
H	-7.342981	-5.430019	-1.177246
H	-6.296620	-5.559663	1.064088
C	-4.221444	-4.120656	1.947251
C	-3.197652	-2.258340	0.080004
H	-4.525459	-2.386863	-2.330315
H	-6.448682	-3.831062	-2.867950
C	-2.664449	-2.381473	1.353721
C	-3.159939	-3.315499	2.288028
H	-1.828493	-1.743351	1.623837
H	-2.704246	-3.389570	3.271177

TS2

B3LYP/BSI SCF energy: -2863.885997a.u.

M06/BSII SCF energy in solution: -2862.87356a.u.

M06/BSII free energy in solution: -2861.845382a.u.

C	-3.204821	-1.291212	-1.349647
H	-2.361379	-1.981533	-1.209028
C	-2.924217	-0.583757	-2.694034
H	-3.742759	0.111498	-2.927060
H	-2.006701	0.008811	-2.629272
C	-2.803089	-1.608769	-3.833469
H	-1.923691	-2.236704	-3.639992
H	-2.622296	-1.092368	-4.784945
C	-4.058858	-2.486858	-3.938237
H	-4.910792	-1.863081	-4.246981
H	-3.932419	-3.247486	-4.719044
C	-4.388703	-3.154878	-2.594979
H	-3.596400	-3.875290	-2.346954
H	-5.321007	-3.729035	-2.673369
C	-4.499422	-2.124132	-1.455035
H	-4.715226	-2.646578	-0.516806
H	-5.357924	-1.469161	-1.648763
C	-3.669677	-1.132954	1.559203
H	-4.713118	-1.389933	1.326848
C	-2.885750	-2.449509	1.755414
H	-2.908717	-3.055914	0.844377
H	-1.828358	-2.206580	1.931309
C	-3.423256	-3.272823	2.938008
H	-4.448983	-3.599619	2.714616
H	-2.827806	-4.186578	3.058722
C	-3.423781	-2.459615	4.239208
H	-3.852489	-3.047430	5.060162
H	-2.385710	-2.234595	4.524460
C	-4.193883	-1.144085	4.063046
H	-4.142866	-0.544955	4.980866
H	-5.257313	-1.368486	3.897271
C	-3.661894	-0.324498	2.874792
H	-2.633394	0.000993	3.088525
H	-4.260335	0.587123	2.774341
C	-4.137710	1.323010	0.010994
H	-4.085585	1.732900	1.031506
C	-5.622606	1.036448	-0.288993
H	-5.715452	0.643044	-1.308738
H	-6.016257	0.263630	0.381146
C	-6.477086	2.311580	-0.167643
H	-7.523103	2.086797	-0.411880
H	-6.468236	2.652346	0.878033
C	-5.947167	3.435523	-1.069722
H	-6.540612	4.347700	-0.930328
H	-6.071547	3.140484	-2.121656
C	-4.461683	3.714536	-0.797469
H	-4.352057	4.127455	0.216143
H	-4.086242	4.481154	-1.486622
C	-3.609454	2.439697	-0.917816
H	-2.561959	2.659798	-0.690789
H	-3.628453	2.095648	-1.959163
C	3.695517	0.073715	0.680310
H	3.128605	0.646602	1.425539
C	4.212768	1.095446	-0.355873
H	4.800506	0.573229	-1.120963
H	3.374673	1.573978	-0.872763
C	5.101651	2.160753	0.307561
H	4.494708	2.751882	1.006973
H	5.470162	2.858886	-0.453310

C	6.275627	1.519988	1.060727
H	6.944426	1.029432	0.338812
H	6.872476	2.289235	1.564996
C	5.780000	0.481514	2.075739
H	5.211294	0.991940	2.866141
H	6.628473	-0.007277	2.569725
C	4.881775	-0.583821	1.420646
H	4.529446	-1.274060	2.193194
H	5.479679	-1.177081	0.718702
C	2.210195	-2.427085	1.265432
H	3.230043	-2.776060	1.479564
C	1.614314	-1.861641	2.573296
H	2.210910	-1.017689	2.940690
H	0.610981	-1.469633	2.359987
C	1.524248	-2.939774	3.666541
H	2.539798	-3.253393	3.948449
H	1.069303	-2.513406	4.568941
C	0.728397	-4.162783	3.190021
H	0.726179	-4.939048	3.964623
H	-0.318845	-3.872294	3.033602
C	1.299023	-4.717392	1.878367
H	0.684920	-5.552101	1.519948
H	2.301455	-5.129114	2.067736
C	1.390030	-3.642410	0.781557
H	0.394862	-3.307452	0.471614
H	1.850102	-4.084130	-0.108142
C	3.003184	-1.957591	-1.561403
H	2.204710	-2.697384	-1.694549
C	4.350398	-2.695890	-1.429889
H	4.364706	-3.334858	-0.539296
H	5.162152	-1.966941	-1.307523
C	4.633535	-3.546117	-2.681936
H	5.606764	-4.041843	-2.580904
H	3.880826	-4.343913	-2.750799
C	4.592116	-2.698858	-3.961621
H	5.421249	-1.976559	-3.942584
H	4.752395	-3.333327	-4.841502
C	3.262320	-1.940648	-4.083647
H	2.442948	-2.659735	-4.219714
H	3.268167	-1.302049	-4.975071
C	2.974187	-1.085836	-2.837626
H	3.722384	-0.286528	-2.773522
H	1.995172	-0.605904	-2.934345
F	-0.072608	-1.818456	-1.327491
Ni	0.468499	-0.205990	-0.654315
P	-2.930737	-0.138266	0.126594
P	2.373811	-1.071462	-0.028214
O	-0.194466	1.752700	-1.440561
C	0.495349	1.584097	-0.424586
C	1.449699	3.274323	2.795738
C	1.644295	4.585681	2.425117
C	1.481244	4.998658	1.075163
C	1.092550	4.037986	0.080429
C	0.913602	2.670422	0.492392
C	1.100131	2.316891	1.819855
H	1.980667	7.068335	1.457397
H	1.566817	2.971655	3.831960
H	1.923969	5.330827	3.165711
C	1.686676	6.352161	0.694342
C	0.926619	4.484431	-1.259181
H	0.944104	1.280913	2.104661
C	1.135284	5.805847	-1.592206
C	1.517867	6.750546	-0.611528
H	0.618119	3.772883	-2.014349
H	1.001224	6.126501	-2.621336
H	1.676488	7.787668	-0.892338

IM2

B3LYP/BSI SCF energy: -2863.9167086a.u.

M06/BSII SCF energy in solution: -2862.91319a.u.

M06/BSII free energy in solution: -2861.882269a.u.

C	-2.775365	-1.916822	-1.336050
H	-2.235302	-2.802384	-0.978843
C	-2.186314	-1.603283	-2.728823
H	-2.648829	-0.703481	-3.149386
H	-1.117074	-1.392494	-2.637756
C	-2.414996	-2.781401	-3.690419
H	-1.850006	-3.652897	-3.330737
H	-2.013598	-2.534994	-4.680887
C	-3.902657	-3.147642	-3.794991
H	-4.447410	-2.314361	-4.262191
H	-4.038513	-4.015102	-4.452218
C	-4.506113	-3.431163	-2.411443
H	-4.046254	-4.338352	-1.994490
H	-5.580218	-3.637168	-2.497173
C	-4.275501	-2.260249	-1.438208
H	-4.689869	-2.511838	-0.455195

H	-4.832241	-1.385087	-1.797848	H	6.111488	2.221253	-1.637340
C	-2.870055	-1.478645	1.588940	H	5.877218	3.836213	-0.979140
H	-3.966533	-1.425798	1.572386	C	5.430621	2.231034	0.414972
C	-2.482655	-2.966146	1.744130	H	4.876236	2.906252	1.082312
H	-2.899153	-3.554968	0.920367	H	6.448906	2.164132	0.817629
H	-1.395812	-3.065110	1.668974	C	4.769147	0.839963	0.454925
C	-3.001381	-3.538492	3.074909	H	4.753657	0.491202	1.491954
H	-4.101453	-3.546841	3.064996	H	5.386900	0.127805	-0.107117
H	-2.684905	-4.584252	3.170656	C	2.870241	-1.478791	1.588774
C	-2.519997	-2.723747	4.282881	H	3.966722	-1.426047	1.571979
H	-2.936055	-3.132343	5.211825	C	2.374061	-0.668533	2.806455
H	-1.426840	-2.809093	4.364132	H	2.658895	0.386702	2.719216
C	-2.898667	-1.244635	4.131536	H	1.276635	-0.696542	2.814495
H	-2.506832	-0.658537	4.971994	C	2.899358	-1.244696	4.131367
H	-3.993130	-1.143666	4.165016	H	3.993837	-1.143835	4.164649
C	-2.373541	-0.668486	2.806549	H	2.507732	-0.658520	4.971868
H	-1.276117	-0.696644	2.814381	C	2.520564	-2.723760	4.282842
H	-2.658247	0.386790	2.719394	H	2.936744	-3.132359	5.211730
C	-3.343369	0.885386	-0.140321	H	1.427412	-2.808998	4.364288
H	-2.765943	1.601114	0.462245	C	3.001655	-3.538594	3.074814
C	-4.768989	0.840263	0.455622	H	2.685108	-4.584323	3.170655
H	-5.386900	0.128134	-0.106287	H	4.101725	-3.547037	3.064698
H	-4.753274	0.491493	1.492643	C	2.482733	-2.966251	1.744109
C	-5.430413	2.231358	0.415864	H	1.395867	-3.065124	1.669165
H	-6.448599	2.164497	0.818779	H	2.899020	-3.555149	0.920294
H	-4.875825	2.906533	1.083079	C	2.775014	-1.917102	-1.336181
C	-5.450849	2.826348	-0.998386	H	2.235053	-2.802661	-0.978825
H	-5.877297	3.836594	-0.978080	C	4.275114	-2.260545	-1.438684
H	-6.111821	2.221666	-1.636267	H	4.689679	-2.512164	-0.455758
C	-4.043042	2.847190	-1.607268	H	4.831800	-1.385392	-1.798422
H	-3.408485	3.550077	-1.050187	C	4.505495	-3.431447	-2.411990
H	-4.079172	3.214214	-2.640148	H	5.579579	-3.637456	-2.497966
C	-3.395959	1.452738	-1.579138	H	4.045725	-4.338639	-1.994944
H	-2.394983	1.500215	-2.013732	C	3.901717	-3.147906	-3.795395
H	-3.991317	0.779291	-2.208918	H	4.446344	-2.314602	-4.262699
C	3.343383	0.885127	-0.140668	H	4.037443	-4.015349	-4.452672
H	2.766131	1.600883	0.462033	C	2.414073	-2.781708	-3.690463
C	3.395610	1.452469	-1.579497	H	1.849194	-3.653227	-3.330660
H	3.990751	0.778992	-2.209450	H	2.012428	-2.535302	-4.680832
H	2.394522	1.500010	-2.013831	C	2.185575	-1.603611	-2.728799
C	4.042749	2.846888	-1.607808	H	2.647888	-0.703766	-3.149491
H	3.408373	3.549805	-1.050561	H	1.116342	-1.392932	-2.637411
H	4.078620	3.213907	-2.640700	F	-0.000017	-2.355370	0.072452
C	5.450715	2.825987	-0.999301	Ni	-0.000005	-0.486883	-0.084790

P	-2.278029	-0.678655	-0.015488
P	2.277968	-0.678848	-0.015577
O	-0.000378	1.523995	-1.785715
C	-0.000076	1.327899	-0.565429
C	0.000247	6.664953	-0.573172
C	0.000454	6.256679	0.740410
C	0.000431	4.876099	1.076797
C	0.000192	3.887464	0.030650
C	-0.000022	4.349594	-1.316513
C	0.000004	5.698813	-1.604659
H	0.000803	5.232756	3.210331
H	0.000266	7.723078	-0.819070
H	0.000637	6.986688	1.546158
C	0.000632	4.467577	2.437745
C	0.000180	2.492657	0.406352
H	-0.000213	3.614583	-2.109125
H	-0.000161	6.022887	-2.641812
C	0.000374	2.160736	1.751740
C	0.000600	3.134091	2.773418
H	0.000346	1.106174	2.009177
H	0.000745	2.826577	3.815278

TS3

B3LYP/BSI SCF energy: -1816.671402a.u.

M06/BSII SCF energy in solution: -1816.06610a.u.

M06/BSII free energy in solution: -1815.499322a.u.

C	-1.668942	-1.025720	-1.501311
H	-1.342762	-0.390837	-2.334881
C	-0.750402	-2.267559	-1.536431
H	-0.980521	-2.934851	-0.696920
H	0.293288	-1.954862	-1.427962
C	-0.928348	-3.039576	-2.855247
H	-0.571499	-2.413707	-3.684667
H	-0.296295	-3.935611	-2.846642
C	-2.395125	-3.422946	-3.100321
H	-2.716166	-4.142247	-2.332916
H	-2.499392	-3.931782	-4.065938
C	-3.308718	-2.190189	-3.049302
H	-3.065404	-1.522685	-3.887670
H	-4.357522	-2.484090	-3.177619
C	-3.142954	-1.418258	-1.727433
H	-3.788271	-0.532044	-1.729299
H	-3.485687	-2.055530	-0.901757
C	-2.224113	1.707740	-0.429098
H	-3.298568	1.497169	-0.334896
C	-1.959814	2.230611	-1.859806
H	-2.320767	1.506210	-2.598091
H	-0.878956	2.317563	-2.016197
C	-2.664910	3.576179	-2.102680
H	-3.754762	3.427750	-2.079307
H	-2.422354	3.934185	-3.110189
C	-2.281198	4.629404	-1.055340
H	-2.825316	5.564194	-1.235955
H	-1.211738	4.862952	-1.151400
C	-2.560177	4.114337	0.362580
H	-2.242449	4.850623	1.110605
H	-3.643564	3.981497	0.496224
C	-1.845895	2.778347	0.621176
H	-0.759915	2.938228	0.580480
H	-2.073846	2.427831	1.634948
C	-2.072194	-0.514369	1.550890
H	-1.615109	0.167261	2.283185
C	-3.603433	-0.401958	1.712505
H	-3.945899	0.615308	1.497953
H	-4.104965	-1.061127	0.993564
C	-4.033868	-0.786481	3.140085
H	-5.125850	-0.728463	3.222938
H	-3.628241	-0.047955	3.846000
C	-3.539588	-2.185431	3.533336
H	-4.042774	-2.935987	2.906862
H	-3.818275	-2.408085	4.570057
C	-2.020644	-2.309443	3.349102
H	-1.507182	-1.646803	4.058901
H	-1.689487	-3.329137	3.578521
C	-1.593926	-1.936324	1.919831
H	-2.028608	-2.661728	1.220050
H	-0.506055	-2.009373	1.824955
F	0.903849	0.959084	-1.702100
Ni	0.870111	0.467486	0.046220
P	-1.312415	0.108082	-0.055078
O	1.504564	-0.159322	2.775668
C	1.406055	0.139383	1.639043
C	5.778764	-2.097308	-0.601447
C	6.107324	-0.770170	-0.443488
C	5.135806	0.176490	-0.020540
C	3.795020	-0.264243	0.238804
C	3.493700	-1.642150	0.068816

C	4.458987	-2.536021	-0.339696
H	6.475527	1.874617	-0.050067
H	6.530161	-2.811676	-0.925030
H	7.119508	-0.425525	-0.640012
C	5.457782	1.549840	0.151804
C	2.823937	0.700997	0.658399
H	2.482910	-1.986437	0.265997
H	4.207488	-3.585531	-0.462877
C	3.188780	2.024576	0.833082
C	4.509456	2.455652	0.570765
H	2.452989	2.748319	1.174263
H	4.770147	3.501875	0.701869

IM4

B3LYP/BSI SCF energy: -1816.679435a.u.

M06/BSII SCF energy in solution: -1816.07015a.u.

M06/BSII free energy in solution: -1815.503573a.u.

C	-1.593586	-1.093877	-1.464307
H	-1.047413	-0.564420	-2.254572
C	-0.854059	-2.437101	-1.276958
H	-1.317947	-3.019557	-0.471427
H	0.184924	-2.249482	-0.989466
C	-0.892623	-3.260307	-2.575727
H	-0.319878	-2.730211	-3.348527
H	-0.389977	-4.221995	-2.418542
C	-2.330555	-3.483471	-3.066067
H	-2.866850	-4.114699	-2.342632
H	-2.328738	-4.031545	-4.015610
C	-3.078814	-2.151952	-3.224523
H	-2.615122	-1.568858	-4.032218
H	-4.118785	-2.329776	-3.523942
C	-3.046053	-1.324279	-1.926303
H	-3.565849	-0.371870	-2.081549
H	-3.602335	-1.864524	-1.149089
C	-2.054821	1.734724	-0.606249
H	-3.143847	1.600997	-0.665904
C	-1.551913	2.168318	-2.002243
H	-1.845322	1.428522	-2.754398
H	-0.457075	2.188066	-2.007982
C	-2.120692	3.540899	-2.401473
H	-3.210107	3.462422	-2.531581
H	-1.711671	3.832037	-3.375965
C	-1.817688	4.617429	-1.351124
H	-2.262232	5.575423	-1.645643
H	-0.731719	4.777075	-1.298001
C	-2.334178	4.193263	0.029627
H	-2.077820	4.944778	0.785833
H	-3.431909	4.135197	0.006364
C	-1.762423	2.828568	0.447237
H	-0.674395	2.918327	0.571137
H	-2.167602	2.544289	1.425731
C	-2.334363	-0.361297	1.480426
H	-1.961129	0.368594	2.215217
C	-3.866985	-0.189089	1.411200
H	-4.134141	0.810604	1.054076
H	-4.288520	-0.902796	0.693215
C	-4.507742	-0.421099	2.791645
H	-5.596914	-0.321242	2.713564
H	-4.171396	0.368047	3.479026
C	-4.136337	-1.792425	3.373745
H	-4.583784	-2.581821	2.752911
H	-4.562581	-1.907014	4.377215
C	-2.613731	-1.986584	3.415318
H	-2.172882	-1.281437	4.133675
H	-2.366662	-2.992430	3.774618
C	-1.980147	-1.760349	2.032549
H	-2.353113	-2.528402	1.343570
H	-0.893601	-1.890747	2.090069
F	1.026373	0.412107	-1.558435
Ni	0.960996	0.359921	0.237801
P	-1.325343	0.095348	-0.045173
O	1.116285	0.315718	3.114654
C	1.055757	0.329031	1.965358
C	5.798172	-2.320674	-0.149312
C	6.182420	-1.002219	-0.055141
C	5.223114	0.032228	0.117691
C	3.829510	-0.313585	0.192882
C	3.473238	-1.686115	0.084498
C	4.427029	-2.665954	-0.078791
H	6.659420	1.652781	0.160531
H	6.544556	-3.099152	-0.280853
H	7.234082	-0.730927	-0.111782
C	5.604284	1.397251	0.219849
C	2.863973	0.724358	0.366070
H	2.419579	-1.949327	0.122498
H	4.129171	-3.707639	-0.160557
C	3.280279	2.034740	0.483095

C	4.655070	2.376042	0.397546
H	2.555066	2.832500	0.628187
H	4.952315	3.418651	0.477554

CO

B3LYP/BSI SCF energy: -113.306914a.u.

M06/BSII SCF energy in solution: -113.281391a.u.

M06/BSII free energy in solution: -113.295493a.u.

C	0.000000	0.000000	-0.650137
O	0.000000	0.000000	0.487603

IM5

B3LYP/BSI SCF energy: -1703.336156a.u.

M06/BSII SCF energy in solution: -1702.74832a.u.

M06/BSII free energy in solution: -1702.185051a.u.

C	1.705393	1.642148	-0.521339
H	2.279930	1.333994	-1.403694
C	0.670049	2.667271	-1.034283
H	0.005610	2.983307	-0.221535
H	0.045691	2.196974	-1.800064
C	1.374011	3.901341	-1.624235
H	1.928400	3.599409	-2.523480
H	0.623864	4.631242	-1.950476
C	2.343124	4.542449	-0.620778
H	1.773323	4.943871	0.229609
H	2.858697	5.394104	-1.079935
C	3.364979	3.519230	-0.105776
H	4.011596	3.201347	-0.935537
H	4.021423	3.975796	0.644706
C	2.673063	2.283054	0.496296
H	3.428800	1.561023	0.826558
H	2.117634	2.590489	1.391559
C	2.417966	-1.174328	0.133896
H	2.993053	-0.843516	1.009793
C	3.351845	-1.133426	-1.096321
H	3.777323	-0.131536	-1.215839
H	2.766678	-1.330445	-2.001154
C	4.505264	-2.143267	-0.959914
H	5.160899	-1.839415	-0.130568
H	5.119136	-2.113526	-1.867724
C	4.000509	-3.568375	-0.701672
H	4.845394	-4.255342	-0.573505
H	3.438355	-3.919743	-1.577992
C	3.089864	-3.606822	0.531614
H	2.694247	-4.617280	0.688772
H	3.677075	-3.358190	1.427448
C	1.922473	-2.615463	0.393668
H	1.290963	-2.923224	-0.450209
H	1.292659	-2.656589	1.290166
C	0.208694	0.070818	1.717677
H	-0.384433	-0.852353	1.737696
C	1.194246	0.024940	2.907404
H	1.870830	-0.831406	2.825400
H	1.822255	0.924221	2.913192
C	0.430849	-0.067123	4.242146
H	1.146966	-0.071359	5.072633
H	-0.100531	-1.028309	4.283358
C	-0.578678	1.075990	4.409237
H	-0.036542	2.029314	4.489298
H	-1.135390	0.955109	5.345953
C	-1.542999	1.140467	3.217040
H	-2.173312	0.240956	3.203183
H	-2.221998	1.995135	3.318449
C	-0.785602	1.241533	1.882466
H	-0.237598	2.192262	1.858681
H	-1.498010	1.256132	1.052890
F	0.869266	-0.417835	-2.901706
Ni	-0.335508	-0.660720	-1.600351
P	0.956678	0.001833	-0.006473
C	-5.471260	1.177985	-1.006283
C	-5.511882	-0.061337	-0.408203
C	-4.337698	-0.851336	-0.273225
C	-3.086654	-0.344572	-0.769918
C	-3.090986	0.941548	-1.382804
C	-4.245417	1.685050	-1.499450
H	-5.316396	-2.512419	0.714874
H	-6.378050	1.768607	-1.102643
H	-6.451135	-0.457766	-0.029205
C	-4.368933	-2.132311	0.340330
C	-1.883567	-1.129120	-0.649289
H	-2.152822	1.333425	-1.767511
H	-4.217988	2.662078	-1.973977
C	-1.984810	-2.368571	-0.027398
C	-3.217337	-2.875729	0.457129
H	-1.097732	-2.987401	0.092415
H	-3.247229	-3.858060	0.92261

IM6

B3LYP/BSI SCF energy: -2750.576843a.u.

M06/BSII SCF energy in solution: -2749.59816a.u.

M06/BSII free energy in solution: -2748.572252a.u.

C	2.745827	1.743392	-1.330055
H	2.190737	2.617696	-0.967401
C	2.173876	1.436369	-2.731225
H	2.643652	0.539285	-3.150595
H	1.102731	1.225118	-2.648887
C	2.404416	2.619028	-3.687165
H	1.827654	3.484385	-3.331540
H	2.017567	2.372798	-4.683566
C	3.889733	2.999548	-3.771067
H	4.449450	2.172293	-4.231142
H	4.025018	3.868645	-4.426085
C	4.469608	3.288325	-2.378796
H	3.991804	4.188490	-1.966886
H	5.541836	3.508901	-2.449062
C	4.241565	2.111681	-1.412364
H	4.636528	2.366377	-0.422374
H	4.816888	1.246166	-1.765036
C	2.807048	1.281364	1.588428
H	3.904069	1.245950	1.586213
C	2.401942	2.762410	1.755797
H	2.809458	3.364869	0.937174
H	1.314220	2.847043	1.686685
C	2.918190	3.327119	3.091058
H	4.018212	3.343366	3.080089
H	2.594413	4.369782	3.196324
C	2.443250	2.498309	4.292112
H	2.858602	2.900576	5.224157
H	1.349889	2.577624	4.375855
C	2.829053	1.022425	4.127028
H	2.438323	0.426637	4.961049
H	3.923961	0.926287	4.161936
C	2.309930	0.455481	2.795496
H	1.212417	0.477021	2.801567
H	2.600208	-0.597164	2.699465
C	3.375723	-1.053160	-0.146272
H	2.792723	-1.797672	0.412920
C	4.769366	-0.967151	0.516335
H	5.383778	-0.218341	-0.000175
H	4.693324	-0.646092	1.558901
C	5.490069	-2.327944	0.482091
H	6.484501	-2.226533	0.934168
H	4.933948	-3.039301	1.108934
C	5.601136	-2.890461	-0.940105
H	6.070853	-3.881373	-0.921353
H	6.261231	-2.243440	-1.536148
C	4.222264	-2.960878	-1.608342
H	3.595548	-3.695859	-1.085510
H	4.315220	-3.310764	-2.643690
C	3.514462	-1.595104	-1.588309
H	2.531659	-1.684458	-2.056375
H	4.101153	-0.888305	-2.189420
C	-3.351733	-1.169621	-0.312429
H	-2.703472	-1.964828	0.080670
C	-3.531388	-1.448809	-1.821616
H	-4.186549	-0.684665	-2.259051
H	-2.570047	-1.386770	-2.335679
C	-4.156560	-2.832053	-2.064689
H	-3.459934	-3.605564	-1.714715
H	-4.285731	-2.993292	-3.142035
C	-5.500672	-2.976260	-1.338943
H	-6.228029	-2.281603	-1.783720
H	-5.907349	-3.985060	-1.479180
C	-5.354714	-2.665185	0.156343
H	-4.726294	-3.435216	0.625510
H	-6.330613	-2.713029	0.655044
C	-4.716665	-1.285296	0.404023
H	-4.609678	-1.138360	1.482455
H	-5.396900	-0.501652	0.044913
C	-2.842676	0.910178	1.753487
H	-3.939082	0.848602	1.764231
C	-2.299901	-0.069676	2.816007
H	-2.570846	-1.104099	2.576868
H	-1.203993	-0.027131	2.796540
C	-2.788041	0.290266	4.228278
H	-3.880653	0.176343	4.278106
H	-2.368622	-0.415172	4.955928
C	-2.408991	1.731049	4.594522
H	-2.798285	1.990062	5.586602
H	-1.314073	1.809640	4.656843
C	-2.927383	2.718894	3.541023
H	-2.607199	3.739236	3.784648
H	-4.027095	2.724421	3.567384

C	-2.455123	2.359378	2.120892
H	-1.371422	2.477957	2.026286
H	-2.901157	3.065753	1.413742
C	-2.874788	1.803013	-1.059363
H	-2.333880	2.628784	-0.582247
C	-4.382960	2.123770	-1.041607
H	-4.753154	2.204127	-0.013315
H	-4.943208	1.305731	-1.512392
C	-4.678285	3.431422	-1.798437
H	-5.758513	3.622207	-1.804326
H	-4.215649	4.269635	-1.258491
C	-4.133080	3.392762	-3.233267
H	-4.681261	2.631713	-3.807452
H	-4.315015	4.351253	-3.734264
C	-2.634359	3.056615	-3.249893
H	-2.073781	3.872880	-2.773243
H	-2.271351	2.988871	-4.282745
C	-2.336894	1.743615	-2.505507
H	-2.792800	0.911898	-3.054638
H	-1.257537	1.562926	-2.482304
F	-0.061469	2.050846	0.158007
Ni	-0.019719	0.213548	-0.129455
P	2.257805	0.476335	-0.031755
P	-2.305000	0.374419	0.021838
C	-0.059431	-1.913639	-1.999651
C	0.012456	-1.628169	-0.638997
C	0.106179	-2.755452	0.250356
C	0.106618	-4.103218	-0.259348
C	0.019538	-4.315074	-1.660615
C	-0.057397	-3.236280	-2.511840
H	0.218093	-1.574890	2.048295
H	-0.118382	-1.096596	-2.717605
C	0.209970	-2.587680	1.660941
C	0.199991	-5.191690	0.651880
H	0.020245	-5.332661	-2.043699
H	-0.118096	-3.393224	-3.586650
C	0.295330	-4.981854	2.009019
C	0.303037	-3.661506	2.520067
H	0.197076	-6.203515	0.252208
H	0.366879	-5.826172	2.689337
H	0.381850	-3.498343	3.591704

TS4

B3LYP/BSI SCF energy: -1703.326522a.u.

M06/BSII SCF energy in solution: -1702.74288a.u.

M06/BSII free energy in solution: -1702.180642a.u.

C	1.656149	1.682751	-0.534946
H	2.222288	1.409540	-1.436371
C	0.573427	2.682208	-1.002111
H	-0.063144	2.974257	-0.158475
H	-0.078081	2.201198	-1.738978
C	1.213965	3.939087	-1.615030
H	1.736114	3.659978	-2.540871
H	0.428612	4.647447	-1.903023
C	2.207723	4.603502	-0.651694
H	1.663517	4.988738	0.222497
H	2.681518	5.468841	-1.129684
C	3.276007	3.606433	-0.181067
H	3.898003	3.307464	-1.036522
H	3.949619	4.079310	0.543573
C	2.642344	2.351683	0.445824
H	3.428715	1.651380	0.749837
H	2.108866	2.644148	1.358559
C	2.459597	-1.119641	0.021463
H	3.160318	-0.701162	0.757519
C	3.177885	-1.176973	-1.347002
H	3.507224	-0.180576	-1.658579
H	2.472629	-1.527377	-2.112961
C	4.399521	-2.111899	-1.303384
H	5.153015	-1.687533	-0.624319
H	4.861879	-2.150760	-2.296418
C	4.028175	-3.522665	-0.829094
H	4.925047	-4.149195	-0.759505
H	3.371997	-3.994537	-1.573482
C	3.304448	-3.473669	0.522717
H	2.991684	-4.479278	0.827422
H	3.997791	-3.114263	1.296677
C	2.077015	-2.548520	0.470098
H	1.351386	-2.959106	-0.244190
H	1.583596	-2.535443	1.447952
C	0.324110	0.062146	1.753321
H	-0.210476	-0.894331	1.822069
C	1.381364	0.091433	2.879855
H	2.116309	-0.709822	2.754713
H	1.938570	1.035164	2.850688
C	0.706970	-0.052515	4.256874
H	1.468381	-0.005514	5.044646

H	0.246045	-1.047755	4.327358
C	-0.366417	1.020470	4.483812
H	0.115503	2.007428	4.537339
H	-0.860653	0.863348	5.449732
C	-1.400041	1.022932	3.348485
H	-1.972273	0.085477	3.367233
H	-2.124699	1.832805	3.492555
C	-0.730251	1.170122	1.971979
H	-0.245756	2.153626	1.916537
H	-1.486928	1.136475	1.183076
F	-0.376945	-0.657652	-3.421621
Ni	-0.351406	-0.599769	-1.648415
P	0.954881	0.013669	-0.013266
C	-5.471700	1.013427	-0.874887
C	-5.401885	-0.138674	-0.125262
C	-4.190907	-0.875494	-0.019244
C	-3.017759	-0.397052	-0.702676
C	-3.135973	0.791613	-1.478361
C	-4.326491	1.479667	-1.563281
H	-5.007399	-2.432142	1.246639
H	-6.406600	1.562131	-0.947557
H	-6.280917	-0.509066	0.397120
C	-4.115680	-2.075471	0.737262
C	-1.787864	-1.129499	-0.586120
H	-2.267147	1.138544	-2.029976
H	-4.390902	2.378672	-2.169753
C	-1.770968	-2.296569	0.157889
C	-2.935124	-2.775609	0.812964
H	-0.857467	-2.877549	0.246894
H	-2.883357	-3.702542	1.378928

IM7

B3LYP/BSI SCF energy: -1703.32833a.u.

M06/BSII SCF energy in solution: -1702.74450a.u.

M06/BSII free energy in solution: -1702.183309a.u.

C	1.696265	1.681223	-0.601768
H	2.269663	1.387074	-1.492959
C	0.615065	2.667234	-1.100824
H	-0.015897	2.990036	-0.264841
H	-0.047134	2.166431	-1.815467
C	1.257822	3.901290	-1.756452
H	1.782884	3.590556	-2.670797
H	0.474410	4.600633	-2.070637
C	2.249884	4.597036	-0.813007
H	1.702355	5.013395	0.044508
H	2.727046	5.444368	-1.319074
C	3.314393	3.615395	-0.302667
H	3.941165	3.287792	-1.144181
H	3.984290	4.112560	0.409005
C	2.676578	2.382184	0.361586
H	3.460593	1.692380	0.693930
H	2.137033	2.703717	1.260983
C	2.510359	-1.082784	0.089822
H	3.179877	-0.639794	0.839872
C	3.280667	-1.170931	-1.247634
H	3.619456	-0.181145	-1.570039
H	2.605596	-1.545020	-2.030985
C	4.501000	-2.102661	-1.142364
H	5.229237	-1.661499	-0.446781
H	4.998346	-2.162310	-2.117401
C	4.113778	-3.502594	-0.649976
H	5.007986	-4.126477	-0.536638
H	3.483394	-3.991871	-1.405423
C	3.345803	-3.423759	0.675506
H	3.024349	-4.422766	0.992483
H	4.013654	-3.046096	1.463059
C	2.119500	-2.502192	0.562656
H	1.413946	-2.932291	-0.160598
H	1.597283	-2.464248	1.524592
C	0.312990	0.134823	1.704364
H	-0.225104	-0.818822	1.787018
C	1.333065	0.202940	2.862295
H	2.074042	-0.599246	2.786403
H	1.888311	1.147671	2.819641
C	0.614424	0.100833	4.221082
H	1.349644	0.175806	5.031367
H	0.155087	-0.893862	4.307916
C	-0.470128	1.175384	4.379952
H	0.006321	2.165606	4.421522
H	-0.995864	1.043614	5.332973
C	-1.464174	1.141509	3.210816
H	-2.036210	0.204261	3.236349
H	-2.193889	1.954125	3.305601
C	-0.745972	1.249988	1.855439
H	-0.255763	2.230356	1.792697
H	-1.475603	1.199546	1.042432
F	-0.891364	-1.177788	-3.261025

Ni	-0.335546	-0.730418	-1.661671
P	0.993108	0.025214	-0.042512
C	-5.411634	1.088661	-0.819446
C	-5.345576	-0.025362	-0.014053
C	-4.162537	-0.810284	0.060434
C	-3.014950	-0.419757	-0.715993
C	-3.128929	0.729963	-1.547702
C	-4.291924	1.466134	-1.598982
H	-4.964775	-2.266799	1.449104
H	-6.325135	1.675020	-0.866707
H	-6.206118	-0.327869	0.578208
C	-4.091230	-1.974359	0.871790
C	-1.815008	-1.195427	-0.622421
H	-2.279903	1.000497	-2.167775
H	-4.356437	2.334131	-2.249199
C	-1.797817	-2.331868	0.163747
C	-2.939548	-2.724124	0.911394
H	-0.906980	-2.951245	0.220384
H	-2.893222	-3.625603	1.517569

TS5

B3LYP/BSI SCF energy: -2226.12648a.u.

M06/BSII SCF energy in solution: -2225.37347a.u.

M06/BSII free energy in solution: -2224.667129a.u.

C	-2.301813	1.519614	-0.473623
H	-1.642351	1.720855	-1.329025
C	-1.975487	2.584065	0.598079
H	-2.633260	2.440085	1.465196
H	-0.946509	2.476986	0.949254
C	-2.190613	4.003527	0.047719
H	-1.472548	4.184008	-0.763295
H	-1.967277	4.738526	0.829966
C	-3.622086	4.193075	-0.472084
H	-4.324012	4.137309	0.372578
H	-3.742239	5.190917	-0.910598
C	-3.986387	3.114774	-1.501800
H	-3.371240	3.251989	-2.402162
H	-5.030888	3.224100	-1.818260
C	-3.759132	1.691586	-0.956912
H	-4.007019	0.970457	-1.741388
H	-4.454659	1.506742	-0.128877
C	-2.711708	-1.355107	-1.108452
H	-3.763356	-1.049103	-1.026480
C	-2.277020	-1.176745	-2.580268
H	-2.326187	-0.126553	-2.886496
H	-1.223275	-1.472359	-2.672806
C	-3.123020	-2.040011	-3.530672
H	-4.164091	-1.687041	-3.508708
H	-2.771485	-1.906389	-4.560778
C	-3.077392	-3.521965	-3.134649
H	-3.726897	-4.112514	-3.791565
H	-2.056603	-3.903181	-3.277633
C	-3.484570	-3.712467	-1.667504
H	-3.393154	-4.766486	-1.380326
H	-4.544877	-3.446654	-1.547839
C	-2.632440	-2.849148	-0.720008
H	-1.591746	-3.188879	-0.757092
H	-2.974771	-3.002567	0.308290
C	-2.379751	-0.644652	1.746351
H	-2.192414	-1.726606	1.777684
C	-3.884487	-0.421815	2.001049
H	-4.486862	-0.883244	1.210265
H	-4.105487	0.652797	1.978102
C	-4.304999	-0.988383	3.369443
H	-5.369363	-0.787525	3.541468
H	-4.192130	-2.081593	3.355983
C	-3.458046	-0.404718	4.509223
H	-3.666113	0.671132	4.599268
H	-3.744830	-0.858296	5.465268
C	-1.958287	-0.609934	4.250321
H	-1.727561	-1.684131	4.276542
H	-1.366862	-0.144564	5.047765
C	-1.531811	-0.037621	2.887563
H	-1.642963	1.052384	2.904915
H	-0.469826	-0.242331	2.712375
F	0.226249	-2.463802	0.816379
Ni	0.527704	-0.638534	-0.016828
P	-1.735396	-0.206913	0.030796
C	3.380292	-1.170549	-0.905437
C	4.749376	-1.026618	-0.686937
C	5.223197	-0.894321	0.626482
C	4.317723	-0.927595	1.699530
C	2.963276	-1.084207	1.449772
C	2.432566	-1.218921	0.138795
H	3.041607	-1.256374	-1.934882
H	5.429915	-1.008279	-1.530533
H	4.707502	-0.835529	2.708688

H	2.292279	-1.140907	2.304872
B	1.351169	-3.015369	0.084673
O	1.118751	-3.319666	-1.257234
H	0.759033	-2.568635	-1.742441
O	2.034033	-3.929969	0.854097
H	2.641031	-4.437965	0.304635
O	6.533400	-0.740928	0.963517
C	7.496458	-0.670115	-0.077065
H	8.460520	-0.530118	0.414486
H	7.524088	-1.594799	-0.667611
H	7.305432	0.177378	-0.747210
C	0.914912	0.897721	-2.365356
C	1.018935	0.902558	-0.981199
C	1.514742	2.095654	-0.352703
C	1.862459	3.241864	-1.150967
C	1.725709	3.175010	-2.563357
C	1.265699	2.022500	-3.155518
H	1.426433	1.336274	1.666001
H	0.555287	0.011272	-2.883764
C	1.677621	2.199449	1.057993
C	2.339315	4.417166	-0.507304
H	1.992915	4.042682	-3.161543
H	1.166797	1.965304	-4.237214
C	2.477155	4.476376	0.860833
C	2.143108	3.352081	1.653028
H	2.597644	5.275980	-1.122891
H	2.844936	5.382325	1.334804
H	2.260166	3.398566	2.732280

IM8

B3LYP/BSI SCF energy: -2226.160003a.u.

M06/BSII SCF energy in solution: -2225.39119a.u.

M06/BSII free energy in solution: -2224.681488a.u.

C	-2.145489	-1.716827	1.459715
H	-2.691999	-0.835032	1.820855
C	-1.121150	-2.074717	2.561651
H	-0.547718	-2.961152	2.270627
H	-0.395709	-1.264046	2.688924
C	-1.836338	-2.368397	3.891261
H	-2.338289	-1.456165	4.243134
H	-1.098469	-2.634299	4.657200
C	-2.870229	-3.492661	3.732958
H	-2.347952	-4.431241	3.498083
H	-3.400309	-3.659666	4.677829
C	-3.871929	-3.178378	2.612028
H	-4.484653	-2.313984	2.903998
H	-4.564103	-4.017183	2.471626
C	-3.164326	-2.862574	1.281340
H	-3.909841	-2.608932	0.520289
H	-2.646932	-3.763499	0.927298
C	-2.828925	-0.517151	-1.174136
H	-3.351258	-1.448638	-1.431959
C	-3.845505	0.395274	-0.455211
H	-4.234646	-0.093010	0.444490
H	-3.347378	1.311896	-0.127176
C	-5.019068	0.749578	-1.385922
H	-5.588545	-0.162496	-1.617644
H	-5.707430	1.421615	-0.860257
C	-4.537727	1.392518	-2.693815
H	-5.390325	1.601398	-3.350894
H	-4.065869	2.358668	-2.469765
C	-3.521836	0.490300	-3.407531
H	-3.144402	0.978977	-4.313359
H	-4.020192	-0.433952	-3.735048
C	-2.341514	0.137826	-2.487016
H	-1.789763	1.052817	-2.246177
H	-1.641638	-0.518232	-3.016712
C	-0.581031	-2.451692	-1.113827
H	0.065694	-1.888200	-1.798234
C	-1.509392	-3.342881	-1.971060
H	-2.160381	-2.737789	-2.607876
H	-2.165666	-3.938835	-1.324037
C	-0.678646	-4.285001	-2.863871
H	-1.351924	-4.923658	-3.447998
H	-0.115537	-3.679657	-3.587756
C	0.301253	-5.141993	-2.051805
H	-0.265955	-5.840518	-1.419884
H	0.913760	-5.755702	-2.722489
C	1.194286	-4.268992	-1.159699
H	1.855999	-3.654829	-1.785421
H	1.842401	-4.897054	-0.536963
C	0.348225	-3.347983	-0.265741
H	-0.257599	-3.972449	0.403070
H	0.997534	-2.746721	0.378630
Ni	0.181820	0.493849	0.227152
P	-1.369455	-1.049534	-0.114338
C	4.423110	0.838079	1.094854

C	5.736606	0.642658	1.506679
C	6.724079	0.310395	0.567685
C	6.378401	0.183735	-0.782524
C	5.050108	0.386862	-1.170227
C	4.037571	0.713067	-0.255567
H	3.676154	1.113082	1.835393
H	6.028419	0.747540	2.547368
H	7.123327	-0.066796	-1.529458
H	4.795562	0.290617	-2.223726
B	2.527123	0.872613	-0.753781
O	2.281561	1.424641	-2.032708
H	2.834413	2.200277	-2.172289
O	1.711708	-0.406196	-0.671210
H	2.182976	-1.030360	-0.106098
F	1.734252	1.684556	0.311210
O	7.985971	0.134922	1.068298
C	9.023822	-0.194082	0.162395
H	9.932040	-0.284264	0.761208
H	8.833648	-1.148206	-0.347218
H	9.168627	0.588583	-0.594177
C	-1.422251	1.592763	2.363984
C	-0.979234	1.736173	1.059854
C	-1.267223	2.970727	0.377902
C	-2.043122	3.987317	1.038354
C	-2.482288	3.771942	2.372402
C	-2.163937	2.606137	3.025340
H	-0.169142	2.518040	-1.440555
H	-1.196096	0.689748	2.923528
C	-0.806852	3.243544	-0.943633
C	-2.347442	5.191689	0.346710
H	-3.062954	4.547138	2.866512
H	-2.482578	2.449480	4.053217
C	-1.901937	5.407286	-0.937321
C	-1.116365	4.424137	-1.584649
H	-2.938659	5.947694	0.858541
H	-2.140990	6.334451	-1.450981
H	-0.744833	4.606712	-2.589235

TS6

B3LYP/BSI SCF energy: -2226.138388a.u.

M06/BSII SCF energy in solution: -2225.38394a.u.

M06/BSII free energy in solution: -2224.675872a.u.

C	-1.518986	-0.849560	1.924411
H	-0.995743	-0.014647	2.409990
C	-0.637843	-2.102015	2.138910
H	-1.130320	-2.982642	1.713731
H	0.317856	-1.999129	1.615301
C	-0.412057	-2.348797	3.639656
H	0.152038	-1.507617	4.065890
H	0.206338	-3.243346	3.779442
C	-1.746681	-2.502767	4.384665
H	-2.246010	-3.419473	4.039573
H	-1.572080	-2.629664	5.459484
C	-2.671228	-1.301522	4.137422
H	-2.236121	-0.406069	4.602661
H	-3.642524	-1.462172	4.620340
C	-2.877938	-1.032022	2.634868
H	-3.513861	-0.150042	2.505759
H	-3.417492	-1.877587	2.188501
C	-2.608798	1.322331	0.209033
H	-3.617020	0.992841	0.494053
C	-2.147967	2.349250	1.265084
H	-2.137578	1.899219	2.263411
H	-1.123669	2.664563	1.048943
C	-3.072755	3.579599	1.272098
H	-4.078420	3.279713	1.601737
H	-2.706306	4.303419	2.009379
C	-3.166184	4.229880	-0.115029
H	-3.855418	5.082322	-0.089950
H	-2.180709	4.625986	-0.394465
C	-3.616453	3.210396	-1.170351
H	-3.630582	3.669080	-2.165958
H	-4.648302	2.894639	-0.957196
C	-2.697089	1.977840	-1.188032
H	-1.693165	2.282155	-1.501413
H	-3.051888	1.260858	-1.936787
C	-2.629722	-1.418726	-0.914260
H	-2.320460	-1.125196	-1.925599
C	-4.166823	-1.275597	-0.829366
H	-4.477892	-0.238797	-0.979194
H	-4.519332	-1.570705	0.167429
C	-4.853771	-2.151240	-1.895370
H	-5.941923	-2.051540	-1.803823
H	-4.587777	-1.769317	-2.890735
C	-4.441234	-3.625415	-1.793921
H	-4.823825	-4.046124	-0.852877
H	-4.900101	-4.204610	-2.603520

C	-2.914306	-3.775790	-1.827132
H	-2.535212	-3.477562	-2.814296
H	-2.630463	-4.825368	-1.684952
C	-2.252108	-2.907865	-0.743832
H	-2.594347	-3.257568	0.238027
H	-1.165735	-3.048584	-0.753813
Ni	0.410673	-0.056050	-0.802972
P	-1.578834	-0.249648	0.145431
C	3.664593	-0.287580	-1.437311
C	4.684336	-0.575100	-0.539797
C	4.690346	-1.798432	0.146446
C	3.665283	-2.725365	-0.083716
C	2.655419	-2.410353	-0.997243
C	2.611304	-1.193053	-1.703576
H	3.667522	0.670504	-1.949053
H	5.485697	0.130716	-0.344243
H	3.650629	-3.681796	0.426795
H	1.885135	-3.162069	-1.171273
B	1.496805	-0.886281	-2.866148
O	1.671760	-1.535406	-4.113076
H	2.607906	-1.630411	-4.314486
O	0.102949	-1.243243	-2.331482
H	0.042070	-2.196325	-2.201197
F	1.362673	0.559895	-2.926911
O	5.732777	-1.993545	1.007661
C	5.792282	-3.213879	1.725038
H	6.690408	-3.158710	2.342653
H	4.916971	-3.347152	2.374692
H	5.870931	-4.078450	1.052766
C	1.564558	0.757349	1.674039
C	1.093207	1.189827	0.444049
C	1.321625	2.565855	0.081727
C	1.983741	3.448423	1.007750
C	2.433847	2.941325	2.255780
C	2.242990	1.618491	2.573563
H	0.492791	2.443630	-1.914584
H	1.443871	-0.280619	1.968297
C	0.927898	3.107390	-1.176428
C	2.182871	4.810803	0.653258
H	2.936762	3.614262	2.946111
H	2.606376	1.224059	3.519519
C	1.766314	5.298759	-0.564054
C	1.139484	4.432965	-1.491243
H	2.681114	5.463443	1.366594
H	1.929109	6.341918	-0.820755
H	0.837546	4.811569	-2.463848

IM9

B3LYP/BSI SCF energy: -2226.146821a.u.

M06/BSII SCF energy in solution: -2225.39781a.u.

M06/BSII free energy in solution: -2224.689051a.u.

C	-1.843811	-0.183788	1.995187
H	-1.097374	0.512463	2.400562
C	-1.441113	-1.590458	2.494138
H	-2.166613	-2.333319	2.145632
H	-0.472027	-1.883199	2.077337
C	-1.399332	-1.628460	4.031419
H	-0.609280	-0.952689	4.387587
H	-1.127224	-2.635209	4.370567
C	-2.745521	-1.207291	4.640310
H	-3.506744	-1.958279	4.384457
H	-2.680373	-1.191263	5.734602
C	-3.194130	0.163531	4.114788
H	-2.505978	0.937602	4.482322
H	-4.185994	0.416550	4.508084
C	-3.219665	0.206467	2.575705
H	-3.523016	1.204751	2.243601
H	-3.983099	-0.492551	2.211285
C	-2.078699	1.869552	-0.135494
H	-3.151548	1.927641	0.092997
C	-1.361194	2.872677	0.793026
H	-1.547783	2.628693	1.844420
H	-0.280881	2.807958	0.640616
C	-1.830979	4.311906	0.515113
H	-2.894052	4.407857	0.781587
H	-1.283117	5.003285	1.166090
C	-1.639779	4.698538	-0.957535
H	-2.011735	5.714771	-1.135112
H	-0.566835	4.707668	-1.191058
C	-2.349593	3.702053	-1.884031
H	-2.165682	3.956345	-2.934485
H	-3.436661	3.772751	-1.731551
C	-1.888038	2.259072	-1.618905
H	-0.828316	2.166621	-1.878858
H	-2.430466	1.570814	-2.276634
C	-2.935990	-0.870824	-0.821748
H	-2.535641	-0.798098	-1.840625

C	-4.369931	-0.295594	-0.842050
H	-4.369130	0.763190	-1.115445
H	-4.818503	-0.363430	0.156893
C	-5.249112	-1.063798	-1.847963
H	-6.267554	-0.657635	-1.828690
H	-4.862662	-0.888678	-2.861682
C	-5.270932	-2.572786	-1.568561
H	-5.780965	-2.757239	-0.612028
H	-5.854060	-3.092618	-2.337571
C	-3.848756	-3.145344	-1.497526
H	-3.377350	-3.080598	-2.488135
H	-3.877617	-4.208910	-1.232468
C	-2.995156	-2.376317	-0.474850
H	-3.445053	-2.505721	0.517262
H	-1.990295	-2.809334	-0.413452
Ni	0.417245	-0.603690	-0.590403
P	-1.608207	0.069046	0.146954
C	3.373107	-0.930583	-1.612406
C	4.411173	-1.094172	-0.715787
C	4.283945	-2.007921	0.349393
C	3.113597	-2.761508	0.486631
C	2.084797	-2.587711	-0.445389
C	2.163579	-1.669924	-1.519027
H	3.478351	-0.221118	-2.427068
H	5.334701	-0.529835	-0.799542
H	3.000795	-3.481372	1.288919
H	1.213104	-3.235005	-0.363065
B	1.082459	-1.734317	-2.779972
O	1.031224	-2.996338	-3.456882
H	1.838004	-3.143443	-3.960884
O	-0.289750	-1.575481	-2.133025
H	-0.688101	-2.452709	-2.079603
F	1.296023	-0.612268	-3.609028
O	5.359511	-2.092921	1.176532
C	5.297062	-2.983022	2.280472
H	6.247944	-2.878745	2.805103
H	4.477156	-2.722493	2.961491
H	5.177025	-4.024015	1.954360
C	1.610364	0.301137	1.909771
C	1.380016	0.554329	0.567479
C	1.968913	1.742138	0.001839
C	2.714972	2.646197	0.836291
C	2.894489	2.336184	2.211328
C	2.367337	1.178362	2.730082
H	1.356523	1.362175	-2.047490
H	1.213820	-0.600327	2.368378
C	1.855860	2.062381	-1.382931
C	3.266753	3.826526	0.266274
H	3.462309	3.021168	2.836359
H	2.519813	0.930323	3.778169
C	3.113769	4.111398	-1.071665
C	2.408046	3.212440	-1.906704
H	3.823805	4.502011	0.911799
H	3.545177	5.015965	-1.491574
H	2.312778	3.422424	-2.968435

IM9_tran

B3LYP/BSI SCF energy: -2226.140028a.u.

M06/BSII SCF energy in solution: -2225.38830a.u.

M06/BSII free energy in solution: -2224.681458a.u.

C	-1.071119	1.463679	-1.272061
H	-2.002878	1.220280	-0.742271
C	-0.999444	0.506533	-2.485385
H	-0.059009	0.653648	-3.026103
H	-1.012442	-0.531392	-2.140517
C	-2.169528	0.742404	-3.456931
H	-3.108248	0.447269	-2.972938
H	-2.055208	0.085493	-4.327360
C	-2.260345	2.207933	-3.903195
H	-1.373648	2.464729	-4.500587
H	-3.128340	2.353965	-4.557122
C	-2.340227	3.148505	-2.693381
H	-3.279428	2.966940	-2.151672
H	-2.364956	4.195348	-3.019309
C	-1.155314	2.933451	-1.735480
H	-1.246710	3.609733	-0.878482
H	-0.228984	3.205986	-2.256306
C	-0.184614	2.259157	1.465416
H	-0.090176	3.278092	1.066492
C	-1.622054	2.093307	2.003147
H	-2.357562	2.201212	1.198850
H	-1.739844	1.086889	2.419770
C	-1.914550	3.126331	3.106094
H	-1.876318	4.139198	2.678898
H	-2.935517	2.982930	3.479183
C	-0.907102	3.018994	4.259452
H	-1.101657	3.794386	5.010003

H	-1.039422	2.051471	4.761768
C	0.535182	3.125556	3.745458
H	1.245312	2.977729	4.567669
H	0.713035	4.139375	3.357777
C	0.816634	2.100945	2.633038
H	0.718957	1.087823	3.043553
H	1.850783	2.203374	2.288139
C	1.930603	1.712253	-0.535414
H	2.587500	1.226344	0.196536
C	2.199462	3.232920	-0.461138
H	1.937135	3.639534	0.519354
H	1.582334	3.762796	-1.196701
C	3.684706	3.532736	-0.740459
H	3.852139	4.615982	-0.703522
H	4.293118	3.095414	0.063549
C	4.144726	2.964735	-2.089739
H	3.628244	3.498408	-2.900698
H	5.216754	3.145903	-2.231604
C	3.834844	1.465602	-2.195693
H	4.444814	0.906924	-1.473189
H	4.105256	1.088747	-3.189146
C	2.348048	1.178734	-1.924205
H	1.750057	1.675269	-2.698840
H	2.155678	0.106114	-2.004354
Ni	0.163773	-0.973553	0.914579
P	0.234873	1.099327	0.036566
C	-3.371285	-0.895573	1.062474
C	-4.259083	-0.728180	-0.004929
C	-4.101066	-1.509846	-1.155847
C	-3.052206	-2.440937	-1.222988
C	-2.192243	-2.591453	-0.141387
C	-2.314673	-1.825800	1.044524
H	-3.524203	-0.310007	1.963871
H	-5.069238	-0.011841	0.075634
H	-2.954820	-3.046313	-2.119216
H	-1.419266	-3.355151	-0.202333
B	-1.544614	-2.253604	2.447330
O	-1.918645	-3.543276	2.937588
H	-2.875943	-3.623848	2.991567
O	-4.906486	-1.441827	-2.257730
C	-6.045741	-0.596701	-2.207651
H	-6.563237	-0.731665	-3.158741
H	-6.718483	-0.873995	-1.386402
H	-5.765277	0.459141	-2.098592
C	2.870130	-0.968500	1.810022
C	2.013239	-1.317696	0.782679
C	2.521081	-2.074328	-0.323089
C	3.919319	-2.415888	-0.362329
C	4.764767	-2.005204	0.702427
C	4.248232	-1.304245	1.767336
H	0.638941	-2.270125	-1.367930
H	2.493081	-0.433958	2.676774
C	1.695972	-2.519172	-1.396136
C	4.416000	-3.166654	-1.463296
H	5.819455	-2.266339	0.667315
H	4.892773	-1.007688	2.591111
C	3.585671	-3.575797	-2.481804
C	2.208414	-3.249277	-2.446191
H	5.473803	-3.418439	-1.482760
H	3.982812	-4.152137	-3.312606
H	1.555215	-3.578625	-3.249454
F	-1.705575	-1.176534	3.363128
O	-0.047159	-2.345832	2.188654
H	0.237838	-3.252197	2.021322

TS7

B3LYP/BSI SCF energy: -2226.134596a.u.

M06/BSII SCF energy in solution: -2225.38294a.u.

M06/BSII free energy in solution: -2224.674872a.u.

C	-2.171425	-0.174474	1.855680
H	-1.611852	0.703491	2.207677
C	-1.594108	-1.382836	2.628287
H	-2.127594	-2.298271	2.349325
H	-0.543478	-1.539754	2.363406
C	-1.740067	-1.175824	4.145205
H	-1.133223	-0.312524	4.451336
H	-1.339475	-2.045578	4.679671
C	-3.205619	-0.937727	4.539133
H	-3.783531	-1.853156	4.345934
H	-3.284461	-0.742769	5.615241
C	-3.820346	0.223188	3.743495
H	-3.331403	1.162980	4.035914
H	-4.883011	0.334579	3.990951
C	-3.655837	0.026763	2.225013
H	-4.081833	0.884874	1.694801
H	-4.233963	-0.853476	1.914047
C	-2.473774	1.459110	-0.596786

H	-3.562311	1.348372	-0.500499
C	-2.067316	2.702382	0.224046
H	-2.351981	2.582714	1.274735
H	-0.980426	2.819557	0.203695
C	-2.730025	3.974104	-0.334812
H	-3.820302	3.904723	-0.205123
H	-2.400994	4.841442	0.249562
C	-2.408757	4.178345	-1.821423
H	-2.921412	5.069579	-2.203133
H	-1.331401	4.357804	-1.935682
C	-2.805099	2.943476	-2.642254
H	-2.525962	3.076115	-3.694427
H	-3.898793	2.827832	-2.621847
C	-2.146703	1.666338	-2.093230
H	-1.060179	1.741289	-2.212528
H	-2.466918	0.802500	-2.687387
C	-2.749229	-1.460814	-0.900148
H	-2.223652	-1.490281	-1.863838
C	-4.236512	-1.161448	-1.193363
H	-4.358464	-0.179177	-1.657677
H	-4.806663	-1.139447	-0.255978
C	-4.835524	-2.227840	-2.130224
H	-5.896071	-2.010046	-2.304895
H	-4.338869	-2.159836	-3.108314
C	-4.667910	-3.649280	-1.576254
H	-5.275915	-3.757814	-0.666695
H	-5.048395	-4.384909	-2.294593
C	-3.200264	-3.943551	-1.235589
H	-2.606275	-3.964929	-2.160162
H	-3.106196	-4.935906	-0.778319
C	-2.630099	-2.874811	-0.287987
H	-3.192880	-2.909850	0.652709
H	-1.592000	-3.110942	-0.025339
Ni	0.539256	-0.533471	-0.328425
P	-1.729250	-0.156872	0.028014
C	3.586191	-0.458805	-0.769233
C	4.868031	-0.802555	-0.330666
C	5.028548	-1.871841	0.558725
C	3.901360	-2.597140	0.978641
C	2.644231	-2.245409	0.509446
C	2.429616	-1.163469	-0.383677
H	3.492292	0.383870	-1.447556
H	5.721426	-0.227855	-0.673097
H	4.045069	-3.427947	1.663077
H	1.797197	-2.843190	0.845947
B	1.528409	-1.840984	-2.221614
O	2.168382	-3.035284	-2.485081
H	3.070612	-2.895568	-2.792816
O	0.189781	-1.978523	-1.730097
H	0.068130	-2.873980	-1.386795
F	1.708840	-0.765150	-3.038177
O	6.225188	-2.292468	1.061752
C	7.395034	-1.577684	0.697005
H	7.339592	-0.525942	1.005281
H	8.220812	-2.062984	1.220009
H	7.577800	-1.622923	-0.384551
C	1.640100	2.002349	2.866961
C	1.975494	3.191218	2.263436
C	1.931312	3.303038	0.848233
C	1.520381	2.167944	0.063772
C	1.129382	0.941207	0.708522
C	1.224443	0.890000	2.091470
H	2.593145	5.361556	0.795703
H	1.693556	1.906003	3.949234
H	2.289379	4.049640	2.852360
C	2.291623	4.510671	0.188613
C	1.526029	2.310047	-1.354250
H	0.993029	-0.032602	2.616601
C	1.889002	3.492079	-1.965128
C	2.269287	4.610050	-1.184232
H	1.258033	1.448988	-1.959954
H	1.890973	3.564584	-3.049400
H	2.551311	5.540084	-1.670412

TS8

B3LYP/BSI SCF energy: -2226.12707a.u.

M06/BSII SCF energy in solution: -2225.37498a.u.

M06/BSII free energy in solution: -2224.665474a.u.

C	-1.022407	1.619475	-1.288172
H	-1.934773	1.535134	-0.684398
C	-1.212626	0.646520	-2.474327
H	-0.334448	0.670365	-3.128832
H	-1.315400	-0.377559	-2.107752
C	-2.457166	1.027849	-3.295235
H	-3.350052	0.890747	-2.670615
H	-2.562641	0.341113	-4.143560
C	-2.394200	2.480071	-3.788633

H	-1.568863	2.583817	-4.507880
H	-3.311849	2.740997	-4.329633
C	-2.169990	3.452502	-2.622070
H	-3.052044	3.443083	-1.965965
H	-2.068315	4.479855	-2.992719
C	-0.926614	3.073810	-1.797538
H	-0.811540	3.778390	-0.966707
H	-0.037249	3.184541	-2.429860
C	0.110839	2.355739	1.342153
H	0.334822	3.325518	0.878510
C	-1.304191	2.448276	1.949057
H	-2.056232	2.624139	1.173061
H	-1.549271	1.494866	2.429925
C	-1.381768	3.576226	2.994061
H	-1.215987	4.543184	2.497157
H	-2.392705	3.614001	3.417544
C	-0.343824	3.391288	4.109035
H	-0.381733	4.233996	4.809713
H	-0.593131	2.490462	4.686717
C	1.068820	3.241022	3.528346
H	1.790630	3.035920	4.327967
H	1.377068	4.190291	3.066318
C	1.131624	2.120282	2.476422
H	0.901507	1.161008	2.956442
H	2.150720	2.035823	2.086354
C	2.009343	1.486085	-0.753164
H	2.656550	0.931601	-0.064087
C	2.479399	2.959477	-0.739000
H	2.358884	3.407805	0.251083
H	1.875778	3.558193	-1.431606
C	3.962458	3.055294	-1.147205
H	4.273408	4.107250	-1.150724
H	4.573349	2.551817	-0.384992
C	4.231033	2.413153	-2.514822
H	3.723396	2.999239	-3.294756
H	5.302327	2.449635	-2.746201
C	3.719825	0.966892	-2.558146
H	4.309176	0.342715	-1.873282
H	3.854851	0.543541	-3.560620
C	2.237525	0.885593	-2.158565
H	1.646430	1.444977	-2.895105
H	1.904816	-0.154277	-2.197477
Ni	0.051022	-0.944004	0.857987
P	0.295726	1.085426	-0.049378
C	-3.126994	-0.398800	0.759230
C	-4.335651	-0.611807	0.080903
C	-4.429477	-1.653071	-0.848505
C	-3.312922	-2.475250	-1.070063
C	-2.135423	-2.240281	-0.372423
C	-1.976041	-1.186344	0.568194
H	-3.109917	0.398723	1.495487
H	-5.186427	0.027748	0.290243
H	-3.403261	-3.292373	-1.779862
H	-1.306965	-2.924063	-0.558320
B	-1.530700	-2.022937	2.566005
O	-2.368617	-3.109380	2.654775
H	-3.271107	-2.850183	2.870149
O	-5.547630	-1.960839	-1.568922
C	-6.706012	-1.164664	-1.383261
H	-7.465731	-1.575802	-2.050074
H	-7.071078	-1.212379	-0.348966
H	-6.523971	-0.114813	-1.648014
C	2.783456	-1.039333	1.923515
C	1.950282	-1.337651	0.855007
C	2.491337	-2.177601	-0.182390
C	3.849164	-2.653115	-0.107910
C	4.652178	-2.282301	1.002636
C	4.123777	-1.496931	2.000406
H	0.690421	-2.235983	-1.378625
H	2.407308	-0.442455	2.749565
C	1.714798	-2.590822	-1.305461
C	4.351954	-3.493613	-1.139617
H	5.678255	-2.638525	1.054859
H	4.731697	-1.226574	2.861055
C	3.564510	-3.868670	-2.204342
C	2.227471	-3.411183	-2.287311
H	5.379637	-3.843030	-1.067538
H	3.964709	-4.515033	-2.980612
H	1.606488	-3.707967	-3.128276
F	-1.745991	-0.915127	3.327585
O	-0.164906	-2.308868	2.309222
H	-0.012334	-3.223937	2.038254

IM10

B3LYP/BSI SCF energy: -1949.616359a.u.

M06/BSII SCF energy in solution: -1948.87131a.u.

M06/BSII free energy in solution: -1948.200463a.u.

C	1.486605	-2.546126	0.437107
H	1.184191	-2.679196	1.486179
C	0.427450	-3.288378	-0.411452
H	0.652381	-3.168865	-1.478695
H	-0.566051	-2.847825	-0.252473
C	0.387246	-4.787193	-0.066866
H	0.031349	-4.907481	0.966198
H	-0.342304	-5.295022	-0.708350
C	1.770027	-5.440466	-0.205204
H	2.072816	-5.427279	-1.262098
H	1.722947	-6.494865	0.091507
C	2.823591	-4.698555	0.629720
H	2.586344	-4.808677	1.697495
H	3.813501	-5.147056	0.482877
C	2.871895	-3.201867	0.273257
H	3.620464	-2.695077	0.892889
H	3.202300	-3.100844	-0.767898
C	2.309848	0.000757	1.713920
H	3.306242	-0.464357	1.701914
C	1.622191	-0.370651	3.047527
H	1.523957	-1.457090	3.148662
H	0.605005	0.041722	3.048420
C	2.396939	0.180708	4.256950
H	3.379062	-0.310768	4.312109
H	1.866893	-0.079272	5.181145
C	2.593947	1.699273	4.159543
H	3.186191	2.061583	5.008343
H	1.616076	2.196086	4.221546
C	3.266750	2.080862	2.834464
H	3.353255	3.170470	2.749926
H	4.292191	1.683176	2.818780
C	2.486968	1.534717	1.626254
H	1.499119	2.006915	1.589635
H	3.003786	1.817033	0.703608
C	2.346585	-0.098497	-1.258835
H	2.075084	0.966779	-1.292317
C	3.887795	-0.184216	-1.202095
H	4.274822	0.268738	-0.283948
H	4.204353	-1.233350	-1.190053
C	4.517178	0.511778	-2.423059
H	5.609375	0.423561	-2.376162
H	4.288584	1.585876	-2.382298
C	3.990368	-0.070160	-3.742633
H	4.329218	-1.111809	-3.838905
H	4.414488	0.474530	-4.594421
C	2.456056	-0.031559	-3.796206
H	2.117462	1.013253	-3.824298
H	2.094294	-0.504819	-4.716912
C	1.829358	-0.723433	-2.573598
H	2.084122	-1.791320	-2.598248
H	0.736320	-0.659805	-2.624676
Ni	-0.910806	-0.155003	0.107801
P	1.356007	-0.673166	0.237118
C	-2.753459	-0.294654	-0.068738
C	-3.486640	-0.845906	0.997417
C	-3.435800	-0.136562	-1.295357
C	-4.809910	-1.281601	0.849811
H	-3.026891	-0.944417	1.979765
C	-4.749895	-0.561392	-1.461711
H	-2.933848	0.331045	-2.138878
C	-5.443830	-1.142259	-0.389610
H	-5.329719	-1.711405	1.699164
H	-5.267167	-0.447126	-2.409988
O	-6.731158	-1.527770	-0.654612
C	-7.489234	-2.091371	0.400017
H	-8.471211	-2.318385	-0.019382
H	-7.037510	-3.018611	0.777820
H	-7.609222	-1.389804	1.236396
C	-1.304728	3.448509	2.143833
C	-0.972111	4.408097	1.214786
C	-0.716535	4.037243	-0.132171
C	-0.791389	2.649676	-0.506403
C	-1.089996	1.658789	0.487933
C	-1.375838	2.080321	1.777868
H	-0.340544	6.049203	-0.831298
H	-1.521650	3.735703	3.170185
H	-0.917992	5.457835	1.492289
C	-0.397309	5.003607	-1.125692
C	-0.560551	2.315648	-1.870594
H	-1.658284	1.356179	2.537578
C	-0.260470	3.276675	-2.812350
C	-0.172295	4.637930	-2.433684
H	-0.641690	1.270941	-2.158418
H	-0.100013	2.992854	-3.849012
H	0.064778	5.392304	-3.178905

IM10_tran

B3LYP/BSI SCF energy: -1949.608739a.u.

M06/BSII SCF energy in solution: -1948.86604a.u.

M06/BSII free energy in solution: -1948.19339a.u.

C	0.366689	1.824944	1.583666
H	1.425276	1.970948	1.333179
C	0.337929	0.795880	2.735865
H	-0.697814	0.572219	3.016617
H	0.789668	-0.142000	2.398076
C	1.090428	1.328715	3.967169
H	2.157280	1.426427	3.721031
H	1.025796	0.598757	4.782680
C	0.547324	2.689928	4.424142
H	-0.485015	2.566533	4.781584
H	1.128012	3.066945	5.274353
C	0.564494	3.709231	3.276346
H	1.605612	3.922904	2.995225
H	0.128446	4.661391	3.601838
C	-0.195086	3.186851	2.042942
H	-0.141850	3.926091	1.235166
H	-1.255108	3.078743	2.302449
C	0.211746	2.397163	-1.336220
H	-0.330853	3.322292	-1.099255
C	1.718546	2.726456	-1.331843
H	2.026545	3.117721	-0.356232
H	2.292594	1.807895	-1.498589
C	2.066903	3.760717	-2.417420
H	1.577450	4.716469	-2.180045
H	3.146375	3.952772	-2.404528
C	1.622356	3.298561	-3.811377
H	1.845305	4.069955	-4.558032
H	2.198682	2.407808	-4.098023
C	0.126573	2.957741	-3.824840
H	-0.170918	2.574069	-4.807942
H	-0.457810	3.874149	-3.657903
C	-0.225695	1.925381	-2.741330
H	0.281790	0.977133	-2.963777
H	-1.300525	1.715564	-2.765371
C	-2.201846	1.263437	-0.042468
H	-2.446971	0.636693	-0.908887
C	-2.837999	2.652549	-0.273075
H	-2.428541	3.132278	-1.167617
H	-2.616952	3.317985	0.569963
C	-4.365933	2.530751	-0.432523
H	-4.800115	3.529036	-0.567072
H	-4.584309	1.969213	-1.351670
C	-5.016809	1.818483	0.760833
H	-4.906986	2.443815	1.658864
H	-6.094154	1.704354	0.591478
C	-4.365064	0.452232	1.013010
H	-4.574640	-0.220051	0.170244
H	-4.797693	-0.019790	1.903037
C	-2.842139	0.577272	1.184620
H	-2.637468	1.168558	2.086771
H	-2.405624	-0.413073	1.337667
Ni	0.439984	-0.821228	-0.457821
P	-0.316038	1.144139	-0.031641
C	3.414161	-0.020451	0.415726
C	4.654217	-0.673745	0.453883
C	4.779142	-1.976313	-0.047527
C	3.659338	-2.626009	-0.588104
C	2.445539	-1.944647	-0.613033
C	2.281688	-0.642499	-0.113479
H	3.362566	0.990239	0.815583
H	5.511291	-0.161299	0.876920
H	3.769611	-3.633654	-0.976315
H	1.574354	-2.476085	-1.049137
O	5.942450	-2.697582	-0.058214
C	7.108118	-2.096139	0.476273
H	7.905694	-2.833436	0.369012
H	7.384746	-1.185316	-0.071500
H	6.988268	-1.848732	1.539539
C	-1.686858	-1.652890	-2.286960
C	-1.169796	-1.763777	-0.999977
C	-1.760333	-2.771156	-0.153283
C	-2.832254	-3.605355	-0.628225
C	-3.306445	-3.427265	-1.955530
C	-2.740118	-2.473238	-2.768475
H	-0.491903	-2.363392	1.549857
H	-1.275581	-0.912612	-2.971723
C	-1.303827	-2.985763	1.180001
C	-3.387279	-4.589450	0.235095
H	-4.116843	-4.057298	-2.315027
H	-3.098583	-2.343892	-3.787482
C	-2.914877	-4.761229	1.516892
C	-1.858760	-3.948916	1.995035
H	-4.197236	-5.211731	-0.139505
H	-3.349115	-5.519494	2.162867
H	-1.485776	-4.088857	3.006099

$FB(OH)_2$

B3LYP/BSI SCF energy: -276.510348a.u.

M06/BSII SCF energy in solution: -276.501819a.u.

M06/BSII free energy in solution: -276.491137a.u.

F	0.593972	1.211761	-0.000004
B	-0.014989	0.019080	0.000008
O	0.718034	-1.133414	-0.000001
H	1.666693	-0.962694	0.000010
O	-1.371687	-0.007554	0.000006
H	-1.708273	-0.910811	-0.000049

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B3LYP/BSI SCF energy: -1949.604432a.u.

M06/BSII SCF energy in solution: -1948.86676a.u.

M06/BSII free energy in solution: -1948.194345a.u.

C	-2.425512	0.807291	0.424628
H	-1.822872	1.304425	1.198756
C	-2.452173	1.770404	-0.782624
H	-3.060894	1.334103	-1.586030
H	-1.442629	1.909113	-1.181333
C	-3.054857	3.129384	-0.389155
H	-2.391297	3.617412	0.337501
H	-3.090178	3.785445	-1.267122
C	-4.457211	2.972243	0.216115
H	-5.145659	2.602836	-0.557845
H	-4.846181	3.945417	0.539090
C	-4.450605	1.986260	1.393412
H	-3.862023	2.411382	2.218774
H	-5.467915	1.842596	1.777891
C	-3.847959	0.625461	0.996617
H	-3.842627	-0.037500	1.868049
H	-4.496166	0.153437	0.248974
C	-1.719291	-1.835799	1.581598
H	-2.802873	-2.008332	1.639713
C	-1.267225	-1.144698	2.888190
H	-1.783270	-0.188064	3.021826
H	-0.196108	-0.911471	2.809876
C	-1.504384	-2.033040	4.121118
H	-2.584958	-2.184436	4.257075
H	-1.147031	-1.517237	5.020445
C	-0.815526	-3.395941	3.975660
H	-1.033276	-4.029324	4.843858
H	0.273814	-3.250663	3.958249
C	-1.252432	-4.095123	2.681830
H	-0.714911	-5.042941	2.558130
H	-2.320098	-4.349057	2.749479
C	-1.021843	-3.207884	1.446116
H	0.057473	-3.049445	1.308629
H	-1.375685	-3.737623	0.555293
C	-2.090198	-1.716466	-1.351641
H	-1.555431	-2.671613	-1.241480
C	-3.599973	-2.029597	-1.340047
H	-3.907262	-2.451737	-0.376328
H	-4.165750	-1.098850	-1.470916
C	-3.973254	-2.999642	-2.475919
H	-5.054027	-3.186345	-2.465712
H	-3.487835	-3.969385	-2.294753
C	-3.536422	-2.461136	-3.846025
H	-4.115793	-1.556088	-4.078678
H	-3.769208	-3.189418	-4.632114
C	-2.039340	-2.118837	-3.860441
H	-1.455247	-3.044229	-3.751990
H	-1.757563	-1.684522	-4.827198
C	-1.664732	-1.151298	-2.725093
H	-2.154013	-0.185636	-2.901294
H	-0.586708	-0.956912	-2.727965
Ni	0.773118	-0.198669	-0.156319
P	-1.376156	-0.729946	0.091897
C	2.643461	-0.046429	-0.255139
C	3.099901	-0.920525	-1.266249
C	3.512900	0.174577	0.837977
C	4.323940	-1.588796	-1.174523
H	2.494828	-1.089324	-2.153356
C	4.737599	-0.473178	0.933234
H	3.236072	0.874310	1.618631
C	5.151303	-1.365534	-0.067456
H	4.621031	-2.264962	-1.968345
H	5.399105	-0.300887	1.776910
O	6.371496	-1.950683	0.124761
C	6.846563	-2.848434	-0.863460
H	7.823207	-3.191023	-0.517176
H	6.181960	-3.714823	-0.979517
H	6.962670	-2.356087	-1.837999
C	1.585580	3.055713	-2.599275
C	1.420136	4.121260	-1.741389

C	1.283773	3.893662	-0.346662
C	1.323100	2.548908	0.162186
C	1.505871	1.437294	-0.749731
C	1.646424	1.735056	-2.108507
H	1.062873	5.983236	0.161959
H	1.688999	3.227607	-3.667968
H	1.393804	5.141314	-2.115339
C	1.084576	4.971410	0.560254
C	1.126365	2.365740	1.558957
H	1.825458	0.932441	-2.816880
C	0.928800	3.431252	2.413591
C	0.914954	4.752139	1.908866
H	1.116174	1.350396	1.945878
H	0.782023	3.256077	3.475841
H	0.765214	5.589577	2.584824

2a

B3LYP/BSI SCF energy: -731.475401a.u.

M06/BSII SCF energy in solution: -731.106884a.u.

M06/BSII free energy in solution: -730.887115a.u.

C	0.671096	0.383187	-0.116114
C	1.588176	0.968002	0.766087
C	1.168378	-0.548136	-1.048764
C	2.947246	0.644384	0.739011
H	1.231341	1.683334	1.501656
C	2.515698	-0.879528	-1.090110
H	0.488071	-1.003192	-1.762420
C	3.417579	-0.286599	-0.193515
H	3.618882	1.116050	1.446719
H	2.898531	-1.590382	-1.815283
O	4.718913	-0.681058	-0.312506
C	5.675877	-0.108107	0.563615
H	6.634830	-0.555645	0.297688
H	5.739724	0.980745	0.439151
H	5.451599	-0.334892	1.614052
C	-2.419243	2.582220	-0.234752
C	-3.452741	1.680995	-0.137802
C	-3.186930	0.293325	0.005800
C	-1.827240	-0.169292	0.040317
C	-0.762350	0.787815	-0.097344
C	-1.080258	2.131438	-0.217448
H	-5.268218	-0.285057	0.097181
H	-2.624230	3.643650	-0.341385
H	-4.486416	2.016247	-0.163975
C	-4.244136	-0.648371	0.133370
C	-1.599624	-1.559190	0.246780
H	-0.275117	2.851743	-0.330123
C	-2.647761	-2.443889	0.375315
C	-3.985468	-1.988112	0.308492
H	-0.579846	-1.920275	0.315659
H	-2.446369	-3.499162	0.536516
H	-4.803881	-2.695557	0.406985

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B3LYP/BSI SCF energy: -2339.472807a.u.

M06/BSII SCF energy in solution: -2338.69442a.u.

M06/BSII free energy in solution: -2337.980134a.u.

C	2.049490	1.486168	-0.821475
H	1.372894	2.101440	-0.210913
C	1.547439	1.586865	-2.278694
H	2.208342	1.001779	-2.930542
H	0.545090	1.157851	-2.369048
C	1.543418	3.046159	-2.764981
H	0.813453	3.618963	-2.177474
H	1.204633	3.085951	-3.807188
C	2.931914	3.686406	-2.630280
H	3.628811	3.186328	-3.318269
H	2.897799	4.739647	-2.933138
C	3.464017	3.562526	-1.196212
H	2.838358	4.166182	-0.523763
H	4.479313	3.971394	-1.127825
C	3.461485	2.102467	-0.706864
H	3.823939	2.069789	0.324335
H	4.171236	1.521167	-1.307392
C	2.814718	-0.206009	1.500198
H	3.843172	0.041683	1.201734
C	2.323744	0.884564	2.481230
H	2.320486	1.870695	2.003131
H	1.286283	0.675071	2.763468
C	3.199701	0.933041	3.744686
H	4.218238	1.245941	3.471653
H	2.812530	1.697543	4.428946
C	3.257764	-0.431901	4.443571
H	3.921537	-0.386320	5.315347
H	2.258115	-0.686899	4.821277
C	3.723168	-1.526289	3.473945

H	3.708487	-2.505091	3.967416
H	4.767689	-1.336419	3.186059
C	2.847440	-1.579454	2.210128
H	1.829650	-1.880535	2.483089
H	3.232243	-2.355390	1.540234
C	2.619936	-1.546521	-1.139052
H	2.556641	-2.416603	-0.472063
C	4.106282	-1.338745	-1.495518
H	4.693124	-1.089657	-0.604599
H	4.205204	-0.491190	-2.185956
C	4.688126	-2.596893	-2.165936
H	5.737195	-2.422263	-2.433833
H	4.683527	-3.423259	-1.441480
C	3.879230	-3.004026	-3.405900
H	3.987374	-2.227934	-4.177423
H	4.283715	-3.928019	-3.835701
C	2.390683	-3.178902	-3.070111
H	2.265277	-4.035482	-2.393587
H	1.820902	-3.412259	-3.977515
C	1.809379	-1.921534	-2.401275
H	1.828592	-1.094794	-3.121278
H	0.758693	-2.087297	-2.140655
F	0.244054	-2.912272	0.544843
Ni	-0.337840	-0.958553	0.257436
P	1.788100	-0.228958	-0.081460
C	-3.287409	-1.427683	0.972803
C	-4.587485	-1.629527	0.508321
C	-4.784511	-2.243857	-0.735821
C	-3.673950	-2.665057	-1.486382
C	-2.393678	-2.468654	-0.990074
C	-2.143487	-1.842380	0.260049
H	-3.162195	-0.943791	1.937859
H	-5.428768	-1.303163	1.109232
H	-3.849521	-3.154864	-2.439535
H	-1.557490	-2.847415	-1.574600
B	-0.904977	-2.985985	1.449023
O	-0.791027	-2.342210	2.682545
H	-0.782962	-1.372371	2.639646
O	-1.418174	-4.270158	1.429822
H	-1.998615	-4.389577	2.189743
C	-1.069299	0.620695	0.856818
O	-1.056373	0.687723	2.090333
O	-6.002329	-2.484114	-1.297231
C	-7.164589	-2.090948	-0.583213
H	-7.188672	-1.006993	-0.413533
H	-8.012480	-2.375766	-1.208203
H	-7.239479	-2.605811	0.382992
C	-1.709635	4.847113	2.107707
C	-1.513033	3.529092	1.753036
C	-1.829017	3.068706	0.444000
C	-2.364990	4.019907	-0.492045
C	-2.553376	5.369915	-0.090081
C	-2.232691	5.779980	1.183072
H	-1.462963	5.171943	3.114724
H	-1.132007	2.819044	2.474089
C	-1.630243	1.711926	-0.005149
C	-2.710160	3.601110	-1.805286
H	-2.959732	6.073997	-0.811914
H	-2.382223	6.813878	1.480597
C	-2.528979	2.296617	-2.202590
C	-1.976284	1.362857	-1.301448
H	-3.127438	4.334307	-2.491255
H	-2.806024	1.980870	-3.203928
H	-1.832994	0.331624	-1.608779

IM11

B3LYP/BSI SCF energy: -2339.500992a.u.

M06/BSII SCF energy in solution: -2338.70657a.u.

M06/BSII free energy in solution: -2337.995782a.u.

C	-3.220665	-0.460746	0.505641
H	-3.307330	0.276253	-0.302676
C	-3.151116	0.331547	1.829628
H	-3.074949	-0.366880	2.673572
H	-2.256891	0.962799	1.854497
C	-4.407325	1.199106	2.017332
H	-4.433070	1.964365	1.229812
H	-4.347069	1.734656	2.972211
C	-5.688659	0.356070	1.955913
H	-5.715332	-0.324896	2.818936
H	-6.572692	0.999057	2.039685
C	-5.751289	-0.466602	0.661483
H	-5.849835	0.212748	-0.196589
H	-6.642604	-1.105550	0.657250
C	-4.493768	-1.335596	0.470997
H	-4.572112	-1.879479	-0.475352
H	-4.458648	-2.089686	1.266246
C	-2.004659	-2.361560	-1.427202

H	-2.814018	-3.031939	-1.103910
C	-2.524510	-1.507343	-2.607710
H	-3.387900	-0.905118	-2.307936
H	-1.747546	-0.793204	-2.903406
C	-2.903902	-2.388436	-3.809238
H	-3.757792	-3.026826	-3.537882
H	-3.242008	-1.751023	-4.634795
C	-1.732547	-3.271928	-4.256991
H	-2.038682	-3.920429	-5.086755
H	-0.922188	-2.634383	-4.635847
C	-1.205291	-4.113792	-3.087504
H	-0.336205	-4.703529	-3.401701
H	-1.978550	-4.833889	-2.781183
C	-0.815305	-3.236897	-1.885072
H	0.032539	-2.598197	-2.155682
H	-0.470805	-3.880600	-1.068464
C	-1.033166	-2.487613	1.387664
H	-0.227217	-3.020952	0.865434
C	-2.063979	-3.535885	1.854792
H	-2.514874	-4.048740	0.998169
H	-2.880161	-3.032344	2.387699
C	-1.414673	-4.565025	2.797879
H	-2.170941	-5.282150	3.138549
H	-0.665489	-5.143253	2.239019
C	-0.741652	-3.885821	3.999168
H	-1.511768	-3.410025	4.623175
H	-0.247405	-4.633310	4.630514
C	0.267635	-2.821467	3.544969
H	1.102046	-3.313011	3.024387
H	0.699941	-2.309626	4.412779
C	-0.380767	-1.792365	2.603669
H	-1.134839	-1.224095	3.160676
H	0.365825	-1.063813	2.266850
Ni	0.102034	0.027032	-0.471642
P	-1.590790	-1.280572	0.057346
C	4.302803	0.657208	0.248358
C	5.575384	0.758242	0.799251
C	6.570554	-0.161779	0.438928
C	6.273879	-1.174320	-0.480368
C	4.985703	-1.252994	-1.019791
C	3.965606	-0.353967	-0.674618
H	3.552203	1.393492	0.524771
H	5.830132	1.544521	1.503678
H	7.026640	-1.894556	-0.780984
H	4.769901	-2.041292	-1.738010
B	2.496382	-0.534453	-1.282208
O	2.352320	-0.997404	-2.607813
H	2.958343	-0.534624	-3.195161
O	1.568460	-1.367396	-0.427188
H	1.959535	-1.460951	0.449880
F	1.747860	0.840339	-1.137610
O	7.790290	0.017342	1.034676
C	8.836105	-0.875246	0.695043
H	9.707366	-0.554743	1.269336
H	8.591181	-1.911901	0.962607
H	9.076261	-0.833458	-0.375672
O	-1.786839	1.634019	-1.580990
C	-0.919344	1.576845	-0.719619
C	-1.299703	6.862657	-0.916550
C	-0.619951	6.549143	0.237343
C	-0.347253	5.197378	0.579490
C	-0.792372	4.141436	-0.289289
C	-1.489052	4.504535	-1.475155
C	-1.732423	5.827887	-1.776787
H	0.681935	5.698021	2.414474
H	-1.501272	7.899508	-1.169921
H	-0.275296	7.333188	0.906919
C	0.359829	4.883001	1.770981
C	-0.492927	2.780957	0.085087
H	-1.831881	3.719918	-2.135027
H	-2.264280	6.078275	-2.690454
C	0.214195	2.537881	1.253056
C	0.637075	3.578493	2.105867
H	0.440451	1.507296	1.516010
H	1.180921	3.344783	3.016235

TS11

B3LYP/BSI SCF energy: -2339.477795a.u.

M06/BSII SCF energy in solution: -2338.69971a.u.

M06/BSII free energy in solution: -2337.985406a.u.

C	-1.887447	1.897786	0.419658
H	-1.318406	2.246231	-0.453519
C	-1.111663	2.349512	1.677188
H	-1.670790	2.050582	2.573319
H	-0.134737	1.860514	1.728440
C	-0.932395	3.877098	1.692712
H	-0.299773	4.170706	0.844386

H	-0.394465	4.175215	2.600451	Ni	-0.008378	-0.962850	-0.473051
C	-2.281939	4.603818	1.607056	P	-1.865968	0.031732	0.162526
H	-2.857151	4.407970	2.523563	C	2.861809	-2.254023	-1.451799
H	-2.129416	5.688565	1.561486	C	4.173069	-1.930381	-1.117997
C	-3.092156	4.130092	0.392508	C	4.674283	-2.255233	0.149396
H	-2.581151	4.441629	-0.529223	C	3.844153	-2.905139	1.074259
H	-4.078004	4.610277	0.379397	C	2.532199	-3.219794	0.711059
C	-3.264652	2.599926	0.375508	C	1.991206	-2.909579	-0.551577
H	-3.828510	2.311181	-0.515670	H	2.491444	-1.998536	-2.440578
H	-3.866261	2.297262	1.241057	H	4.830455	-1.428031	-1.821028
C	-3.147207	-0.274061	-1.184956	H	4.210240	-3.177402	2.057996
H	-4.095084	0.129114	-0.799814	H	1.921647	-3.752111	1.440863
C	-2.789004	0.479059	-2.487047	B	0.482149	-3.369468	-0.984100
H	-2.670746	1.551731	-2.299790	O	0.250444	-4.757695	-1.138214
H	-1.819006	0.125941	-2.852668	H	1.013415	-5.184400	-1.540937
C	-3.863491	0.263841	-3.566273	O	-0.535292	-2.819576	0.023305
H	-4.809814	0.718872	-3.237494	H	-0.319423	-3.121809	0.913138
H	-3.567406	0.788703	-4.482272	F	0.126435	-2.550613	-2.144606
C	-4.089519	-1.226764	-3.851304	O	5.974006	-1.905724	0.385860
H	-4.887008	-1.356926	-4.592818	C	6.543278	-2.241120	1.639046
H	-3.176679	-1.652691	-4.289063	H	7.575743	-1.888904	1.606531
C	-4.428909	-1.984339	-2.561415	H	6.021981	-1.746893	2.469963
H	-4.535355	-3.056406	-2.763668	H	6.538320	-3.325331	1.811913
H	-5.401890	-1.638567	-2.181584	O	0.488477	0.894720	-2.320016
C	-3.352361	-1.777558	-1.482043	C	0.766729	0.584455	-1.169515
H	-2.407314	-2.217649	-1.817379	C	3.267478	5.259868	-1.203937
H	-3.643415	-2.319395	-0.576164	C	3.715577	4.569282	-0.102157
C	-2.540095	-0.870770	1.666812	C	3.237693	3.262403	0.185736
H	-2.646083	-1.886594	1.263783	C	2.271549	2.651092	-0.687232
C	-3.922124	-0.423247	2.187539	C	1.835433	3.394539	-1.819962
H	-4.651085	-0.372761	1.371514	C	2.319491	4.662292	-2.065828
H	-3.847443	0.587102	2.608985	H	4.450008	3.032363	1.961294
C	-4.431924	-1.381550	3.279585	H	3.640423	6.257892	-1.415253
H	-5.401342	-1.032032	3.654358	H	4.446339	5.013362	0.569153
H	-4.607072	-2.371109	2.834998	C	3.709846	2.555143	1.323654
C	-3.428113	-1.511573	4.433797	C	1.790704	1.332655	-0.352037
H	-3.348507	-0.546222	4.954053	H	1.128621	2.936290	-2.498045
H	-3.791530	-2.234463	5.173491	H	1.971429	5.206684	-2.939265
C	-2.040005	-1.924510	3.922970	C	2.282237	0.694786	0.777108
H	-2.093536	-2.943588	3.513817	C	3.248391	1.292475	1.612748
H	-1.323101	-1.958108	4.752051	H	1.925246	-0.304874	1.010989
C	-1.529882	-0.966634	2.832513	H	3.621194	0.751010	2.476715
H	-1.370493	0.023698	3.274527				
H	-0.553590	-1.298280	2.461367	**IM12**			

B3LYP/BSI SCF energy: -2339.489866a.u.

M06/BSII SCF energy in solution: -2338.71487a.u.

M06/BSII free energy in solution: -2337.999324a.u.

C	-1.126835	2.069172	-1.085096
H	-0.226284	1.725493	-1.609359
C	-0.683569	3.161693	-0.085815
H	-1.564745	3.559326	0.433984
H	-0.022002	2.744356	0.677930
C	0.023610	4.318854	-0.809388
H	0.952707	3.944603	-1.260406
H	0.316152	5.085338	-0.081830
C	-0.870511	4.927596	-1.897902
H	-1.737064	5.411983	-1.424911
H	-0.332363	5.714087	-2.440150
C	-1.363845	3.851883	-2.875624
H	-0.508669	3.458411	-3.442698
H	-2.050076	4.289079	-3.610936
C	-2.061131	2.683248	-2.153046
H	-2.356478	1.935418	-2.894509
H	-2.983820	3.046644	-1.684415
C	-2.630490	-0.447357	-1.572710
H	-3.320255	0.285122	-2.014878
C	-1.662026	-0.926801	-2.678915
H	-1.070094	-0.094509	-3.073332
H	-0.939103	-1.625558	-2.242775
C	-2.420659	-1.617210	-3.824709
H	-3.064335	-0.882725	-4.331276
H	-1.703445	-1.971375	-4.574742
C	-3.283402	-2.778330	-3.312984
H	-3.847252	-3.227782	-4.139399
H	-2.631049	-3.565218	-2.910580
C	-4.237516	-2.305525	-2.208961
H	-4.814129	-3.150732	-1.815373
H	-4.966321	-1.600740	-2.636795
C	-3.480743	-1.627590	-1.052717
H	-2.845341	-2.363868	-0.552614
H	-4.207034	-1.283194	-0.308438
C	-3.000428	0.864637	1.071244
H	-3.376926	-0.143933	1.282445
C	-4.189400	1.733738	0.611780
H	-4.624748	1.341713	-0.314153
H	-3.840807	2.750695	0.391299
C	-5.274009	1.804137	1.702132
H	-6.093606	2.450802	1.366530
H	-5.704695	0.803176	1.845016
C	-4.706294	2.308286	3.036343
H	-4.386573	3.354004	2.921713
H	-5.485981	2.303857	3.806976
C	-3.508101	1.460015	3.486949
H	-3.852016	0.441392	3.716046
H	-3.082902	1.862013	4.414395
C	-2.419461	1.392236	2.401866
H	-1.990408	2.390736	2.260869
H	-1.599619	0.745145	2.733771
Ni	-0.142457	-0.908205	0.597072
P	-1.695058	0.485306	-0.226827
C	0.916343	-3.577326	-0.492499
C	2.201251	-3.525139	-0.993077
C	3.237302	-2.940967	-0.231505
C	2.958030	-2.412518	1.026432
C	1.638452	-2.470368	1.516459
C	0.582270	-3.060634	0.789423
H	0.131759	-4.054099	-1.072625
H	2.451861	-3.929957	-1.968861
H	3.734442	-1.961176	1.632217
H	1.459630	-2.137497	2.537132
B	-0.884871	-3.330462	1.461020
O	-0.800601	-3.908328	2.771549
H	-1.497611	-4.567910	2.861021
O	-1.517381	-1.916668	1.606364
H	-1.546367	-1.744740	2.556929
F	-1.715845	-4.048569	0.577646
O	4.466078	-2.953244	-0.816973
C	5.549211	-2.355318	-0.119298
H	6.422197	-2.472092	-0.763378
H	5.370495	-1.288113	0.058505
H	5.738491	-2.857182	0.838340
O	1.445189	-0.231865	-1.495471
C	1.265349	-0.047517	-0.298517
C	5.833404	2.628752	-0.841103
C	5.386288	2.846570	0.441191
C	4.178902	2.257411	0.904731
C	3.407345	1.424686	0.019150
C	3.905398	1.219244	-1.299590
C	5.083810	1.805418	-1.712367
H	4.331579	3.117026	2.883780
H	6.758097	3.083728	-1.184416

H	5.952419	3.473994	1.125147
C	3.732734	2.483338	2.234257
C	2.187095	0.840606	0.521055
H	3.336088	0.592790	-1.971954
H	5.440664	1.630633	-2.723573
C	1.810310	1.094331	1.831040
C	2.569486	1.911836	2.693815
H	0.889140	0.646106	2.197053
H	2.232695	2.084633	3.711745

TS12

B3LYP/BSI SCF energy: -2339.477284a.u.

M06/BSII SCF energy in solution: -2338.70034a.u.

M06/BSII free energy in solution: -2337.985319a.u.

C	2.018307	1.859093	0.210935
H	1.183746	2.061985	0.896565
C	1.695267	2.577282	-1.118245
H	2.525101	2.428019	-1.821454
H	0.799862	2.151903	-1.579480
C	1.500761	4.086578	-0.897935
H	0.618708	4.243362	-0.262570
H	1.285904	4.575372	-1.855794
C	2.732618	4.720848	-0.238138
H	3.581039	4.673337	-0.936304
H	2.554474	5.783989	-0.037323
C	3.105132	3.990417	1.059629
H	2.312229	4.148303	1.804092
H	4.022450	4.413318	1.487074
C	3.287880	2.476749	0.839707
H	3.526681	2.003264	1.796093
H	4.150708	2.310535	0.182960
C	2.783044	-0.626659	1.634294
H	3.775372	-0.153618	1.648001
C	2.015768	-0.176497	2.899671
H	1.888857	0.910970	2.914451
H	1.002836	-0.592066	2.875309
C	2.739364	-0.622575	4.181288
H	3.708260	-0.106267	4.252842
H	2.155869	-0.311808	5.056154
C	2.973010	-2.138613	4.203506
H	3.527641	-2.427763	5.104501
H	2.003181	-2.652592	4.250340
C	3.722396	-2.594040	2.944502
H	3.840310	-3.684313	2.942813
H	4.737481	-2.170148	2.951888
C	2.993040	-2.157734	1.661694
H	2.023371	-2.663023	1.609194
H	3.569045	-2.489490	0.791114
C	3.056978	-0.625012	-1.314983
H	3.068484	-1.704765	-1.114754
C	4.520241	-0.137183	-1.302138
H	4.968550	-0.272768	-0.311899
H	4.552218	0.938308	-1.518623
C	5.357584	-0.882802	-2.357275
H	6.386752	-0.504156	-2.350440
H	5.414417	-1.945947	-2.083883
C	4.749929	-0.751026	-3.761154
H	4.807207	0.298883	-4.082377
H	5.335518	-1.330047	-4.484938
C	3.282056	-1.203367	-3.779752
H	3.234366	-2.283821	-3.580144
H	2.848564	-1.050353	-4.775393
C	2.447584	-0.455797	-2.725276
H	2.406947	0.606250	-2.992534
H	1.410696	-0.812638	-2.734717
Ni	-0.134302	-0.984563	-0.145627
P	1.927335	-0.020573	0.065017
C	-2.785317	-2.050870	0.821358
C	-4.159729	-2.262728	0.681576
C	-4.713174	-2.348541	-0.601813
C	-3.877341	-2.236045	-1.726183
C	-2.515967	-2.039396	-1.553246
C	-1.904970	-1.942556	-0.275156
H	-2.381187	-1.969605	1.826869
H	-4.782055	-2.345791	1.565609
H	-4.324773	-2.312651	-2.712713
H	-1.899252	-1.982091	-2.449609
B	-0.411549	-3.444693	-0.073601
O	-0.929453	-4.523546	-0.768557
H	-1.674898	-4.919513	-0.304095
C	-1.043206	0.448982	0.638088
O	-1.007918	0.511471	1.864364
O	-6.035710	-2.548060	-0.866587
C	-6.933816	-2.645264	0.227848
H	-6.934540	-1.730157	0.833420
H	-7.924272	-2.789590	-0.206905
H	-6.695563	-3.500462	0.873368

C	-3.334334	3.953609	2.215962
C	-2.626309	2.862993	1.756630
C	-2.506414	2.599452	0.362366
C	-3.151586	3.509809	-0.547082
C	-3.872262	4.622825	-0.035890
C	-3.964381	4.845256	1.318159
H	-3.410156	4.128444	3.285784
H	-2.149913	2.182990	2.448669
C	-1.781785	1.479412	-0.191089
C	-3.066153	3.291766	-1.948079
H	-4.352360	5.296949	-0.741055
H	-4.518504	5.699015	1.697936
C	-2.372191	2.217693	-2.452622
C	-1.737844	1.322102	-1.566716
H	-3.563998	3.991705	-2.614848
H	-2.312700	2.052166	-3.524442
H	-1.191513	0.471506	-1.963352
F	-0.259139	-3.511169	1.283300
O	0.685947	-2.792175	-0.733840
H	0.621253	-2.955277	-1.684482

IM13

B3LYP/BSI SCF energy: -2062.962795a.u.

M06/BSII SCF energy in solution: -2062.19422a.u.

M06/BSII free energy in solution: -2061.515359a.u.

C	-2.339652	0.435164	-1.165480
H	-2.155338	-0.646548	-1.083327
C	-1.802665	0.865454	-2.548479
H	-1.967784	1.942376	-2.687019
H	-0.720642	0.700381	-2.603679
C	-2.511662	0.100860	-3.679016
H	-2.251836	-0.964231	-3.604684
H	-2.138895	0.446257	-4.650876
C	-4.036766	0.264252	-3.604773
H	-4.297753	1.312539	-3.809753
H	-4.521881	-0.334790	-4.384471
C	-4.575802	-0.126177	-2.220782
H	-4.428118	-1.203892	-2.063280
H	-5.656793	0.051102	-2.168647
C	-3.866884	0.650457	-1.095822
H	-4.265248	0.339081	-0.124915
H	-4.099640	1.715890	-1.200806
C	-2.172113	0.603049	1.813831
H	-3.112417	1.173648	1.841984
C	-2.518277	-0.903253	1.854836
H	-3.123676	-1.195096	0.990852
H	-1.590750	-1.483436	1.804922
C	-3.268606	-1.267220	3.147882
H	-4.240303	-0.752359	3.161101
H	-3.485010	-2.342108	3.154072
C	-2.466746	-0.875274	4.396210
H	-3.040260	-1.099014	5.303776
H	-1.552631	-1.482453	4.442116
C	-2.082179	0.610017	4.360560
H	-1.455755	0.862861	5.224210
H	-2.990680	1.224346	4.442818
C	-1.338228	0.972961	3.063509
H	-0.385004	0.431407	3.022113
H	-1.097914	2.042082	3.074280
C	-1.285215	2.970422	0.281136
H	-0.939259	3.165584	1.306676
C	-2.635936	3.693381	0.108309
H	-3.393391	3.277427	0.782357
H	-3.003617	3.540551	-0.914094
C	-2.487392	5.205444	0.355634
H	-3.454292	5.701780	0.209072
H	-2.206160	5.373651	1.404889
C	-1.423576	5.823990	-0.563042
H	-1.766448	5.758588	-1.605707
H	-1.303558	6.890971	-0.341462
C	-0.077691	5.097321	-0.426653
H	0.327000	5.267812	0.580890
H	0.654316	5.511680	-1.129616
C	-0.219861	3.583169	-0.657524
H	-0.495773	3.400573	-1.704047
H	0.751783	3.096122	-0.501313
Ni	0.922434	0.472258	0.081000
P	-1.265859	1.084727	0.236967
C	3.668107	0.277715	1.002693
C	5.032743	0.581318	0.942264
C	5.574816	1.090267	-0.244123
C	4.744629	1.283633	-1.356350
C	3.388733	0.974449	-1.274015
C	2.801722	0.481701	-0.084799
H	3.270386	-0.138962	1.925780
H	5.657256	0.412602	1.813002
H	5.185335	1.669263	-2.271356

H	2.778221	1.130799	-2.162855
C	0.947138	-1.285008	0.599366
O	1.051237	-1.521914	1.794361
O	6.893560	1.419558	-0.421198
C	7.779917	1.224137	0.665522
H	8.764257	1.541214	0.315507
H	7.496930	1.829032	1.537521
H	7.828793	0.169550	0.968162
C	-0.655098	-6.326928	0.358536
C	-0.433958	-5.911555	-0.933874
C	0.028813	-4.596824	-1.210954
C	0.265318	-3.683453	-0.124988
C	0.033493	-4.152525	1.198662
C	-0.414989	-5.436003	1.429324
H	0.090891	-4.893705	-3.352171
H	-1.007208	-7.334870	0.558559
H	-0.607180	-6.586206	-1.768636
C	0.266286	-4.182361	-2.548756
C	0.715853	-2.350034	-0.444268
H	0.235415	-3.485117	2.025066
H	-0.580278	-5.768621	2.450399
C	0.930763	-2.002593	-1.768147
C	0.717319	-2.912791	-2.824640
H	1.289858	-0.999861	-1.977907
H	0.912270	-2.606173	-3.848052

TS13

B3LYP/BSI SCF energy: -2062.952274a.u.

M06/BSII SCF energy in solution: -2062.18644a.u.

M06/BSII free energy in solution: -2061.506835a.u.

C	-0.418432	2.596102	1.031660
H	-1.513190	2.510770	0.971391
C	-0.042009	2.228685	2.484449
H	1.045775	2.278734	2.614102
H	-0.334234	1.194155	2.698378
C	-0.710872	3.186511	3.485767
H	-1.800454	3.048193	3.442257
H	-0.404950	2.928471	4.506601
C	-0.373657	4.653947	3.181628
H	0.701229	4.818813	3.343979
H	-0.899016	5.317132	3.878879
C	-0.725245	5.018578	1.732292
H	-1.815165	4.971040	1.598457
H	-0.429729	6.052238	1.515685
C	-0.051447	4.063352	0.730947
H	-0.333790	4.336013	-0.292127
H	1.036283	4.188007	0.802129
C	-0.756492	1.798820	-1.810956
H	-0.386975	2.794636	-2.093079
C	-2.289094	1.886463	-1.634238
H	-2.548189	2.639932	-0.882373
H	-2.666469	0.926202	-1.261699
C	-2.992848	2.239146	-2.956135
H	-2.701812	3.254088	-3.264261
H	-4.077146	2.260941	-2.795667
C	-2.636266	1.250422	-4.073481
H	-3.119635	1.545276	-5.012589
H	-3.027046	0.256477	-3.815681
C	-1.116242	1.163574	-4.260395
H	-0.864862	0.418749	-5.024845
H	-0.739392	2.128873	-4.628915
C	-0.404236	0.807603	-2.944440
H	-0.700130	-0.203032	-2.632555
H	0.678435	0.779408	-3.112766
C	1.948229	1.458694	-0.637252
H	2.107650	0.573804	-1.271672
C	2.399232	2.688735	-1.454274
H	1.789057	2.804887	-2.355625
H	2.261410	3.601305	-0.862831
C	3.881806	2.570104	-1.853931
H	4.186035	3.465574	-2.409336
H	4.001181	1.721219	-2.542015
C	4.787821	2.362978	-0.631822
H	4.761449	3.266625	-0.005631
H	5.829553	2.235079	-0.949220
C	4.330728	1.157290	0.200354
H	4.473231	0.234783	-0.378022
H	4.949726	1.057795	1.100037
C	2.851053	1.276038	0.602777
H	2.735176	2.141750	1.268158
H	2.546818	0.392240	1.173550
Ni	-0.498684	-0.927516	0.322323
P	0.111270	1.288685	-0.218649
O	-0.243287	-3.483148	-0.786112
C	0.045276	-2.613380	0.009308
C	-2.312647	-1.391775	0.480268
C	-3.030762	-2.318638	-0.281638

C	-3.041305	-0.618321	1.409794
C	-4.420238	-2.455809	-0.163760
H	-2.496110	-2.962535	-0.975177
C	-4.421510	-0.752574	1.551705
H	-2.534143	0.111302	2.040556
C	-5.121185	-1.670733	0.757668
H	-4.935458	-3.182055	-0.783410
H	-4.977163	-0.156885	2.270528
O	-6.477460	-1.725293	0.962358
C	-7.225307	-2.650560	0.196009
H	-8.264494	-2.538185	0.511694
H	-7.152990	-2.443408	-0.880473
H	-6.904710	-3.685355	0.377405
C	2.498006	-2.295840	2.918401
C	3.723172	-2.477812	2.318634
C	3.824753	-2.719644	0.920911
C	2.630529	-2.786820	0.127015
C	1.365355	-2.577059	0.776138
C	1.318392	-2.329121	2.139682
H	5.984462	-2.848926	0.901040
H	2.429799	-2.124695	3.988668
H	4.635767	-2.443901	2.908497
C	5.085840	-2.901198	0.291468
C	2.753804	-3.047998	-1.265164
H	0.350333	-2.182422	2.611561
C	3.994139	-3.216339	-1.842742
C	5.171680	-3.140508	-1.061442
H	1.853568	-3.135338	-1.861540
H	4.069048	-3.418896	-2.907305
H	6.141238	-3.278653	-1.531233

IM14

B3LYP/BSI SCF energy: -2062.952328a.u.

M06/BSII SCF energy in solution: -2062.19225a.u.

M06/BSII free energy in solution: -2061.514682a.u.

C	0.316216	2.605832	-0.919747
H	1.391239	2.407747	-1.041245
C	-0.300614	2.493842	-2.332919
H	-1.380884	2.670269	-2.285170
H	-0.172011	1.478084	-2.722760
C	0.330541	3.516342	-3.293420
H	1.393631	3.272205	-3.434369
H	-0.140294	3.438866	-4.280638
C	0.209110	4.949376	-2.754443
H	-0.851954	5.235612	-2.727813
H	0.704535	5.654693	-3.432141
C	0.797476	5.065759	-1.341007
H	1.883253	4.898310	-1.384176
H	0.654754	6.080456	-0.950244
C	0.167344	4.042515	-0.379085
H	0.623481	4.136412	0.612815
H	-0.897539	4.277225	-0.258997
C	0.893842	1.421940	1.740735
H	0.633088	2.383227	2.203330
C	2.396400	1.456433	1.389304
H	2.617009	2.293020	0.717873
H	2.666007	0.540764	0.848545
C	3.275143	1.576474	2.646341
H	3.095281	2.551201	3.122597
H	4.332100	1.562591	2.354512
C	2.984304	0.458329	3.655737
H	3.594448	0.590831	4.557163
H	3.273869	-0.507201	3.218132
C	1.494022	0.424906	4.018731
H	1.283332	-0.407558	4.700529
H	1.230152	1.345222	4.559615
C	0.611552	0.298711	2.766092
H	0.801859	-0.672546	2.288373
H	-0.444095	0.298566	3.059307
C	-1.940151	1.479254	0.880587
H	-2.131030	0.520156	1.380977
C	-2.161124	2.596351	1.922815
H	-1.444958	2.515656	2.746938
H	-2.000566	3.579150	1.463270
C	-3.592217	2.534914	2.490413
H	-3.738951	3.351254	3.208351
H	-3.712973	1.598740	3.053288
C	-4.653349	2.597381	1.382212
H	-4.615056	3.585979	0.901644
H	-5.656650	2.500222	1.813963
C	-4.416711	1.510888	0.324558
H	-4.571406	0.518944	0.768956
H	-5.145761	1.606110	-0.489109
C	-2.990845	1.582281	-0.247349
H	-2.870887	2.537749	-0.774892
H	-2.843620	0.780849	-0.977465
Ni	0.059595	-0.959045	-0.741048

P	-0.196749	1.191673	0.218431
O	0.644332	-3.640581	-1.665877
C	0.802803	-2.469853	-1.413014
C	-1.612739	-1.778526	-0.445104
C	-2.059385	-2.087035	0.855398
C	-2.486059	-2.087471	-1.498877
C	-3.316867	-2.642354	1.092342
H	-1.416069	-1.899673	1.712896
C	-3.760040	-2.630934	-1.280930
H	-2.178986	-1.914689	-2.527551
C	-4.179996	-2.912053	0.022799
H	-3.647780	-2.881473	2.099209
H	-4.397968	-2.843458	-2.132053
O	-5.397989	-3.451833	0.356042
C	-6.284305	-3.783060	-0.695701
H	-7.172338	-4.208438	-0.223804
H	-6.577783	-2.898944	-1.278684
H	-5.849478	-4.525887	-1.378107
C	5.468519	-2.729803	0.979142
C	5.526372	-1.621883	0.161638
C	4.423271	-1.266347	-0.657839
C	3.242120	-2.076739	-0.624265
C	3.215851	-3.217296	0.219822
C	4.305037	-3.532953	1.005647
H	5.372047	0.472234	-1.537417
H	6.318938	-2.992353	1.601701
H	6.420694	-1.004600	0.131681
C	4.465568	-0.127495	-1.514889
C	2.131987	-1.714671	-1.465965
H	2.332069	-3.845274	0.225284
H	4.272151	-4.409895	1.645472
C	2.213063	-0.584420	-2.270419
C	3.391716	0.206208	-2.303441
H	1.388561	-0.348739	-2.939381
H	3.441243	1.066792	-2.964248

TS14

B3LYP/BSI SCF energy: -2062.95098a.u.

M06/BSII SCF energy in solution: -2062.18617a.u.

M06/BSII free energy in solution: -2061.505406a.u.

C	-2.390487	-1.171069	-1.321724
H	-1.511004	-1.823456	-1.428307
C	-2.470742	-0.330221	-2.614535
H	-3.340535	0.338268	-2.565329
H	-1.586031	0.311038	-2.706554
C	-2.608004	-1.228762	-3.855591
H	-1.691423	-1.824510	-3.970526
H	-2.692524	-0.608747	-4.756302
C	-3.815175	-2.170518	-3.739475
H	-4.739282	-1.574746	-3.749789
H	-3.864341	-2.835700	-4.609765
C	-3.758983	-2.991490	-2.443320
H	-2.899914	-3.676041	-2.483965
H	-4.653207	-3.619631	-2.350668
C	-3.626049	-2.089807	-1.201962
H	-3.565959	-2.712840	-0.304093
H	-4.535039	-1.486031	-1.102653
C	-2.086501	-1.304341	1.634709
H	-3.141620	-1.612873	1.671632
C	-1.210822	-2.568678	1.467220
H	-1.453860	-3.097515	0.539299
H	-0.160555	-2.263596	1.398257
C	-1.378456	-3.526802	2.658947
H	-2.412659	-3.900800	2.685808
H	-0.733586	-4.402193	2.516860
C	-1.051674	-2.833092	3.987696
H	-1.215975	-3.518951	4.827671
H	0.012721	-2.563604	3.999000
C	-1.893507	-1.561824	4.163676
H	-1.611208	-1.041540	5.086846
H	-2.952892	-1.837727	4.271967
C	-1.734640	-0.605977	2.968425
H	-0.696827	-0.253740	2.917333
H	-2.368527	0.273539	3.128642
C	-3.176671	1.209770	0.494931
H	-2.943749	1.488444	1.532655
C	-4.665595	0.813229	0.449336
H	-4.854105	-0.072154	1.066817
H	-4.941254	0.546039	-0.578594
C	-5.562751	1.975083	0.912890
H	-6.616722	1.678001	0.851224
H	-5.359742	2.186784	1.972234
C	-5.314999	3.243291	0.083341
H	-5.633081	3.063258	-0.953718
H	-5.930848	4.069374	0.458254
C	-3.830703	3.637158	0.096092
H	-3.544589	3.938282	1.113848

H	-3.661683	4.510233	-0.545357
C	-2.926895	2.476817	-0.354975
H	-3.118112	2.261016	-1.413722
H	-1.873482	2.775289	-0.283830
Ni	0.118687	0.773261	0.065056
P	-1.887398	-0.132733	0.173142
C	1.989430	2.456908	1.336833
C	2.626328	3.687819	1.300468
C	3.163086	4.163811	0.091035
C	3.062876	3.386570	-1.070150
C	2.407640	2.152190	-1.017377
C	1.827542	1.676973	0.170621
H	1.630387	2.058442	2.281838
H	2.745810	4.295137	2.192614
H	3.493116	3.723045	-2.006554
H	2.360175	1.554386	-1.922767
C	1.634838	-0.180602	0.585750
O	1.701793	-0.418885	1.799819
O	3.779477	5.378157	0.158959
C	4.368469	5.902842	-1.020080
H	4.795329	6.867343	-0.740289
H	5.166582	5.251511	-1.398826
H	3.624198	6.054320	-1.812536
C	5.700081	-3.552557	0.362796
C	5.123533	-3.544920	-0.885661
C	3.996247	-2.725560	-1.165653
C	3.447314	-1.896981	-0.125629
C	4.071439	-1.932114	1.153771
C	5.167020	-2.734926	1.386460
H	3.836328	-3.357005	-3.228848
H	6.562667	-4.181573	0.564388
H	5.524473	-4.165042	-1.683750
C	3.410209	-2.717661	-2.459499
C	2.314150	-1.065469	-0.440006
H	3.656554	-1.322810	1.945250
H	5.626477	-2.741281	2.371059
C	1.794664	-1.088185	-1.723577
C	2.328493	-1.914809	-2.735554
H	0.938727	-0.450801	-1.940035
H	1.884160	-1.909923	-3.727011

TS15

B3LYP/BSI SCF energy: -2062.947824a.u.

M06/BSII SCF energy in solution: -2062.18921a.u.

M06/BSII free energy in solution: -2061.510284a.u.

C	-0.475995	2.354098	1.027129
H	-1.528699	2.069138	1.168192
C	0.202396	2.170286	2.404291
H	1.265469	2.424391	2.337135
H	0.157164	1.119101	2.710192
C	-0.459021	3.065157	3.466178
H	-1.497833	2.738439	3.618909
H	0.052228	2.939555	4.428082
C	-0.450172	4.542408	3.045805
H	0.588689	4.900102	3.008822
H	-0.963966	5.155549	3.795662
C	-1.098150	4.733835	1.667017
H	-2.168524	4.491522	1.732065
H	-1.035206	5.784119	1.357648
C	-0.442982	3.836172	0.601626
H	-0.945013	3.979050	-0.361902
H	0.598759	4.151216	0.462053
C	-1.090757	1.361628	-1.700737
H	-0.847171	2.343082	-2.127867
C	-2.581274	1.387578	-1.301692
H	-2.774055	2.196935	-0.589614
H	-2.844242	0.452851	-0.794719
C	-3.490236	1.575230	-2.529638
H	-3.316604	2.572853	-2.958680
H	-4.539756	1.551202	-2.212887
C	-3.231640	0.511432	-3.604806
H	-3.862655	0.697594	-4.482238
H	-3.517242	-0.474800	-3.214352
C	-1.751291	0.487370	-4.008212
H	-1.565532	-0.308759	-4.739136
H	-1.492892	1.433453	-4.505518
C	-0.839800	0.288963	-2.785838
H	-1.029137	-0.703393	-2.355001
H	0.209750	0.296834	-3.102106
C	1.766477	1.547591	-0.950850
H	2.050246	0.617149	-1.460746
C	1.830235	2.686859	-1.991872
H	1.117771	2.520921	-2.805933
H	1.555447	3.640900	-1.524390
C	3.244876	2.804877	-2.590697
H	3.272741	3.637333	-3.304511
H	3.464831	1.894073	-3.165207

C	4.316984	2.989102	-1.508791
H	4.172044	3.962707	-1.018096
H	5.314020	3.016082	-1.964567
C	4.237345	1.875059	-0.456349
H	4.499183	0.911481	-0.913099
H	4.968513	2.051139	0.341871
C	2.827522	1.771401	0.149448
H	2.606725	2.703087	0.687000
H	2.797285	0.955103	0.876459
Ni	0.020299	-1.049105	0.727674
P	0.075484	1.079823	-0.245192
O	-0.576389	-3.325644	2.395861
C	-0.527038	-2.367722	1.706092
C	1.811700	-1.654252	0.434447
C	2.249586	-1.947487	-0.874929
C	2.742741	-1.878337	1.460840
C	3.538213	-2.407460	-1.145254
H	1.571951	-1.818141	-1.718189
C	4.048607	-2.325563	1.212639
H	2.458122	-1.708454	2.496992
C	4.451171	-2.593313	-0.099216
H	3.858105	-2.631780	-2.159112
H	4.726197	-2.474045	2.046577
O	5.697000	-3.040916	-0.462883
C	6.642063	-3.274457	0.563951
H	7.547910	-3.630680	0.069279
H	6.875951	-2.357321	1.122064
H	6.295763	-4.039086	1.272412
C	-4.796382	-3.028850	-1.401236
C	-5.227837	-2.187435	-0.400705
C	-4.312784	-1.648434	0.544050
C	-2.920598	-1.984479	0.442398
C	-2.512273	-2.861131	-0.600863
C	-3.425751	-3.370883	-1.498315
H	-5.796039	-0.534206	1.659398
H	-5.506042	-3.438723	-2.114011
H	-6.279875	-1.926775	-0.315109
C	-4.740409	-0.784503	1.588833
C	-1.997613	-1.434074	1.393736
H	-1.463931	-3.133946	-0.677669
H	-3.094482	-4.044703	-2.283134
C	-2.471523	-0.621889	2.411011
C	-3.842253	-0.283712	2.504670
H	-1.783034	-0.246866	3.163888
H	-4.183261	0.364405	3.307317

IM15

B3LYP/BSI SCF energy: -2062.962102a.u.

M06/BSII SCF energy in solution: -2062.20135a.u.

M06/BSII free energy in solution: -2061.519955a.u.

C	0.416945	2.339768	-0.971446
H	1.483788	2.119980	-1.111087
C	-0.233748	2.213942	-2.368480
H	-1.308543	2.411037	-2.304390
H	-0.128696	1.189710	-2.743419
C	0.396677	3.210988	-3.355864
H	1.453261	2.950066	-3.509780
H	-0.092541	3.124383	-4.333372
C	0.301530	4.653506	-2.836990
H	-0.755408	4.953362	-2.795132
H	0.792919	5.342240	-3.534353
C	0.918792	4.784976	-1.437319
H	2.000998	4.603104	-1.499322
H	0.795671	5.807169	-1.059643
C	0.297595	3.785458	-0.444670
H	0.783340	3.887373	0.531858
H	-0.759713	4.038870	-0.297319
C	1.022053	1.253916	1.721597
H	0.658232	2.180523	2.182934
C	2.519719	1.468768	1.414891
H	2.656266	2.315790	0.734531
H	2.929945	0.590445	0.910461
C	3.309501	1.730205	2.710695
H	2.977648	2.680385	3.154444
H	4.371999	1.852982	2.469778
C	3.121051	0.601164	3.733201
H	3.666172	0.829640	4.656939
H	3.552772	-0.325550	3.331846
C	1.633215	0.374526	4.034729
H	1.505387	-0.467579	4.725476
H	1.223774	1.259875	4.542548
C	0.835761	0.111891	2.746302
H	1.183000	-0.826075	2.298151
H	-0.224743	-0.027143	2.987452
C	-1.817471	1.335377	0.909598
H	-2.117031	0.348520	1.285478
C	-1.930755	2.333152	2.085005

H	-1.257846	2.062170	2.903083
H	-1.639718	3.339553	1.757305
C	-3.369446	2.373656	2.635215
H	-3.427994	3.105835	3.449834
H	-3.606967	1.395891	3.077266
C	-4.400464	2.697928	1.547065
H	-4.243313	3.727394	1.193506
H	-5.414422	2.663271	1.963200
C	-4.271014	1.731100	0.363102
H	-4.545597	0.716227	0.679060
H	-4.968671	2.009948	-0.436050
C	-2.836432	1.710936	-0.189993
H	-2.599759	2.707820	-0.583032
H	-2.775385	1.006784	-1.022777
Ni	0.140732	-1.079664	-0.822695
P	-0.084752	0.972340	0.219164
O	0.293502	-3.494212	-2.434162
C	0.240331	-2.552216	-1.779190
C	-1.725248	-1.638654	-0.514202
C	-2.069654	-2.216758	0.725820
C	-2.742901	-1.591550	-1.477718
C	-3.355813	-2.676972	1.001177
H	-1.318787	-2.308497	1.509888
C	-4.047014	-2.043356	-1.225006
H	-2.534030	-1.188777	-2.467790
C	-4.357897	-2.588915	0.024403
H	-3.607176	-3.113951	1.963430
H	-4.795563	-1.974217	-2.006705
O	-5.590547	-3.064994	0.387130
C	-6.631434	-3.013192	-0.571692
H	-7.513148	-3.435553	-0.086197
H	-6.850767	-1.982012	-0.880350
H	-6.393970	-3.606863	-1.464580
C	4.893502	-3.149467	1.151073
C	5.343878	-2.320388	0.148438
C	4.438191	-1.569471	-0.649816
C	3.025210	-1.665940	-0.395235
C	2.604685	-2.543469	0.645708
C	3.504816	-3.267595	1.397950
H	5.962699	-0.662663	-1.896276
H	5.599500	-3.719493	1.748541
H	6.409002	-2.232369	-0.053713
C	4.894993	-0.732969	-1.703300
C	2.085725	-0.900377	-1.172768
H	1.538863	-2.642104	0.837580
H	3.150115	-3.933925	2.179415
C	2.599154	-0.138268	-2.211610
C	3.990505	-0.043336	-2.474955
H	1.927156	0.414867	-2.863102
H	4.337201	0.580514	-3.295648

TS16

B3LYP/BSI SCF energy: -2062.944061a.u.

M06/BSII SCF energy in solution: -2062.18795a.u.

M06/BSII free energy in solution: -2061.508244a.u.

C	2.402455	2.031990	0.126637
H	2.284462	2.448164	-0.884828
C	1.650202	2.997635	1.070688
H	1.748956	2.657790	2.108217
H	0.579559	2.996137	0.841280
C	2.214220	4.424826	0.959263
H	2.019689	4.809588	-0.051743
H	1.683860	5.088703	1.652359
C	3.724226	4.459839	1.237276
H	3.902683	4.196101	2.289685
H	4.114147	5.475493	1.100703
C	4.481696	3.473260	0.336978
H	4.412234	3.806384	-0.708222
H	5.548663	3.466536	0.591049
C	3.910390	2.047397	0.449732
H	4.464347	1.374882	-0.214260
H	4.071701	1.685129	1.473039
C	2.535984	-0.448048	-1.467360
H	3.589821	-0.447157	-1.155715
C	2.433321	0.343643	-2.789894
H	2.772009	1.376792	-2.656981
H	1.379934	0.395186	-3.095198
C	3.256446	-0.317584	-3.908767
H	4.323362	-0.272143	-3.646894
H	3.140085	0.254055	-4.837410
C	2.849355	-1.781025	-4.125357
H	3.481803	-2.242664	-4.893158
H	1.818514	-1.816422	-4.504987
C	2.930602	-2.575358	-2.814713
H	2.580434	-3.602958	-2.968588
H	3.981704	-2.647622	-2.499055
C	2.104356	-1.913975	-1.698404

H	1.043728	-1.938935	-1.969099
H	2.200657	-2.499612	-0.778518
C	1.926401	-0.732478	1.416128
H	1.261997	-1.589407	1.236911
C	3.364302	-1.278357	1.570011
H	3.707940	-1.759199	0.649479
H	4.057084	-0.452363	1.768087
C	3.448132	-2.288572	2.729388
H	4.478807	-2.650455	2.828905
H	2.830984	-3.164987	2.486699
C	2.965453	-1.678240	4.052163
H	3.659668	-0.881753	4.357235
H	2.986588	-2.430992	4.849231
C	1.553483	-1.093195	3.908939
H	0.838190	-1.905873	3.728148
H	1.247441	-0.603332	4.841536
C	1.473265	-0.089963	2.745816
H	2.120420	0.765838	2.976053
H	0.453924	0.302051	2.655865
Ni	-0.694260	0.706844	-0.649560
P	1.542641	0.359700	-0.080211
O	-0.695787	3.208566	-2.194131
C	-0.654962	2.280135	-1.508273
C	-2.618024	0.595900	-0.300778
C	-3.702736	0.663508	-1.189296
C	-2.844956	1.072189	1.010581
C	-4.939433	1.192637	-0.816799
H	-3.595801	0.281514	-2.199792
C	-4.068196	1.613654	1.394083
H	-2.045252	1.058503	1.745829
C	-5.130706	1.674381	0.484261
H	-5.741676	1.217011	-1.545671
H	-4.223198	1.988632	2.401284
O	-6.300019	2.202502	0.959674
C	-7.401602	2.287080	0.072949
H	-8.216777	2.735332	0.643822
H	-7.178669	2.922429	-0.794609
H	-7.714857	1.296655	-0.283384
C	-1.614536	-2.715361	-2.474169
C	-1.648050	-3.754453	-1.572360
C	-1.644429	-3.483528	-0.177664
C	-1.573182	-2.123927	0.291268
C	-1.516164	-1.042652	-0.665027
C	-1.578188	-1.378173	-2.022594
H	-1.760548	-5.563550	0.395579
H	-1.632023	-2.915458	-3.542758
H	-1.696774	-4.786600	-1.908968
C	-1.708076	-4.543124	0.768015
C	-1.573933	-1.915124	1.695441
H	-1.605978	-0.586680	-2.768238
C	-1.649320	-2.964166	2.589374
C	-1.713842	-4.296149	2.121990
H	-1.533386	-0.901180	2.069650
H	-1.665701	-2.764567	3.657165
H	-1.772373	-5.118395	2.829630

IM16

B3LYP/BSI SCF energy: -2063.002432a.u.

M06/BSII SCF energy in solution: -2062.24293a.u.

M06/BSII free energy in solution: -2061.562755a.u.

C	-2.532591	0.297113	-1.360211
H	-2.458435	1.383151	-1.213142
C	-1.697561	-0.018379	-2.621404
H	-1.745276	-1.094829	-2.831330
H	-0.644328	0.230430	-2.452845
C	-2.228138	0.748969	-3.844224
H	-2.087472	1.824248	-3.673371
H	-1.635897	0.489649	-4.730394
C	-3.713842	0.452559	-4.092752
H	-3.830174	-0.603173	-4.377790
H	-4.086715	1.045227	-4.936820
C	-4.553640	0.729172	-2.837601
H	-4.539831	1.807667	-2.624339
H	-5.602812	0.460445	-3.012259
C	-4.020105	-0.032470	-1.609528
H	-4.632239	0.218549	-0.736663
H	-4.143003	-1.108760	-1.775727
C	-3.053482	-0.134053	1.518332
H	-3.955266	-0.643542	1.151368
C	-3.393859	1.360153	1.713176
H	-3.704468	1.812807	0.764750
H	-2.484329	1.889112	2.031052
C	-4.496528	1.568526	2.765092
H	-5.434129	1.127837	2.396960
H	-4.687388	2.641014	2.893809
C	-4.125422	0.924445	4.107282
H	-4.944735	1.041877	4.826514

H	-3.257496	1.448392	4.532331
C	-3.779911	-0.559339	3.926357
H	-3.465132	-0.997592	4.880885
H	-4.681991	-1.105695	3.615114
C	-2.675032	-0.765566	2.875866
H	-1.739927	-0.316328	3.234571
H	-2.482251	-1.837665	2.765500
C	-1.521555	-2.226155	0.100569
H	-1.288419	-2.475782	1.145657
C	-2.754498	-3.058518	-0.304497
H	-3.636765	-2.765208	0.275812
H	-2.994241	-2.871033	-1.358688
C	-2.485482	-4.563594	-0.120896
H	-3.364466	-5.140128	-0.434317
H	-2.338370	-4.774664	0.947864
C	-1.243179	-5.014540	-0.903256
H	-1.442656	-4.918332	-1.980354
H	-1.042721	-6.076615	-0.717947
C	-0.014684	-4.167017	-0.540471
H	0.264900	-4.357894	0.505127
H	0.846731	-4.464215	-1.150633
C	-0.287016	-2.663619	-0.720048
H	-0.452948	-2.455932	-1.784224
H	0.590578	-2.082562	-0.416674
Ni	0.266634	0.542745	0.869498
P	-1.701384	-0.347912	0.215034
O	1.435600	-1.253936	2.842132
C	1.032791	-0.526390	2.032130
C	2.656289	1.703058	-0.277360
C	1.654665	2.090430	0.677722
C	2.383883	1.878634	-1.627203
C	0.400589	2.599724	0.223015
H	1.954884	2.243346	1.708896
C	1.187506	2.477565	-2.080387
H	3.141998	1.613455	-2.358445
C	0.217111	2.852525	-1.170969
H	-0.254156	3.082703	0.941615
H	1.027856	2.675142	-3.134954
O	-0.911652	3.442972	-1.679765
C	-1.704946	4.244888	-0.813948
H	-2.456295	4.718651	-1.448418
H	-2.212550	3.647580	-0.047451
H	-1.103939	5.021764	-0.324992
C	5.966870	1.585166	1.575283
C	6.526286	0.403773	1.148530
C	5.825594	-0.438143	0.245637
C	4.527830	-0.045657	-0.230442
C	3.975614	1.210604	0.203098
C	4.697542	1.982534	1.100901
H	7.365752	-1.953638	0.175708
H	6.502736	2.227551	2.268355
H	7.507664	0.095046	1.499292
C	6.379507	-1.674174	-0.186639
C	3.833218	-0.943453	-1.089704
H	4.287655	2.935159	1.424698
C	4.395899	-2.138310	-1.482053
C	5.686989	-2.506053	-1.035380
H	2.838644	-0.678545	-1.428906
H	3.841965	-2.806960	-2.135119
H	6.122630	-3.448631	-1.354570

IM17

B3LYP/BSI SCF energy: -2062.974216a.u.

M06/BSII SCF energy in solution: -2062.21656a.u.

M06/BSII free energy in solution: -2061.534651a.u.

C	-1.739831	-1.904731	-1.247607
H	-0.683835	-2.211146	-1.289031
C	-2.051395	-1.225938	-2.598730
H	-3.101711	-0.906430	-2.615269
H	-1.444747	-0.320239	-2.716225
C	-1.809718	-2.185936	-3.775795
H	-0.738105	-2.425255	-3.830451
H	-2.066674	-1.689769	-4.719503
C	-2.613101	-3.485247	-3.618203
H	-3.686116	-3.255706	-3.688345
H	-2.388026	-4.175537	-4.439921
C	-2.328623	-4.154658	-2.266311
H	-1.282683	-4.492205	-2.241953
H	-2.947455	-5.052317	-2.147278
C	-2.575104	-3.193363	-1.088631
H	-2.336030	-3.701491	-0.149104
H	-3.642166	-2.946897	-1.048116
C	-1.545896	-1.762739	1.707748
H	-2.388224	-2.468943	1.707528
C	-0.228578	-2.570825	1.658400
H	-0.186799	-3.193424	0.757568
H	0.612797	-1.868340	1.594242

C	-0.053860	-3.461061	2.900454
H	-0.840399	-4.229823	2.912409
H	0.902556	-3.993452	2.837101
C	-0.124911	-2.640822	4.194842
H	-0.041754	-3.297566	5.069199
H	0.730963	-1.953401	4.232845
C	-1.427215	-1.832177	4.258133
H	-1.447247	-1.208447	5.160080
H	-2.280298	-2.521765	4.337454
C	-1.608445	-0.942735	3.015575
H	-0.817750	-0.181097	2.993291
H	-2.561272	-0.407462	3.094556
C	-3.400567	0.136832	0.394228
H	-3.292071	0.588480	1.391222
C	-4.636729	-0.783560	0.440060
H	-4.484382	-1.614742	1.137736
H	-4.798586	-1.227923	-0.549972
C	-5.898294	0.004645	0.835667
H	-6.768658	-0.662857	0.839991
H	-5.784276	0.374870	1.864524
C	-6.139632	1.191683	-0.108361
H	-6.375266	0.810431	-1.112454
H	-7.014174	1.766862	0.218697
C	-4.903171	2.099181	-0.192208
H	-4.741441	2.580001	0.783632
H	-5.073275	2.907762	-0.913595
C	-3.638807	1.312624	-0.578901
H	-3.752157	0.934745	-1.602808
H	-2.764588	1.972995	-0.583087
Ni	-0.082853	0.784704	0.060774
P	-1.700118	-0.661659	0.182497
C	0.615549	2.407954	1.061516
C	-0.135377	3.569039	0.728089
C	0.030662	4.172118	-0.511167
C	0.962108	3.642629	-1.443967
C	1.710380	2.529908	-1.130958
C	1.588847	1.883330	0.142975
H	0.662962	2.090347	2.099062
H	-0.815482	3.979173	1.465589
H	1.073927	4.146407	-2.398428
H	2.441634	2.164701	-1.844062
C	2.516960	0.829380	0.643600
O	2.605369	0.588858	1.851861
O	-0.634723	5.284268	-0.936590
C	-1.568745	5.882764	-0.052684
H	-1.980022	6.742837	-0.583372
H	-2.382224	5.191331	0.202769
H	-1.087028	6.224503	0.872536
C	7.530057	-0.650897	0.313779
C	6.906654	-1.157204	-0.802547
C	5.521065	-0.935582	-1.029594
C	4.763082	-0.173724	-0.076460
C	5.441551	0.331616	1.068607
C	6.786751	0.100530	1.254282
H	5.464592	-2.044173	-2.887032
H	8.589777	-0.826061	0.476355
H	7.465947	-1.735704	-1.533668
C	4.877912	-1.459455	-2.182824
C	3.368941	0.063237	-0.340175
H	4.877789	0.886509	1.807065
H	7.282268	0.496362	2.136313
C	2.793643	-0.461782	-1.485630
C	3.540347	-1.233028	-2.404529
H	1.736056	-0.290210	-1.670486
H	3.051054	-1.639799	-3.284938

2b

B3LYP/BSI SCF energy: -844.801874a.u.

M06/BSII SCF energy in solution: -844.41289a.u.

M06/BSII free energy in solution: -844.18584a.u.

C	2.403276	-1.063535	0.873825
C	3.722990	-0.793760	0.527069
C	3.996697	0.203446	-0.422537
C	2.938226	0.914908	-1.010217
C	1.628189	0.644718	-0.643244
C	1.335885	-0.346569	0.313012
H	2.173230	-1.843109	1.592565
H	4.523833	-1.357937	0.989966
H	3.172695	1.668640	-1.754553
H	0.821641	1.193605	-1.116900
C	-0.051867	-0.736175	0.710199
O	-0.256583	-1.832292	1.226739
O	5.242449	0.549360	-0.841254
C	6.359055	-0.144184	-0.300686
H	7.239635	0.289728	-0.776202
H	6.431307	-0.008611	0.785579
H	6.316437	-1.216474	-0.528303

C	-5.037456	-0.974928	-0.905880
C	-4.803980	0.334686	-0.557063
C	-3.529926	0.747001	-0.081092
C	-2.474377	-0.219318	0.038312
C	-2.753084	-1.565431	-0.329595
C	-3.999431	-1.929054	-0.790457
H	-4.105368	2.813340	0.199837
H	-6.014945	-1.279379	-1.268724
H	-5.592094	1.078644	-0.641555
C	-3.289824	2.099266	0.282515
C	-1.184930	0.229346	0.491950
H	-1.974837	-2.309748	-0.224113
H	-4.188743	-2.962920	-1.064833
C	-1.001378	1.562492	0.823975
C	-2.054387	2.499497	0.733022
H	-0.032342	1.890926	1.185607
H	-1.879449	3.532310	1.019091

Ph[Ni]F

B3LYP/BSI SCF energy: -2596.935836a.u.

M06/BSII SCF energy in solution: -2596.03614a.u.

M06/BSII free energy in solution: -2595.055982a.u.

C	0.000007	1.743802	-0.807251
C	-0.000039	1.894489	-2.210434
H	-0.000105	1.010768	-2.845502
C	-0.000008	3.151679	-2.826700
H	-0.000047	3.220268	-3.912788
C	0.000075	4.315329	-2.054481
H	0.000099	5.293174	-2.528575
C	0.000129	4.201125	-0.662127
C	0.000094	2.938355	-0.057569
C	2.795709	-0.798350	1.750960
H	2.251118	-1.749771	1.780547
C	2.226682	0.040548	2.917012
H	2.690938	1.033289	2.940110
H	1.152722	0.191483	2.769354
C	2.477315	-0.658744	4.263950
H	1.910664	-1.599901	4.289038
H	2.091311	-0.038719	5.082348
C	3.968318	-0.957072	4.479185
H	4.518199	-0.008636	4.565244
H	4.118831	-1.490793	5.425367
C	4.547052	-1.770565	3.312520
H	4.080077	-2.765427	3.297806
H	5.622605	-1.932419	3.455236
C	4.297963	-1.079857	1.958824
H	4.695707	-1.703124	1.149658
H	4.860182	-0.137025	1.933854
C	2.836406	-1.539176	-1.117964
H	3.933941	-1.511995	-1.133141
C	2.411865	-2.958854	-0.683627
H	2.837763	-3.198570	0.296262
H	1.325570	-2.986042	-0.556108
C	2.877870	-4.016665	-1.699610
H	3.977086	-4.061019	-1.700184
H	2.528948	-5.006698	-1.381655
C	2.391276	-3.711039	-3.122855
H	2.776572	-4.458016	-3.827501
H	1.294870	-3.786321	-3.154896
C	2.811085	-2.300279	-3.554529
H	2.416369	-2.069337	-4.551512
H	3.906916	-2.255756	-3.635202
C	2.331585	-1.242354	-2.548020
H	1.233758	-1.229372	-2.532957
H	2.646893	-0.245811	-2.877567
C	3.333388	1.308472	-0.456492
H	2.736337	1.729111	-1.276970
C	4.750807	1.033984	-1.006235
H	5.383975	0.608178	-0.217021
H	4.725299	0.299977	-1.817144
C	5.396433	2.328944	-1.535632
H	6.410043	2.113852	-1.895856
H	4.823804	2.679035	-2.406089
C	5.428567	3.437365	-0.474900
H	5.840142	4.359601	-0.902552
H	6.107240	3.140657	0.337951
C	4.029522	3.690241	0.102559
H	3.374928	4.106265	-0.674936
H	4.077974	4.437871	0.903853
C	3.401100	2.394342	0.640632
H	2.401985	2.604258	1.030831
H	4.008941	2.029671	1.478650
C	-3.333388	1.308448	-0.456451
H	-2.736397	1.729025	-1.276999
C	-3.400972	2.394408	0.640600
H	-4.008732	2.029822	1.478717
H	-2.401807	2.604339	1.030667

C	-4.029429	3.690273	0.102485	H	-2.690679	1.033466	2.940074
H	-3.374902	4.106237	-0.675101	H	-1.152539	0.191494	2.769340
H	-4.077793	4.437960	0.903731	F	-0.000032	-1.677102	0.765422
C	-5.428531	3.437374	-0.474829	Ni	-0.000011	0.024552	0.010243
H	-6.107140	3.140756	0.338108	P	2.276991	-0.173006	0.057458
H	-5.840130	4.359577	-0.902530	P	-2.276949	-0.172994	0.057535
C	-5.396509	2.328864	-1.535466	H	0.000195	5.096265	-0.043484
H	-4.823968	2.678877	-2.406014	H	0.000147	2.888314	1.030484
H	-6.410156	2.113744	-1.895571				
C	-4.750840	1.033934	-1.006051	**IM1^{con}-F**			
H	-4.725387	0.299898	-1.816937	B3LYP/BSI SCF energy: -1549.693079a.u.			
H	-5.383948	0.608162	-0.216770	M06/BSII SCF energy in solution: -1549.18516a.u.			
C	-2.836418	-1.539174	-1.117838	M06/BSII free energy in solution: -1548.665224a.u.			
H	-3.933960	-1.511995	-1.132914				
C	-2.331742	-1.242338	-2.547950	C	2.378743	0.517335	-1.136037
H	-2.647043	-0.245771	-2.877427	C	3.076848	1.445804	-0.336834
H	-1.233907	-1.229404	-2.532996	H	2.532891	2.242588	0.167465
C	-2.811424	-2.300193	-3.554440	C	4.465011	1.381572	-0.183520
H	-3.907259	-2.255556	-3.635015	H	4.977588	2.119095	0.429983
H	-2.416777	-2.069241	-4.551448	C	5.195166	0.374023	-0.818468
C	-2.391706	-3.711005	-3.122872	H	6.273788	0.320417	-0.697370
H	-2.777208	-4.457910	-3.827484	C	4.528456	-0.566191	-1.606702
H	-1.295317	-3.786420	-3.155096	C	3.138958	-0.498600	-1.753921
C	-2.878095	-4.016627	-1.699551	C	0.528354	-0.651804	1.423900
H	-2.529204	-5.006701	-1.381689	H	1.359373	0.062304	1.495446
H	-3.977316	-4.060888	-1.699943	C	1.148458	-2.023730	1.077912
C	-2.411851	-2.958878	-0.683623	H	0.350404	-2.770876	0.980957
H	-1.325528	-2.986107	-0.556325	H	1.667963	-1.972364	0.116899
H	-2.837543	-3.198619	0.296347	C	2.125834	-2.482227	2.172753
C	-2.795628	-0.798266	1.751071	H	2.978825	-1.790840	2.203541
H	-2.251057	-1.749696	1.780691	H	2.531916	-3.466867	1.912617
C	-4.297875	-1.079717	1.959006	C	1.449476	-2.527796	3.549238
H	-4.695659	-1.703037	1.149899	H	0.673649	-3.307088	3.546630
H	-4.860081	-0.136880	1.933966	H	2.173039	-2.811529	4.322517
C	-4.546940	-1.770309	3.312767	C	0.808796	-1.176652	3.893551
H	-5.622487	-1.932152	3.455530	H	1.599083	-0.422448	4.014418
H	-4.079960	-2.765168	3.298115	H	0.283621	-1.233988	4.854496
C	-3.968163	-0.956718	4.479342	C	-0.169755	-0.704608	2.801790
H	-4.518001	-0.008250	4.565310	H	-0.564535	0.277829	3.079176
H	-4.118689	-1.490335	5.425580	H	-1.025579	-1.389714	2.764505
C	-2.477150	-0.658475	4.264055	C	-1.445073	1.487065	0.744671
H	-1.910541	-1.599654	4.289223	H	-1.907066	1.100660	1.663218
H	-2.091108	-0.038390	5.082389	C	-0.487096	2.637774	1.130093
C	-2.226506	0.040680	2.917054	H	0.291086	2.283375	1.816539

H	0.026203	2.980911	0.221839
C	-1.239332	3.820508	1.761886
H	-1.676780	3.505226	2.720226
H	-0.529634	4.623768	1.992954
C	-2.351174	4.331701	0.836913
H	-2.900739	5.149759	1.317582
H	-1.900349	4.747354	-0.074765
C	-3.309476	3.196032	0.456315
H	-4.074271	3.558985	-0.240280
H	-3.843651	2.859940	1.357358
C	-2.573490	2.001890	-0.176642
H	-2.150240	2.275274	-1.149429
H	-3.299311	1.204301	-0.368674
C	-1.750714	-1.141412	-0.647874
H	-2.351156	-0.472736	-1.277833
C	-2.673924	-1.787491	0.405029
H	-3.114130	-1.026294	1.059570
H	-2.089689	-2.458135	1.048103
C	-3.791209	-2.601070	-0.274028
H	-4.415711	-3.079209	0.490169
H	-4.446102	-1.916098	-0.830436
C	-3.220643	-3.652346	-1.236700
H	-2.661696	-4.403971	-0.660621
H	-4.035965	-4.187701	-1.737373
C	-2.287643	-3.010434	-2.273570
H	-2.869626	-2.342702	-2.923593
H	-1.853300	-3.778838	-2.923826
C	-1.162699	-2.201468	-1.606088
H	-0.501343	-2.885939	-1.061598
H	-0.556287	-1.703930	-2.370043
F	-0.817183	1.220170	-2.681468
Ni	0.622450	0.777282	-1.709305
P	-0.469969	0.064135	-0.001196
H	5.088702	-1.354989	-2.103394
H	2.643384	-1.250249	-2.367282

IM2^{con}-F

B3LYP/BSI SCF energy: -2057.210066a.u.

M06/BSII SCF energy in solution: -2056.57333a.u.

M06/BSII free energy in solution: -2055.94881a.u.

C	-1.431174	1.351797	-0.280116
C	-1.754509	2.171615	0.814855
H	-1.667062	1.786293	1.827660
C	-2.205826	3.484515	0.634967
H	-2.457171	4.091263	1.501976
C	-2.336787	4.013931	-0.649824
H	-2.685729	5.033205	-0.791225
C	-2.020030	3.216581	-1.751909
C	-1.570794	1.904563	-1.566711
C	1.832682	1.762933	-0.021896
H	0.996495	2.343703	0.387970
C	1.949087	2.142478	-1.515647
H	2.784879	1.594976	-1.969038
H	1.042314	1.854443	-2.053253
C	2.194420	3.650849	-1.681725
H	1.314432	4.196425	-1.315262
H	2.290684	3.892397	-2.747064
C	3.445674	4.103570	-0.917004
H	4.334589	3.645642	-1.374550
H	3.575796	5.188856	-1.003052
C	3.370932	3.694761	0.560361
H	2.560169	4.252715	1.049417
H	4.296165	3.969325	1.081286
C	3.111768	2.186308	0.734313
H	3.031965	1.964308	1.802796
H	3.975580	1.623743	0.359536
C	1.672220	-0.408440	2.014809
H	2.727771	-0.133134	2.144138
C	0.828584	0.444440	2.989028
H	0.925884	1.512179	2.764007
H	-0.230443	0.192571	2.845579
C	1.215997	0.180581	4.453436
H	2.250593	0.512630	4.621208
H	0.584127	0.784225	5.115707
C	1.095419	-1.308218	4.804298
H	1.417577	-1.484476	5.837357
H	0.039243	-1.607413	4.749865
C	1.915603	-2.169356	3.834808
H	1.780260	-3.233613	4.060706
H	2.984647	-1.954330	3.976815
C	1.535661	-1.906590	2.366604
H	0.507368	-2.236897	2.181925
H	2.175001	-2.514708	1.718922
C	2.244845	-1.212874	-0.794938
H	1.943730	-2.168112	-0.347976
C	3.777494	-1.083349	-0.671776
H	4.088895	-1.065373	0.379323

H	4.105116	-0.134025	-1.113588
C	4.487421	-2.238669	-1.400680
H	5.574017	-2.108752	-1.327357
H	4.250714	-3.183819	-0.891767
C	4.053708	-2.330141	-2.870379
H	4.396515	-1.431943	-3.404040
H	4.540013	-3.184705	-3.355940
C	2.527427	-2.441108	-2.992671
H	2.196931	-3.395053	-2.557892
H	2.228919	-2.460610	-4.047451
C	1.801642	-1.290247	-2.274245
H	2.024654	-0.349627	-2.791339
H	0.721608	-1.454173	-2.331074
F	-0.511837	-2.338622	-0.076032
Ni	-0.923429	-0.450422	-0.118830
P	1.231959	-0.004721	0.226856
H	-2.125127	3.613128	-2.759254
H	-1.340227	1.302858	-2.443578
C	-3.155119	-1.278757	0.810090
C	-4.157330	-0.366357	1.159479
C	-4.865091	0.249154	0.138797
C	-4.614981	-0.013980	-1.209076
C	-3.616159	-0.921922	-1.533490
C	-2.855450	-1.585362	-0.540196
H	-2.641415	-1.822940	1.598434
H	-4.396468	-0.139617	2.193048
H	-5.202401	0.494392	-1.966515
H	-3.412721	-1.154309	-2.574544
F	-5.836908	1.127554	0.455677
B	-1.859764	-2.811028	-0.912902
O	-2.251149	-4.034337	-0.319554
H	-1.566634	-4.706790	-0.416503
O	-1.457891	-2.792680	-2.280225
H	-1.318783	-3.687570	-2.606430

TS^{con}-F

B3LYP/BSI SCF energy: -2057.191511a.u.

M06/BSII SCF energy in solution: -2056.55572a.u.

M06/BSII free energy in solution: -2055.932319a.u.

C	-1.217545	1.514632	0.564740
C	-1.034652	1.937689	1.893689
H	-0.725594	1.225789	2.655716
C	-1.240497	3.269822	2.272375
H	-1.094839	3.563164	3.309778
C	-1.629295	4.218608	1.325855
H	-1.788113	5.253406	1.616600
C	-1.822910	3.817463	0.001689
C	-1.627880	2.483342	-0.369324
C	2.115487	1.569400	0.039065
H	1.514162	2.051863	0.821896
C	1.865116	2.363418	-1.263043
H	2.460522	1.928178	-2.076158
H	0.813460	2.294172	-1.554730
C	2.261362	3.839327	-1.093800
H	1.598000	4.302859	-0.351568
H	2.096979	4.374518	-2.036791
C	3.723379	3.981519	-0.648424
H	4.383096	3.632348	-1.455956
H	3.971081	5.036124	-0.479149
C	4.001772	3.161778	0.619079
H	3.438139	3.591183	1.459138
H	5.062536	3.225296	0.890464
C	3.599593	1.684350	0.451969
H	3.793056	1.155393	1.390028
H	4.240204	1.220496	-0.308151
C	2.170756	-1.072731	1.408351
H	3.253954	-0.952010	1.271188
C	1.793267	-0.449642	2.770908
H	2.002338	0.625204	2.786448
H	0.709573	-0.553211	2.918595
C	2.525199	-1.143292	3.931923
H	3.605456	-0.962944	3.836526
H	2.217690	-0.692549	4.883014
C	2.259122	-2.654713	3.942229
H	2.831329	-3.136844	4.743533
H	1.197761	-2.833810	4.164632
C	2.602831	-3.284959	2.586104
H	2.352052	-4.352073	2.587284
H	3.687770	-3.219191	2.419716
C	1.868468	-2.588500	1.426729
H	0.789446	-2.751632	1.528719
H	2.165246	-3.057847	0.483450
C	1.919512	-1.091127	-1.543457
H	1.593244	-2.111360	-1.300836
C	3.438323	-1.135811	-1.808469
H	3.984620	-1.443750	-0.909600
H	3.794961	-0.130211	-2.064496

C	3.768461	-2.094039	-2.967466
H	4.848234	-2.084687	-3.158905
H	3.513296	-3.120315	-2.668005
C	2.994355	-1.730560	-4.242496
H	3.341629	-0.754226	-4.610129
H	3.209563	-2.455937	-5.035881
C	1.483078	-1.662960	-3.977664
H	1.111467	-2.665819	-3.724989
H	0.950975	-1.352691	-4.884698
C	1.150089	-0.698983	-2.826082
H	1.411027	0.321817	-3.127217
H	0.071822	-0.704211	-2.632893
F	-0.892524	-2.247162	-0.358575
Ni	-0.939791	-0.270708	0.049135
P	1.346908	-0.149139	-0.016759
H	-2.139571	4.542047	-0.745129
H	-1.815281	2.194564	-1.400904
C	-3.870946	-0.173630	0.876832
C	-5.166843	0.208386	0.538802
C	-5.523226	0.214323	-0.806636
C	-4.636244	-0.163966	-1.809531
C	-3.351615	-0.555229	-1.436874
C	-2.920320	-0.576233	-0.088367
H	-3.593761	-0.167729	1.927723
H	-5.894207	0.508511	1.286297
H	-4.962273	-0.156747	-2.844729
H	-2.671697	-0.883496	-2.220635
F	-6.773497	0.589820	-1.148623
B	-2.124764	-2.455924	0.378926
O	-2.006918	-2.516689	1.766713
H	-1.542291	-1.753849	2.128657
O	-2.920646	-3.382089	-0.256134
H	-3.627194	-3.673068	0.331014

IM1^{sw}-F

B3LYP/BSI SCF energy: -1549.685233a.u.

M06/BSII SCF energy in solution: -1549.18119a.u.

M06/BSII free energy in solution: -1548.662938a.u.

C	2.381266	0.504543	-1.071294
C	2.918438	1.248940	-0.012793
H	2.320240	2.003713	0.490619
C	4.239311	1.040387	0.403568
H	4.643699	1.631169	1.222247
C	5.034960	0.084902	-0.230007
H	6.058633	-0.078234	0.095537
C	4.509206	-0.649725	-1.295254
C	3.194338	-0.435571	-1.721950
C	0.365031	-0.681385	1.433552
H	1.190593	0.026733	1.586444
C	1.017519	-2.035384	1.074740
H	0.235284	-2.788588	0.913946
H	1.585472	-1.948457	0.144075
C	1.943380	-2.511826	2.206668
H	2.783139	-1.809879	2.296693
H	2.376282	-3.483926	1.942880
C	1.199809	-2.603040	3.546370
H	0.440240	-3.395954	3.486406
H	1.889812	-2.893955	4.347192
C	0.514886	-1.274004	3.894559
H	1.281241	-0.508038	4.078968
H	-0.058928	-1.370611	4.824096
C	-0.413026	-0.792796	2.763427
H	-0.857240	0.167411	3.044880
H	-1.241659	-1.502337	2.655237
C	-1.513360	1.519709	0.706839
H	-2.165074	1.108167	1.489957
C	-0.567451	2.559479	1.350625
H	0.050868	2.096543	2.127226
H	0.121511	2.930122	0.579650
C	-1.342808	3.745692	1.947868
H	-1.962236	3.390527	2.784042
H	-0.635982	4.469752	2.369796
C	-2.238377	4.417963	0.899271
H	-2.815784	5.230673	1.355095
H	-1.607281	4.876805	0.125445
C	-3.179320	3.397948	0.246235
H	-3.776591	3.875105	-0.539367
H	-3.891064	3.026629	0.997538
C	-2.408661	2.206806	-0.349640
H	-1.781743	2.561722	-1.180482
H	-3.124377	1.496499	-0.776251
C	-1.839497	-1.068320	-0.716310
H	-2.434560	-0.385393	-1.340428
C	-2.804950	-1.718638	0.295189
H	-3.237879	-0.965166	0.962792
H	-2.251920	-2.423378	0.928916
C	-3.927879	-2.483732	-0.428349

H	-4.584092	-2.960755	0.309387
H	-4.550924	-1.769480	-0.984951
C	-3.361347	-3.529931	-1.398827
H	-2.837682	-4.307765	-0.824824
H	-4.176552	-4.032623	-1.932212
C	-2.383667	-2.893216	-2.397175
H	-2.932362	-2.200449	-3.050828
H	-1.950687	-3.659552	-3.050359
C	-1.257494	-2.125389	-1.684017
H	-0.630464	-2.834946	-1.131447
H	-0.606605	-1.640622	-2.420977
F	1.072737	1.323203	-3.382341
Ni	0.677358	0.771042	-1.767594
P	-0.526930	0.093728	-0.026247
H	5.126208	-1.384361	-1.807122
H	2.809923	-0.991483	-2.572197

IM2^{sw}-F

B3LYP/BSI SCF energy: -2057.225684a.u.

M06/BSII SCF energy in solution: -2056.57589a.u.

M06/BSII free energy in solution: -2055.951354a.u.

C	0.578357	-2.324849	0.570099
C	0.659837	-3.378710	-0.360548
H	0.276229	-3.242407	-1.369324
C	1.207438	-4.616319	-0.010752
H	1.254495	-5.413144	-0.749366
C	1.683231	-4.834045	1.284729
H	2.107244	-5.796085	1.559274
C	1.598508	-3.807011	2.224200
C	1.055496	-2.566200	1.867678
C	2.257734	0.743172	1.539091
H	2.680423	-0.260520	1.682250
C	1.340695	1.007131	2.755812
H	0.894493	2.004415	2.680871
H	0.508929	0.294958	2.771572
C	2.143378	0.924140	4.065572
H	2.515307	-0.101510	4.198012
H	1.484178	1.129938	4.916964
C	3.328624	1.900447	4.060327
H	2.946526	2.931315	4.051855
H	3.913812	1.793589	4.981055
C	4.227162	1.685098	2.833592
H	4.712828	0.701989	2.906937
H	5.031845	2.429597	2.813348
C	3.427054	1.750476	1.519569
H	4.094560	1.560993	0.672056
H	3.033713	2.766677	1.389298
C	2.640999	0.015657	-1.323880
H	3.269541	0.903878	-1.470396
C	3.568183	-1.126957	-0.855646
H	4.083726	-0.850960	0.070413
H	2.973364	-2.017914	-0.634209
C	4.613622	-1.463037	-1.934432
H	5.285582	-0.603446	-2.073669
H	5.238778	-2.293886	-1.586924
C	3.955309	-1.812646	-3.275817
H	4.720390	-2.018109	-4.033838
H	3.369887	-2.735261	-3.161014
C	3.029691	-0.682394	-3.744884
H	2.524326	-0.960385	-4.677071
H	3.631112	0.210430	-3.969898
C	1.979111	-0.334543	-2.676993
H	1.308914	-1.191326	-2.535474
H	1.350742	0.491075	-3.029652
C	0.727305	2.199737	-0.732642
H	-0.001706	1.877223	-1.486741
C	1.755969	3.113251	-1.437033
H	2.294724	2.571362	-2.219079
H	2.508145	3.463097	-0.718521
C	1.056381	4.327210	-2.077361
H	1.805789	4.973745	-2.549330
H	0.398666	3.971942	-2.882807
C	0.226800	5.122744	-1.061743
H	0.900036	5.585730	-0.325873
H	-0.300299	5.943638	-1.561543
C	-0.770670	4.214202	-0.329527
H	-1.522353	3.844292	-1.040245
H	-1.313330	4.780827	0.436386
C	-0.055739	3.017173	0.319265
H	0.638183	3.397033	1.079892
H	-0.777011	2.385903	0.850445
Ni	-0.404347	-0.822593	-0.002474
P	1.331338	0.528931	-0.077122
H	1.951171	-3.968051	3.240394
H	0.992701	-1.794693	2.630068
C	-4.580905	-0.828323	0.917439
C	-5.839848	-0.546856	1.452080

C	-6.771157	0.101886	0.649778
C	-6.485098	0.467677	-0.660440
C	-5.219506	0.172757	-1.170172
C	-4.235970	-0.474922	-0.399980
H	-3.853043	-1.351130	1.532208
H	-6.109216	-0.825217	2.465999
H	-7.243633	0.967118	-1.254783
H	-4.986945	0.447874	-2.196350
F	-7.993895	0.382666	1.157743
B	-2.780022	-0.734856	-1.021159
O	-2.677076	-1.044801	-2.394512
H	-3.330919	-1.706250	-2.642370
O	-1.796801	0.389322	-0.746303
H	-2.181837	0.990031	-0.097107
F	-2.078243	-1.834590	-0.185476

TS1^{sw}-F

B3LYP/BSI SCF energy: -2057.206233a.u.

M06/BSII SCF energy in solution: -2056.57087a.u.

M06/BSII free energy in solution: -2055.943843a.u.

C	1.245163	1.547881	0.010834
C	1.529463	2.500052	-0.988973
H	1.317666	2.271517	-2.030674
C	2.113859	3.730282	-0.672846
H	2.331161	4.443087	-1.464959
C	2.420560	4.043035	0.653830
H	2.871802	4.999997	0.901490
C	2.146959	3.112651	1.656856
C	1.560278	1.882520	1.337586
C	-1.527378	0.245754	1.902558
H	-1.110138	1.254042	2.029309
C	-0.656467	-0.697982	2.762687
H	-1.031638	-1.724479	2.690072
H	0.371924	-0.716183	2.387385
C	-0.685619	-0.264699	4.238520
H	-0.219148	0.725890	4.334227
H	-0.079689	-0.953881	4.838229
C	-2.122036	-0.207459	4.779344
H	-2.540345	-1.224058	4.798669
H	-2.124885	0.149554	5.815749
C	-3.014532	0.688399	3.908128
H	-2.674986	1.730404	3.990301
H	-4.048446	0.668146	4.272722
C	-2.978583	0.265315	2.427902
H	-3.603797	0.941837	1.835196
H	-3.418985	-0.735611	2.331987
C	-2.307392	1.387351	-0.736851
H	-3.361292	1.152187	-0.535268
C	-2.035017	2.789414	-0.150148
H	-2.251000	2.806288	0.923555
H	-0.976101	3.038941	-0.264243
C	-2.895079	3.854573	-0.853814
H	-3.957161	3.668262	-0.637189
H	-2.660997	4.841592	-0.438097
C	-2.680637	3.848861	-2.373413
H	-3.327159	4.593992	-2.851851
H	-1.645121	4.143142	-2.593114
C	-2.946637	2.456666	-2.961398
H	-2.740304	2.447803	-4.037925
H	-4.012332	2.211095	-2.845903
C	-2.096727	1.378649	-2.268749
H	-1.036198	1.555051	-2.484251
H	-2.333672	0.394531	-2.688713
C	-2.223692	-1.567902	-0.519153
H	-1.782229	-1.710965	-1.513532
C	-3.757667	-1.492256	-0.691228
H	-4.042121	-0.641178	-1.316218
H	-4.241073	-1.345765	0.282990
C	-4.297488	-2.780998	-1.340803
H	-5.388555	-2.715956	-1.428455
H	-3.905534	-2.852211	-2.364836
C	-3.897374	-4.038998	-0.558762
H	-4.395142	-4.031860	0.421569
H	-4.248605	-4.937083	-1.079835
C	-2.377950	-4.100852	-0.352121
H	-1.880834	-4.232514	-1.323092
H	-2.110043	-4.970397	0.259739
C	-1.857864	-2.816453	0.314957
H	-2.309372	-2.735120	1.311696
H	-0.775609	-2.880953	0.473105
Ni	0.754801	-0.144101	-0.626824
P	-1.323522	-0.005605	0.055136
H	2.393590	3.339478	2.691490
H	1.377048	1.174834	2.141206
C	4.036098	-0.252245	-0.986607
C	5.005500	-0.081249	0.002000
C	5.039287	-0.982632	1.058993

C	4.144387	-2.043998	1.150864
C	3.190794	-2.192197	0.143717
C	3.100822	-1.307667	-0.953533
H	3.988327	0.457826	-1.806443
H	5.719275	0.735506	-0.028444
H	4.211065	-2.730265	1.989077
H	2.507465	-3.038035	0.211163
F	5.969939	-0.828569	2.027122
B	2.057039	-1.565958	-2.197999
O	2.373555	-2.634652	-3.074061
H	3.323515	-2.684236	-3.219560
O	0.659367	-1.828962	-1.621285
H	0.653173	-2.674424	-1.157953
F	1.839630	-0.279777	-2.825549

IM3^{sw}-F

B3LYP/BSI SCF energy: -2057.212042a.u.

M06/BSII SCF energy in solution: -2056.58000a.u.

M06/BSII free energy in solution: -2055.95431a.u.

C	1.592554	1.088630	-0.057151
C	2.120233	1.524215	-1.289418
H	2.010133	0.903939	-2.176641
C	2.803684	2.738552	-1.408670
H	3.202588	3.040093	-2.374601
C	2.976630	3.560157	-0.292524
H	3.506306	4.504716	-0.381374
C	2.470015	3.147326	0.939666
C	1.787427	1.929753	1.051094
C	-1.660612	1.268469	1.386236
H	-1.015651	2.130938	1.170496
C	-1.198983	0.714979	2.753684
H	-1.814858	-0.144083	3.041077
H	-0.168598	0.350592	2.686862
C	-1.320784	1.794429	3.842422
H	-0.632141	2.619407	3.612323
H	-1.005644	1.383741	4.808956
C	-2.755097	2.336740	3.935896
H	-3.421008	1.535873	4.287982
H	-2.811419	3.137863	4.682077
C	-3.252917	2.844975	2.574966
H	-2.671138	3.730422	2.282991
H	-4.298019	3.168931	2.647407
C	-3.116387	1.773392	1.477497
H	-3.452100	2.183143	0.518713
H	-3.783285	0.933464	1.710989
C	-1.738793	1.123734	-1.589339
H	-2.835967	1.155033	-1.582910
C	-1.248252	2.586903	-1.612004
H	-1.623713	3.132796	-0.740233
H	-0.156768	2.613549	-1.557481
C	-1.716445	3.300217	-2.893206
H	-2.813601	3.378190	-2.889503
H	-1.331946	4.326923	-2.897306
C	-1.266550	2.555464	-4.157458
H	-1.638777	3.066228	-5.053429
H	-0.169600	2.575822	-4.216555
C	-1.744941	1.097294	-4.138192
H	-1.374474	0.559094	-5.018408
H	-2.842877	1.074820	-4.197820
C	-1.290389	0.369328	-2.862445
H	-0.197106	0.284149	-2.859566
H	-1.675305	-0.656822	-2.864270
C	-2.460144	-1.330272	-0.102463
H	-1.931349	-2.005543	-0.786401
C	-3.877523	-1.095341	-0.671164
H	-3.834171	-0.617126	-1.653611
H	-4.444152	-0.421946	-0.015472
C	-4.635966	-2.429402	-0.810349
H	-5.646378	-2.237043	-1.190505
H	-4.130449	-3.046583	-1.565931
C	-4.700551	-3.203202	0.512672
H	-5.314962	-2.642497	1.231647
H	-5.197761	-4.168749	0.364037
C	-3.298330	-3.407973	1.101761
H	-2.717281	-4.070299	0.445227
H	-3.361234	-3.907105	2.076005
C	-2.560884	-2.066649	1.251959
H	-3.114841	-1.445755	1.966811
H	-1.568142	-2.226649	1.686970
Ni	0.831118	-0.646721	-0.020396
P	-1.263340	0.137802	-0.058714
H	2.608630	3.769176	1.821192
H	1.423691	1.634635	2.031659
C	3.803303	-1.371985	-0.838995
C	4.806935	-0.607819	-0.261836
C	4.767608	-0.386000	1.116697
C	3.770042	-0.909206	1.923067

C	2.769487	-1.679431	1.316321
C	2.753140	-1.935879	-0.075127
H	3.818939	-1.564017	-1.907812
H	5.614918	-0.177766	-0.844697
H	3.787811	-0.723134	2.991707
H	2.025472	-2.149512	1.956331
F	5.742122	0.356271	1.679449
B	1.713476	-3.013272	-0.739658
O	1.901272	-4.334945	-0.224651
H	1.657922	-4.968646	-0.909817
O	0.305601	-2.505445	-0.302764
H	0.053242	-3.046846	0.455754
F	1.733037	-2.926401	-2.142232

TS2^{sw}-F

B3LYP/BSI SCF energy: -2057.198648a.u.

M06/BSII SCF energy in solution: -2056.56612a.u.

M06/BSII free energy in solution: -2055.941182a.u.

C	1.327650	1.455922	0.108975
C	1.569691	2.337649	-0.963712
H	1.496485	1.976578	-1.988164
C	1.913833	3.676507	-0.751746
H	2.094249	4.328236	-1.604036
C	2.031051	4.175965	0.547524
H	2.300040	5.215094	0.716576
C	1.812595	3.316836	1.625138
C	1.470592	1.976977	1.406205
C	-1.800828	0.515427	1.722886
H	-1.359577	1.522173	1.737492
C	-1.072271	-0.284614	2.826774
H	-1.474303	-1.302628	2.881902
H	-0.008533	-0.380211	2.584891
C	-1.253320	0.392034	4.196262
H	-0.763950	1.375708	4.178406
H	-0.746863	-0.195559	4.971300
C	-2.739178	0.565922	4.545254
H	-3.194804	-0.425169	4.683948
H	-2.847170	1.093729	5.500120
C	-3.492204	1.315802	3.436616
H	-3.126036	2.350631	3.384472
H	-4.561232	1.375098	3.674248
C	-3.300013	0.647815	2.062506
H	-3.830476	1.223159	1.295899
H	-3.761562	-0.348438	2.082890
C	-2.217292	1.219919	-1.131256
H	-3.294623	1.026348	-1.045138
C	-1.990614	2.694519	-0.732205
H	-2.354764	2.876236	0.284516
H	-0.920484	2.919316	-0.729576
C	-2.714074	3.645784	-1.702460
H	-3.801081	3.504361	-1.610896
H	-2.509859	4.683424	-1.413079
C	-2.295529	3.404512	-3.159403
H	-2.848274	4.072807	-3.830496
H	-1.231319	3.652367	-3.274983
C	-2.520355	1.940843	-3.560588
H	-2.172522	1.765102	-4.585487
H	-3.598588	1.724459	-3.555739
C	-1.802790	0.977497	-2.601062
H	-0.718230	1.114581	-2.691837
H	-2.007483	-0.058315	-2.896597
C	-2.264947	-1.650857	-0.441620
H	-1.735346	-1.954847	-1.354291
C	-3.770471	-1.587162	-0.781788
H	-3.967723	-0.837492	-1.553283
H	-4.345597	-1.287383	0.103399
C	-4.279053	-2.952715	-1.282698
H	-5.353646	-2.889813	-1.492154
H	-3.788822	-3.184891	-2.238601
C	-3.995266	-4.081336	-0.282682
H	-4.589199	-3.917454	0.627869
H	-4.316847	-5.044835	-0.695044
C	-2.507089	-4.129248	0.089921
H	-1.918502	-4.416835	-0.792740
H	-2.328187	-4.897958	0.851302
C	-2.020344	-2.763207	0.602458
H	-2.564426	-2.523257	1.524287
H	-0.961140	-2.816068	0.881638
Ni	0.896351	-0.333415	-0.314568
P	-1.363847	-0.037267	-0.018004
H	1.917428	3.685063	2.643509
H	1.336503	1.330969	2.270269
C	3.922510	-0.057750	-0.837866
C	5.220512	-0.074180	-0.327219
C	5.464163	-0.786753	0.841876
C	4.460284	-1.493096	1.496213
C	3.178833	-1.476952	0.946555

C	2.860048	-0.761825	-0.231942
H	3.730449	0.513804	-1.741035
H	6.033722	0.462218	-0.806056
H	4.693815	-2.041603	2.403313
H	2.406521	-2.053783	1.454439
F	6.714756	-0.802132	1.353108
B	2.011105	-2.002296	-1.743490
O	2.791577	-3.142026	-1.699293
H	3.658826	-2.995939	-2.092713
O	0.700460	-2.164957	-1.178970
H	0.702455	-2.929043	-0.586815
F	2.043243	-1.185576	-2.835096

IM4-F

B3LYP/BSI SCF energy: -1780.681501a.u.

M06/BSII SCF energy in solution: -1780.05344a.u.

M06/BSII free energy in solution: -1779.465679a.u.

C	-1.284630	1.918331	-0.033612
C	-1.175069	2.538264	1.223439
H	-1.146205	1.936838	2.129566
C	-1.096993	3.931889	1.334188
H	-1.006644	4.388417	2.317490
C	-1.139999	4.733947	0.192436
H	-1.082986	5.815552	0.278429
C	-1.275077	4.130896	-1.060669
C	-1.358851	2.739246	-1.172670
C	2.180207	1.034152	0.366645
H	1.575047	1.639055	1.057089
C	2.329613	1.866585	-0.926323
H	2.934004	1.306680	-1.652322
H	1.350348	2.043095	-1.380605
C	3.017325	3.211601	-0.640257
H	2.362199	3.816518	0.000656
H	3.137372	3.769812	-1.576444
C	4.378182	3.016404	0.042197
H	5.066710	2.521885	-0.658435
H	4.827076	3.986619	0.285991
C	4.248908	2.159222	1.309559
H	3.663153	2.708191	2.060256
H	5.235750	1.981178	1.753869
C	3.559836	0.811144	1.023864
H	3.466211	0.246267	1.957145
H	4.199597	0.216011	0.361221
C	1.309090	-1.510355	1.657958
H	2.380485	-1.728555	1.766549
C	0.838110	-0.734106	2.909805
H	1.393384	0.203837	3.016653
H	-0.216932	-0.457806	2.775835
C	0.983453	-1.570868	4.192171
H	2.049189	-1.764581	4.380550
H	0.615586	-0.994929	5.049529
C	0.235789	-2.906188	4.082468
H	0.388872	-3.504921	4.987989
H	-0.843812	-2.712349	4.013414
C	0.689871	-3.688332	2.843792
H	0.112456	-4.614711	2.741960
H	1.740499	-3.987554	2.967755
C	0.552317	-2.854257	1.558248
H	-0.513181	-2.654831	1.370877
H	0.915135	-3.444859	0.710409
C	1.711373	-1.551758	-1.283350
H	1.136863	-2.475966	-1.120795
C	3.205058	-1.933714	-1.259804
H	3.492562	-2.323670	-0.276657
H	3.814182	-1.037959	-1.433667
C	3.528585	-2.971784	-2.349693
H	4.600356	-3.203395	-2.334548
H	3.003889	-3.910427	-2.121122
C	3.106815	-2.479414	-3.741696
H	3.720646	-1.610135	-4.017896
H	3.305482	-3.252005	-4.493732
C	1.624487	-2.078720	-3.767593
H	1.004093	-2.972575	-3.609409
H	1.353710	-1.682546	-4.753352
C	1.297241	-1.039332	-2.682014
H	1.822296	-0.104477	-2.910359
H	0.226671	-0.803175	-2.692913
Ni	-1.193046	0.068516	-0.159946
P	1.064011	-0.462228	0.111304
H	-1.327666	4.745209	-1.956719
H	-1.485796	2.294490	-2.156124
C	-4.016544	0.302730	0.597113
C	-5.342311	-0.115919	0.472539
C	-5.701116	-0.880369	-0.633515
C	-4.783307	-1.229656	-1.615004
C	-3.459125	-0.798853	-1.471197
C	-3.037482	-0.046159	-0.353871

H	-3.741910	0.919045	1.449192
H	-6.097120	0.143362	1.208689
H	-5.108056	-1.813112	-2.471090
H	-2.750520	-1.059392	-2.256885
F	-6.986935	-1.286772	-0.761114

TS^{con}-F[B2]

B3LYP/BSI SCF energy: -2255.672599a.u.

M06/BSII SCF energy in solution: -2255.04837a.u.

M06/BSII free energy in solution: -2254.442765a.u.

C	-1.067511	1.525635	0.308700
C	-1.115238	2.049327	1.613140
H	-0.942966	1.399821	2.467786
C	-1.393870	3.401461	1.845739
H	-1.428782	3.775084	2.866784
C	-1.628031	4.267602	0.776503
H	-1.842413	5.317648	0.955502
C	-1.594635	3.764424	-0.525974
C	-1.323182	2.411084	-0.754415
C	2.254826	1.607044	0.148911
H	1.557677	2.127307	0.819141
C	2.172382	2.322331	-1.218378
H	2.871836	1.850464	-1.920106
H	1.169371	2.223329	-1.641137
C	2.533877	3.810142	-1.081828
H	1.779566	4.303133	-0.454185
H	2.485676	4.292408	-2.065539
C	3.927139	3.995190	-0.465887
H	4.685135	3.610818	-1.163618
H	4.145802	5.060394	-0.325346
C	4.047793	3.249580	0.870673
H	3.382111	3.719250	1.608333
H	5.065981	3.338407	1.268479
C	3.674004	1.760671	0.740544
H	3.744641	1.290411	1.725987
H	4.408373	1.258625	0.098019
C	2.171121	-0.961387	1.653244
H	3.255813	-0.789793	1.666839
C	1.560403	-0.309785	2.915107
H	1.730307	0.772493	2.920250
H	0.471510	-0.451514	2.888989
C	2.119012	-0.932475	4.204951
H	3.193701	-0.712433	4.279165
H	1.644536	-0.463366	5.075050
C	1.907019	-2.451800	4.230698
H	2.351768	-2.884868	5.134402
H	0.829863	-2.665715	4.278355
C	2.497668	-3.109918	2.976788
H	2.295900	-4.187460	2.979056
H	3.591446	-2.997179	2.990371
C	1.940408	-2.489172	1.683525
H	0.868802	-2.704292	1.603604
H	2.417281	-2.970263	0.823739
C	2.220953	-1.126985	-1.319398
H	1.874544	-2.136872	-1.062164
C	3.758882	-1.169585	-1.429419
H	4.211493	-1.437863	-0.467770
H	4.137456	-0.172341	-1.687514
C	4.204839	-2.169426	-2.511844
H	5.298154	-2.157758	-2.597745
H	3.927019	-3.185384	-2.197700
C	3.555779	-1.862983	-3.869185
H	3.930321	-0.897130	-4.238246
H	3.854298	-2.615140	-4.608924
C	2.025436	-1.802666	-3.756146
H	1.636934	-2.797973	-3.499997
H	1.581668	-1.534989	-4.722128
C	1.572938	-0.796508	-2.684263
H	1.853508	0.213982	-3.002519
H	0.481514	-0.810712	-2.596830
F	-0.604155	-2.250676	-0.335592
Ni	-0.737755	-0.297597	-0.017055
P	1.510859	-0.121949	0.100329
H	-1.788044	4.423707	-1.369192
H	-1.324705	2.043103	-1.778141
C	-3.579127	-0.464317	0.866346
C	-4.834498	0.119884	0.830163
C	-5.284802	0.526421	-0.423577
C	-4.533208	0.362038	-1.583244
C	-3.286928	-0.231429	-1.437567
C	-2.741479	-0.704225	-0.231469
H	-5.430747	0.268511	1.721525
H	-4.897872	0.702888	-2.544268
F	-6.493761	1.103440	-0.515431
B	-2.034758	-2.574301	-0.336142
O	-2.490644	-3.227408	0.801809
H	-2.442168	-2.686203	1.596887

O	-2.387266	-3.093876	-1.570158
H	-3.185814	-3.625020	-1.477209
F	-3.124729	-0.847045	2.096228
F	-2.536356	-0.344031	-2.554372

TS1^{con}-F$^{[B2]}$

B3LYP/BSI SCF energy: -2255.677501a.u.

M06/BSII SCF energy in solution: -2255.05452a.u.

M06/BSII free energy in solution: -2254.447728a.u.

C	1.086576	1.574726	0.228836
C	1.491428	2.531056	-0.724653
H	1.377035	2.320105	-1.784549
C	2.074950	3.739899	-0.333471
H	2.386750	4.456349	-1.089688
C	2.262019	4.025562	1.021039
H	2.712314	4.966334	1.325934
C	1.870613	3.089603	1.978939
C	1.283504	1.881372	1.585598
C	-1.878781	0.329068	1.845310
H	-1.450468	1.329530	1.994501
C	-1.125660	-0.619896	2.805777
H	-1.520241	-1.637241	2.712591
H	-0.065134	-0.674285	2.538871
C	-1.292533	-0.158384	4.263305
H	-0.813858	0.822772	4.390772
H	-0.768227	-0.850704	4.932397
C	-2.774590	-0.058505	4.654306
H	-3.217582	-1.064797	4.646810
H	-2.873766	0.316887	5.679455
C	-3.551913	0.841389	3.682932
H	-3.198050	1.877050	3.783646
H	-4.617815	0.850102	3.940008
C	-3.375356	0.392150	2.220916
H	-3.920566	1.073217	1.558528
H	-3.827280	-0.599873	2.093636
C	-2.392118	1.403424	-0.891031
H	-3.462124	1.175914	-0.795205
C	-2.171236	2.819845	-0.318184
H	-2.488148	2.868009	0.729233
H	-1.104776	3.063635	-0.338674
C	-2.951675	3.867555	-1.131838
H	-4.030929	3.686376	-1.021931
H	-2.759417	4.864641	-0.718647
C	-2.579844	3.822926	-2.619978
H	-3.170415	4.555716	-3.182456
H	-1.526110	4.110939	-2.737626
C	-2.787354	2.415889	-3.196777
H	-2.468243	2.378997	-4.244753
H	-3.860368	2.174980	-3.188261
C	-2.020932	1.353729	-2.391224
H	-0.941861	1.519023	-2.495931
H	-2.218742	0.359780	-2.808101
C	-2.331603	-1.545775	-0.592216
H	-1.811052	-1.682749	-1.548609
C	-3.848202	-1.496941	-0.883631
H	-4.100647	-0.645974	-1.522711
H	-4.410245	-1.370132	0.050543
C	-4.305249	-2.791390	-1.583995
H	-5.387386	-2.750578	-1.756693
H	-3.832751	-2.842937	-2.574579
C	-3.938285	-4.048001	-0.783019
H	-4.515027	-4.062941	0.153022
H	-4.224461	-4.948110	-1.339354
C	-2.439922	-4.077668	-0.451019
H	-1.858004	-4.188022	-1.376038
H	-2.204482	-4.946546	0.174885
C	-2.006889	-2.788333	0.266890
H	-2.545785	-2.724613	1.220720
H	-0.941129	-2.831147	0.514422
Ni	0.620626	-0.091359	-0.484814
P	-1.500887	0.031780	0.034776
H	2.023055	3.295729	3.035849
H	1.002590	1.169520	2.356439
C	3.997132	-0.172690	-0.761719
C	4.920031	0.007791	0.263884
C	4.849486	-0.862034	1.343768
C	3.908033	-1.882779	1.413407
C	3.028703	-1.987350	0.343957
C	2.995704	-1.157111	-0.783901
H	5.661565	0.795555	0.220259
H	3.870142	-2.565637	2.252787
F	5.725886	-0.719793	2.355083
B	1.964408	-1.420857	-2.078810
O	2.372880	-2.419747	-2.987978
H	3.275365	-2.268840	-3.286995
O	0.612721	-1.787747	-1.496121
H	0.720656	-2.583272	-0.957854

F	1.681612	-0.127289	-2.645853
F	4.094902	0.671726	-1.806839
F	2.115192	-3.007079	0.425395

TS2^{con}-F$^{[B2]}$

B3LYP/BSI SCF energy: -2255.676171a.u.

M06/BSII SCF energy in solution: -2255.05633a.u.

M06/BSII free energy in solution: -2254.450686a.u.

C	1.173581	1.467210	0.230493
C	1.435687	2.423647	-0.769613
H	1.345168	2.150792	-1.817736
C	1.836332	3.725531	-0.451504
H	2.034296	4.437026	-1.250182
C	1.988163	4.111857	0.881918
H	2.300087	5.122566	1.130811
C	1.746609	3.177267	1.889333
C	1.348745	1.874892	1.564900
C	-2.015071	0.626384	1.662368
H	-1.537372	1.616273	1.680119
C	-1.386594	-0.175261	2.825381
H	-1.842528	-1.169358	2.885056
H	-0.318362	-0.333853	2.648820
C	-1.612077	0.549641	4.162727
H	-1.082647	1.512345	4.144502
H	-1.173217	-0.034285	4.980520
C	-3.106938	0.790000	4.423057
H	-3.607207	-0.178791	4.565183
H	-3.246707	1.351107	5.354540
C	-3.769850	1.532611	3.253341
H	-3.364643	2.552426	3.194235
H	-4.847619	1.635221	3.428328
C	-3.526031	0.820397	1.909728
H	-3.990080	1.393448	1.099760
H	-4.024008	-0.158138	1.927548
C	-2.279452	1.239837	-1.238938
H	-3.359986	1.048282	-1.211848
C	-2.077338	2.727153	-0.877811
H	-2.497159	2.942976	0.110417
H	-1.009669	2.955638	-0.822461
C	-2.746202	3.641308	-1.920024
H	-3.836184	3.497096	-1.886952
H	-2.563101	4.689303	-1.654808
C	-2.242355	3.352845	-3.340961
H	-2.758922	3.993347	-4.065749
H	-1.174698	3.604914	-3.404440
C	-2.435761	1.874554	-3.704320
H	-2.025064	1.666341	-4.699295
H	-3.511495	1.652440	-3.757980
C	-1.776652	0.946304	-2.671020
H	-0.687836	1.077866	-2.699826
H	-1.964758	-0.099559	-2.940605
C	-2.396616	-1.605393	-0.455609
H	-1.811920	-1.950163	-1.317919
C	-3.876507	-1.537541	-0.894415
H	-4.016471	-0.813762	-1.702384
H	-4.504183	-1.203570	-0.058139
C	-4.364858	-2.915158	-1.382915
H	-5.423386	-2.850703	-1.662275
H	-3.816906	-3.180053	-2.298005
C	-4.155223	-4.015029	-0.333657
H	-4.807422	-3.822064	0.530245
H	-4.455718	-4.988246	-0.739162
C	-2.695519	-4.059320	0.138911
H	-2.048597	-4.374299	-0.691510
H	-2.573736	-4.804913	0.933740
C	-2.236694	-2.680803	0.642351
H	-2.848231	-2.406201	1.510765
H	-1.202957	-2.730536	1.001553
Ni	0.733398	-0.306831	-0.263435
P	-1.507217	0.014671	-0.036868
H	1.875991	3.455621	2.933002
H	1.195359	1.167546	2.375828
C	3.767147	-0.039493	-0.837448
C	5.042699	0.079030	-0.293980
C	5.284199	-0.588272	0.901122
C	4.317340	-1.364984	1.535693
C	3.084184	-1.433378	0.908161
C	2.724314	-0.800891	-0.289575
H	5.808990	0.679164	-0.768757
H	4.525267	-1.882364	2.463932
F	6.501296	-0.489453	1.464184
B	1.851030	-2.092182	-1.604075
O	2.616017	-3.248947	-1.524504
H	3.395775	-3.191520	-2.087314
O	0.559324	-2.200074	-0.966589
H	0.632480	-2.832949	-0.237569
F	1.813203	-1.394610	-2.775167

F	3.543307	0.622586	-1.989205
F	2.135421	-2.209833	1.516653

Ph[Ni]Cl

B3LYP/BSI SCF energy: -2957.300888a.u.

M06/BSII SCF energy in solution: -2956.40839a.u.

M06/BSII free energy in solution: -2955.427202a.u.

C	-0.000008	1.669105	-0.591348
C	-0.000004	1.933463	-1.976172
H	0.000012	1.108269	-2.683080
C	-0.000025	3.238641	-2.483411
H	-0.000026	3.397952	-3.559727
C	-0.000040	4.332781	-1.615921
H	-0.000055	5.347100	-2.005497
C	-0.000032	4.101620	-0.238054
C	-0.000017	2.792965	0.258922
C	3.070648	-0.940087	1.628708
H	2.639309	-1.946941	1.589905
C	2.537738	-0.316601	2.938453
H	2.905043	0.709485	3.054638
H	1.445176	-0.272476	2.902625
C	2.984556	-1.147470	4.153807
H	2.509565	-2.136660	4.102158
H	2.625755	-0.675805	5.076812
C	4.510362	-1.314283	4.200080
H	4.977404	-0.332645	4.367465
H	4.800566	-1.945416	5.048770
C	5.045861	-1.908868	2.889598
H	4.672463	-2.936538	2.778625
H	6.140518	-1.975320	2.918197
C	4.606360	-1.079771	1.668362
H	4.982095	-1.548182	0.751572
H	5.075082	-0.089421	1.728992
C	2.919951	-1.334803	-1.306144
H	4.007103	-1.194042	-1.366134
C	2.672003	-2.837993	-1.058974
H	3.143315	-3.159266	-0.124909
H	1.599961	-3.020155	-0.936366
C	3.224174	-3.685130	-2.219305
H	4.319107	-3.586719	-2.255696
H	3.014586	-4.744555	-2.028945
C	2.636386	-3.260305	-3.571793
H	3.076831	-3.851373	-4.383879
H	1.557685	-3.472844	-3.579156
C	2.855900	-1.762250	-3.820908
H	2.380525	-1.454965	-4.760470
H	3.931611	-1.566696	-3.938251
C	2.309442	-0.913723	-2.661148
H	1.219968	-1.038372	-2.605017
H	2.488034	0.148556	-2.860756
C	3.244761	1.436279	-0.318385
H	2.562213	1.918610	-1.028157
C	4.625830	1.341688	-1.006828
H	5.351984	0.863394	-0.337945
H	4.576368	0.725977	-1.909307
C	5.139938	2.740390	-1.398076
H	6.128827	2.650133	-1.864315
H	4.471651	3.162508	-2.161710
C	5.198483	3.694242	-0.197655
H	5.517606	4.692395	-0.521140
H	5.959829	3.337735	0.511275
C	3.840769	3.767800	0.513024
H	3.100444	4.237802	-0.147767
H	3.912067	4.400803	1.406224
C	3.340662	2.369426	0.909767
H	2.369634	2.451581	1.404479
H	4.039217	1.942878	1.639735
C	-3.244779	1.436367	-0.318148
H	-2.562263	1.918707	-1.027944
C	-3.340569	2.369508	0.910019
H	-4.039110	1.943000	1.640020
H	-2.369514	2.451612	1.404687
C	-3.840623	3.767910	0.513308
H	-3.100302	4.237878	-0.147512
H	-3.911853	4.400911	1.406515
C	-5.198369	3.694424	-0.197317
H	-5.959705	3.337947	0.511640
H	-5.517457	4.692597	-0.520775
C	-5.139923	2.740586	-1.397754
H	-4.471644	3.162680	-2.161409
H	-6.128835	2.650387	-1.863955
C	-4.625873	1.341851	-1.006547
H	-4.576461	0.726151	-1.909038
H	-5.352028	0.863578	-0.337651
C	-2.919965	-1.334588	-1.306218
H	-4.007159	-1.194057	-1.365992
C	-2.309794	-0.913089	-2.661240

H	-2.488686	0.149185	-2.860606
H	-1.220280	-1.037475	-2.605320
C	-2.856234	-1.761523	-3.821077
H	-3.932015	-1.566222	-3.938202
H	-2.381096	-1.453928	-4.760657
C	-2.636291	-3.259569	-3.572298
H	-3.076714	-3.850590	-4.384431
H	-1.557536	-3.471828	-3.579876
C	-3.223754	-3.684816	-2.219802
H	-3.013869	-4.744226	-2.029690
H	-4.318718	-3.586674	-2.255998
C	-2.671620	-2.837772	-1.059385
H	-1.599514	-3.019698	-0.936968
H	-3.142718	-3.159349	-0.125318
C	-3.070669	-0.940305	1.628670
H	-2.639230	-1.947110	1.589754
C	-4.606365	-1.080181	1.668240
H	-4.982011	-1.548478	0.751354
H	-5.075207	-0.089902	1.729027
C	-5.045810	-1.909543	2.889316
H	-6.140460	-1.976135	2.917861
H	-4.672280	-2.937148	2.778182
C	-4.510434	-1.315114	4.199920
H	-4.977604	-0.333563	4.367452
H	-4.800595	-1.946427	5.048491
C	-2.984645	-1.148105	4.153736
H	-2.509530	-2.137228	4.101940
H	-2.625939	-0.676554	5.076835
C	-2.537878	-0.316976	2.938542
H	-2.905310	0.709043	3.054893
H	-1.445321	-0.272718	2.902765
Ni	-0.000009	-0.090151	0.147882
P	2.329277	-0.181270	0.072165
P	-2.329301	-0.181227	0.072238
H	-0.000034	4.941083	0.453931
H	-0.000004	2.651024	1.337934
Cl	-0.000026	-2.156981	1.116277

$ClB(OH)_2$

B3LYP/BSI SCF energy: -636.848083a.u.

M06/BSII SCF energy in solution: -636.833076a.u.

M06/BSII free energy in solution: -636.825a.u.

B	-0.452160	-0.004416	0.000005
O	-1.124835	1.177001	-0.000002
H	-0.547985	1.948923	-0.000012
O	-1.107143	-1.187037	0.000024
H	-2.064813	-1.059599	0.000012
Cl	1.337025	-0.046292	-0.000012

TS^{con}-Cl[B1]

B3LYP/BSI SCF energy: -2417.522682a.u.

M06/BSII SCF energy in solution: -2416.89716a.u.

M06/BSII free energy in solution: -2416.275307a.u.

C	-1.161634	1.512709	0.609233
C	-0.994459	1.899578	1.951273
H	-0.731244	1.162312	2.706199
C	-1.156893	3.230493	2.355988
H	-1.024048	3.494038	3.403033
C	-1.486860	4.214601	1.423823
H	-1.612202	5.248066	1.734794
C	-1.667903	3.849569	0.087051
C	-1.517146	2.517315	-0.309252
C	2.070229	1.619514	-0.034975
H	1.420479	2.112208	0.699435
C	1.838336	2.342315	-1.381185
H	2.481427	1.898337	-2.151747
H	0.802582	2.214363	-1.708490
C	2.165231	3.840863	-1.269534
H	1.456793	4.308112	-0.572901
H	2.012813	4.323534	-2.242553
C	3.602276	4.067776	-0.780765
H	4.306647	3.708210	-1.544895
H	3.799386	5.139139	-0.655889
C	3.862684	3.323549	0.535189
H	3.247696	3.768002	1.330143
H	4.907933	3.445895	0.844264
C	3.530194	1.823214	0.428105
H	3.706175	1.356361	1.401637
H	4.223385	1.349745	-0.278608
C	2.282098	-0.962638	1.410285
H	3.342946	-0.711649	1.281255
C	1.819854	-0.378671	2.763591
H	1.887173	0.714289	2.768068
H	0.757572	-0.620275	2.906258
C	2.624938	-0.960491	3.937403
H	3.674229	-0.644937	3.846914

H	2.255054	-0.542522	4.881213
C	2.553511	-2.493102	3.963280
H	3.175676	-2.890511	4.773782
H	1.521623	-2.803402	4.179637
C	2.986636	-3.087107	2.616532
H	2.876435	-4.177797	2.627256
H	4.055313	-2.883246	2.456726
C	2.178323	-2.502949	1.443945
H	1.128778	-2.803434	1.538557
H	2.542431	-2.939089	0.508395
C	2.009965	-1.080370	-1.536580
H	1.745662	-2.114248	-1.276292
C	3.531516	-1.044355	-1.790151
H	4.086361	-1.306416	-0.882126
H	3.834928	-0.025429	-2.060936
C	3.923558	-2.002761	-2.929725
H	5.002746	-1.936664	-3.113284
H	3.723490	-3.036504	-2.614308
C	3.141351	-1.705440	-4.217053
H	3.434859	-0.716431	-4.597262
H	3.405515	-2.429567	-4.996659
C	1.626701	-1.720763	-3.964698
H	1.311470	-2.739199	-3.698035
H	1.084874	-1.456745	-4.880589
C	1.231021	-0.756993	-2.832975
H	1.439133	0.270052	-3.151459
H	0.153068	-0.817305	-2.649083
Ni	-0.940824	-0.278751	0.051008
P	1.376080	-0.139423	-0.031518
H	-1.943176	4.601202	-0.649334
H	-1.701853	2.257021	-1.348658
C	-3.880208	0.166071	0.774957
C	-5.171568	0.499587	0.373290
C	-5.514972	0.324796	-0.964086
C	-4.617208	-0.185701	-1.894933
C	-3.340782	-0.538083	-1.457502
C	-2.925100	-0.377110	-0.114684
H	-3.609284	0.322435	1.815062
H	-5.903416	0.903299	1.065767
H	-4.929455	-0.315843	-2.926243
H	-2.659637	-0.979856	-2.181136
F	-6.760627	0.653569	-1.367612
B	-2.445513	-2.314281	0.746497
O	-2.160144	-2.088413	2.078467
H	-1.488508	-1.405738	2.200229
O	-3.497176	-3.115408	0.397565
H	-4.187387	-3.065173	1.070912
Cl	-0.955467	-2.625349	-0.424813

TS^{con}-Cl[B2]

B3LYP/BSI SCF energy: -2615.999749a.u.

M06/BSII SCF energy in solution: -2615.38672a.u.

M06/BSII free energy in solution: -2614.782367a.u.

C	2.210437	1.659775	-0.013756
H	1.497134	2.193693	0.626521
C	2.091656	2.279768	-1.424268
H	2.804893	1.791995	-2.100165
H	1.091682	2.111771	-1.832361
C	2.394106	3.787085	-1.393726
H	1.625300	4.291758	-0.793755
H	2.320218	4.197143	-2.408267
C	3.782875	4.068515	-0.804221
H	4.551808	3.664360	-1.478485
H	3.960776	5.148662	-0.741504
C	3.936021	3.424599	0.579475
H	3.252213	3.916723	1.285071
H	4.950295	3.582552	0.965807
C	3.624597	1.916006	0.554818
H	3.720347	1.523666	1.571248
H	4.378652	1.401903	-0.054431
C	2.339020	-0.813653	1.622016
H	3.403727	-0.552115	1.563752
C	1.745625	-0.144551	2.882034
H	1.804796	0.947062	2.814884
H	0.676804	-0.391164	2.936722
C	2.445706	-0.627312	4.162931
H	3.494433	-0.297325	4.148304
H	1.983063	-0.153732	5.037018
C	2.395677	-2.155637	4.290239
H	2.946059	-2.483000	5.180206
H	1.352908	-2.472481	4.433038
C	2.960976	-2.832166	3.034026
H	2.868794	-3.921779	3.112729
H	4.036223	-2.614705	2.957774
C	2.253498	-2.349551	1.754998
H	1.203660	-2.661681	1.779669
H	2.704470	-2.842725	0.887683

C	2.289126	-1.132270	-1.332012
H	2.019333	-2.151159	-1.023637
C	3.824949	-1.090162	-1.475371
H	4.313527	-1.282298	-0.513300
H	4.139186	-0.088206	-1.792661
C	4.306923	-2.117599	-2.516042
H	5.396031	-2.049181	-2.625765
H	4.093327	-3.130393	-2.146366
C	3.616782	-1.917418	-3.873087
H	3.929252	-0.952316	-4.297324
H	3.943477	-2.688539	-4.580746
C	2.087821	-1.936137	-3.730250
H	1.761123	-2.938145	-3.419544
H	1.611973	-1.740749	-4.698400
C	1.599967	-0.905204	-2.698103
H	1.821653	0.101322	-3.069329
H	0.512912	-0.970806	-2.588291
Ni	-0.739744	-0.336030	0.046289
P	1.542993	-0.107967	0.060829
C	-3.638193	-0.076277	0.877081
C	-4.876124	0.511669	0.671183
C	-5.254141	0.700091	-0.655842
C	-4.452986	0.317581	-1.728227
C	-3.234531	-0.266705	-1.414504
C	-2.758160	-0.527627	-0.117800
H	-5.509372	0.827132	1.490788
H	-4.764202	0.483426	-2.752129
F	-6.441630	1.272805	-0.910967
B	-2.520200	-2.590291	0.112596
O	-2.839855	-2.848979	1.425624
H	-2.552502	-2.171110	2.046753
O	-3.237812	-3.200506	-0.889311
H	-4.112017	-3.437264	-0.554406
Cl	-0.645321	-2.658903	-0.339475
F	-3.254207	-0.241246	2.173396
F	-2.442484	-0.610934	-2.455128
C	-1.023596	1.505236	0.388959
C	-1.292967	2.401373	-0.661604
C	-1.016585	2.026797	1.695120
C	-1.518614	3.761186	-0.421899
H	-1.339193	2.038867	-1.686232
C	-1.248071	3.385600	1.940022
H	-0.838632	1.370600	2.542463
C	-1.493852	4.261924	0.881835
H	-1.723533	4.427237	-1.257084
H	-1.238856	3.756001	2.962801
H	-1.673784	5.316773	1.070184

TS1^{sw}-Cl$^{[B1]}$

B3LYP/BSI SCF energy: -2417.545791a.u.

M06/BSII SCF energy in solution: -2416.91441a.u.

M06/BSII free energy in solution: -2416.291085a.u.

C	1.205446	1.548327	-0.107336
C	1.490754	2.395529	-1.196314
H	1.271272	2.068172	-2.208169
C	2.088424	3.644483	-1.002361
H	2.307649	4.274216	-1.861394
C	2.408205	4.081444	0.285440
H	2.872137	5.052464	0.435804
C	2.129808	3.257624	1.376068
C	1.526580	2.009579	1.180527
C	-1.699597	0.643975	1.821032
H	-1.260091	1.649415	1.770680
C	-0.927531	-0.114941	2.924588
H	-1.339011	-1.122803	3.044302
H	0.123367	-0.239481	2.644791
C	-1.042699	0.625275	4.268002
H	-0.553017	1.605463	4.184116
H	-0.501320	0.070865	5.043574
C	-2.510460	0.818728	4.677591
H	-2.958769	-0.163402	4.885213
H	-2.573187	1.391954	5.609860
C	-3.314929	1.517121	3.571730
H	-2.955982	2.549533	3.457588
H	-4.372470	1.584627	3.853425
C	-3.184052	0.791074	2.219880
H	-3.748656	1.335167	1.455385
H	-3.641005	-0.203648	2.300504
C	-2.314020	1.208201	-1.035944
H	-3.375409	1.002514	-0.842565
C	-2.081989	2.704998	-0.737664
H	-2.337616	2.938017	0.301607
H	-1.023131	2.948235	-0.865041
C	-2.927425	3.585540	-1.675503
H	-3.994902	3.423472	-1.465307
H	-2.725146	4.641546	-1.461296
C	-2.649045	3.275439	-3.152560

H	-3.287866	3.890370	-3.797493
H	-1.610733	3.546026	-3.388781
C	-2.864000	1.786106	-3.453574
H	-2.609909	1.564263	-4.496394
H	-3.929649	1.541808	-3.332696
C	-2.027645	0.892900	-2.522374
H	-0.961244	1.045031	-2.725144
H	-2.227952	-0.161201	-2.744418
C	-2.241853	-1.638507	-0.215661
H	-1.734168	-1.983481	-1.125334
C	-3.759571	-1.617928	-0.506828
H	-3.998739	-0.914203	-1.308515
H	-4.310750	-1.285639	0.382031
C	-4.251199	-3.018697	-0.921297
H	-5.333034	-2.988159	-1.097299
H	-3.786374	-3.286049	-1.880214
C	-3.909715	-4.090354	0.122626
H	-4.482127	-3.898720	1.041594
H	-4.217555	-5.079557	-0.235225
C	-2.410977	-4.084720	0.453569
H	-1.837602	-4.400961	-0.428546
H	-2.192554	-4.808190	1.248044
C	-1.947395	-2.683102	0.884691
H	-2.482555	-2.406812	1.801628
H	-0.883152	-2.696001	1.146377
Ni	0.739033	-0.229730	-0.464861
P	-1.376085	0.019955	0.079760
H	2.383479	3.581472	2.382726
H	1.334786	1.387335	2.049888
C	4.176376	-0.568464	-0.831519
C	5.113472	-0.116379	0.096116
C	5.032866	-0.577882	1.405096
C	4.054602	-1.479852	1.805771
C	3.133915	-1.920660	0.854132
C	3.157388	-1.481102	-0.488589
H	4.221371	-0.195325	-1.849601
H	5.891375	0.589656	-0.175380
H	4.029739	-1.824362	2.834557
H	2.385009	-2.644187	1.172612
F	5.932289	-0.142032	2.313737
B	2.111174	-2.136903	-1.551228
O	2.407406	-3.412587	-2.054744
H	3.352867	-3.515873	-2.204136
O	0.720761	-2.143363	-0.976775
H	0.654618	-2.834696	-0.305921
Cl	1.804244	-0.755758	-2.990533

TS1^{sw}-Cl$^{[B2]}$

B3LYP/BSI SCF energy: -2616.013003a.u.

M06/BSII SCF energy in solution: -2615.39595a.u.

M06/BSII free energy in solution: -2614.789555a.u.

C	1.097179	1.553567	0.113957
C	1.478465	2.471782	-0.885204
H	1.332135	2.222953	-1.932048
C	2.076607	3.691669	-0.554952
H	2.370104	4.377181	-1.346366
C	2.301517	4.028871	0.781902
H	2.763936	4.978264	1.037903
C	1.930248	3.133325	1.784941
C	1.328209	1.913842	1.453073
C	-1.896199	0.464330	1.838026
H	-1.449256	1.463604	1.932320
C	-1.165283	-0.436154	2.859926
H	-1.577312	-1.450073	2.831238
H	-0.104798	-0.526258	2.602993
C	-1.328186	0.122868	4.283839
H	-0.832245	1.101594	4.347894
H	-0.818676	-0.533284	4.999266
C	-2.809427	0.274692	4.661143
H	-3.270330	-0.721871	4.716655
H	-2.904900	0.717431	5.659412
C	-3.566851	1.123768	3.630268
H	-3.195079	2.157349	3.666005
H	-4.633364	1.167692	3.881111
C	-3.393132	0.578748	2.200562
H	-3.922971	1.226470	1.494028
H	-3.864951	-0.410292	2.134607
C	-2.370284	1.418627	-0.941865
H	-3.444157	1.212950	-0.839339
C	-2.132241	2.853747	-0.424896
H	-2.448148	2.947767	0.619576
H	-1.063738	3.086216	-0.456364
C	-2.903634	3.875498	-1.279474
H	-3.984410	3.709571	-1.161010
H	-2.701121	4.886416	-0.906569
C	-2.534741	3.768407	-2.765042
H	-3.119563	4.483913	-3.355161

H	-1.478705	4.042234	-2.895152
C	-2.755520	2.341473	-3.285681
H	-2.436300	2.259840	-4.331036
H	-3.830954	2.111665	-3.268584
C	-1.998414	1.305397	-2.438353
H	-0.918852	1.454578	-2.551021
H	-2.202696	0.297302	-2.816103
C	-2.397592	-1.518489	-0.501641
H	-1.835699	-1.775436	-1.408359
C	-3.890971	-1.405056	-0.884282
H	-4.049643	-0.611537	-1.619681
H	-4.489211	-1.144421	-0.001250
C	-4.403969	-2.732327	-1.475330
H	-5.470169	-2.636995	-1.713206
H	-3.887127	-2.919070	-2.426759
C	-4.169614	-3.919113	-0.531549
H	-4.789485	-3.795561	0.368293
H	-4.493895	-4.851631	-1.007751
C	-2.694675	-4.013810	-0.118631
H	-2.079924	-4.258488	-0.995277
H	-2.551017	-4.826172	0.603659
C	-2.204461	-2.689115	0.488462
H	-2.778748	-2.491355	1.402471
H	-1.157472	-2.779606	0.795165
Ni	0.615793	-0.172401	-0.429684
P	-1.515962	0.065213	0.044927
H	2.108613	3.379533	2.829101
H	1.061495	1.235972	2.258932
C	4.019813	-0.392645	-0.670807
C	4.871117	0.031267	0.344824
C	4.686625	-0.511696	1.608190
C	3.702066	-1.457095	1.866929
C	2.896413	-1.821910	0.797518
C	2.965568	-1.312565	-0.511191
H	5.651288	0.755937	0.149091
H	3.579196	-1.899438	2.847422
F	5.493666	-0.124589	2.611131
B	1.968133	-1.923563	-1.693022
O	2.366948	-3.135548	-2.272247
H	3.291102	-3.116291	-2.541181
O	0.595424	-2.048288	-1.108309
H	0.638176	-2.714438	-0.407616
F	4.253942	0.131338	-1.884720
F	1.958879	-2.782780	1.076570
Cl	1.597428	-0.490812	-3.013253

TS2^{sw}-Cl$^{[B1]}$

B3LYP/BSI SCF energy: -2417.530366a.u.

M06/BSII SCF energy in solution: -2416.89954a.u.

M06/BSII free energy in solution: -2416.277566a.u.

C	1.229564	1.553192	0.121068
C	1.475969	2.371938	-0.999204
H	1.459763	1.941076	-1.998392
C	1.753817	3.736052	-0.862795
H	1.939807	4.339006	-1.749101
C	1.798253	4.323239	0.403848
H	2.016310	5.382100	0.513275
C	1.574046	3.526956	1.527662
C	1.298450	2.161840	1.385732
C	-1.897772	0.560455	1.735240
H	-1.492914	1.582218	1.716042
C	-1.161869	-0.166788	2.883623
H	-1.522830	-1.198008	2.968998
H	-0.089845	-0.225504	2.667175
C	-1.398570	0.551239	4.223391
H	-0.946829	1.551999	4.179720
H	-0.886895	0.011928	5.029466
C	-2.896945	0.680577	4.535412
H	-3.318792	-0.321660	4.699036
H	-3.045477	1.236317	5.468729
C	-3.651715	1.363062	3.385347
H	-3.320695	2.407722	3.302674
H	-4.727015	1.392950	3.598962
C	-3.407235	0.652535	2.041320
H	-3.940389	1.179955	1.242851
H	-3.834812	-0.357810	2.090402
C	-2.281607	1.135753	-1.151130
H	-3.353569	0.912125	-1.070518
C	-2.105341	2.630976	-0.807178
H	-2.488161	2.840384	0.197273
H	-1.042785	2.889142	-0.801235
C	-2.845112	3.521628	-1.821373
H	-3.928422	3.349894	-1.737424
H	-2.676506	4.575313	-1.569481
C	-2.399849	3.237795	-3.262447
H	-2.963424	3.862226	-3.965988
H	-1.342131	3.513507	-3.374039

C	-2.574931	1.753280	-3.608773
H	-2.209163	1.549016	-4.622016
H	-3.646250	1.504679	-3.607569
C	-1.840764	0.849208	-2.604966
H	-0.759740	1.012796	-2.689724
H	-2.012066	-0.202605	-2.862301
C	-2.249141	-1.707018	-0.346405
H	-1.690327	-2.034185	-1.233322
C	-3.747627	-1.706452	-0.722933
H	-3.950219	-0.995836	-1.529177
H	-4.353132	-1.390077	0.135925
C	-4.200312	-3.107329	-1.177995
H	-5.271115	-3.088364	-1.413729
H	-3.680630	-3.361981	-2.112368
C	-3.904317	-4.184686	-0.126108
H	-4.525744	-4.005114	0.762911
H	-4.183398	-5.174303	-0.506316
C	-2.425099	-4.167035	0.283325
H	-1.805277	-4.468673	-0.572803
H	-2.240304	-4.898279	1.079449
C	-1.997449	-2.765655	0.750691
H	-2.575200	-2.505506	1.646285
H	-0.945734	-2.770877	1.060929
Ni	0.880238	-0.274547	-0.188868
P	-1.408476	-0.048069	0.025976
H	1.622726	3.964586	2.522503
H	1.158239	1.567166	2.284803
C	3.919041	0.091732	-0.533581
C	5.193836	0.072240	0.032858
C	5.388251	-0.643770	1.208984
C	4.355978	-1.347628	1.819706
C	3.098759	-1.328283	1.216064
C	2.832283	-0.611718	0.025687
H	3.766694	0.670635	-1.439578
H	6.026523	0.609662	-0.410046
H	4.548320	-1.896451	2.736243
H	2.304667	-1.901677	1.694035
F	6.616504	-0.662612	1.772141
B	2.060285	-2.022923	-1.517247
O	2.920644	-3.080917	-1.369217
H	3.758572	-2.950296	-1.826164
O	0.777309	-2.195276	-0.926700
H	0.829005	-2.907401	-0.272503
Cl	2.046500	-1.101165	-3.097725

TS2^{sw}-Cl$^{[B2]}$

B3LYP/BSI SCF energy: -2616.007202a.u.

M06/BSII SCF energy in solution: -2615.3885a.u.

M06/BSII free energy in solution: -2614.783649a.u.

C	1.078422	1.573272	0.153765
C	1.329469	2.448034	-0.920407
H	1.292645	2.076614	-1.940694
C	1.648950	3.793176	-0.708492
H	1.840520	4.440664	-1.561275
C	1.727808	4.304307	0.588931
H	1.976306	5.348950	0.755391
C	1.496540	3.451532	1.668815
C	1.180141	2.105198	1.451410
C	-2.035805	0.577695	1.721766
H	-1.612674	1.592110	1.737068
C	-1.334918	-0.196301	2.862075
H	-1.724628	-1.218498	2.917576
H	-0.261856	-0.283174	2.662040
C	-1.576233	0.496704	4.213990
H	-1.103372	1.488636	4.200375
H	-1.088391	-0.071857	5.014635
C	-3.076554	0.649069	4.506289
H	-3.519912	-0.348142	4.640678
H	-3.228898	1.186472	5.449681
C	-3.800933	1.372406	3.361450
H	-3.449840	2.412471	3.309037
H	-4.878678	1.416990	3.559401
C	-3.549055	0.690923	2.003536
H	-4.057793	1.250416	1.211084
H	-3.998351	-0.310952	2.018561
C	-2.365237	1.238863	-1.155227
H	-3.437687	1.008624	-1.109881
C	-2.210533	2.723943	-0.760729
H	-2.619651	2.899477	0.239789
H	-1.151694	2.992463	-0.721398
C	-2.936171	3.635872	-1.766638
H	-4.019106	3.450240	-1.712962
H	-2.785506	4.683532	-1.480564
C	-2.455195	3.399330	-3.204785
H	-3.010349	4.038196	-3.901993
H	-1.398679	3.690123	-3.284945
C	-2.604679	1.923950	-3.599603

H	-2.211337	1.754184	-4.608805
H	-3.672650	1.663510	-3.633110
C	-1.885078	0.998528	-2.604857
H	-0.804572	1.176738	-2.657886
H	-2.036583	-0.047455	-2.895855
C	-2.389803	-1.628959	-0.427101
H	-1.774674	-1.979674	-1.265649
C	-3.854899	-1.575237	-0.915958
H	-3.969923	-0.864906	-1.739276
H	-4.510681	-1.230066	-0.106071
C	-4.323265	-2.961252	-1.399287
H	-5.371852	-2.903402	-1.715155
H	-3.744252	-3.238381	-2.291306
C	-4.146519	-4.044136	-0.327027
H	-4.827150	-3.839766	0.512019
H	-4.431103	-5.024397	-0.726981
C	-2.702970	-4.076367	0.192823
H	-2.028031	-4.401982	-0.610549
H	-2.604866	-4.808786	1.003096
C	-2.262437	-2.689552	0.689662
H	-2.898540	-2.403098	1.536527
H	-1.240140	-2.736240	1.078179
Ni	0.722738	-0.251363	-0.192559
P	-1.535066	0.009855	0.004184
H	1.569255	3.829300	2.686381
H	1.028931	1.465173	2.317215
C	3.778485	0.076477	-0.640293
C	5.034303	0.216405	-0.055933
C	5.236410	-0.403847	1.170461
C	4.246475	-1.154654	1.800530
C	3.037020	-1.247750	1.132962
C	2.716185	-0.668804	-0.104110
H	5.814103	0.802323	-0.526466
H	4.418902	-1.633750	2.756185
F	6.432692	-0.281841	1.771540
B	1.903596	-2.165131	-1.344035
O	2.720570	-3.251646	-1.103969
H	3.486819	-3.272419	-1.686958
O	0.624317	-2.224884	-0.701562
H	0.729762	-2.750791	0.106930
Cl	1.818841	-1.514280	-3.054128
F	3.599758	0.705972	-1.816059
F	2.068504	-2.002069	1.745777

Ph[Ni]Br

B3LYP/BSI SCF energy: -2510.486612a.u.

M06/BSII SCF energy in solution: -2509.56454a.u.

M06/BSII free energy in solution: -2508.582785a.u.

C	-0.000007	1.817245	-0.223208
C	-0.000013	2.359284	-1.524209
H	-0.000012	1.698102	-2.386138
C	-0.000021	3.740956	-1.751131
H	-0.000026	4.118196	-2.771606
C	-0.000025	4.633155	-0.676861
H	-0.000032	5.705878	-0.849243
C	-0.000020	4.122985	0.623988
C	-0.000010	2.739941	0.841533
C	3.169154	-1.109273	1.376125
H	2.761531	-2.105674	1.171467
C	2.687617	-0.747897	2.799737
H	3.040651	0.249963	3.083404
H	1.593993	-0.727783	2.822642
C	3.209644	-1.772238	3.821791
H	2.755419	-2.749596	3.609236
H	2.883588	-1.488124	4.829787
C	4.739516	-1.897441	3.772708
H	5.191935	-0.948995	4.097422
H	5.083243	-2.663340	4.478407
C	5.225916	-2.227261	2.354369
H	4.874073	-3.230008	2.074200
H	6.322012	-2.260818	2.323086
C	4.708350	-1.206716	1.323614
H	5.050283	-1.492775	0.322385
H	5.155858	-0.228759	1.540552
C	2.905798	-0.950142	-1.573455
H	3.985826	-0.767548	-1.635014
C	2.705462	-2.479589	-1.616149
H	3.206305	-2.960940	-0.770580
H	1.642048	-2.718053	-1.515425
C	3.253457	-3.067625	-2.928895
H	4.343223	-2.923015	-2.967583
H	3.083341	-4.150788	-2.941883
C	2.615211	-2.412498	-4.161198
H	3.051544	-2.819427	-5.081400
H	1.544107	-2.659421	-4.186634
C	2.779625	-0.887549	-4.120225
H	2.267759	-0.422337	-4.971571

H	3.844795	-0.633678	-4.221470
C	2.241654	-0.298202	-2.805894
H	1.159070	-0.471555	-2.747707
H	2.381079	0.788305	-2.801671
C	3.228163	1.587502	-0.091495
H	2.506071	2.188347	-0.655663
C	4.566232	1.646226	-0.864458
H	5.333790	1.060291	-0.343955
H	4.465524	1.215005	-1.864128
C	5.052693	3.099856	-1.013066
H	6.010518	3.112070	-1.547715
H	4.337922	3.651505	-1.639841
C	5.185610	3.806479	0.341370
H	5.484244	4.851953	0.198084
H	5.988584	3.328845	0.921326
C	3.872723	3.726459	1.131781
H	3.095039	4.305804	0.617047
H	3.996706	4.178196	2.123807
C	3.394226	2.272732	1.284522
H	2.452315	2.252067	1.839183
H	4.131326	1.723690	1.882793
C	-3.228156	1.587514	-0.091495
H	-2.506049	2.188356	-0.655647
C	-3.394229	2.272736	1.284525
H	-4.131348	1.723703	1.882780
H	-2.452327	2.252050	1.839201
C	-3.872698	3.726472	1.131787
H	-3.094997	4.305808	0.617069
H	-3.996688	4.178205	2.123815
C	-5.185572	3.806520	0.341358
H	-5.988563	3.328897	0.921299
H	-5.484186	4.852001	0.198074
C	-5.052649	3.099904	-1.013081
H	-4.337860	3.651546	-1.639842
H	-6.010466	3.112137	-1.547743
C	-4.566214	1.646265	-0.864477
H	-4.465500	1.215052	-1.864148
H	-5.333789	1.060339	-0.343989
C	-2.905801	-0.950138	-1.573455
H	-3.985824	-0.767523	-1.635031
C	-2.241623	-0.298226	-2.805891
H	-2.381020	0.788284	-2.801681
H	-1.159044	-0.471607	-2.747687
C	-2.779590	-0.887573	-4.120224
H	-3.844752	-0.633678	-4.221486
H	-2.267701	-0.422382	-4.971568
C	-2.615212	-2.412527	-4.161180
H	-3.051543	-2.819455	-5.081384
H	-1.544114	-2.659476	-4.186599
C	-3.253490	-3.067626	-2.928879
H	-3.083399	-4.150794	-2.941853
H	-4.343251	-2.922993	-2.967582
C	-2.705499	-2.479590	-1.616131
H	-1.642092	-2.718076	-1.515390
H	-3.206363	-2.960919	-0.770563
C	-3.169157	-1.109272	1.376124
H	-2.761529	-2.105671	1.171465
C	-4.708353	-1.206727	1.323615
H	-5.050285	-1.492788	0.322387
H	-5.155869	-0.228775	1.540557
C	-5.225908	-2.227279	2.354369
H	-6.322004	-2.260846	2.323089
H	-4.874056	-3.230023	2.074198
C	-4.739509	-1.897457	3.772708
H	-5.191934	-0.949015	4.097425
H	-5.083229	-2.663359	4.478407
C	-3.209637	-1.772242	3.821790
H	-2.755405	-2.749596	3.609233
H	-2.883583	-1.488126	4.829785
C	-2.687620	-0.747896	2.799735
H	-3.040658	0.249961	3.083405
H	-1.593995	-0.727776	2.822637
Ni	0.000000	-0.047302	0.161634
P	2.344141	-0.095500	0.018989
P	-2.344147	-0.095497	0.018989
H	-0.000023	4.801447	1.474264
H	-0.000006	2.378778	1.868249
Br	-0.000010	-2.427296	0.839111

$BrB(OH)_2$

B3LYP/BSI SCF energy: -190.024764a.u.

M06/BSII SCF energy in solution: -189.983104a.u.

M06/BSII free energy in solution: -189.97693a.u.

B	-0.982242	-0.004083	0.000006
O	-1.667123	1.165496	0.000001
H	-1.107536	1.949922	-0.000008
O	-1.602696	-1.200736	0.000018

H	-2.564764	-1.103020	0.000025
Br	0.992630	-0.015559	-0.000006

TS^{con}-Br[B1]

B3LYP/BSI SCF energy: -1970.700171a.u.

M06/BSII SCF energy in solution: -1970.04720a.u.

M06/BSII free energy in solution: -1969.427127a.u.

C	-1.011820	1.760169	0.535941
C	-0.833824	2.202694	1.858963
H	-0.635190	1.489621	2.655661
C	-0.902660	3.561509	2.191725
H	-0.762827	3.869077	3.225739
C	-1.149391	4.516609	1.205340
H	-1.201975	5.571341	1.460584
C	-1.342775	4.095851	-0.113231
C	-1.284771	2.737296	-0.438560
C	2.203946	1.652218	-0.171715
H	1.583170	2.231623	0.523108
C	1.997988	2.273135	-1.571611
H	2.616303	1.739133	-2.303956
H	0.956342	2.166030	-1.887292
C	2.396128	3.758619	-1.584714
H	1.718347	4.314378	-0.923415
H	2.256710	4.167202	-2.592969
C	3.847396	3.953295	-1.125431
H	4.525116	3.495369	-1.860527
H	4.099107	5.019988	-1.092562
C	4.082071	3.310046	0.247060
H	3.496384	3.849997	1.004097
H	5.134651	3.405316	0.540399
C	3.674673	1.824475	0.269141
H	3.834058	1.435979	1.279096
H	4.339157	1.257559	-0.394666
C	2.325363	-0.800996	1.477122
H	3.391951	-0.604289	1.309307
C	1.909428	-0.079356	2.777901
H	2.006048	1.006888	2.679348
H	0.844254	-0.276226	2.962211
C	2.723546	-0.572430	3.985306
H	3.778715	-0.296893	3.845925
H	2.385749	-0.058300	4.892997
C	2.610447	-2.093208	4.155547
H	3.242701	-2.432501	4.984488
H	1.576516	-2.350268	4.425885
C	2.990210	-2.824586	2.860643
H	2.847526	-3.905284	2.977357
H	4.060010	-2.671334	2.657903
C	2.170291	-2.326428	1.656464
H	1.114558	-2.578772	1.805007
H	2.492625	-2.861049	0.757130
C	2.021336	-1.153814	-1.446748
H	1.712356	-2.151234	-1.106147
C	3.542521	-1.206102	-1.700259
H	4.087889	-1.415705	-0.773187
H	3.890590	-0.228375	-2.055550
C	3.887455	-2.272893	-2.755760
H	4.968358	-2.273665	-2.941210
H	3.638582	-3.266440	-2.356828
C	3.118877	-2.045367	-4.065564
H	3.459379	-1.106183	-4.524674
H	3.347133	-2.842939	-4.782309
C	1.605469	-1.966881	-3.817498
H	1.241320	-2.944699	-3.472198
H	1.076460	-1.750652	-4.753229
C	1.257105	-0.898373	-2.766970
H	1.513523	0.089409	-3.165015
H	0.177494	-0.893439	-2.583239
Ni	-0.901917	-0.067524	0.076045
P	1.430428	-0.070012	-0.020465
H	-1.555566	4.825500	-0.891235
H	-1.477093	2.436539	-1.465452
C	-3.802659	0.637582	0.730065
C	-5.087091	0.972349	0.305834
C	-5.451375	0.673242	-1.003285
C	-4.580145	0.040286	-1.882953
C	-3.312074	-0.311181	-1.421140
C	-2.875679	-0.030559	-0.103902
H	-3.516267	0.893321	1.745988
H	-5.795887	1.472053	0.958610
H	-4.906494	-0.183110	-2.893714
H	-2.655250	-0.845603	-2.103135
F	-6.689698	1.000969	-1.429469
B	-2.628666	-1.940438	1.027405
O	-2.276746	-1.576284	2.301748
H	-1.510254	-0.988949	2.319394
O	-3.773442	-2.628488	0.768997
H	-4.451858	-2.414732	1.423097

Br	-1.079285	-2.641326	-0.225632

TS^{con}-Br$^{[B2]}$

B3LYP/BSI SCF energy: -2169.176936a.u.

M06/BSII SCF energy in solution: -2168.53592a.u.

M06/BSII free energy in solution: -2167.933779a.u.

C	2.310335	1.720015	-0.083838
H	1.613297	2.303272	0.530130
C	2.212861	2.280026	-1.520838
H	2.911497	1.740706	-2.172261
H	1.209000	2.123643	-1.924184
C	2.562557	3.777022	-1.558119
H	1.810464	4.332815	-0.982818
H	2.501830	4.142325	-2.590508
C	3.959314	4.041061	-0.979663
H	4.715409	3.581793	-1.632923
H	4.171577	5.116741	-0.966405
C	4.089699	3.456831	0.432509
H	3.420503	4.002469	1.112265
H	5.107778	3.600296	0.814553
C	3.730681	1.959584	0.476805
H	3.811935	1.614776	1.511446
H	4.470149	1.393636	-0.103634
C	2.384644	-0.678169	1.654498
H	3.451501	-0.432701	1.577106
C	1.812310	0.051323	2.890417
H	1.882309	1.138102	2.773886
H	0.741546	-0.180902	2.968743
C	2.523477	-0.382582	4.182790
H	3.574404	-0.061875	4.142065
H	2.075132	0.131703	5.041248
C	2.463575	-1.903691	4.376910
H	3.022801	-2.196340	5.273458
H	1.420260	-2.205441	4.546429
C	3.006531	-2.639262	3.144307
H	2.905605	-3.723541	3.271448
H	4.082624	-2.435621	3.044582
C	2.285274	-2.205265	1.855646
H	1.233039	-2.504442	1.910009
H	2.717935	-2.740764	1.003991
C	2.306980	-1.122587	-1.282851
H	2.011812	-2.121875	-0.936390
C	3.843235	-1.125311	-1.428121
H	4.328425	-1.293623	-0.459911
H	4.182186	-0.144251	-1.782699
C	4.297922	-2.203804	-2.428669
H	5.388266	-2.166838	-2.541419
H	4.060056	-3.195952	-2.019721
C	3.611246	-2.040091	-3.792249
H	3.947539	-1.101023	-4.254980
H	3.917085	-2.846968	-4.468714
C	2.082538	-2.013971	-3.647994
H	1.731279	-2.994473	-3.297461
H	1.610131	-1.845247	-4.622858
C	1.622940	-0.930980	-2.657102
H	1.870236	0.054003	-3.067456
H	0.534757	-0.964152	-2.544785
Ni	-0.713375	-0.160525	0.081099
P	1.588479	-0.024424	0.070039
C	-3.592886	0.285933	0.892109
C	-4.817939	0.888757	0.655380
C	-5.193455	1.012819	-0.680204
C	-4.403250	0.553615	-1.730424
C	-3.197967	-0.040265	-1.385818
C	-2.725019	-0.242848	-0.076408
H	-5.442745	1.263168	1.456501
H	-4.712434	0.670659	-2.761685
F	-6.368115	1.596954	-0.965589
B	-2.773382	-2.351253	0.275460
O	-3.094928	-2.489465	1.597667
H	-2.698969	-1.831905	2.180519
O	-3.555000	-2.918089	-0.694584
H	-4.444879	-3.069511	-0.349311
Br	-0.737672	-2.685225	-0.222216
F	-3.212175	0.177167	2.194957
F	-2.415690	-0.457804	-2.406924
C	-0.916848	1.704274	0.352312
C	-1.153656	2.571867	-0.729327
C	-0.874515	2.272404	1.638201
C	-1.315425	3.948467	-0.538598
H	-1.222165	2.175012	-1.739739
C	-1.042210	3.648519	1.833846
H	-0.717702	1.640418	2.507689
C	-1.257289	4.495409	0.745367
H	-1.496553	4.591981	-1.396641
H	-1.007017	4.055551	2.842016
H	-1.387839	5.563572	0.895409

TS1^{sw}-Br$^{[B1]}$

B3LYP/BSI SCF energy: -1970.731009a.u.

M06/BSII SCF energy in solution: -1970.07067a.u.

M06/BSII free energy in solution: -1969.448189a.u.

C	-1.148169	1.157287	1.007949
C	-1.520085	0.967182	2.352862
H	-1.388393	-0.005028	2.816830
C	-2.093806	2.004699	3.094238
H	-2.382518	1.828744	4.127722
C	-2.300223	3.258585	2.513870
H	-2.744564	4.064269	3.091975
C	-1.935806	3.464655	1.183525
C	-1.358688	2.426127	0.442665
C	1.919330	1.804386	-0.736389
H	1.447815	2.473381	-0.003216
C	1.257634	2.113914	-2.098475
H	1.706846	1.495046	-2.882629
H	0.192645	1.861719	-2.073843
C	1.452283	3.593743	-2.469343
H	0.927988	4.222125	-1.736016
H	0.989326	3.795922	-3.442448
C	2.940787	3.972081	-2.498716
H	3.433447	3.430621	-3.319082
H	3.058657	5.039909	-2.716409
C	3.634682	3.621408	-1.174661
H	3.233646	4.258295	-0.373905
H	4.707849	3.837551	-1.236734
C	3.424790	2.145038	-0.789306
H	3.909844	1.944471	0.171569
H	3.920411	1.506237	-1.531840
C	2.292015	0.074976	1.660797
H	3.370569	0.044633	1.454841
C	2.039540	1.314265	2.546377
H	2.363039	2.228159	2.036328
H	0.968126	1.421217	2.738058
C	2.789458	1.187327	3.885354
H	3.873630	1.196144	3.700145
H	2.572462	2.064989	4.505509
C	2.413270	-0.100938	4.630009
H	2.986229	-0.182213	5.561291
H	1.353422	-0.057029	4.915761
C	2.647815	-1.335885	3.749557
H	2.324048	-2.245213	4.268470
H	3.726020	-1.448267	3.562812
C	1.905571	-1.221852	2.407988
H	0.824013	-1.228908	2.583639
H	2.113642	-2.105267	1.794544
C	2.344488	-1.264841	-0.980959
H	1.775211	-2.141730	-0.646305
C	3.833601	-1.530503	-0.664099
H	3.996607	-1.636739	0.411411
H	4.446422	-0.682778	-0.996498
C	4.317208	-2.816758	-1.361880
H	5.381936	-2.968179	-1.148427
H	3.787045	-3.675514	-0.927636
C	4.077222	-2.786269	-2.877461
H	4.721914	-2.021014	-3.332942
H	4.366381	-3.743768	-3.325599
C	2.611575	-2.467101	-3.203609
H	1.972455	-3.296190	-2.869221
H	2.472171	-2.378686	-4.287578
C	2.164609	-1.167373	-2.512700
H	2.776884	-0.341897	-2.896273
H	1.129729	-0.924013	-2.780422
Ni	-0.688705	-0.338697	-0.021541
P	1.471780	0.123609	-0.030369
H	-2.101868	4.432193	0.715615
H	-1.100291	2.613637	-0.595009
C	-4.139611	-0.650111	-0.297697
C	-4.934993	0.457821	-0.574429
C	-4.608983	1.262764	-1.662745
C	-3.523737	0.985076	-2.482456
C	-2.743295	-0.134456	-2.185983
C	-3.018157	-0.982003	-1.087954
H	-4.369691	-1.264232	0.566912
H	-5.790429	0.714022	0.041780
H	-3.307472	1.630472	-3.327471
H	-1.908081	-0.360818	-2.845552
F	-5.372537	2.342072	-1.931183
B	-2.119259	-2.311718	-0.925286
O	-2.487789	-3.492524	-1.550613
H	-3.445109	-3.594372	-1.581833
O	-0.685351	-2.022195	-1.108194
H	-0.436173	-2.086026	-2.038996
Br	-1.964471	-2.617379	1.408255

TS1^{sw}-Br$^{[B2]}$

B3LYP/BSI SCF energy: -2169.196335a.u.

M06/BSII SCF energy in solution: -2168.54985a.u.

M06/BSII free energy in solution: -2167.944574a.u.

C	-1.066766	1.442058	0.571148
C	-1.597784	1.520969	1.873945
H	-1.580353	0.646644	2.518556
C	-2.175214	2.704514	2.344489
H	-2.585750	2.738105	3.350852
C	-2.226169	3.838789	1.529966
H	-2.670489	4.759209	1.898880
C	-1.703648	3.778570	0.237722
C	-1.124348	2.593821	-0.232322
C	2.141892	1.494535	-1.210038
H	1.690743	2.394709	-0.770872
C	1.546229	1.358038	-2.629705
H	1.952361	0.470035	-3.125501
H	0.461455	1.214297	-2.575233
C	1.878999	2.596034	-3.480425
H	1.383712	3.477020	-3.048054
H	1.469107	2.471292	-4.489585
C	3.393295	2.845172	-3.545772
H	3.872534	2.016374	-4.086177
H	3.604766	3.754558	-4.120221
C	4.002551	2.951055	-2.141018
H	3.615924	3.851615	-1.643615
H	5.090432	3.072700	-2.203808
C	3.668412	1.719271	-1.280000
H	4.093012	1.844965	-0.278311
H	4.151260	0.836324	-1.717481
C	2.250867	0.723634	1.657830
H	3.337730	0.590845	1.572299
C	2.005127	2.206663	2.010807
H	2.413664	2.864898	1.236877
H	0.930204	2.400772	2.061472
C	2.653147	2.558988	3.362415
H	3.746164	2.469986	3.277514
H	2.444119	3.608479	3.601232
C	2.156262	1.643068	4.488957
H	2.658259	1.892720	5.431291
H	1.083223	1.816911	4.647993
C	2.382029	0.166474	4.137736
H	1.973523	-0.481828	4.921366
H	3.462410	-0.035943	4.096154
C	1.740132	-0.197238	2.788850
H	0.652304	-0.100802	2.862045
H	1.930123	-1.250408	2.556706
C	2.460804	-1.473387	-0.336070
H	1.791405	-2.180446	0.170566
C	3.874372	-1.644249	0.264454
H	3.881382	-1.408390	1.331398
H	4.576170	-0.952757	-0.219816
C	4.372451	-3.090556	0.081299
H	5.385601	-3.181475	0.490850
H	3.734434	-3.761082	0.673039
C	4.346279	-3.532444	-1.387569
H	5.084508	-2.948131	-1.955748
H	4.647644	-4.582892	-1.473071
C	2.956231	-3.323730	-2.002961
H	2.231891	-3.994033	-1.521791
H	2.967359	-3.583129	-3.068364
C	2.485202	-1.870065	-1.829332
H	3.174647	-1.210964	-2.372330
H	1.501376	-1.736998	-2.287099
Ni	-0.589604	-0.242787	-0.084451
P	1.573794	0.168827	-0.007802
H	-1.743935	4.652634	-0.408068
H	-0.728527	2.576895	-1.244364
C	-3.952599	-0.576656	0.013182
C	-4.757902	0.482174	-0.388629
C	-4.523981	1.032105	-1.641881
C	-3.539135	0.543624	-2.490144
C	-2.775906	-0.511685	-2.011341
C	-2.887891	-1.111900	-0.741289
H	-5.544607	0.856212	0.254176
H	-3.384113	0.952448	-3.480454
F	-5.287366	2.055419	-2.057049
B	-1.935275	-2.407864	-0.379106
O	-2.357565	-3.665997	-0.792586
H	-3.290450	-3.816219	-0.607050
O	-0.554468	-2.112259	-0.823900
H	-0.546861	-2.140854	-1.791917
F	-4.239796	-1.110768	1.208244
F	-1.849122	-1.007384	-2.889204
Br	-1.501566	-2.370702	1.840029

TS2^{sw}-Br$^{[B1]}$

B3LYP/BSI SCF energy: -1970.709537a.u.

M06/BSII SCF energy in solution: -1970.05107a.u.

M06/BSII free energy in solution: -1969.431425a.u.

C	-0.858216	1.616771	0.923765
C	-0.831747	1.478167	2.323993
H	-0.801701	0.487906	2.771559
C	-0.852332	2.593360	3.170184
H	-0.833049	2.450266	4.248521
C	-0.901862	3.882570	2.637488
H	-0.917966	4.749492	3.292431
C	-0.947482	4.041610	1.250347
C	-0.935033	2.923858	0.409547
C	2.448138	1.400283	0.501312
H	1.810412	1.723532	1.334836
C	2.438087	2.549401	-0.531683
H	3.080392	2.283988	-1.381648
H	1.427436	2.701481	-0.920839
C	2.959336	3.855970	0.088207
H	2.265436	4.176015	0.876630
H	2.960164	4.648831	-0.669695
C	4.367040	3.676121	0.672494
H	5.075736	3.478089	-0.145014
H	4.701815	4.601223	1.156631
C	4.408767	2.510598	1.670105
H	3.799317	2.764853	2.548505
H	5.431475	2.354898	2.034594
C	3.875941	1.202027	1.056056
H	3.898601	0.419528	1.820257
H	4.552498	0.878299	0.255021
C	2.130712	-1.508170	1.010659
H	3.226801	-1.438242	1.016353
C	1.627572	-1.302924	2.457303
H	1.889344	-0.305965	2.828055
H	0.532077	-1.356409	2.457298
C	2.185179	-2.376404	3.406228
H	3.277569	-2.269933	3.475936
H	1.791757	-2.213804	4.416742
C	1.839667	-3.789073	2.917249
H	2.285950	-4.542219	3.577575
H	0.751449	-3.931411	2.966856
C	2.310839	-4.002348	1.472408
H	2.007962	-4.993676	1.114797
H	3.410150	-3.982646	1.442790
C	1.759887	-2.925065	0.520356
H	0.670487	-3.018231	0.453674
H	2.156090	-3.106060	-0.484492
C	2.145665	-0.629782	-1.812544
H	1.700505	-1.629485	-1.915246
C	3.671324	-0.791133	-1.973327
H	4.082479	-1.415588	-1.172713
H	4.154483	0.189924	-1.885778
C	4.024035	-1.401896	-3.341843
H	5.113154	-1.475897	-3.445367
H	3.636381	-2.429648	-3.387783
C	3.431747	-0.583802	-4.498247
H	3.911815	0.404797	-4.524693
H	3.655374	-1.064243	-5.457895
C	1.915706	-0.401240	-4.334205
H	1.422257	-1.379892	-4.428640
H	1.517736	0.227219	-5.139762
C	1.566846	0.217114	-2.969286
H	1.967077	1.235938	-2.928686
H	0.479509	0.317163	-2.862497
Ni	-0.796716	0.095539	-0.188061
P	1.512201	-0.120074	-0.110109
H	-1.007641	5.038445	0.818919
H	-1.007187	3.078869	-0.664582
C	-3.742824	0.477620	0.476088
C	-4.990369	1.038843	0.200285
C	-5.229874	1.531371	-1.077957
C	-4.268120	1.469670	-2.080692
C	-3.036820	0.887271	-1.779035
C	-2.728937	0.369262	-0.499222
H	-3.553214	0.114125	1.481714
H	-5.765657	1.111829	0.956530
H	-4.492977	1.866718	-3.065661
H	-2.299000	0.834249	-2.579388
F	-6.432632	2.080813	-1.356904
B	-2.277773	-1.878439	-0.790125
O	-3.225707	-2.211070	-1.710971
H	-4.101071	-2.350105	-1.332992
O	-0.967017	-1.676025	-1.270814
H	-1.000923	-1.540563	-2.230260
Br	-2.374604	-2.710465	1.046160

TS2^{sw}-Br$^{[B2]}$

B3LYP/BSI SCF energy: -2169.185217a.u.

M06/BSII SCF energy in solution: -2168.53818a.u.

M06/BSII free energy in solution: -2167.934603a.u.

C	0.876387	1.694446	-0.472442
C	1.129933	1.969288	-1.829389
H	1.174148	1.156116	-2.548546
C	1.349452	3.274992	-2.280838
H	1.545126	3.452327	-3.336019
C	1.324290	4.346060	-1.384989
H	1.495352	5.360603	-1.734478
C	1.091955	4.093430	-0.032471
C	0.876170	2.784598	0.415285
C	-2.304813	1.330455	1.212987
H	-1.945226	2.246343	0.723381
C	-1.659037	1.313769	2.617195
H	-1.994647	0.433954	3.176718
H	-0.570406	1.233523	2.535461
C	-2.050951	2.575453	3.404797
H	-1.636682	3.459195	2.899928
H	-1.598921	2.544793	4.403369
C	-3.576859	2.717125	3.515243
H	-3.970822	1.894166	4.128886
H	-3.836775	3.645642	4.037103
C	-4.246197	2.679884	2.133529
H	-3.956714	3.574995	1.565174
H	-5.337384	2.716112	2.236981
C	-3.840214	1.427900	1.334249
H	-4.316188	1.452144	0.347913
H	-4.225232	0.536353	1.846245
C	-2.438370	0.419743	-1.609194
H	-3.491710	0.130838	-1.499190
C	-2.421731	1.910270	-2.012500
H	-2.919432	2.522081	-1.252723
H	-1.390646	2.267672	-2.081442
C	-3.127014	2.115352	-3.365428
H	-4.193394	1.865672	-3.263270
H	-3.080898	3.175343	-3.642039
C	-2.508592	1.247146	-4.469921
H	-3.048651	1.389436	-5.413587
H	-1.474136	1.572252	-4.647436
C	-2.510897	-0.235020	-4.072255
H	-2.018200	-0.840572	-4.841993
H	-3.549126	-0.592608	-4.010831
C	-1.815062	-0.456893	-2.719289
H	-0.750412	-0.211732	-2.809946
H	-1.860610	-1.518417	-2.449307
C	-2.352628	-1.678403	0.476168
H	-1.652631	-2.347103	-0.041001
C	-3.773664	-2.022198	-0.025353
H	-3.864333	-1.847327	-1.101201
H	-4.514406	-1.376095	0.463600
C	-4.110878	-3.498918	0.261071
H	-5.131687	-3.712822	-0.077676
H	-3.444380	-4.135337	-0.337610
C	-3.953171	-3.859485	1.744102
H	-4.710216	-3.321175	2.332290
H	-4.142867	-4.928426	1.896357
C	-2.557130	-3.483885	2.258648
H	-1.800624	-4.108381	1.763892
H	-2.478689	-3.685828	3.333684
C	-2.249266	-2.003267	1.983331
H	-2.971135	-1.389377	2.536357
H	-1.262374	-1.743648	2.380237
Ni	0.651089	-0.095077	0.094461
P	-1.632430	0.022497	0.045507
H	1.086986	4.913604	0.682098
H	0.725053	2.622159	1.479525
C	3.714064	0.245329	-0.298620
C	4.931681	0.685644	0.214161
C	5.073306	0.697555	1.595842
C	4.060009	0.274975	2.453363
C	2.893177	-0.158807	1.847241
C	2.634643	-0.217419	0.470153
H	5.727751	1.025086	-0.436954
H	4.183747	0.288006	3.529049
F	6.231394	1.125628	2.127903
B	1.990952	-2.243484	0.053981
O	2.883991	-2.991049	0.779082
H	3.699592	-3.177060	0.301741
O	0.697755	-2.086934	0.618325
H	0.787258	-2.134506	1.584427
F	3.595886	0.263846	-1.638999
F	1.901768	-0.595219	2.693193
Br	1.944251	-2.529287	-1.950365

^{PPh2Me}Naph[Ni]F

B3LYP/BSI SCF energy: -2458.651426a.u.

M06/BSII SCF energy in solution: -2457.88418a.u.

M06/BSII free energy in solution: -2457.366718a.u.

F	-0.622287	-2.330469	-1.788157
Ni	-0.213535	-0.800317	-0.776046
P	1.910736	-1.533718	-0.854056
P	-2.434747	-0.394585	-0.867010
O	0.141361	0.399255	1.571716
C	0.180558	0.632847	0.361799
C	-2.990149	-0.673790	-2.605233
H	-2.509254	-1.603521	-2.913643
H	-4.076848	-0.755855	-2.687366
H	-2.625824	0.134538	-3.245305
C	-3.371538	-1.675793	0.082724
C	-4.445517	-1.359027	0.926735
C	-2.988280	-3.021177	-0.066476
C	-5.124578	-2.368811	1.612327
H	-4.755334	-0.327636	1.054650
C	-3.677577	-4.023768	0.615678
H	-2.151385	-3.257833	-0.717818
C	-4.743962	-3.701920	1.458526
H	-5.953157	-2.109235	2.265475
H	-3.376064	-5.060239	0.490346
H	-5.274615	-4.485443	1.992439
C	-3.202357	1.199577	-0.363414
C	-4.067913	1.912560	-1.207398
C	-2.906233	1.732424	0.904528
C	-4.622893	3.126485	-0.796573
H	-4.317661	1.527767	-2.190256
C	-3.468152	2.940937	1.314281
H	-2.226155	1.208191	1.568005
C	-4.326518	3.642353	0.464811
H	-5.288836	3.665536	-1.464568
H	-3.224267	3.339212	2.294765
H	-4.758047	4.587019	0.783181
C	2.134192	-2.985207	0.260416
C	3.399281	-3.562583	0.454370
C	1.023700	-3.535807	0.915007
C	3.548185	-4.675175	1.281028
H	4.272280	-3.135538	-0.031464
C	1.176492	-4.648559	1.744892
H	0.043085	-3.094200	0.772853
C	2.435776	-5.220022	1.927835
H	4.531895	-5.113446	1.424452
H	0.309216	-5.064258	2.249713
H	2.553331	-6.084377	2.575505
C	3.366009	-0.477424	-0.454827
C	3.477510	0.062285	0.839170
C	4.355671	-0.171689	-1.400759
C	4.553927	0.881273	1.173921
H	2.714748	-0.150278	1.581550
C	5.432627	0.651545	-1.062227
H	4.297616	-0.573783	-2.406702
C	5.534923	1.178511	0.224541
H	4.622522	1.292950	2.176589
H	6.190772	0.877206	-1.806992
H	6.371783	1.819472	0.486812
C	2.261178	-2.216071	-2.530805
H	3.193405	-2.785949	-2.560698
H	1.406517	-2.851829	-2.766078
H	2.296645	-1.405893	-3.264275
C	0.841580	3.339382	-2.208848
C	1.147015	4.449065	-1.456493
C	1.159275	4.386911	-0.037206
C	0.848575	3.150408	0.628205
C	0.530007	1.999671	-0.181076
C	0.535568	2.124392	-1.561498
H	1.708979	6.463389	0.210048
H	0.834593	3.392382	-3.293710
H	1.385160	5.394685	-1.937660
C	1.477074	5.538356	0.732346
C	0.875083	3.137771	2.051193
H	0.294092	1.244185	-2.154273
C	1.188361	4.275274	2.765554
C	1.492649	5.488522	2.106943
H	0.643520	2.211286	2.558329
H	1.201676	4.237775	3.851583
H	1.737165	6.374942	2.685505

PPh_2Me

B3LYP/BSI SCF energy: -844.571767a.u.

M06/BSII SCF energy in solution: -844.285993a.u.

M06/BSII free energy in solution: -844.106234a.u.

P	-0.042096	1.372785	0.692726
C	-0.069696	2.579653	-0.729593
H	-1.003249	3.145360	-0.665669
H	0.758133	3.288291	-0.632251
H	-0.021992	2.096610	-1.710473

C	-1.438431	0.257015	0.190072
C	-2.633436	0.339999	0.920377
C	-1.370922	-0.639475	-0.888732
C	-3.739206	-0.440748	0.575150
H	-2.695017	1.018013	1.767993
C	-2.471648	-1.424884	-1.230534
H	-0.449227	-0.729817	-1.456739
C	-3.659393	-1.325250	-0.500741
H	-4.657429	-0.362947	1.150787
H	-2.403482	-2.116071	-2.066344
H	-4.515544	-1.938634	-0.767454
C	1.434111	0.328996	0.296557
C	1.672762	-0.796216	1.107193
C	2.370189	0.635004	-0.702885
C	2.794851	-1.598085	0.911626
H	0.969021	-1.046850	1.897360
C	3.502983	-0.162286	-0.891894
H	2.225606	1.497958	-1.344811
C	3.717537	-1.281937	-0.089614
H	2.954039	-2.466506	1.544936
H	4.215267	0.093810	-1.671647
H	4.597110	-1.901711	-0.238479

^{PPh2Me}TS10^{con}

B3LYP/BSI SCF energy: -2136.8364a.u.

M06/BSII SCF energy in solution: -2136.17750a.u.

M06/BSII free energy in solution: -2135.722449a.u.

F	0.291979	-3.015306	1.142244
Ni	0.022111	-1.071608	0.580122
P	2.215564	-0.598237	0.603171
C	-3.026508	-1.080773	0.857901
C	-4.258079	-1.161528	0.207757
C	-4.356940	-1.888213	-0.986758
C	-3.223382	-2.539971	-1.500714
C	-2.016378	-2.456777	-0.823094
C	-1.865115	-1.725502	0.384596
H	-2.973561	-0.508125	1.780325
H	-5.121286	-0.657310	0.627265
H	-3.327511	-3.112384	-2.417589
H	-1.168861	-3.012533	-1.219770
B	-0.983893	-2.857726	1.851133
O	-0.971406	-2.102935	3.024625
H	-0.794969	-1.157937	2.901178
O	-1.648310	-4.070888	1.867363
H	-2.339061	-4.043585	2.538675
C	-0.544975	0.661495	0.853007
O	-0.649732	0.904357	2.059121
O	-5.499729	-2.030090	-1.714488
C	-6.680414	-1.394493	-1.248763
H	-6.559847	-0.305014	-1.196947
H	-7.458524	-1.635987	-1.974635
H	-6.979284	-1.768949	-0.261512
C	2.829713	1.115676	0.331214
C	3.509375	1.486896	-0.838311
C	2.555308	2.098741	1.297824
C	3.918483	2.807927	-1.029883
H	3.726523	0.745614	-1.600114
C	2.968130	3.416120	1.103403
H	2.000274	1.845275	2.195641
C	3.653142	3.774120	-0.059465
H	4.446485	3.078763	-1.939785
H	2.746360	4.164107	1.858829
H	3.972606	4.801232	-0.209776
C	3.183234	-1.649400	-0.554175
C	4.583367	-1.741393	-0.482982
C	2.501886	-2.400275	-1.522756
C	5.282587	-2.568956	-1.360091
H	5.131977	-1.160119	0.252479
C	3.203033	-3.229153	-2.401125
H	1.419015	-2.340346	-1.581640
C	4.592663	-3.315331	-2.319541
H	6.364911	-2.632810	-1.294601
H	2.661928	-3.809360	-3.142623
H	5.138863	-3.962413	-2.999790
C	2.883492	-1.042287	2.270799
H	2.618754	-2.083183	2.470759
H	3.966666	-0.911755	2.333952
H	2.399026	-0.417969	3.025168
C	-1.894622	5.765161	0.335571
C	-1.789880	5.237093	-0.930284
C	-1.443185	3.873243	-1.126382
C	-1.196765	3.032193	0.013178
C	-1.317986	3.612071	1.306268
C	-1.656702	4.940449	1.458591
H	-1.536875	3.990450	-3.283396
H	-2.161278	6.808958	0.474628
H	-1.972381	5.856791	-1.804724

C	-1.340988	3.335743	-2.437615
C	-0.839739	1.654754	-0.225423
H	-1.145430	2.985903	2.170794
H	-1.744895	5.358112	2.457841
C	-0.754585	1.187211	-1.527489
C	-1.005602	2.017136	-2.638647
H	-0.497181	0.142651	-1.676712
H	-0.935332	1.611474	-3.643371

^{PPh2Me}TS11^{sw}

B3LYP/BSI SCF energy: -2136.842213a.u.

M06/BSII SCF energy in solution: -2136.18334a.u.

M06/BSII free energy in solution: -2135.726951a.u.

Ni	-0.713134	-0.577856	-1.092551
P	-2.030530	1.066185	-0.543152
C	1.472197	-2.969816	-1.142627
C	2.486116	-3.249838	-0.234960
C	2.169624	-3.559005	1.095915
C	0.827683	-3.580112	1.500943
C	-0.170828	-3.297300	0.565205
C	0.103598	-2.986504	-0.781692
H	1.733981	-2.730291	-2.169688
H	3.531733	-3.234175	-0.526710
H	0.556404	-3.823607	2.522186
H	-1.206056	-3.346511	0.901914
B	-1.082484	-2.827860	-1.914046
O	-1.682908	-4.021552	-2.380882
H	-1.024161	-4.716073	-2.480791
O	-2.165460	-1.901564	-1.374589
H	-2.630594	-2.290417	-0.624872
F	-0.511437	-1.964133	-2.939940
O	3.230117	-3.824803	1.914039
C	2.969708	-4.170385	3.263254
H	3.943120	-4.348582	3.723344
H	2.461738	-3.358715	3.801223
H	2.362831	-5.081976	3.340547
O	0.810866	1.084134	-2.382653
C	0.761166	0.548958	-1.280000
C	5.500439	2.846798	-0.671477
C	5.176751	2.252603	0.526316
C	3.956475	1.542441	0.682905
C	3.044023	1.444309	-0.423727
C	3.414286	2.067646	-1.647307
C	4.608653	2.748407	-1.763188
H	4.338405	1.019431	2.745894
H	6.436815	3.386245	-0.781384
H	5.852793	2.315373	1.375403
C	3.632623	0.930269	1.923584
C	1.813324	0.716096	-0.225554
H	2.740042	1.995074	-2.489430
H	4.868131	3.213091	-2.710415
C	1.556808	0.131791	1.005070
C	2.456892	0.236220	2.084810
H	0.634383	-0.427899	1.127123
H	2.218472	-0.234537	3.033644
C	-1.466388	2.613413	0.282698
C	-1.882125	2.953386	1.578823
C	-0.581936	3.471062	-0.395311
C	-1.429309	4.128644	2.181105
H	-2.564957	2.307158	2.119944
C	-0.136764	4.645416	0.209698
H	-0.223145	3.216145	-1.387109
C	-0.558984	4.978295	1.498472
H	-1.762635	4.379195	3.184168
H	0.546691	5.297019	-0.326675
H	-0.208915	5.893025	1.967907
C	-3.453555	0.490524	0.468653
C	-3.216692	-0.431834	1.501663
C	-4.764508	0.936783	0.246569
C	-4.266322	-0.892339	2.297679
H	-2.206754	-0.793791	1.676449
C	-5.814689	0.468444	1.037954
H	-4.975154	1.647442	-0.545727
C	-5.568293	-0.444849	2.064293
H	-4.068264	-1.604858	3.093189
H	-6.826020	0.816718	0.849737
H	-6.387600	-0.809570	2.676781
C	-2.746587	1.656671	-2.138128
H	-1.912058	1.925925	-2.790100
H	-3.283760	0.826553	-2.603241
H	-3.405645	2.519438	-2.012043

^{PPh2Me}TS12^{sw}

B3LYP/BSI SCF energy: -2136.843317a.u.

M06/BSII SCF energy in solution: -2136.18497a.u.

M06/BSII free energy in solution: -2135.73003a.u.

Ni	-0.339297	-1.029932	-0.435592
P	-2.318000	0.005869	-0.688618
C	2.476746	-1.939392	-1.042239
C	3.800523	-2.146129	-0.645083
C	4.076131	-2.439289	0.696022
C	3.018543	-2.535718	1.616691
C	1.714484	-2.337179	1.189207
C	1.382939	-2.035087	-0.157878
H	2.286776	-1.703891	-2.085850
H	4.597936	-2.068997	-1.375726
H	3.253017	-2.772638	2.650244
H	0.920578	-2.446386	1.926581
B	-0.003116	-3.430215	-0.939096
O	0.307086	-4.612147	-0.284161
H	1.141104	-4.978202	-0.597892
C	0.643357	0.507065	-0.815005
O	0.740216	0.755869	-2.016568
O	5.322710	-2.658362	1.203516
C	6.433532	-2.555177	0.326556
H	6.514635	-1.550732	-0.107790
H	7.317235	-2.756555	0.934344
H	6.379030	-3.291842	-0.485343
C	-2.587824	1.810137	-0.408617
C	-3.491545	2.289173	0.551494
C	-1.854024	2.735521	-1.172362
C	-3.661791	3.661957	0.741621
H	-4.069099	1.594270	1.151472
C	-2.032344	4.105173	-0.981670
H	-1.128247	2.390213	-1.901260
C	-2.935807	4.572936	-0.025139
H	-4.366223	4.015971	1.489105
H	-1.456002	4.806735	-1.577667
H	-3.069358	5.640651	0.123320
C	-3.645419	-0.810892	0.291099
C	-4.915343	-1.100047	-0.228577
C	-3.360653	-1.172287	1.618958
C	-5.875882	-1.736356	0.560188
H	-5.161260	-0.834484	-1.251396
C	-4.323668	-1.799702	2.410157
H	-2.377561	-0.958468	2.031178
C	-5.583406	-2.085642	1.879552
H	-6.853199	-1.959260	0.141930
H	-4.088696	-2.069655	3.435730
H	-6.332172	-2.581202	2.490575
C	-2.798274	-0.218754	-2.458201
H	-2.845321	-1.288899	-2.674549
H	-3.747207	0.263869	-2.705594
H	-2.001431	0.215157	-3.067390
C	3.821198	4.745406	-0.419066
C	3.434533	4.404068	0.856135
C	2.577696	3.294491	1.087919
C	2.105254	2.516346	-0.025447
C	2.529424	2.897998	-1.329238
C	3.362855	3.980853	-1.516130
H	2.553230	3.554505	3.234876
H	4.477218	5.595359	-0.584732
H	3.781296	4.978899	1.711440
C	2.185398	2.949968	2.409271
C	1.239468	1.394459	0.245857
H	2.179608	2.319288	-2.172862
H	3.672910	4.248904	-2.522559
C	0.900978	1.103050	1.556658
C	1.361363	1.874562	2.643268
H	0.255750	0.247331	1.734539
H	1.067580	1.614110	3.655904
F	0.220594	-3.307710	-2.278985
O	-1.252633	-2.850471	-0.519386
H	-1.531243	-3.221708	0.328344

^{PPh2Me}TS13

B3LYP/BSI SCF energy: -1860.31542a.u.

M06/BSII SCF energy in solution: -1859.66730a.u.

M06/BSII free energy in solution: -1859.247121a.u.

Ni	0.694658	-0.004406	-0.233898
P	-0.828763	-1.484921	0.742753
O	1.400085	0.577150	-2.873979
C	0.817278	0.796389	-1.836147
C	2.545486	-0.090306	0.039515
C	3.543718	-0.397554	-0.889590
C	2.932630	0.044110	1.390481
C	4.873830	-0.604491	-0.501544
H	3.284466	-0.463570	-1.943290
C	4.253990	-0.144808	1.791665
H	2.198103	0.300763	2.153962
C	5.232306	-0.477987	0.845072
H	5.614208	-0.851522	-1.254734
H	4.550928	-0.040150	2.831344

O	6.501390	-0.651714	1.336988
C	7.527870	-0.985445	0.421505
H	8.442577	-1.077811	1.010488
H	7.329771	-1.939691	-0.085315
H	7.667964	-0.205068	-0.338704
C	-2.733751	2.062350	-2.418731
C	-2.809042	3.173926	-1.607946
C	-1.691119	3.593293	-0.837385
C	-0.472357	2.837326	-0.895958
C	-0.426350	1.678463	-1.739814
C	-1.537003	1.315207	-2.487103
H	-2.672737	5.318958	0.023472
H	-3.591309	1.756156	-3.010838
H	-3.726664	3.754424	-1.553621
C	-1.746882	4.750344	-0.013651
C	0.645991	3.286181	-0.138483
H	-1.477725	0.443093	-3.131382
C	0.554356	4.412037	0.650405
C	-0.651784	5.150207	0.717330
H	1.574831	2.728136	-0.188658
H	1.417527	4.739951	1.222199
H	-0.706894	6.037004	1.342118
C	0.044700	-2.715286	1.815690
H	0.866752	-3.133840	1.230675
H	0.472183	-2.210645	2.686150
H	-0.613842	-3.526180	2.138111
C	-2.243938	-0.896100	1.763276
C	-2.575538	-1.437945	3.014430
C	-3.002527	0.180274	1.269875
C	-3.642974	-0.919359	3.751667
H	-2.005415	-2.264178	3.426195
C	-4.073312	0.688638	2.002763
H	-2.754354	0.623925	0.309504
C	-4.395161	0.141449	3.247319
H	-3.884652	-1.347555	4.720353
H	-4.648663	1.519696	1.605493
H	-5.223962	0.543861	3.822562
C	-1.599626	-2.555856	-0.547693
C	-0.871833	-2.802561	-1.723776
C	-2.862092	-3.146632	-0.389452
C	-1.394355	-3.633516	-2.716046
H	0.101461	-2.338731	-1.863424
C	-3.383896	-3.971418	-1.386950
H	-3.441773	-2.958085	0.508993
C	-2.651488	-4.217550	-2.550186
H	-0.821200	-3.816149	-3.620416
H	-4.364130	-4.420875	-1.254938
H	-3.060990	-4.858504	-3.325727

^{PPh2Me}TS14

B3LYP/BSI SCF energy: -1860.314122a.u.

M06/BSII SCF energy in solution: -1859.66864a.u.

M06/BSII free energy in solution: -1859.245271a.u.

Ni	0.013663	0.367995	0.023710
P	2.027184	-0.478840	-0.093187
C	-1.697590	2.510596	-0.662389
C	-2.450935	3.578846	-0.177046
C	-3.279780	3.383454	0.937796
C	-3.350134	2.118266	1.542763
C	-2.585568	1.066749	1.052919
C	-1.714391	1.248147	-0.044424
H	-1.106747	2.634320	-1.565943
H	-2.405050	4.539209	-0.677765
H	-4.014723	1.987938	2.391329
H	-2.664336	0.097143	1.534347
C	-1.222721	-0.112811	-1.283635
O	-0.930901	0.336496	-2.403262
O	-4.067709	4.346950	1.493071
C	-4.049860	5.646227	0.922415
H	-4.735153	6.247648	1.521822
H	-3.048143	6.092815	0.962460
H	-4.395640	5.636214	-0.119119
C	-2.457012	-4.165578	1.978398
C	-3.225711	-4.298529	0.845738
C	-3.130134	-3.367117	-0.224621
C	-2.216054	-2.260832	-0.121878
C	-1.434875	-2.165616	1.064109
C	-1.550717	-3.084510	2.084532
H	-4.608374	-4.360463	-1.452452
H	-2.541791	-4.884834	2.787970
H	-3.923917	-5.126246	0.748375
C	-3.918593	-3.522132	-1.394414
C	-2.125587	-1.336270	-1.217518
H	-0.726557	-1.341316	1.155749
H	-0.942876	-2.975988	2.978825
C	-2.903702	-1.550912	-2.345181
C	-3.804648	-2.631335	-2.436315

H	-2.799781	-0.852282	-3.168256
H	-4.405435	-2.754639	-3.333045
C	3.050884	-0.282742	1.428879
C	3.633209	-1.359538	2.112551
C	3.207520	1.012706	1.954079
C	4.357753	-1.146359	3.288708
H	3.525900	-2.371631	1.736709
C	3.936474	1.224933	3.122201
H	2.756929	1.859369	1.441619
C	4.512963	0.143692	3.794578
H	4.801542	-1.992108	3.806426
H	4.049915	2.232775	3.511081
H	5.076500	0.307348	4.708541
C	3.081104	0.240009	-1.428752
C	2.446963	0.806437	-2.546517
C	4.483212	0.203808	-1.376541
C	3.211660	1.320866	-3.596246
H	1.360897	0.837697	-2.596158
C	5.240621	0.724479	-2.425724
H	4.984973	-0.221154	-0.511884
C	4.605463	1.283156	-3.537613
H	2.713462	1.755293	-4.458337
H	6.325548	0.696000	-2.374130
H	5.196740	1.689642	-4.353498
C	2.094517	-2.290071	-0.471866
H	1.592887	-2.436311	-1.431540
H	3.120875	-2.660045	-0.548205
H	1.544918	-2.853334	0.286619

^{PEt3}Naph[Ni]F

B3LYP/BSI SCF energy: -1927.606937a.u.

M06/BSII SCF energy in solution: -1927.10248a.u.

M06/BSII free energy in solution: -1926.61749a.u.

F	2.962106	0.039307	0.406135
Ni	1.158514	0.025531	-0.087976
P	1.302423	-2.213551	-0.093902
P	1.387295	2.257041	-0.060224
O	-0.822670	0.107625	-1.899324
C	-0.621909	0.040222	-0.683362
C	-0.107628	-3.159923	-2.395686
H	0.811122	-3.490070	-2.891104
H	-0.924845	-3.784797	-2.771105
H	-0.306590	-2.127113	-2.691080
C	-0.004119	-3.288616	-0.868793
H	-0.954357	-3.001510	-0.404024
H	0.185049	-4.330195	-0.580919
C	2.892706	-2.722710	-0.901520
H	3.645464	-2.084700	-0.430394
H	2.824287	-2.382108	-1.940852
C	3.267313	-4.207656	-0.842534
H	4.223307	-4.377159	-1.349670
H	3.378778	-4.560774	0.187424
H	2.521050	-4.841357	-1.333001
C	1.387021	-2.903949	1.633888
H	0.450609	-2.601080	2.117132
H	1.371152	-3.999438	1.581251
C	2.593104	-2.414005	2.448556
H	2.709425	-1.330491	2.371839
H	2.480971	-2.695002	3.501114
H	3.523443	-2.860821	2.084165
C	2.570734	2.676271	-1.429832
H	3.402064	1.979850	-1.280101
H	2.078304	2.372006	-2.360210
C	3.066595	4.124378	-1.528272
H	3.739508	4.234893	-2.385463
H	2.244175	4.833968	-1.665430
H	3.624300	4.425881	-0.636632
C	-0.664313	3.540438	-1.612973
H	-1.022732	2.560149	-1.933494
H	-1.516996	4.227414	-1.596907
H	0.036727	3.905791	-2.369919
C	-0.012501	3.477805	-0.223747
H	0.358245	4.468136	0.068964
H	-0.759779	3.187391	0.523318
C	2.268256	2.815744	1.474554
H	3.184762	2.219760	1.491456
H	2.539454	3.872398	1.367624
C	1.479833	2.594068	2.770976
H	0.526520	3.132845	2.775827
H	1.270337	1.531060	2.920940
H	2.058726	2.943001	3.632624
C	-4.994922	-0.129611	-1.685961
C	-3.645288	-0.077811	-1.407187
C	-3.174199	-0.078190	-0.063669
C	-4.152934	-0.137083	0.989718
C	-5.534980	-0.188949	0.663128
C	-5.952428	-0.184822	-0.647436

H	-5.327188	-0.127478	-2.720522
H	-2.915444	-0.033423	-2.203529
C	-1.778092	-0.025239	0.299736
C	-3.733314	-0.142229	2.347083
H	-6.258255	-0.232245	1.473785
H	-7.011537	-0.224262	-0.885891
C	-2.398105	-0.092391	2.672412
C	-1.434412	-0.035901	1.643321
H	-4.491063	-0.185642	3.125736
H	-2.082056	-0.094498	3.711701
H	-0.377194	0.008596	1.895541

PEt_3

B3LYP/BSI SCF energy: -579.04767a.u.

M06/BSII SCF energy in solution: -578.89050a.u.

M06/BSII free energy in solution: -578.727456a.u.

P	-0.001518	-0.001238	-0.505413
C	0.236947	1.638093	0.380241
H	-0.675188	2.222343	0.209498
H	0.304985	1.469510	1.463635
C	1.298332	-1.023686	0.384721
H	2.259371	-0.521820	0.220736
H	1.112959	-1.003324	1.467346
C	-1.537918	-0.610441	0.386708
H	-1.584710	-1.694420	0.227742
H	-1.427370	-0.454652	1.468531
C	-2.834137	0.035197	-0.120337
H	-3.707058	-0.379362	0.395781
H	-2.841227	1.117572	0.046823
H	-2.967510	-0.133530	-1.193745
C	1.451128	2.432587	-0.118020
H	1.523439	3.399177	0.392582
H	2.389386	1.897841	0.064145
H	1.384618	2.625346	-1.193609
C	1.387767	-2.469892	-0.119908
H	2.185649	-3.016577	0.394625
H	0.455327	-3.018531	0.050608
H	1.597393	-2.502151	-1.193927

$^{PEt3}TS10^{con}$

B3LYP/BSI SCF energy: -1871.316078a.u.

M06/BSII SCF energy in solution: -1870.78662a.u.

M06/BSII free energy in solution: -1870.346209a.u.

F	2.743491	1.674758	-0.206601
Ni	1.204496	0.332631	-0.014820
P	2.563203	-1.387702	0.460813
C	-0.980755	2.237985	-1.018033
C	-2.017534	3.110885	-0.686518
C	-1.980691	3.784681	0.541906
C	-0.893990	3.588904	1.410463
C	0.132188	2.730124	1.045595
C	0.134174	2.018885	-0.183227
H	-1.035877	1.721636	-1.973165
H	-2.842311	3.252386	-1.375792
H	-0.878241	4.133421	2.349840
H	0.980017	2.631736	1.720985
B	1.902894	2.296318	-1.230055
O	1.781015	1.629061	-2.450781
H	1.282615	0.797261	-2.417146
O	2.136307	3.657568	-1.250904
H	1.780936	4.029019	-2.065976
C	-0.198208	-0.666284	-0.666571
O	-0.103998	-0.835041	-1.885491
O	-2.937565	4.650324	0.979461
C	-4.063411	4.888843	0.148669
H	-4.631761	3.968599	-0.036897
H	-4.692635	5.596895	0.690364
H	-3.770974	5.328862	-0.813203
C	3.948431	-0.796840	1.553194
H	4.428991	0.031009	1.023381
H	4.686227	-1.604251	1.643992
C	3.483160	-0.324713	2.937362
H	3.031150	-1.135922	3.516979
H	4.330651	0.059465	3.513680
H	2.746666	0.480617	2.851876
C	1.979236	-2.916828	1.351792
H	2.866110	-3.405387	1.775539
H	1.366867	-2.578517	2.194244
C	1.186414	-3.918683	0.500746
H	0.854183	-4.755029	1.124090
H	0.296728	-3.465941	0.057363
H	1.794801	-4.333763	-0.307841
C	3.444449	-2.080161	-1.024163
H	4.078555	-2.911635	-0.689249
H	2.667039	-2.505451	-1.667857
C	4.265826	-1.053537	-1.817848

H	4.715720	-1.536759	-2.691264
H	3.647364	-0.224430	-2.171379
H	5.080138	-0.633584	-1.220047
C	-4.502315	-3.720349	-1.228111
C	-4.437234	-3.342747	0.093009
C	-3.388792	-2.506752	0.562674
C	-2.380121	-2.048488	-0.354757
C	-2.481669	-2.458204	-1.713604
C	-3.514271	-3.270608	-2.133279
H	-4.107903	-2.473852	2.601549
H	-5.308498	-4.359133	-1.577178
H	-5.190158	-3.677988	0.801923
C	-3.331689	-2.118554	1.928147
C	-1.326863	-1.206141	0.159944
H	-1.733518	-2.113358	-2.413956
H	-3.569421	-3.567389	-3.176987
C	-1.325944	-0.858492	1.502240
C	-2.322937	-1.306781	2.392479
H	-0.532283	-0.207494	1.858284
H	-2.291836	-1.005756	3.435341

^{PEt3}TS11^{sw}

B3LYP/BSI SCF energy: -1871.319702a.u.

M06/BSII SCF energy in solution: -1870.79256a.u.

M06/BSII free energy in solution: -1870.350914a.u.

Ni	-1.324500	-0.287619	-0.460349
P	-2.807452	1.025979	0.449968
C	1.212525	-2.115999	-1.488761
C	2.503779	-2.210229	-0.984226
C	2.718206	-2.738906	0.296394
C	1.623581	-3.170010	1.058350
C	0.337189	-3.066749	0.523162
C	0.078590	-2.540894	-0.757156
H	1.064006	-1.701368	-2.482065
H	3.364323	-1.879618	-1.557626
H	1.762910	-3.589906	2.048284
H	-0.490018	-3.434007	1.131019
B	-1.416404	-2.542963	-1.430153
O	-1.910240	-3.779079	-1.909203
H	-1.202707	-4.294868	-2.308699
O	-2.424099	-1.960895	-0.436212
H	-2.451361	-2.499664	0.363105
F	-1.398857	-1.456715	-2.411378
O	4.019592	-2.797402	0.706524
C	4.296721	-3.328960	1.990134
H	5.380890	-3.286101	2.107982
H	3.825012	-2.737250	2.785951
H	3.966698	-4.372325	2.079548
O	-0.363881	1.784036	-1.806571
C	-0.139008	1.101680	-0.816837
C	4.623275	3.411699	-1.086950
C	4.541498	2.794594	0.139810
C	3.377337	2.073716	0.517741
C	2.266900	1.991590	-0.391883
C	2.388547	2.639351	-1.652110
C	3.536019	3.328064	-1.986018
H	4.152650	1.517943	2.458257
H	5.518852	3.958708	-1.367193
H	5.370644	2.845482	0.841013
C	3.302313	1.436587	1.785643
C	1.102138	1.247778	0.023873
H	1.559135	2.587149	-2.343857
H	3.604480	3.812501	-2.956016
C	1.093190	0.634594	1.267583
C	2.183625	0.728668	2.156730
H	0.213164	0.066396	1.555088
H	2.134335	0.239735	3.125040
C	-2.702293	2.864165	0.202387
H	-2.426900	2.994817	-0.848926
H	-3.709629	3.275496	0.333354
C	-4.408619	0.576987	-0.384411
H	-4.419451	-0.514836	-0.442278
H	-4.289385	0.922065	-1.418533
C	-3.115658	0.831937	2.274746
H	-3.967429	1.465961	2.548371
H	-2.238602	1.244321	2.784359
C	-1.708865	3.610391	1.102560
H	-1.677112	4.667552	0.821104
H	-1.996267	3.561281	2.157452
H	-0.694943	3.214304	1.007494
C	-3.350666	-0.614654	2.726491
H	-2.473693	-1.237655	2.524303
H	-3.542772	-0.651397	3.803486
H	-4.209947	-1.065692	2.220742
C	-5.705840	1.121330	0.225976
H	-5.713969	2.214179	0.289607
H	-6.558676	0.826137	-0.393775

H	-5.882603	0.725914	1.231163

^{PEt3}TS12^{sw}

B3LYP/BSI SCF energy: -1871.322267a.u.

M06/BSII SCF energy in solution: -1870.79471a.u.

M06/BSII free energy in solution: -1870.354631a.u.

Ni	1.218685	0.495688	0.091073
P	2.841168	-1.054659	-0.006781
C	-1.013906	2.182922	-1.033526
C	-2.280768	2.766829	-0.946452
C	-2.804592	3.083225	0.312989
C	-2.044294	2.822529	1.465984
C	-0.785224	2.254148	1.345439
C	-0.209833	1.914248	0.092932
H	-0.633472	1.930704	-2.019813
H	-2.847258	2.957205	-1.851213
H	-2.466651	3.080037	2.432716
H	-0.218917	2.087365	2.261024
B	1.656548	2.903534	-0.185968
O	1.462253	4.134910	0.414586
H	0.855014	4.684358	-0.092886
C	-0.030672	-0.689387	-0.621291
O	0.003005	-0.868564	-1.836437
O	-4.026434	3.649881	0.526666
C	-4.854611	3.905780	-0.596831
H	-5.092869	2.983738	-1.141967
H	-5.775103	4.337855	-0.200783
H	-4.390328	4.619939	-1.289203
C	4.298045	-0.673594	1.085708
H	4.605527	0.348085	0.844277
H	5.125301	-1.339711	0.809781
C	3.994616	-0.790383	2.585882
H	3.729943	-1.813682	2.870035
H	4.867403	-0.499667	3.179412
H	3.161767	-0.141390	2.877945
C	2.523908	-2.854022	0.385358
H	3.489372	-3.306598	0.645595
H	1.907338	-2.872478	1.290251
C	1.846990	-3.677960	-0.720371
H	1.644062	-4.689584	-0.354218
H	0.900099	-3.240852	-1.041634
H	2.488242	-3.769617	-1.601656
C	3.571790	-1.109269	-1.714554
H	4.316011	-1.915330	-1.751569
H	2.743634	-1.390282	-2.373151
C	4.179007	0.219448	-2.186591
H	4.530108	0.120246	-3.218940
H	3.445819	1.029104	-2.155306
H	5.037076	0.517098	-1.575607
C	-4.340768	-3.771711	-1.022745
C	-4.061906	-3.636169	0.317304
C	-2.958509	-2.857258	0.758866
C	-2.118743	-2.201869	-0.208122
C	-2.440387	-2.363804	-1.585329
C	-3.520558	-3.126523	-1.976442
H	-3.325965	-3.229674	2.857543
H	-5.187445	-4.368946	-1.349239
H	-4.684963	-4.122531	1.063873
C	-2.679860	-2.722137	2.145327
C	-1.011694	-1.412346	0.273475
H	-1.812486	-1.878305	-2.319415
H	-3.744640	-3.232350	-3.034404
C	-0.799659	-1.308489	1.638497
C	-1.619707	-1.962686	2.581348
H	0.032512	-0.695563	1.976898
H	-1.414706	-1.858420	3.642905
F	1.822634	2.815028	-1.539766
O	2.528311	2.024449	0.547417
H	2.519366	2.282409	1.479200

^{PEt3}TS13

B3LYP/BSI SCF energy: -1594.793711a.u.

M06/BSII SCF energy in solution: -1594.27492a.u.

M06/BSII free energy in solution: -1593.870598a.u.

Ni	-0.374011	-0.097585	0.059771
P	0.302753	2.126345	-0.245050
O	0.247436	-2.476787	-1.268179
C	0.383446	-1.665379	-0.379091
C	-2.138417	-0.724572	-0.029859
C	-2.695802	-1.663348	-0.913802
C	-3.016079	-0.054356	0.838389
C	-4.067520	-1.895581	-0.953565
H	-2.038930	-2.223869	-1.573613
C	-4.399801	-0.287086	0.822810
H	-2.637065	0.676527	1.553605
C	-4.928561	-1.209260	-0.085137

H	-4.498753	-2.613950	-1.645069
H	-5.039472	0.251800	1.513412
O	-6.261679	-1.514135	-0.201610
C	-7.170459	-0.859903	0.662151
H	-8.161565	-1.240582	0.407309
H	-6.962884	-1.080105	1.718352
H	-7.158267	0.229756	0.520582
C	2.582851	-1.350519	2.727924
C	3.856215	-1.316938	2.207029
C	4.075531	-1.403866	0.804845
C	2.951762	-1.535815	-0.078862
C	1.632572	-1.553744	0.491399
C	1.468376	-1.455049	1.864382
H	6.230802	-1.269950	0.934472
H	2.426440	-1.297875	3.801324
H	4.717956	-1.229125	2.864028
C	5.386113	-1.367996	0.257135
C	3.194355	-1.635105	-1.476388
H	0.462252	-1.481123	2.274879
C	4.479833	-1.593595	-1.972570
C	5.586695	-1.458017	-1.101522
H	2.352361	-1.768036	-2.145356
H	4.646270	-1.675672	-3.042833
H	6.593593	-1.431065	-1.507989
C	2.606019	3.917085	-0.212336
H	3.681100	3.985973	-0.015514
H	2.442943	4.232882	-1.247036
H	2.108015	4.640337	0.440993
C	0.022332	2.673594	-2.003120
H	0.326831	3.720927	-2.115055
H	0.704887	2.072370	-2.615610
C	-1.422037	2.476774	-2.485676
H	-2.123489	3.109706	-1.932738
H	-1.506718	2.742124	-3.544466
H	-1.743106	1.438372	-2.364870
C	2.113374	2.485532	0.035426
H	2.656555	1.777546	-0.601325
H	2.329644	2.178282	1.064687
C	-0.587361	3.430404	0.746091
H	-1.649833	3.322929	0.502810
H	-0.280564	4.424622	0.399743
C	-0.384506	3.294372	2.260603
H	0.662393	3.439328	2.545858
H	-0.978223	4.041528	2.796833
H	-0.691819	2.305145	2.615517

^{PEt3}TS14

B3LYP/BSI SCF energy: -1594.792509a.u.

M06/BSII SCF energy in solution: -1594.27751a.u.

M06/BSII free energy in solution: -1593.87035a.u.

Ni	1.253821	0.257393	-0.128315
P	2.903941	-1.166213	-0.352253
C	-0.139324	2.504853	-1.091551
C	-0.442457	3.851629	-0.889771
C	-0.814240	4.287183	0.390591
C	-0.889173	3.365573	1.447690
C	-0.576610	2.029334	1.230667
C	-0.158560	1.574132	-0.038920
H	0.086214	2.150136	-2.093884
H	-0.408961	4.540074	-1.726518
H	-1.203772	3.723677	2.423188
H	-0.664692	1.331795	2.058044
C	-0.465758	-0.210903	-0.694655
O	-0.595147	-0.261504	-1.923306
O	-1.143405	5.572332	0.704818
C	-1.104322	6.549949	-0.322963
H	-1.390721	7.492289	0.146767
H	-0.097828	6.650504	-0.748995
H	-1.812424	6.319288	-1.129133
C	-5.254220	-2.447605	-0.726754
C	-4.691803	-2.732653	0.495319
C	-3.391073	-2.266208	0.828385
C	-2.650939	-1.488590	-0.129166
C	-3.265959	-1.214813	-1.383642
C	-4.531419	-1.679782	-1.669210
H	-3.392713	-3.155653	2.800516
H	-6.249936	-2.808090	-0.969375
H	-5.236371	-3.318771	1.231612
C	-2.818611	-2.560434	2.094588
C	-1.342070	-1.014940	0.241564
H	-2.711058	-0.643247	-2.115306
H	-4.979208	-1.454688	-2.633233
C	-0.841506	-1.321102	1.495855
C	-1.565759	-2.099192	2.423998
H	0.149040	-0.950986	1.755038
H	-1.132189	-2.325269	3.394120
C	2.940784	-2.079185	-1.978985

H	3.855123	-2.686710	-2.011631
H	3.038233	-1.307199	-2.750915
C	1.701338	-2.938362	-2.261478
H	1.795088	-3.420150	-3.240457
H	1.578499	-3.733379	-1.518729
H	0.794745	-2.328415	-2.268605
C	4.620185	-0.419118	-0.345267
H	5.351235	-1.212011	-0.142199
H	4.801909	-0.080909	-1.372314
C	4.804898	0.760703	0.618894
H	5.818418	1.168464	0.539387
H	4.099798	1.566736	0.390679
H	4.644732	0.470270	1.661078
C	3.026698	-2.574109	0.866964
H	2.076195	-3.114124	0.798740
H	3.812125	-3.260676	0.525024
C	3.280530	-2.153433	2.319675
H	3.241799	-3.023542	2.983351
H	4.265235	-1.692266	2.442072
H	2.530015	-1.435142	2.665238

^{PBu3}Naph[Ni]F

B3LYP/BSI SCF energy: -2399.398935a.u.

M06/BSII SCF energy in solution: -2398.60803a.u.

M06/BSII free energy in solution: -2397.808958a.u.

F	-0.001362	-2.711349	-0.126720
Ni	-0.000565	-0.840442	-0.181272
P	-2.229165	-1.062658	-0.183984
P	2.227836	-1.064794	-0.183997
O	0.000724	1.316297	-1.714350
C	0.000424	0.997928	-0.520933
C	-3.507742	1.349045	-1.124429
H	-3.894531	0.852922	-2.024374
H	-2.503511	1.702410	-1.379093
C	-3.435965	0.340102	0.034256
H	-3.131969	0.859707	0.950873
H	-4.430440	-0.083082	0.228141
C	-2.694679	-1.880929	-1.783489
H	-2.005531	-2.729820	-1.858116
H	-2.406580	-1.181630	-2.577838
C	-4.149782	-2.335333	-1.970965
H	-4.422795	-3.053614	-1.187502
H	-4.832246	-1.482400	-1.858297
C	-2.747033	-2.279064	1.117593
H	-3.813949	-2.507262	1.003194
H	-2.169481	-3.179819	0.888706
C	-2.449969	-1.829194	2.555548
H	-2.978507	-0.892834	2.781632
H	-1.377789	-1.613298	2.646271
C	2.692516	-1.883522	-1.783506
H	2.002598	-2.731789	-1.858098
H	2.405013	-1.183962	-2.577842
C	4.147204	-2.339244	-1.971020
H	4.830427	-1.486919	-1.858352
H	4.419577	-3.057765	-1.187555
C	3.508825	1.345629	-1.124589
H	2.504976	1.700083	-1.379241
H	3.895056	0.849053	-2.024525
C	3.436008	0.336814	0.034143
H	4.430072	-0.087333	0.228041
H	3.132535	0.856769	0.950734
C	2.744532	-2.281687	1.117582
H	2.165686	-3.181675	0.888933
H	3.811106	-2.511326	1.002880
C	2.448515	-1.831303	2.555595
H	2.978607	-0.895792	2.781549
H	1.376706	-1.613677	2.646596
C	0.003428	5.448766	-1.094668
C	0.002443	4.076795	-0.948746
C	0.001930	3.476810	0.343328
C	0.002447	4.349904	1.487055
C	0.003460	5.758153	1.296424
C	0.003952	6.301561	0.032751
H	0.003804	5.879734	-2.092183
H	0.002045	3.426941	-1.812841
C	0.000955	2.050967	0.570451
C	0.001948	3.799928	2.797410
H	0.003846	6.400189	2.173930
H	0.004732	7.379614	-0.100925
C	0.000995	2.438541	2.991151
C	0.000526	1.577630	1.873114
H	0.002345	4.479372	3.646413
H	0.000623	2.023800	3.995106
H	-0.000183	0.499969	2.018642
C	2.839032	-2.889865	3.596915
H	3.910024	-3.115291	3.500903
H	2.308777	-3.824764	3.372326

C	2.534194	-2.458334	5.034751
H	2.824140	-3.230841	5.754377
H	3.072926	-1.540420	5.297058
H	1.463970	-2.263350	5.170598
C	4.381774	-2.989141	-3.343312
H	3.697049	-3.839757	-3.458787
H	4.113064	-2.273238	-4.131656
C	5.825467	-3.459549	-3.546599
H	6.110775	-4.201989	-2.792455
H	5.960385	-3.918337	-4.531479
H	6.530296	-2.623601	-3.470313
C	4.403389	2.548610	-0.791938
H	5.415713	2.195978	-0.549936
H	4.023405	3.035533	0.116057
C	4.470730	3.574383	-1.927840
H	3.477348	3.980690	-2.147511
H	5.124794	4.413621	-1.669147
H	4.857047	3.122947	-2.849028
C	-4.384961	-2.985008	-3.343261
H	-3.700995	-3.836230	-3.458762
H	-4.115629	-2.269333	-4.131600
C	-5.829081	-3.454114	-3.546521
H	-6.533156	-2.617536	-3.470163
H	-5.964450	-3.912731	-4.531418
H	-6.115026	-4.196334	-2.792402
C	-4.400977	2.552989	-0.791715
H	-5.413691	2.201455	-0.549747
H	-4.020473	3.039437	0.116318
C	-4.467181	3.578910	-1.927552
H	-5.120308	4.418860	-1.668803
H	-3.473348	3.984125	-2.147204
H	-4.854003	3.127967	-2.848769
C	-2.841957	-2.887132	3.596948
H	-2.313156	-3.822844	3.372322
H	-3.913305	-3.110928	3.501086
C	-2.536285	-2.456007	5.034731
H	-3.073612	-1.537276	5.297057
H	-2.827298	-3.228049	5.754425
H	-1.465753	-2.262623	5.170432

^{PBu3}TS10^{con}

B3LYP/BSI SCF energy: -2107.212558a.u.

M06/BSII SCF energy in solution: -2106.54107a.u.

M06/BSII free energy in solution: -2105.942804a.u.

F	-2.175611	-2.085539	-0.301278
Ni	-0.681865	-0.692637	-0.136275
P	-2.069107	0.983392	0.411303
C	1.535126	-2.485849	-1.253793
C	2.615554	-3.328066	-0.988853
C	2.650982	-4.039805	0.217882
C	1.592562	-3.910199	1.132795
C	0.522770	-3.079539	0.834015
C	0.445951	-2.333436	-0.371605
H	1.535404	-1.939038	-2.193496
H	3.417483	-3.416346	-1.713081
H	1.633182	-4.482345	2.054873
H	-0.300675	-3.032437	1.544285
B	-1.352367	-2.672093	-1.355001
O	-1.298641	-1.996067	-2.576413
H	-0.852219	-1.136651	-2.546183
O	-1.534214	-4.040761	-1.376824
H	-1.186645	-4.396179	-2.202331
C	0.677760	0.381575	-0.758571
O	0.573915	0.604853	-1.967234
O	3.654906	-4.882251	0.590766
C	4.755264	-5.052302	-0.289521
H	5.283968	-4.106609	-0.464046
H	5.429055	-5.755122	0.203187
H	4.441405	-5.469984	-1.254612
C	-3.350522	0.376416	1.611983
H	-3.860967	-0.460664	1.123787
H	-4.093844	1.170962	1.762125
C	-2.775062	-0.087920	2.959560
H	-2.269648	0.748392	3.460968
H	-2.006278	-0.851655	2.781420
C	-1.434126	2.534091	1.225822
H	-2.270013	3.001823	1.762759
H	-0.707364	2.214412	1.981088
C	-0.779037	3.556730	0.281904
H	-0.043092	3.062892	-0.361391
H	-1.538775	3.979240	-0.387266
C	-3.074381	1.633062	-1.012323
H	-3.728302	2.431556	-0.635330
H	-2.360048	2.100997	-1.699554
C	-3.895027	0.575702	-1.770079
H	-3.234995	-0.220646	-2.132108
H	-4.611690	0.096262	-1.090820

C	4.803819	3.697754	-1.162622
C	4.773933	3.237059	0.133182
C	3.778305	2.316990	0.558749
C	2.788118	1.857322	-0.377971
C	2.853142	2.353008	-1.710523
C	3.833051	3.248386	-2.086844
H	4.517363	2.204556	2.588017
H	5.569141	4.401241	-1.477525
H	5.514274	3.570775	0.855936
C	3.754981	1.847792	1.899762
C	1.786313	0.930899	0.092091
H	2.119864	2.006516	-2.425715
H	3.860958	3.609803	-3.111077
C	1.813903	0.510220	1.412782
C	2.793926	0.959057	2.322067
H	1.055849	-0.197175	1.737007
H	2.786718	0.598449	3.346310
C	-0.088739	4.699290	1.041129
H	-0.818454	5.195972	1.695379
H	0.680033	4.276912	1.701306
C	0.552588	5.728722	0.105092
H	1.037657	6.531310	0.669980
H	1.311917	5.261159	-0.530962
H	-0.195074	6.189090	-0.551184
C	-3.849254	-0.659123	3.896000
H	-4.624760	0.100843	4.063348
H	-4.347720	-1.500837	3.397441
C	-3.284804	-1.120996	5.243001
H	-4.072880	-1.523726	5.887172
H	-2.532128	-1.906063	5.108858
H	-2.808063	-0.292495	5.779379
C	-4.659743	1.179198	-2.957459
H	-5.319780	1.981829	-2.599540
H	-3.943772	1.654644	-3.641568
C	-5.483393	0.137866	-3.721619
H	-6.231182	-0.330302	-3.071436
H	-6.013339	0.590927	-4.565852
H	-4.842901	-0.658637	-4.115444

^{PBu3}TS11^{sw}

B3LYP/BSI SCF energy: -2107.2197a.u.

M06/BSII SCF energy in solution: -2106.54851a.u.

M06/BSII free energy in solution: -2105.951124a.u.

Ni	-0.916006	-0.524510	-0.494590
P	-2.031588	0.999197	0.585234
C	1.203801	-2.622545	-1.635833
C	2.501369	-2.894283	-1.187592
C	2.683148	-3.528316	0.044996
C	1.560605	-3.897772	0.806463
C	0.285373	-3.619396	0.335375
C	0.054772	-2.964825	-0.898896
H	1.076820	-2.124914	-2.593493
H	3.349474	-2.602573	-1.796325
H	1.723046	-4.404264	1.753304
H	-0.563196	-3.938847	0.940347
B	-1.456237	-2.708948	-1.479868
O	-2.183960	-3.837297	-1.924347
H	-1.603394	-4.459650	-2.373675
O	-2.278741	-1.977938	-0.414523
H	-2.328203	-2.511556	0.387254
F	-1.322690	-1.625429	-2.454877
O	3.895006	-3.834930	0.594092
C	5.064608	-3.448777	-0.110715
H	5.907234	-3.773779	0.502092
H	5.126509	-3.935103	-1.092745
H	5.112550	-2.360773	-0.246147
O	0.246842	1.357718	-1.934534
C	0.433813	0.686514	-0.927127
C	5.160455	3.101097	-1.037536
C	5.133815	2.308272	0.086438
C	3.993328	1.520258	0.397703
C	2.848305	1.551446	-0.472298
C	2.914896	2.379097	-1.628186
C	4.039695	3.131338	-1.897868
H	4.855634	0.693299	2.200992
H	6.037516	3.699647	-1.266287
H	5.988344	2.271288	0.757570
C	3.977581	0.701856	1.559648
C	1.704873	0.743154	-0.120648
H	2.064190	2.403919	-2.295049
H	4.064350	3.753577	-2.788124
C	1.750433	-0.036949	1.025165
C	2.879816	-0.066298	1.869416
H	0.887599	-0.652989	1.264667
H	2.878034	-0.699102	2.751474
C	-1.228413	2.323618	1.620417
H	-1.994795	2.696075	2.313309

H	-0.465006	1.827226	2.229905
C	-3.075643	1.940180	-0.625611
H	-2.368435	2.476261	-1.268170
H	-3.655889	2.693538	-0.075076
C	-3.253207	0.248609	1.765617
H	-3.854187	-0.454491	1.180243
H	-3.924823	1.045453	2.112164
C	-0.598555	3.504621	0.861773
H	0.082594	3.142078	0.086007
H	-1.382777	4.068493	0.341481
C	-2.614941	-0.472860	2.962261
H	-2.026376	0.236544	3.558804
H	-1.903455	-1.226124	2.597387
C	-3.994961	1.066253	-1.495431
H	-4.725794	0.543732	-0.864981
H	-3.403870	0.288369	-1.991816
C	0.166164	4.451840	1.797471
H	0.946687	3.884245	2.321401
H	-0.514204	4.827737	2.574199
C	0.803868	5.630013	1.054440
H	0.046584	6.232205	0.539636
H	1.340953	6.289878	1.743358
H	1.518497	5.279557	0.301751
C	-4.743843	1.891645	-2.551928
H	-4.012028	2.400433	-3.193295
H	-5.322857	2.684278	-2.057163
C	-5.675947	1.037194	-3.416663
H	-6.190589	1.645641	-4.167492
H	-5.117697	0.255549	-3.942815
H	-6.440666	0.543169	-2.806410
C	-3.651546	-1.150222	3.870823
H	-4.236322	-1.867174	3.279022
H	-4.366185	-0.396626	4.227956
C	-3.018818	-1.866142	5.068102
H	-3.779620	-2.343279	5.693679
H	-2.321042	-2.645368	4.740820
H	-2.460059	-1.165813	5.699319

^{PBu_3}TS12^{sw}

B3LYP/BSI SCF energy: -2107.218552a.u.

M06/BSII SCF energy in solution: -2106.54762a.u.

M06/BSII free energy in solution: -2105.948943a.u.

Ni	0.659145	0.769668	0.089586
P	2.214220	-0.852973	0.007598
C	-1.535453	2.532691	-0.993643
C	-2.775439	3.167865	-0.880266
C	-3.252489	3.518543	0.388557
C	-2.472099	3.240778	1.523904
C	-1.240096	2.621451	1.376946
C	-0.712915	2.243508	0.114137
H	-1.192676	2.252984	-1.986294
H	-3.358015	3.370445	-1.772099
H	-2.857390	3.526193	2.498292
H	-0.655951	2.444130	2.279349
B	1.187817	3.158130	-0.217617
O	1.056441	4.399688	0.378724
H	0.463198	4.971376	-0.120683
C	-0.642996	-0.370013	-0.601825
O	-0.637921	-0.528833	-1.820472
O	-4.445293	4.134952	0.627986
C	-5.292643	4.411631	-0.476001
H	-5.581148	3.494246	-1.004573
H	-6.184825	4.883237	-0.060697
H	-4.819825	5.100146	-1.188298
C	3.686113	-0.520208	1.094183
H	4.050828	0.476208	0.823981
H	4.477545	-1.237811	0.839941
C	3.385073	-0.571584	2.600446
H	3.037780	-1.574631	2.881258
H	2.556536	0.111759	2.833951
C	1.808743	-2.627202	0.424719
H	2.746524	-3.127974	0.700376
H	1.185631	-2.598780	1.326075
C	1.092227	-3.437193	-0.670012
H	0.230097	-2.883496	-1.053003
H	1.767942	-3.579585	-1.522782
C	2.940570	-0.961218	-1.698806
H	3.666347	-1.785391	-1.725412
H	2.104369	-1.236369	-2.351266
C	3.577356	0.341882	-2.208245
H	2.857012	1.162568	-2.122796
H	4.434492	0.614268	-1.578166
C	-4.821167	-3.640044	-0.961907
C	-4.578305	-3.435592	0.376384
C	-3.519702	-2.591011	0.806836
C	-2.687935	-1.938505	-0.169271
C	-2.973443	-2.170706	-1.544913

C	-4.009273	-2.998580	-1.925174
H	-3.919453	-2.891737	2.911182
H	-5.633203	-4.287867	-1.279707
H	-5.195648	-3.917884	1.130303
C	-3.277750	-2.388387	2.192041
C	-1.620276	-1.089149	0.301360
H	-2.356360	-1.681857	-2.285855
H	-4.205923	-3.156504	-2.982106
C	-1.439234	-0.927577	1.665401
C	-2.256943	-1.571491	2.617489
H	-0.634689	-0.275989	1.996695
H	-2.079203	-1.416131	3.677688
C	0.624564	-4.810311	-0.166094
H	1.486901	-5.374920	0.215056
H	-0.051104	-4.666853	0.687446
C	-0.090003	-5.624546	-1.249554
H	-0.414513	-6.597787	-0.867069
H	-0.976957	-5.095722	-1.614894
H	0.567107	-5.806586	-2.107845
C	4.601823	-0.204493	3.462637
H	5.428931	-0.887660	3.227365
H	4.949735	0.799871	3.185838
C	4.308543	-0.251912	4.965442
H	5.193949	0.011103	5.552824
H	3.510216	0.448501	5.236549
H	3.988749	-1.253188	5.275685
C	4.045467	0.226728	-3.666276
H	4.762173	-0.601434	-3.758080
H	3.186725	-0.039952	-4.296600
C	4.681660	1.518543	-4.188845
H	5.564988	1.792763	-3.600412
H	4.996822	1.414287	-5.232295
H	3.975514	2.354203	-4.133678
F	1.315632	3.054633	-1.573912
O	2.038183	2.248450	0.501989
H	2.062490	2.511911	1.431949

Ni(iPr)$_2$

B3LYP/BSI SCF energy: -2491.143903a.u.

M06/BSII SCF energy in solution: -2489.95253a.u.

M06/BSII free energy in solution: -2488.912051a.u.

Ni	0.000153	-0.000047	0.000160
C	-0.000635	-1.873495	-0.000169
C	-0.635861	-4.088456	-0.229999
C	0.633600	-4.088661	0.230542
H	-1.302084	-4.899817	-0.474419
H	1.299437	-4.900255	0.475248
N	1.014048	-2.754914	0.363391
N	-1.015640	-2.754574	-0.363508
C	-2.343777	-2.427025	-0.817295
C	-3.399554	-2.438651	0.118662
C	-2.569097	-2.252336	-2.198867
C	-4.701787	-2.254770	-0.363036
C	-3.891620	-2.082207	-2.627198
C	-4.949133	-2.082106	-1.721222
H	-5.533346	-2.258196	0.334727
H	-4.096892	-1.953686	-3.685284
H	-5.967801	-1.950728	-2.076014
C	2.342206	-2.427870	0.817415
C	3.398222	-2.439950	-0.118300
C	2.567285	-2.253288	2.199010
C	4.700397	-2.256601	0.363720
C	3.889781	-2.083694	2.627686
C	4.947505	-2.084033	1.721982
H	5.532134	-2.260377	-0.333828
H	4.094781	-1.955312	3.685850
H	5.966151	-1.953065	2.076990
C	-3.165552	-2.701492	1.603332
H	-2.097215	-2.572985	1.797095
C	-3.911323	-1.706476	2.507830
H	-3.667457	-0.674019	2.249184
H	-4.998531	-1.825525	2.440477
H	-3.633512	-1.874078	3.554512
C	-3.543993	-4.151473	1.971280
H	-4.608576	-4.336856	1.788262
H	-2.972760	-4.879783	1.388077
H	-3.347312	-4.341850	3.032263
C	-1.433979	-2.306168	-3.217067
H	-0.497721	-2.152777	-2.673689
C	-1.527144	-1.189939	-4.270973
H	-0.646269	-1.216348	-4.920885
H	-2.407670	-1.299496	-4.913778
H	-1.569752	-0.205642	-3.796677
C	-1.371000	-3.690944	-3.894192
H	-1.228612	-4.490194	-3.160362
H	-2.294643	-3.901840	-4.445362
H	-0.537982	-3.734136	-4.604891

C	1.432065	-2.306663	3.217107	H	-5.966693	1.953821	2.075698
H	0.495678	-2.155309	2.673403	C	3.166132	2.701296	1.602990
C	1.370639	-3.690308	3.896635	H	2.097946	2.572100	1.797154
H	1.229436	-4.490984	3.164110	C	3.912926	1.707090	2.507546
H	2.294387	-3.899169	4.448400	H	3.670029	0.674348	2.249118
H	0.537501	-3.733308	4.607203	H	5.000013	1.827170	2.440072
C	1.523805	-1.188289	4.268853	H	3.635067	1.874592	3.554228
H	2.405025	-1.294828	4.911218	C	3.543702	4.151639	1.970459
H	1.564107	-0.204871	3.792533	H	4.608097	4.337682	1.787017
H	0.643435	-1.215142	4.919438	H	2.971773	4.879418	1.387285
C	3.164478	-2.702861	-1.603002	H	3.347253	4.342125	3.031464
H	2.096282	-2.573678	-1.797114	C	1.433463	2.305791	-3.217033
C	3.541999	-4.153203	-1.970519	H	0.497142	2.153970	-2.673337
H	4.606403	-4.339305	-1.787202	C	1.525263	1.188159	-4.269566
H	2.970115	-4.880949	-1.387246	H	0.644591	1.215041	-4.919742
H	3.345414	-4.343715	-3.031494	H	2.406137	1.295580	-4.912260
C	3.911184	-1.708559	-2.507505	H	1.566264	0.204421	-3.793979
H	3.667930	-0.675886	-2.249153	C	1.371779	3.689843	-3.895743
H	4.998289	-1.828311	-2.439788	H	1.230495	4.490079	-3.162766
H	3.633573	-1.876203	-3.554229	H	2.295462	3.899138	-4.447453
C	0.000710	1.873368	0.000294	H	0.538580	3.733119	-4.606225
C	0.635864	4.088254	-0.230660	C	-1.432726	2.306485	3.217130
C	-0.633588	4.088634	0.229898	H	-0.496584	2.151938	2.673871
H	1.302033	4.899542	-0.475465	C	-1.368407	3.691466	3.893722
H	-1.299493	4.900330	0.474079	H	-1.225057	4.490287	3.159622
N	-1.013936	2.754940	0.363585	H	-2.291922	3.903520	4.444663
N	1.015746	2.754329	-0.363392	H	-0.535462	3.734062	4.604545
C	2.343768	2.426700	-0.817419	C	-1.527099	1.190827	4.271522
C	3.399779	2.438301	0.118289	H	-2.407467	1.301649	4.914323
C	2.568749	2.251964	-2.199033	H	-1.570819	0.206348	3.797693
C	4.701881	2.254363	-0.363736	H	-0.646175	1.216566	4.921388
C	3.891157	2.081757	-2.627695	C	-3.163759	2.703103	-1.603386
C	4.948890	2.081648	-1.721985	H	-2.095413	2.574480	-1.797024
H	5.533614	2.257775	0.333814	C	-3.541997	4.153095	-1.971474
H	4.096147	1.953197	-3.685838	H	-4.606595	4.338614	-1.788690
H	5.967462	1.950206	-2.077034	H	-2.970816	4.881370	-1.388166
C	-2.342270	2.428095	0.817301	H	-3.345066	4.343419	-3.032419
C	-3.397976	2.440385	-0.118724	C	-3.909491	1.708034	-2.507864
C	-2.567813	2.253413	2.198846	H	-3.665550	0.675605	-2.249170
C	-4.700361	2.257284	0.362858	H	-4.996701	1.827000	-2.440470
C	-3.890465	2.083985	2.627054	H	-3.631708	1.875609	-3.554557
C	-4.947918	2.084639	1.721005				
H	-5.531866	2.261261	-0.334968	**iPr**			
H	-4.095887	1.955463	3.685106	B3LYP/BSI SCF energy: -1160.064019a.u.			

M06/BSII SCF energy in solution: -1159.45092a.u.

M06/BSII free energy in solution: -1158.943374a.u.

C	-0.000040	0.000091	-0.334820
C	-0.675640	-0.049644	1.877270
C	0.675626	0.049992	1.877244
H	-1.384045	-0.101951	2.689417
H	1.384058	0.102320	2.689363
N	1.062294	0.077518	0.534340
N	-1.062350	-0.077221	0.534385
C	-2.435948	-0.163120	0.107717
C	-3.209320	1.012604	0.059393
C	-2.963863	-1.424637	-0.239823
C	-4.547221	0.899463	-0.341588
C	-4.303612	-1.480964	-0.640955
C	-5.091100	-0.332665	-0.688174
H	-5.166312	1.790760	-0.388360
H	-4.738925	-2.435195	-0.918967
H	-6.129925	-0.400091	-0.999448
C	2.435921	0.163183	0.107684
C	3.209041	-1.012700	0.059295
C	2.964144	1.424637	-0.239712
C	4.547031	-0.899801	-0.341478
C	4.303969	1.480718	-0.640585
C	5.091224	0.332250	-0.687797
H	5.165941	-1.791223	-0.388254
H	4.739550	2.434885	-0.918390
H	6.130122	0.399507	-0.998867
C	-2.636685	2.384657	0.401347
H	-1.586552	2.252555	0.673813
C	-2.671783	3.322899	-0.820458
H	-2.125394	2.888127	-1.662336
H	-3.698321	3.519131	-1.149041
H	-2.211990	4.286754	-0.575071
C	-3.352176	3.017242	1.610310
H	-4.411546	3.201651	1.400778
H	-3.296196	2.369383	2.491181
H	-2.893048	3.978223	1.866876
C	-2.097799	-2.680442	-0.234252
H	-1.279117	-2.511288	0.472975
C	-1.463363	-2.895586	-1.624503
H	-0.815149	-3.779619	-1.618227
H	-2.237830	-3.049779	-2.384747
H	-0.864969	-2.025017	-1.907142
C	-2.847643	-3.938527	0.235203
H	-3.335811	-3.782482	1.202795
H	-3.613655	-4.254393	-0.481232
H	-2.145380	-4.772150	0.340335
C	2.098283	2.680585	-0.234276
H	1.279637	2.511681	0.473068
C	2.848334	3.938682	0.234796
H	3.336513	3.782850	1.202414
H	3.614351	4.254241	-0.481771
H	2.146185	4.772424	0.339709
C	1.463801	2.895557	-1.624552
H	2.238282	3.049632	-2.384806
H	0.865385	2.024972	-1.907106
H	0.815628	3.779623	-1.618381
C	2.636138	-2.384641	0.401213
H	1.585938	-2.252382	0.673318
C	3.351223	-3.017065	1.610506
H	4.410667	-3.201473	1.401338
H	3.294946	-2.369075	2.491263
H	2.892027	-3.978014	1.867072
C	2.671506	-3.323087	-0.820415
H	2.125416	-2.888398	-1.662530
H	3.698108	-3.519528	-1.148669
H	2.211517	-4.286837	-0.574985

^{iPr}TS1

B3LYP/BSI SCF energy: -3089.578729a.u.

M06/BSII SCF energy in solution: -3088.17024a.u.

M06/BSII free energy in solution: -3086.982165a.u.

F	-0.565082	-1.320069	1.827870
Ni	0.087065	-0.033465	-0.023199
C	-1.576836	-0.655370	0.689005
O	-1.988503	-1.502817	-0.105250
C	-6.419020	-1.002189	2.768427
C	-5.779110	0.022134	3.424946
C	-4.463331	0.419373	3.059842
C	-3.787463	-0.264222	1.986927
C	-4.489898	-1.311994	1.324553
C	-5.764217	-1.669034	1.706515
H	-4.337877	1.983013	4.551073
H	-7.423827	-1.296970	3.058798
H	-6.270436	0.549590	4.239203
C	-3.813052	1.480546	3.742154

C	-2.446958	0.139939	1.653757	C	0.685965	0.798863	4.790623
H	-4.000363	-1.813542	0.501138	H	-0.247313	0.321360	5.101802
H	-6.274693	-2.471977	1.181494	H	1.227661	1.081722	5.701289
C	-1.871083	1.192814	2.338270	H	0.424121	1.714316	4.254434
C	-2.545764	1.869994	3.376268	C	1.945507	-1.365524	4.795413
H	-0.852117	1.467127	2.087629	H	2.418265	-2.156932	4.209824
H	-2.051108	2.684447	3.898039	H	2.655852	-1.036896	5.563604
C	1.695044	-1.399252	0.510922	H	1.079238	-1.804757	5.301498
C	3.281121	-2.491996	1.777023	C	2.333189	-2.826696	-2.592634
C	2.660911	-3.424441	1.029335	H	2.453436	-1.930698	-1.976986
H	4.068151	-2.575949	2.506291	C	3.673748	-3.591580	-2.581041
H	2.800752	-4.489959	0.960779	H	3.963058	-3.878257	-1.565545
N	1.704088	-2.759058	0.268810	H	3.605906	-4.506226	-3.180959
N	2.703684	-1.267006	1.451726	H	4.476132	-2.973127	-2.999367
C	3.271126	-0.073281	2.050521	C	1.994198	-2.358291	-4.017734
C	4.503671	0.398997	1.541723	H	1.908823	-3.195227	-4.718501
C	2.690485	0.466589	3.222685	H	1.053450	-1.800056	-4.040288
C	5.088799	1.508078	2.166916	H	2.787061	-1.706982	-4.395552
C	3.323093	1.575870	3.801362	C	-0.414960	-4.415778	1.477874
C	4.497669	2.103761	3.273979	H	0.024909	-3.519808	1.916301
H	6.028427	1.898754	1.790207	C	0.160969	-5.658794	2.188411
H	2.899255	2.022042	4.693877	H	-0.274351	-6.581684	1.788100
H	4.966839	2.962990	3.745839	H	1.247903	-5.735144	2.084778
C	0.882240	-3.578378	-0.603203	H	-0.068405	-5.620516	3.258982
C	-0.079227	-4.428061	-0.012356	C	-1.930555	-4.319855	1.728046
C	1.226447	-3.672733	-1.968716	H	-2.346404	-3.457720	1.207229
C	-0.705241	-5.371206	-0.838905	H	-2.458943	-5.223083	1.400360
C	0.578156	-4.644676	-2.740084	H	-2.120697	-4.201297	2.800128
C	-0.378195	-5.488777	-2.183969	C	-0.543300	1.382215	-1.194762
H	-1.449696	-6.034195	-0.409904	C	-1.544826	2.565058	-2.904304
H	0.835153	-4.752564	-3.788610	C	-0.344060	3.132913	-2.693552
H	-0.865757	-6.238811	-2.800804	H	-2.325995	2.798862	-3.607042
C	5.270939	-0.308287	0.422985	H	0.138695	3.973779	-3.161361
H	4.570167	-0.948768	-0.120777	N	0.258349	2.420506	-1.660308
C	5.899193	0.660394	-0.592360	N	-1.681276	1.529052	-1.986139
H	5.167225	1.373172	-0.970660	C	-3.000369	0.917479	-1.921277
H	6.728230	1.225765	-0.153044	C	-3.229151	-0.307757	-2.578298
H	6.307956	0.098503	-1.438933	C	-4.053340	1.684773	-1.372654
C	6.386409	-1.205079	1.006529	C	-4.542884	-0.787295	-2.616543
H	7.115067	-0.599100	1.556227	C	-5.347472	1.151358	-1.437982
H	6.001841	-1.964030	1.691165	C	-5.591836	-0.073597	-2.045068
H	6.918761	-1.721826	0.200331	H	-4.749658	-1.733076	-3.103885
C	1.491273	-0.176871	3.916732	H	-6.174270	1.711121	-1.013087
H	0.815871	-0.565867	3.151861	H	-6.602982	-0.469226	-2.083291

C	1.544462	2.894732	-1.201138
C	1.605310	3.682553	-0.029111
C	2.650132	2.758476	-2.068787
C	2.830440	4.279229	0.290152
C	3.837573	3.415543	-1.719305
C	3.935128	4.156039	-0.546788
H	2.912120	4.876799	1.191104
H	4.696006	3.348677	-2.380800
H	4.868438	4.649613	-0.290938
C	-2.115310	-1.057477	-3.299012
H	-1.183616	-0.859811	-2.760390
C	-2.321392	-2.577813	-3.304414
H	-2.460583	-2.953657	-2.289079
H	-3.179941	-2.875048	-3.917989
H	-1.441246	-3.068005	-3.726765
C	-1.962260	-0.536568	-4.745249
H	-2.884267	-0.699389	-5.315353
H	-1.732084	0.532620	-4.777841
H	-1.153405	-1.068303	-5.259467
C	-3.870461	3.090644	-0.796756
H	-2.801305	3.267093	-0.649726
C	-4.553517	3.277696	0.568704
H	-4.314371	4.269310	0.969105
H	-5.644113	3.216780	0.488812
H	-4.224345	2.531475	1.289665
C	-4.399040	4.160421	-1.778283
H	-3.911497	4.111980	-2.755603
H	-5.475648	4.038136	-1.939596
H	-4.233870	5.164432	-1.371698
C	2.586988	1.988085	-3.387413
H	1.631585	1.457449	-3.425422
C	2.652531	2.940526	-4.600110
H	1.851352	3.684503	-4.585254
H	3.604886	3.481303	-4.624865
H	2.565738	2.374447	-5.533771
C	3.699606	0.931186	-3.500340
H	4.695709	1.384964	-3.491826
H	3.650017	0.210020	-2.680504
H	3.599078	0.386178	-4.444020
C	0.365481	3.995292	0.803894
H	-0.329546	3.159310	0.698435
C	-0.337024	5.260432	0.262828
H	0.324410	6.131620	0.333105
H	-0.634379	5.145546	-0.783392
H	-1.239386	5.473606	0.846555
C	0.662067	4.160393	2.302969
H	1.241912	3.320656	2.694589
H	1.217321	5.081500	2.513087
H	-0.278606	4.222470	2.859431

^{iPr}TS1A

B3LYP/BSI SCF energy: -1929.516266a.u.

M06/BSII SCF energy in solution: -1928.69312a.u.

M06/BSII free energy in solution: -1928.051283a.u.

F	-0.057213	-1.458147	-2.729654
Ni	0.523158	-0.172269	-1.200709
C	-1.049728	-0.366244	-2.212431
O	-0.839799	0.725287	-2.750112
C	-6.022226	1.072940	-1.426637
C	-5.952438	-0.274244	-1.159510
C	-4.729904	-0.986361	-1.298101
C	-3.545682	-0.283196	-1.710587
C	-3.658374	1.107848	-1.987328
C	-4.862921	1.763483	-1.849762
H	-5.582017	-2.897205	-0.751102
H	-6.963862	1.604787	-1.323010
H	-6.837263	-0.822344	-0.845275
C	-4.673011	-2.382870	-1.052900
C	-2.322667	-1.032423	-1.840741
H	-2.781642	1.642754	-2.325411
H	-4.922698	2.824714	-2.074989
C	-2.320162	-2.398136	-1.594146
C	-3.494132	-3.075437	-1.207430
H	-1.395560	-2.946786	-1.718004
H	-3.458988	-4.147103	-1.034776
C	1.147701	0.157782	0.533110
C	1.456107	0.679869	2.741362
C	2.684173	0.483787	2.205287
H	1.150875	0.944711	3.740655
H	3.668644	0.540216	2.641381
N	2.485490	0.164395	0.865045
N	0.530510	0.479070	1.718658
C	-0.892077	0.631927	1.900224
C	-1.484864	1.872496	1.591433
C	-1.629267	-0.453785	2.416715
C	-2.867718	1.991402	1.779257
C	-3.006031	-0.274574	2.594364

C	-3.622485	0.930866	2.270254
H	-3.358314	2.929342	1.538256
H	-3.603745	-1.091272	2.986552
H	-4.694649	1.044132	2.401631
C	3.551886	-0.110469	-0.066895
C	3.956516	-1.446780	-0.265089
C	4.160762	0.970207	-0.737925
C	5.002279	-1.680191	-1.166364
C	5.202363	0.678350	-1.627281
C	5.620842	-0.631586	-1.841232
H	5.333327	-2.699163	-1.343407
H	5.686904	1.489637	-2.162244
H	6.429392	-0.836290	-2.537328
C	-0.679374	3.077210	1.112027
H	0.366208	2.771143	1.022548
C	-1.126737	3.563281	-0.278705
H	-1.009670	2.775857	-1.027587
H	-2.175073	3.881522	-0.275586
H	-0.521435	4.422658	-0.588377
C	-0.734841	4.219912	2.146264
H	-1.754978	4.598966	2.271097
H	-0.380774	3.889866	3.128605
H	-0.107075	5.057214	1.822537
C	-0.967370	-1.767693	2.823783
H	0.037042	-1.783860	2.390905
C	-1.709286	-3.003104	2.285167
H	-1.143976	-3.911063	2.522181
H	-2.702493	-3.112603	2.734010
H	-1.835392	-2.947405	1.201350
C	-0.816625	-1.850246	4.357080
H	-0.231074	-1.013941	4.752169
H	-1.795624	-1.830839	4.848632
H	-0.313695	-2.779939	4.645215
C	3.719497	2.417512	-0.541593
H	2.918581	2.430173	0.202470
C	4.865538	3.290259	0.006204
H	5.257826	2.892151	0.947911
H	5.699688	3.352405	-0.700958
H	4.512141	4.310469	0.190471
C	3.139828	3.007574	-1.842173
H	3.889685	3.031737	-2.640396
H	2.287176	2.419973	-2.196068
H	2.799130	4.035132	-1.673926
C	3.300280	-2.622901	0.450646
H	2.509325	-2.228094	1.093670
C	4.304309	-3.363556	1.355187
H	5.119584	-3.806738	0.773319
H	4.751302	-2.688987	2.092894
H	3.804542	-4.174418	1.896208
C	2.630012	-3.585123	-0.549440
H	1.891375	-3.060458	-1.162945
H	3.364307	-4.043766	-1.220807
H	2.120758	-4.393689	-0.013297

Ni(SiPr)$_2$

B3LYP/BSI SCF energy: -2493.549846a.u.

M06/BSII SCF energy in solution: -2492.36095a.u.

M06/BSII free energy in solution: -2491.271662a.u.

Ni	-0.000022	0.000073	0.000011
C	0.000500	1.892450	-0.000477
N	-0.992929	2.736825	0.445922
N	0.994284	2.736222	-0.447142
C	2.309653	2.422568	-0.926581
C	3.383564	2.394852	-0.006392
C	2.542613	2.345128	-2.318780
C	4.681784	2.226336	-0.502881
C	3.861924	2.198082	-2.765791
C	4.924318	2.130989	-1.869754
H	5.515996	2.189063	0.191947
H	4.058630	2.137636	-3.832389
H	5.940556	2.014893	-2.236807
C	-2.308597	2.424026	0.925093
C	-3.382195	2.395976	0.004545
C	-2.542103	2.347783	2.317276
C	-4.680652	2.228287	0.500706
C	-3.861624	2.201576	2.763932
C	-4.923719	2.134126	1.867564
H	-5.514618	2.190739	-0.194402
H	-4.058734	2.142044	3.830508
H	-5.940128	2.018671	2.234343
C	3.177590	2.595880	1.491013
H	2.104696	2.713955	1.663863
C	3.631545	1.369305	2.297144
H	3.099752	0.473701	1.970978
H	4.704904	1.184113	2.180633
H	3.434873	1.518928	3.365025
C	3.880454	3.874719	1.990082

H	4.968548	3.799621	1.886741	H	-5.941543	-2.016547	-2.232798
H	3.558922	4.761094	1.432697	C	2.308790	-2.423162	0.926234
H	3.660166	4.042724	3.050266	C	3.382142	-2.395885	0.005374
C	1.416105	2.452924	-3.340773	C	2.542673	-2.345875	2.318289
H	0.472310	2.478948	-2.788486	C	4.680745	-2.227955	0.501064
C	1.364524	1.227046	-4.269288	C	3.862324	-2.199415	2.764485
H	0.516317	1.306058	-4.957810	C	4.924187	-2.132766	1.867785
H	2.273575	1.140133	-4.874843	H	5.514531	-2.191029	-0.194294
H	1.250359	0.306733	-3.691516	H	4.059722	-2.139076	3.830961
C	1.527942	3.750742	-4.167141	H	5.940708	-2.017133	2.234201
H	1.553183	4.639993	-3.528823	C	-3.176161	-2.594408	1.493669
H	2.441051	3.756656	-4.772889	H	-2.103160	-2.712187	1.666049
H	0.676023	3.846819	-4.849594	C	-3.629868	-1.367295	2.299110
C	-1.415926	2.455911	3.339596	H	-3.098436	-0.471856	1.971917
H	-0.471916	2.481119	2.787637	H	-4.703330	-1.182399	2.183099
C	-1.527538	3.754416	4.164922	H	-3.432526	-1.516041	3.366990
H	-1.552224	4.643184	3.525912	C	-3.878585	-3.872956	1.994119
H	-2.440853	3.761140	4.770351	H	-4.966749	-3.798041	1.891378
H	-0.675817	3.850694	4.847595	H	-3.557309	-4.759721	1.437209
C	-1.365219	1.230751	4.269108	H	-3.657635	-4.040142	3.054295
H	-2.274537	1.144729	4.874389	C	-1.417869	-2.455857	-3.339434
H	-1.251257	0.309918	3.692129	H	-0.473690	-2.480950	-2.787757
H	-0.517232	1.309937	4.957883	C	-1.367266	-1.231237	-4.269663
C	-3.175659	2.595767	-1.492948	H	-0.519354	-1.310819	-4.958487
H	-2.102674	2.713379	-1.665550	H	-2.276638	-1.145572	-4.874911
C	-3.877946	3.874442	-1.993246	H	-1.253258	-0.310051	-3.693262
H	-4.966101	3.799780	-1.890236	C	-1.529979	-3.754791	-4.164031
H	-3.556319	4.761142	-1.436433	H	-1.554578	-4.643223	-3.524551
H	-3.657228	4.041560	-3.053482	H	-2.443520	-3.761679	-4.769120
C	-3.629748	1.368702	-2.298259	H	-0.678521	-3.851571	-4.846962
H	-3.098365	0.473184	-1.971189	C	1.416742	-2.453195	3.340966
H	-4.703207	1.183964	-2.181957	H	0.472597	-2.478452	2.789235
H	-3.432668	1.517404	-3.366194	C	1.528222	-3.751334	4.166890
C	-0.000413	-1.892315	0.000590	H	1.552463	-4.640417	3.528301
N	0.992953	-2.736336	0.447739	H	2.441708	-3.758034	4.772063
N	-0.994003	-2.736402	-0.445961	H	0.676665	-3.847037	4.849849
C	-2.309751	-2.423176	-0.924668	C	1.366600	-1.227579	4.269902
C	-3.383040	-2.394590	-0.003777	H	2.276034	-1.141580	4.875012
C	-2.543678	-2.347027	-2.316786	H	1.252864	-0.306967	3.692521
C	-4.681591	-2.226459	-0.499545	H	0.518694	-1.306153	4.958845
C	-3.863283	-2.200343	-2.763035	C	3.175231	-2.596756	-1.491923
C	-4.925061	-2.132360	-1.866333	H	2.102191	-2.714262	-1.664245
H	-5.515318	-2.188509	0.195829	C	3.877188	-3.875910	-1.991465
H	-4.060718	-2.140882	-3.829554	H	4.965378	-3.801342	-1.888755

H	3.555561	-4.762171	-1.433954
H	3.656204	-4.043742	-3.051532
C	3.629400	-1.370371	-2.298224
H	3.098273	-0.474509	-1.971693
H	4.702923	-1.185780	-2.182292
H	3.432048	-1.519803	-3.366006
C	0.663045	-4.173369	0.377672
H	0.576438	-4.597279	1.385950
H	1.449460	-4.724750	-0.147422
C	-0.664483	-4.173468	-0.374810
H	-0.577976	-4.598163	-1.382763
H	-1.451051	-4.724241	0.150695
C	0.664454	4.173285	-0.377668
H	0.576990	4.596580	-1.386145
H	1.451258	4.725010	0.146468
C	-0.662479	4.173729	0.375807
H	-0.574811	4.597428	1.384096
H	-1.449061	4.725556	-0.148555

SiPr

B3LYP/BSI SCF energy: -1161.270788a.u.

M06/BSII SCF energy in solution: -1160.65379a.u.

M06/BSII free energy in solution: -1160.123456a.u.

C	-0.000087	0.000126	-0.279653
N	-1.076476	0.066270	0.538449
N	1.076475	-0.065563	0.538342
C	2.426708	-0.240338	0.085806
C	2.858082	-1.515831	-0.343818
C	3.304548	0.864135	0.106620
C	4.187532	-1.656946	-0.759137
C	4.628189	0.668740	-0.307618
C	5.068870	-0.578881	-0.736626
H	4.540630	-2.623862	-1.103343
H	5.318465	1.507735	-0.303491
H	6.098042	-0.711625	-1.058900
C	-2.426829	0.240433	0.085965
C	-2.858595	1.515825	-0.343544
C	-3.304225	-0.864372	0.106577
C	-4.188069	1.656569	-0.758835
C	-4.627904	-0.669394	-0.307822
C	-5.069014	0.578145	-0.736571
H	-4.541556	2.623424	-1.102814
H	-5.317844	-1.508668	-0.304002
H	-6.098219	0.710588	-1.058864
C	1.899895	-2.700945	-0.413398
H	1.069761	-2.493784	0.269873
C	1.297007	-2.819837	-1.828561
H	0.767640	-1.899644	-2.090063
H	2.082465	-2.997171	-2.572283
H	0.590255	-3.656579	-1.877169
C	2.536806	-4.027641	0.034851
H	3.306274	-4.373319	-0.663751
H	2.997221	-3.941852	1.024664
H	1.772750	-4.810963	0.081886
C	2.844812	2.258015	0.521168
H	1.796098	2.184827	0.822477
C	2.899136	3.236278	-0.668754
H	2.522318	4.222072	-0.373385
H	3.923852	3.366983	-1.033603
H	2.290106	2.872168	-1.501256
C	3.643677	2.800212	1.721614
H	3.589030	2.122464	2.580156
H	4.702551	2.932374	1.474015
H	3.254145	3.775721	2.033140
C	-2.844133	-2.258073	0.521288
H	-1.795326	-2.184645	0.822203
C	-3.642577	-2.799802	1.722283
H	-3.587670	-2.121635	2.580472
H	-4.701512	-2.932051	1.475012
H	-3.252942	-3.775152	2.034179
C	-2.898876	-3.236865	-0.668114
H	-3.923729	-3.367943	-1.032478
H	-2.290223	-2.873188	-1.501090
H	-2.521835	-4.222460	-0.372374
C	-1.900548	2.701021	-0.413380
H	-1.070652	2.494374	0.270331
C	-2.537748	4.027951	0.033770
H	-3.307062	4.373032	-0.665295
H	-2.998416	3.942756	1.023515
H	-1.773806	4.811399	0.080486
C	-1.297073	2.819006	-1.828372
H	-0.767647	1.898625	-2.089138
H	-2.082208	2.995887	-2.572544
H	-0.590243	3.655662	-1.877227
C	-0.754794	0.139287	1.990329
H	-1.326781	-0.599382	2.559795
H	-1.003254	1.133584	2.382807

C	0.755003	-0.137566	1.990249
H	1.327103	0.601395	2.559235
H	1.003466	-1.131615	2.383389

^{SiPr}TS1

B3LYP/BSI SCF energy: -3091.977069a.u.

M06/BSII SCF energy in solution: -3090.57053a.u.

M06/BSII free energy in solution: -3089.337335a.u.

F	0.542198	1.432889	1.759204
Ni	-0.131678	0.020055	0.026420
C	1.539671	0.680396	0.734229
O	1.988338	1.437843	-0.128311
C	6.362636	1.025048	2.851364
C	5.694827	0.046286	3.548445
C	4.373147	-0.337561	3.190927
C	3.722834	0.307720	2.079428
C	4.452734	1.309472	1.377618
C	5.730796	1.657519	1.755239
H	4.192051	-1.808426	4.768411
H	7.371308	1.311030	3.137084
H	6.167003	-0.452281	4.391704
C	3.688212	-1.339766	3.926554
C	2.377024	-0.083062	1.752731
H	3.982225	1.780929	0.526163
H	6.262513	2.425248	1.199558
C	1.769154	-1.082861	2.485664
C	2.413457	-1.713803	3.571779
H	0.751051	-1.354042	2.231296
H	1.891406	-2.483230	4.133789
C	-1.675147	1.524022	0.333057
N	-1.672749	2.761298	-0.236992
N	-2.711060	1.537094	1.230375
C	-3.163196	0.501476	2.129418
C	-4.342029	-0.214644	1.799369
C	-2.549297	0.332281	3.396075
C	-4.765417	-1.233878	2.661300
C	-3.014355	-0.703136	4.219455
C	-4.088066	-1.503602	3.845242
H	-5.651649	-1.808935	2.412490
H	-2.541469	-0.864468	5.182797
H	-4.425906	-2.304264	4.497725
C	-0.773558	3.410506	-1.160312
C	0.143833	4.359556	-0.643189
C	-0.989990	3.288439	-2.549759
C	0.827624	5.176908	-1.550760
C	-0.285421	4.139709	-3.411421
C	0.608365	5.084265	-2.921042
H	1.533546	5.909981	-1.172498
H	-0.453353	4.069589	-4.482259
H	1.137246	5.742620	-3.604852
C	-5.251433	0.189221	0.639292
H	-4.670635	0.819064	-0.041957
C	-5.797714	-0.994922	-0.170683
H	-4.998123	-1.644392	-0.522297
H	-6.491054	-1.603123	0.420579
H	-6.355085	-0.627895	-1.039475
C	-6.446876	1.016255	1.170239
H	-7.091233	0.391126	1.798209
H	-6.137152	1.870129	1.779233
H	-7.053232	1.392595	0.338561
C	-1.540480	1.327367	3.964566
H	-1.088995	1.869221	3.133689
C	-0.388467	0.680923	4.747811
H	0.341551	1.447554	5.025802
H	-0.734283	0.210884	5.675752
H	0.134006	-0.065110	4.151348
C	-2.275603	2.329544	4.886469
H	-3.110451	2.829677	4.385973
H	-2.684453	1.818890	5.766022
H	-1.580914	3.099809	5.239735
C	-1.986941	2.304059	-3.149708
H	-2.378147	1.684807	-2.337668
C	-3.176656	3.032767	-3.807626
H	-3.681489	3.699721	-3.101145
H	-2.849812	3.642291	-4.657260
H	-3.913497	2.311715	-4.178760
C	-1.300961	1.362754	-4.157650
H	-0.846883	1.918709	-4.984502
H	-0.513389	0.781709	-3.670060
H	-2.025195	0.667163	-4.591609
C	0.378852	4.568020	0.851703
H	-0.118001	3.755364	1.384062
C	-0.198652	5.916458	1.333181
H	0.308831	6.757418	0.847064
H	-1.268895	6.020955	1.125508
H	-0.056675	6.024631	2.414194
C	1.871054	4.479373	1.220095

H	2.289752	3.532190	0.880672
H	2.448042	5.301776	0.780946
H	1.988571	4.541427	2.307496
C	0.453997	-1.428170	-1.096048
N	-0.421840	-2.383599	-1.589249
N	1.590332	-1.558548	-1.870982
C	2.972327	-1.172738	-1.668179
C	3.503082	-0.064352	-2.365081
C	3.824470	-2.059570	-0.960169
C	4.876527	0.188987	-2.266644
C	5.188465	-1.749722	-0.885207
C	5.713556	-0.632032	-1.521734
H	5.295327	1.042472	-2.789741
H	5.851855	-2.405034	-0.330865
H	6.774921	-0.411619	-1.449832
C	-1.668369	-2.896333	-1.079012
C	-1.713743	-3.634732	0.129764
C	-2.788965	-2.878846	-1.950531
C	-2.894448	-4.320661	0.447088
C	-3.926022	-3.615082	-1.599769
C	-3.986609	-4.331853	-0.410062
H	-2.939974	-4.890574	1.369420
H	-4.780433	-3.621787	-2.270150
H	-4.878849	-4.896460	-0.154444
C	2.662637	0.806149	-3.289615
H	1.611850	0.616994	-3.054489
C	2.911572	2.309783	-3.094666
H	2.714600	2.601516	-2.063227
H	3.938485	2.589639	-3.356449
H	2.245303	2.882020	-3.745412
C	2.914501	0.422405	-4.765187
H	3.949577	0.642764	-5.050595
H	2.744548	-0.641622	-4.957277
H	2.257017	0.996292	-5.428189
C	3.354180	-3.390048	-0.371468
H	2.270649	-3.339310	-0.240342
C	3.971743	-3.707363	1.001686
H	3.482650	-4.587718	1.433769
H	5.037860	-3.945929	0.920021
H	3.860964	-2.879456	1.700514
C	3.667730	-4.559703	-1.332919
H	3.202720	-4.442140	-2.315405
H	4.748440	-4.643574	-1.491764
H	3.317133	-5.507292	-0.908271
C	-2.809827	-2.112240	-3.272248
H	-1.852769	-1.593624	-3.375403
C	-2.991951	-3.047346	-4.486664
H	-2.245032	-3.846965	-4.515360
H	-3.977202	-3.525807	-4.473658
H	-2.914113	-2.479534	-5.420242
C	-3.914547	-1.037940	-3.280199
H	-4.907435	-1.484327	-3.166859
H	-3.774787	-0.318494	-2.469082
H	-3.908742	-0.490973	-4.228742
C	-0.515244	-3.814037	1.055672
H	0.249193	-3.089320	0.769550
C	0.082263	-5.229007	0.902363
H	-0.638720	-5.995860	1.207480
H	0.369387	-5.441210	-0.132380
H	0.973379	-5.337838	1.529948
C	-0.866950	-3.543662	2.529607
H	-1.290540	-2.545575	2.666685
H	-1.589924	-4.268806	2.917816
H	0.032757	-3.626992	3.147520
C	-3.304142	2.885486	1.407250
H	-2.892590	3.356629	2.306950
H	-4.387220	2.830726	1.507580
C	-2.848896	3.580897	0.144180
H	-3.600027	3.537100	-0.656809
H	-2.569705	4.623103	0.294149
C	0.206965	-3.265340	-2.601180
H	-0.493604	-3.520229	-3.394775
H	0.547601	-4.196063	-2.126664
C	1.348204	-2.396712	-3.066108
H	2.244477	-2.947088	-3.348753
H	1.050782	-1.760031	-3.910039

^{SiPr}TS1A

B3LYP/BSI SCF energy: -1930.722882a.u.

M06/BSII SCF energy in solution: -1929.89885a.u.

M06/BSII free energy in solution: -1929.234918a.u.

F	-0.087882	-0.753652	-2.949087
Ni	0.527682	0.063368	-1.147949
C	-1.039366	0.224380	-2.191477
O	-0.748283	1.402327	-2.416930
C	-5.943062	1.711164	-1.115269
C	-5.955896	0.339374	-1.211629

C	-4.772557	-0.384648	-1.521917
C	-3.540498	0.328205	-1.722297
C	-3.568473	1.747148	-1.627697
C	-4.737037	2.416399	-1.333323
H	-5.745428	-2.315758	-1.506400
H	-6.855307	2.253492	-0.883142
H	-6.877726	-0.216958	-1.060635
C	-4.801260	-1.797312	-1.653724
C	-2.358211	-0.434862	-2.029885
H	-2.654966	2.297094	-1.805426
H	-4.731276	3.501266	-1.274193
C	-2.441019	-1.814204	-2.156825
C	-3.660825	-2.495924	-1.975627
H	-1.546379	-2.367175	-2.411867
H	-3.690401	-3.575224	-2.091807
C	1.167207	-0.052666	0.602940
N	2.502364	-0.003688	0.872260
N	0.529702	-0.166936	1.797416
C	-0.893192	-0.136639	1.981309
C	-1.552115	1.109868	2.063355
C	-1.590883	-1.355936	2.119390
C	-2.943109	1.106412	2.222222
C	-2.980044	-1.303540	2.283621
C	-3.653887	-0.086169	2.320690
H	-3.476949	2.050931	2.266632
H	-3.541158	-2.228450	2.379819
H	-4.734096	-0.065734	2.432287
C	3.532617	0.067514	-0.126400
C	4.053900	-1.127262	-0.672236
C	4.021655	1.334058	-0.516958
C	5.071648	-1.024864	-1.628050
C	5.038525	1.380467	-1.478360
C	5.561063	0.214715	-2.030051
H	5.482590	-1.928678	-2.068449
H	5.421674	2.344032	-1.801314
H	6.349016	0.271803	-2.775879
C	-0.799630	2.437972	2.026717
H	0.265121	2.216136	1.911524
C	-1.202943	3.312848	0.826103
H	-0.993584	2.804388	-0.118086
H	-2.269339	3.561438	0.850914
H	-0.641542	4.254092	0.839889
C	-0.972588	3.205988	3.353138
H	-2.015754	3.499438	3.512411
H	-0.666494	2.600945	4.213419
H	-0.369151	4.120404	3.347547
C	-0.875284	-2.703669	2.131416
H	0.184854	-2.516015	1.936817
C	-1.375108	-3.645206	1.021589
H	-0.808134	-4.582909	1.035094
H	-2.433553	-3.896200	1.150376
H	-1.258500	-3.185177	0.037542
C	-0.988254	-3.377250	3.514189
H	-0.608421	-2.729417	4.311448
H	-2.029689	-3.617176	3.754816
H	-0.418315	-4.312789	3.534818
C	3.467880	2.635336	0.053907
H	2.728255	2.375766	0.816865
C	4.566005	3.474412	0.736024
H	5.080454	2.906012	1.518322
H	5.323251	3.807730	0.018311
H	4.132239	4.369263	1.195481
C	2.733942	3.452093	-1.027917
H	3.414958	3.746722	-1.833997
H	1.915441	2.875858	-1.469790
H	2.312949	4.366773	-0.595641
C	3.537201	-2.504315	-0.268518
H	2.755094	-2.360197	0.482343
C	4.646214	-3.363343	0.370427
H	5.450304	-3.575704	-0.342289
H	5.095833	-2.863136	1.234936
H	4.240666	-4.324097	0.706098
C	2.886235	-3.234206	-1.459656
H	2.071151	-2.640871	-1.884675
H	3.613484	-3.430228	-2.255054
H	2.478339	-4.198868	-1.137427
C	2.831155	-0.129194	2.304121
H	3.449022	0.711818	2.636826
H	3.393418	-1.052531	2.489650
C	1.438997	-0.143221	2.961330
H	1.278392	-1.020981	3.595740
H	1.253311	0.749650	3.570177

TS^{con}

B3LYP/BSI SCF energy: -2499.793287a.u.

M06/BSII SCF energy in solution: -2499.01833a.u.

M06/BSII free energy in solution: -2498.341879a.u.

Ni	0.353551	-0.002072	0.066000	H	-0.897507	-1.923116	4.634774
P	2.462319	0.638752	0.083872	O	-1.515229	-0.617118	-0.286836
C	3.571668	-0.097449	1.384154	C	-2.123787	-1.379150	-1.343517
C	3.160436	0.099112	-1.560097	H	-3.099704	-0.926850	-1.530974
C	2.810725	2.461672	0.185196	C	-1.356282	-1.359921	-2.650525
C	4.641491	-0.306802	-1.638627	C	-0.311959	-2.244379	-2.951013
C	5.046237	-0.679209	-3.070267	C	-1.730995	-0.398723	-3.601642
C	4.258568	2.935102	-0.017203	C	0.342038	-2.161373	-4.181632
C	4.384266	4.456217	0.140225	H	-0.000969	-2.988680	-2.230442
C	3.204756	0.300683	2.823159	C	-1.072543	-0.314525	-4.828073
C	4.086875	-0.407846	3.857835	H	-2.540592	0.288357	-3.370622
H	2.948315	0.921898	-2.254906	C	-0.032939	-1.199450	-5.120982
H	2.543521	-0.752654	-1.861215	H	1.147368	-2.855444	-4.403971
H	5.290138	0.498536	-1.275527	H	-1.376527	0.433410	-5.554855
H	4.814159	-1.167217	-0.982595	H	0.478226	-1.142852	-6.078017
H	2.435738	2.794937	1.158263	C	-2.443749	-2.764172	-0.783002
H	2.154657	2.932127	-0.554030	F	-3.272988	-2.650968	0.277351
H	4.929066	2.443213	0.698198	F	-1.360543	-3.452662	-0.372505
H	4.608227	2.649070	-1.016150	F	-3.074466	-3.508353	-1.716500
H	4.608049	0.185433	1.168484	C	-0.400422	3.858807	-1.619641
H	3.509660	-1.184061	1.271619	C	-0.484245	2.479767	-1.402613
H	3.300691	1.386865	2.945206	C	-0.465933	1.909667	-0.108897
H	2.154670	0.053767	3.013962	C	-0.368406	2.828280	0.961296
H	4.917016	0.168466	-3.752935	C	-0.280333	4.209001	0.766120
H	4.434553	-1.505619	-3.447772	C	-0.292536	4.729787	-0.531377
H	5.147602	-0.178321	3.703612	H	-0.422226	4.255943	-2.632291
H	3.965825	-1.494481	3.794457	H	-0.577064	1.826198	-2.268453
H	4.090044	4.776200	1.145937	H	-0.371994	2.447394	1.981813
H	3.740643	4.980695	-0.574234	H	-0.207309	4.880531	1.619066
C	1.046806	-1.769158	0.355582	H	-0.228563	5.803059	-0.692009
C	0.787414	-2.401750	1.709618	C	-3.297629	1.368648	2.278921
O	1.680302	-2.417225	-0.476225	C	-4.464423	1.267713	0.072767
C	-0.044503	-1.794238	2.661595	C	-4.328994	2.087748	1.364320
C	0.392146	-3.599091	4.214428	H	-2.767061	2.109010	2.891869
C	1.414259	-3.619110	2.024468	H	-3.824653	0.693929	2.964684
C	1.222788	-4.211572	3.269605	H	-5.118162	1.784982	-0.637607
H	-0.557521	-0.867094	2.423347	H	-4.916582	0.288749	0.294415
H	0.239263	-4.062641	5.185410	B	-2.191196	0.558865	0.227197
H	2.045614	-4.080336	1.271307	O	-3.205767	1.075605	-0.576824
H	1.714699	-5.151267	3.506930	O	-2.332133	0.560765	1.605374
H	3.823683	-0.101704	4.875471	C	-3.890714	3.522022	1.018014
H	6.095419	-0.989344	-3.116880	H	-4.660471	4.018738	0.415864
H	5.414290	4.787511	-0.028187	H	-3.745681	4.114982	1.928060
C	-0.243155	-2.394707	3.906739	H	-2.958321	3.536086	0.452916

C	-5.686872	2.129549	2.087234
H	-5.603960	2.664222	3.040248
H	-6.437203	2.651787	1.483499
H	-6.063030	1.122712	2.300168

TS1^{sw}

B3LYP/BSI SCF energy: -2499.813162a.u.

M06/BSII SCF energy in solution: -2499.03641a.u.

M06/BSII free energy in solution: -2498.359285a.u.

Ni	-0.638431	-0.096583	0.400520
P	-2.715749	-0.340999	-0.242654
C	-3.749161	1.047622	0.429595
C	-2.861824	-0.252378	-2.104637
C	-3.592222	-1.896297	0.267936
C	-4.152918	0.299932	-2.733574
C	-4.102270	0.246274	-4.265653
C	-5.088125	-2.040947	-0.052217
C	-5.667205	-3.336996	0.529683
C	-3.884071	1.031253	1.961830
C	-4.654034	2.250870	2.481049
H	-2.669523	-1.273827	-2.457735
H	-2.010977	0.345530	-2.448046
H	-5.025564	-0.259499	-2.379646
H	-4.301283	1.337854	-2.413660
H	-3.421811	-1.984925	1.346362
H	-3.028391	-2.720281	-0.185590
H	-5.645597	-1.185115	0.347303
H	-5.242382	-2.033343	-1.137155
H	-4.738139	1.026038	-0.042182
H	-3.258259	1.974501	0.114111
H	-4.397272	0.115673	2.280288
H	-2.888128	1.001809	2.416334
H	-3.992505	-0.783628	-4.622935
H	-3.256767	0.824183	-4.654621
H	-5.665628	2.296190	2.061041
H	-4.141664	3.182640	2.217095
H	-5.562009	-3.361560	1.619695
H	-5.152030	-4.216057	0.127314
C	-0.570595	-1.866735	0.971614
C	-0.073637	-2.962441	0.063489
O	-0.899220	-2.116120	2.120279
C	0.266942	-2.701266	-1.270028
C	0.800252	-5.035469	-1.600661
C	0.027627	-4.272779	0.560202
C	0.461251	-5.303172	-0.269178
H	0.217306	-1.683614	-1.643540
H	1.141288	-5.840612	-2.245619
H	-0.240965	-4.453450	1.596251
H	0.537769	-6.315860	0.117089
H	-4.747030	2.219191	3.571090
H	-5.017462	0.656499	-4.704208
H	-6.731429	-3.434779	0.292637
C	0.705933	-3.734616	-2.099842
H	0.984324	-3.521444	-3.127658
O	1.592430	0.668224	-0.300066
C	2.895743	0.731635	-0.823575
H	3.285457	1.750281	-0.712136
C	3.892113	-0.214495	-0.163920
C	3.692677	-1.601902	-0.140515
C	5.028163	0.315866	0.458083
C	4.612311	-2.436131	0.494584
H	2.818337	-2.028910	-0.616358
C	5.950270	-0.518213	1.093037
H	5.185683	1.391344	0.455521
C	5.743651	-1.897743	1.112795
H	4.443286	-3.509251	0.506748
H	6.824210	-0.089192	1.574983
H	6.457317	-2.549781	1.608652
C	2.817502	0.496904	-2.336801
F	2.071485	1.451145	-2.952246
F	2.253938	-0.692031	-2.662151
F	4.041298	0.530712	-2.901420
C	1.610125	-0.172718	3.994140
C	1.710112	0.223231	2.658298
C	0.859719	1.202501	2.108338
C	-0.105814	1.763001	2.975239
C	-0.215487	1.373601	4.309194
C	0.645463	0.399138	4.822897
H	2.283569	-0.930653	4.385921
H	2.464573	-0.235906	2.029280
H	-0.772754	2.529394	2.589309
H	-0.965213	1.829786	4.951382
H	0.563129	0.090522	5.861898
C	-0.579021	2.600694	-1.139356
C	1.506826	3.845964	-0.623191
C	0.017722	4.013792	-0.998352
H	-1.652883	2.668656	-1.359921

H	-0.087466	2.075007	-1.968140
H	1.940357	4.828614	-0.394953
H	2.040709	3.451563	-1.501307
B	1.023093	1.766039	0.588091
O	1.710470	3.019579	0.509652
O	-0.420246	1.864657	0.074751
C	-0.721532	4.812261	0.088244
H	-0.343668	5.839987	0.130905
H	-1.797435	4.861198	-0.120280
H	-0.579395	4.361989	1.072488
C	-0.088693	4.734502	-2.351373
H	-1.136402	4.880170	-2.640311
H	0.378168	5.724614	-2.302364
H	0.406680	4.169998	-3.149341

IM1^{sw}

B3LYP/BSI SCF energy: -2499.823532a.u.

M06/BSII SCF energy in solution: -2499.04878a.u.

M06/BSII free energy in solution: -2498.371496a.u.

Ni	1.185745	-0.087091	0.945326
P	2.136516	-0.877763	-0.890380
C	3.079493	-2.440465	-0.526049
C	0.830632	-1.296837	-2.158642
C	3.357569	0.188364	-1.800140
C	0.972319	-2.615644	-2.937868
C	-0.147518	-2.782521	-3.972816
C	3.987438	-0.390310	-3.076645
C	4.971829	0.592534	-3.723365
C	4.275975	-2.235877	0.419655
C	4.940706	-3.564542	0.797339
H	0.818709	-0.448908	-2.856035
H	-0.128791	-1.263514	-1.634583
H	1.946328	-2.664200	-3.439794
H	0.944435	-3.458800	-2.237566
H	4.138006	0.456719	-1.079864
H	2.829456	1.121113	-2.029105
H	4.511189	-1.326080	-2.847190
H	3.202507	-0.643483	-3.799055
H	3.408601	-2.896647	-1.466965
H	2.366313	-3.137857	-0.074453
H	5.016940	-1.582736	-0.056988
H	3.949953	-1.708316	1.322521
H	-0.110056	-1.987467	-4.725997
H	-1.131633	-2.738975	-3.498320
H	5.302943	-4.098413	-0.088813
H	4.238493	-4.225010	1.318554
H	5.790424	0.840363	-3.038862
H	4.473618	1.528988	-3.997036
C	2.462768	1.260467	1.061860
C	2.254497	2.623709	0.461903
O	3.482999	0.997431	1.684654
C	1.130246	2.907892	-0.324384
C	1.931610	5.162972	-0.667384
C	3.216772	3.622920	0.680904
C	3.055647	4.885922	0.118924
H	0.377698	2.139453	-0.477126
H	1.805885	6.149640	-1.104886
H	4.080404	3.381144	1.292441
H	3.801882	5.656829	0.290514
H	5.796051	-3.399512	1.459931
H	-0.058963	-3.741173	-4.494255
H	5.411714	0.169257	-4.632071
C	0.970158	4.174492	-0.887937
H	0.091433	4.391715	-1.488291
O	-1.849737	-0.294716	-0.066323
C	-3.194561	-0.214214	-0.430211
H	-3.845676	-0.602735	0.363661
C	-3.642204	1.202604	-0.778614
C	-2.841974	2.025221	-1.583288
C	-4.863610	1.695537	-0.309318
C	-3.258150	3.315332	-1.909076
H	-1.894901	1.644182	-1.949335
C	-5.280899	2.989130	-0.631501
H	-5.489621	1.065826	0.317711
C	-4.479034	3.801885	-1.433110
H	-2.633364	3.942074	-2.540217
H	-6.229492	3.360503	-0.254092
H	-4.801364	4.808257	-1.685234
C	-3.411976	-1.134693	-1.640904
F	-3.076903	-2.422517	-1.366686
F	-2.661397	-0.770011	-2.708044
F	-4.702552	-1.136856	-2.034405
C	-0.811145	3.037622	2.708068
C	-1.296048	1.975690	1.956921
C	-0.776597	0.666937	2.096441
C	0.288169	0.503005	3.018435
C	0.801035	1.587656	3.763805

C	0.249106	2.849267	3.612251
H	-1.248119	4.026398	2.592928
H	-2.107460	2.145766	1.256543
H	0.641870	-0.497974	3.259708
H	1.618468	1.422842	4.459921
H	0.628321	3.687917	4.189440
C	-0.438552	-2.898988	0.899029
C	-2.685917	-2.643190	1.938162
C	-1.399891	-3.500936	1.943347
H	0.520512	-3.430251	0.928555
H	-0.869889	-3.011009	-0.105399
H	-3.347433	-2.974573	2.749876
H	-3.217519	-2.822252	0.991450
B	-1.416045	-0.632114	1.328474
O	-2.435485	-1.262749	2.129643
O	-0.196156	-1.522496	1.170024
C	-0.757089	-3.490778	3.340022
H	-1.416618	-3.975519	4.068693
H	0.197164	-4.031708	3.341316
H	-0.577271	-2.469516	3.681623
C	-1.743621	-4.939530	1.527722
H	-0.850151	-5.575200	1.522950
H	-2.459226	-5.385459	2.227469
H	-2.188569	-4.975250	0.526932

TS2^{sw}

B3LYP/BSI SCF energy: -2499.811533a.u.

M06/BSII SCF energy in solution: -2499.0374a.u.

M06/BSII free energy in solution: -2498.362687a.u.

Ni	-0.932615	-0.018083	-0.796943
P	-2.582057	0.006156	0.728273
C	-3.883600	-1.289266	0.413354
C	-1.871911	-0.393702	2.405255
C	-3.542108	1.585734	0.924421
C	-2.733044	-1.124408	3.448539
C	-1.956530	-1.342817	4.753664
C	-4.687831	1.642993	1.945300
C	-5.399054	3.002305	1.928488
C	-4.572823	-1.150740	-0.954280
C	-5.598225	-2.262796	-1.202206
H	-1.514240	0.562303	2.809550
H	-0.973262	-0.982916	2.200098
H	-3.652917	-0.566478	3.657564
H	-3.047574	-2.096266	3.049291
H	-3.911293	1.829980	-0.078694
H	-2.795226	2.354837	1.153734
H	-5.419716	0.852293	1.739365
H	-4.300282	1.451907	2.952748
H	-4.627274	-1.267439	1.218725
H	-3.384260	-2.263287	0.480772
H	-5.069778	-0.175796	-1.021394
H	-3.817215	-1.153263	-1.747954
H	-1.693716	-0.387266	5.220921
H	-1.022621	-1.884121	4.567806
H	-6.386222	-2.257039	-0.440356
H	-5.125470	-3.251650	-1.180844
H	-5.828823	3.210669	0.942578
H	-4.703508	3.815161	2.164333
C	-1.474493	1.598660	-1.538097
C	-0.886258	2.901827	-1.041851
O	-2.339681	1.616818	-2.404398
C	-0.025191	2.935147	0.062987
C	0.117230	5.343633	-0.105192
C	-1.239332	4.102387	-1.675846
C	-0.735805	5.316110	-1.213402
H	0.257120	2.000545	0.542419
H	0.505461	6.291264	0.258420
H	-1.911885	4.053948	-2.526614
H	-1.008385	6.242930	-1.711190
H	-6.078181	-2.144315	-2.178760
H	-2.545729	-1.917575	5.475711
H	-6.211378	3.033045	2.661953
C	0.470049	4.152602	0.534318
H	1.131142	4.172414	1.396637
O	1.685008	-0.342890	0.308222
C	2.808815	-0.655691	1.102446
H	3.193946	-1.652635	0.861814
C	3.933412	0.354987	0.953887
C	3.664322	1.707949	0.721234
C	5.261843	-0.063879	1.084484
C	4.710238	2.624469	0.609412
H	2.637955	2.036775	0.611518
C	6.308292	0.852844	0.978726
H	5.479142	-1.113358	1.265426
C	6.034281	2.200465	0.739597
H	4.489198	3.670931	0.418731
H	7.335550	0.513237	1.075758

H	6.847713	2.914925	0.650162
C	2.323290	-0.727251	2.556613
F	1.400489	-1.714457	2.714498
F	1.744871	0.420951	2.960949
F	3.338497	-1.000396	3.401607
C	2.106445	0.969389	-3.727599
C	1.556505	0.779656	-2.460229
C	0.506385	-0.134407	-2.221552
C	0.023185	-0.830203	-3.358012
C	0.559425	-0.644933	-4.634030
C	1.608954	0.256423	-4.821008
H	2.922211	1.674988	-3.864522
H	1.972321	1.331376	-1.623812
H	-0.816153	-1.515590	-3.258237
H	0.154292	-1.193870	-5.480779
H	2.032895	0.404795	-5.810847
C	-0.651193	-3.058685	-0.658965
C	1.567771	-3.425865	-1.688662
C	0.467065	-4.097234	-0.846401
H	-1.152215	-2.875365	-1.616860
H	-1.401085	-3.426000	0.050547
H	1.186031	-3.204755	-2.695994
H	2.427902	-4.096597	-1.795944
B	1.135065	-1.314314	-0.563289
O	2.037564	-2.228273	-1.092970
O	-0.159880	-1.811660	-0.130199
C	-0.098838	-5.301493	-1.615581
H	0.673445	-6.064238	-1.762316
H	-0.922130	-5.770165	-1.064790
H	-0.474913	-5.011697	-2.603075
C	1.015900	-4.551382	0.518243
H	0.239573	-5.071946	1.090850
H	1.854049	-5.244368	0.385864
H	1.362452	-3.708581	1.119362

IM1[B]

B3LYP/BSI SCF energy: -2715.710521a.u.

M06/BSII SCF energy in solution: -2714.86685a.u.

M06/BSII free energy in solution: -2714.234361a.u.

F	-3.552099	0.615339	-1.500092
Ni	-2.174861	0.226558	-0.288308
P	-2.534261	-1.916406	-0.856709
P	-2.176762	2.440239	0.130655
C	2.432942	-0.111751	-0.717743
C	1.058652	-0.055484	-0.491390
C	0.543091	-0.263102	0.795126
C	1.426408	-0.527461	1.853420
C	2.796778	-0.581046	1.624031
C	3.327689	-0.375478	0.334979
H	2.824639	0.047597	-1.718730
H	0.371039	0.150790	-1.308803
H	1.007575	-0.684309	2.842713
H	3.476531	-0.786421	2.446919
C	-0.945160	-0.200338	1.051787
O	-1.369065	-0.451909	2.180643
B	4.859617	-0.452827	0.082922
O	5.432546	-0.352956	-1.162760
O	5.782822	-0.636513	1.085090
C	6.873529	-0.266814	-0.979595
C	7.238791	1.222405	-1.045083
H	8.319890	1.376232	-0.976263
H	6.892348	1.630773	-1.998392
H	6.756101	1.785569	-0.241412
C	7.068246	-0.896946	0.456224
C	7.246013	-2.421507	0.434409
H	8.221257	-2.709562	0.030549
H	7.171049	-2.800723	1.457187
H	6.466397	-2.903886	-0.161781
C	8.161309	-0.254280	1.307881
H	8.186667	-0.732517	2.291229
H	9.144833	-0.383350	0.843879
H	7.982693	0.811842	1.457568
C	7.550852	-1.024223	-2.120002
H	7.330280	-0.529481	-3.070185
H	8.638013	-1.036033	-1.989067
H	7.195803	-2.053930	-2.187022
C	-3.934016	2.889413	0.468960
H	-4.501173	2.473079	-0.365112
H	-4.271436	2.402995	1.388070
H	-4.079184	3.970723	0.537192
C	-1.751298	3.475099	-1.340896
C	-1.070205	4.697111	-1.233945
C	-2.158640	3.023693	-2.608998
C	-0.793184	5.451938	-2.375495
H	-0.750209	5.062185	-0.263845
C	-1.881590	3.787011	-3.743585
H	-2.703358	2.085778	-2.678762

C	-1.195990	4.998557	-3.632159
H	-0.262570	6.395217	-2.279177
H	-2.202454	3.431286	-4.718957
H	-0.978248	5.587038	-4.519241
C	-1.211735	3.178039	1.511107
C	-1.830781	3.763685	2.625361
C	0.192620	3.113785	1.477732
C	-1.067226	4.273554	3.677833
H	-2.911988	3.825407	2.682778
C	0.953099	3.629779	2.525560
H	0.694837	2.656617	0.631105
C	0.324901	4.209791	3.630149
H	-1.564484	4.721194	4.533661
H	2.036617	3.569429	2.481972
H	0.917922	4.606253	4.449359
C	-4.049388	-2.493081	0.019532
C	-4.963068	-3.387776	-0.556268
C	-4.279475	-2.023399	1.323171
C	-6.089112	-3.802621	0.155293
H	-4.806643	-3.764918	-1.561906
C	-5.402954	-2.449154	2.034350
H	-3.573701	-1.335492	1.781788
C	-6.310724	-3.334781	1.452077
H	-6.792518	-4.491581	-0.303963
H	-5.569240	-2.082072	3.043218
H	-7.187969	-3.659415	2.004715
C	-1.323943	-3.278120	-0.561932
C	-0.970163	-3.606859	0.758315
C	-0.718619	-3.978762	-1.615798
C	-0.045270	-4.617672	1.012536
H	-1.408728	-3.064250	1.589578
C	0.211571	-4.988194	-1.357541
H	-0.967352	-3.747122	-2.645992
C	0.548259	-5.312410	-0.043941
H	0.215518	-4.859120	2.038967
H	0.668881	-5.521084	-2.186564
H	1.270321	-6.098769	0.156690
C	-2.928870	-2.012762	-2.650608
H	-3.684166	-1.246399	-2.827559
H	-2.036667	-1.743690	-3.221725
H	-3.275304	-2.998920	-2.967937

TS1^{B}

B3LYP/BSI SCF energy: -2393.907607a.u.

M06/BSII SCF energy in solution: -2393.17138a.u.

M06/BSII free energy in solution: -2392.59837a.u.

Ni	2.336113	0.851434	-0.725680
P	3.296001	-1.089705	-0.485472
C	0.319639	3.445656	-1.098170
C	-1.023322	3.577569	-0.771428
C	-1.436002	3.430195	0.561347
C	-0.486817	3.155040	1.555181
C	0.858948	3.034928	1.201171
C	1.311388	3.175532	-0.125379
H	0.623867	3.551980	-2.136115
H	-1.776265	3.784181	-1.525672
H	-0.782576	3.040165	2.591991
H	1.587732	2.843036	1.985022
C	2.291639	-2.623121	-0.301177
C	2.082131	-3.196705	0.962272
C	1.685075	-3.209057	-1.424671
C	1.290198	-4.337307	1.097793
H	2.544819	-2.760007	1.841578
C	0.897596	-4.351646	-1.283962
H	1.809582	-2.767794	-2.407979
C	0.698765	-4.919246	-0.024309
H	1.140167	-4.772310	2.081745
H	0.436392	-4.794911	-2.161664
H	0.084219	-5.808403	0.082264
C	4.503509	-1.186319	0.898155
C	5.587313	-2.080108	0.859517
C	4.322787	-0.382207	2.034247
C	6.472640	-2.163168	1.933179
H	5.742657	-2.717736	-0.005301
C	5.208156	-0.473836	3.110900
H	3.507538	0.332436	2.061513
C	6.283059	-1.361444	3.061750
H	7.308931	-2.854861	1.889391
H	5.060167	0.157091	3.982377
H	6.974241	-1.427046	3.897082
C	4.281386	-1.380445	-2.019591
H	5.107093	-0.664684	-2.039225
H	4.669846	-2.399938	-2.081987
H	3.631797	-1.172005	-2.873218
C	-1.966630	-0.353380	0.354713
C	-0.646822	-0.158872	-0.046317
C	-0.322824	-0.138096	-1.408646

C	-1.336934	-0.316043	-2.364922
C	-2.652885	-0.496780	-1.956927
C	-2.993965	-0.516798	-0.590045
H	-2.211957	-0.370327	1.412852
H	0.137705	-0.014567	0.690301
H	-1.066644	-0.301421	-3.416021
H	-3.436872	-0.622311	-2.698771
C	1.090193	0.079047	-1.871834
O	1.411896	-0.133855	-3.032721
B	-4.471427	-0.694367	-0.139111
O	-4.860823	-0.760926	1.178176
O	-5.523972	-0.792910	-1.016440
C	-6.314261	-0.687686	1.209068
C	-6.672680	0.776486	1.498565
H	-7.752466	0.916688	1.605811
H	-6.193251	1.077672	2.434181
H	-6.312770	1.437559	0.705170
C	-6.706080	-1.153426	-0.248545
C	-6.868726	-2.673890	-0.379561
H	-7.777203	-3.027998	0.116806
H	-6.932956	-2.932479	-1.439986
H	-6.011499	-3.204031	0.044959
C	-7.912941	-0.441599	-0.856505
H	-8.082173	-0.810567	-1.872043
H	-8.817283	-0.636785	-0.270507
H	-7.759001	0.637280	-0.912942
C	-6.820138	-1.584837	2.336938
H	-6.471706	-1.196742	3.298413
H	-7.914832	-1.605450	2.357597
H	-6.453451	-2.607544	2.234488
B	2.897933	3.198705	-0.491970
O	3.517519	2.079023	0.312938
O	3.658800	4.377553	-0.292476
F	2.980030	2.704635	-1.888761
H	4.468585	2.063665	0.137623
H	3.277506	5.116808	-0.776936
O	-2.775122	3.573777	0.787496
C	-3.254500	3.400734	2.110171
H	-2.817623	4.133245	2.801518
H	-4.334044	3.554827	2.062916
H	-3.051990	2.388987	2.484481

IM2^{B}

B3LYP/BSI SCF energy: -2393.915441a.u.

M06/BSII SCF energy in solution: -2393.18315a.u.

M06/BSII free energy in solution: -2392.610299a.u.

Ni	2.213164	0.849370	-0.087579
P	3.053682	-1.115441	-0.618824
C	1.444833	3.568308	-0.852450
C	0.134232	4.012575	-1.013280
C	-0.765315	3.897885	0.058197
C	-0.340086	3.337112	1.274731
C	0.968407	2.899122	1.409002
C	1.917998	3.001638	0.354145
H	2.140487	3.661835	-1.681379
H	-0.178487	4.434643	-1.961254
H	-1.057638	3.260321	2.085509
H	1.295254	2.499150	2.365666
B	3.537849	2.822240	0.667756
O	4.095091	3.696170	1.647632
H	4.356137	4.522039	1.226153
O	-2.063560	4.298490	0.018546
C	-2.576313	4.817016	-1.200604
H	-2.509923	4.078605	-2.008876
H	-3.625083	5.049570	-1.009855
H	-2.053135	5.732707	-1.503237
C	1.983001	-2.577056	-0.966278
C	1.845808	-3.615731	-0.033005
C	1.261185	-2.644688	-2.170515
C	1.011835	-4.702122	-0.300766
H	2.396402	-3.585332	0.901278
C	0.433926	-3.735878	-2.434875
H	1.325091	-1.839457	-2.894597
C	0.306818	-4.767338	-1.502809
H	0.919184	-5.499501	0.431071
H	-0.115982	-3.774813	-3.370689
H	-0.339724	-5.614838	-1.711258
C	4.286866	-1.740819	0.594208
C	5.457518	-2.402915	0.190493
C	4.043420	-1.568026	1.967331
C	6.362684	-2.880831	1.138466
H	5.668760	-2.548635	-0.863801
C	4.946686	-2.055280	2.913690
H	3.156554	-1.033843	2.293435
C	6.107994	-2.710195	2.500774
H	7.266757	-3.386354	0.811743
H	4.746987	-1.910923	3.971287

H	6.815105	-3.081030	3.237036
C	3.984194	-0.859609	-2.190331
H	4.826832	-0.192363	-1.992254
H	4.336132	-1.797293	-2.627521
H	3.308029	-0.352043	-2.882479
C	-2.157006	-0.372572	0.722637
C	-0.843188	-0.082575	0.360711
C	-0.541420	0.309726	-0.949487
C	-1.578035	0.417246	-1.891364
C	-2.889361	0.141598	-1.521086
C	-3.204352	-0.261601	-0.208302
H	-2.382381	-0.684408	1.738646
H	-0.039960	-0.160974	1.088413
H	-1.324524	0.714032	-2.904442
H	-3.689093	0.230624	-2.251663
C	0.875934	0.598951	-1.371675
O	1.147225	0.702720	-2.564822
B	-4.671439	-0.576745	0.200493
O	-5.025247	-1.074217	1.431633
O	-5.747618	-0.386799	-0.632976
C	-6.477084	-1.028008	1.523703
C	-6.827618	0.254220	2.289876
H	-7.904184	0.339666	2.465208
H	-6.321682	0.236011	3.259030
H	-6.490762	1.144192	1.751139
C	-6.908757	-0.990781	0.003918
C	-7.074914	-2.384418	-0.616657
H	-7.969797	-2.890010	-0.241743
H	-7.167043	-2.280428	-1.701234
H	-6.206566	-3.016612	-0.410932
C	-8.131062	-0.128328	-0.304801
H	-8.322724	-0.137902	-1.381604
H	-9.021377	-0.517330	0.200415
H	-7.981400	0.908619	0.000804
C	-6.950137	-2.252776	2.304114
H	-6.568684	-2.203997	3.328001
H	-8.043670	-2.286560	2.351943
H	-6.591597	-3.180729	1.855333
O	3.578890	1.405539	1.209898
H	4.481305	1.061972	1.215251
F	4.247795	2.858318	-0.570084

TS2^{B}

B3LYP/BSI SCF energy: -2393.901162a.u.

M06/BSII SCF energy in solution: -2393.16574a.u.

M06/BSII free energy in solution: -2392.593867a.u.

Ni	2.138844	0.619611	-0.116342
P	2.880215	-1.447976	-0.598276
C	1.554266	3.419186	-1.026923
C	0.840274	4.620697	-1.001315
C	0.098607	4.952148	0.139263
C	0.093236	4.081663	1.242415
C	0.823919	2.904272	1.195141
C	1.593949	2.527986	0.064015
H	2.106933	3.171318	-1.929527
H	0.857177	5.273218	-1.867111
H	-0.485567	4.360420	2.117903
H	0.821652	2.267095	2.076724
B	3.687347	2.430692	0.681196
O	3.796025	3.457114	1.587377
H	3.841540	4.309824	1.139844
O	-0.640059	6.090897	0.280830
C	-0.693649	6.997111	-0.808863
H	-1.122819	6.529703	-1.704340
H	-1.337883	7.817504	-0.487918
H	0.299277	7.394901	-1.056116
C	1.726397	-2.870611	-0.830545
C	1.637696	-3.913362	0.103373
C	0.882547	-2.890423	-1.954704
C	0.729797	-4.956759	-0.085215
H	2.281211	-3.920143	0.976909
C	-0.018723	-3.938282	-2.140255
H	0.913401	-2.082053	-2.677827
C	-0.098319	-4.973992	-1.207662
H	0.675526	-5.758312	0.646065
H	-0.664103	-3.939062	-3.013826
H	-0.802988	-5.787538	-1.353929
C	4.161250	-2.094607	0.559704
C	5.311663	-2.768424	0.117223
C	3.979389	-1.906526	1.941753
C	6.252752	-3.242349	1.031796
H	5.476799	-2.928770	-0.943091
C	4.918503	-2.389077	2.855874
H	3.104008	-1.373379	2.301514
C	6.057493	-3.055815	2.402008
H	7.138208	-3.759256	0.673162
H	4.762122	-2.235257	3.919500

H	6.792051	-3.424802	3.111845
C	3.734965	-1.323180	-2.231482
H	4.640650	-0.722397	-2.111978
H	3.984118	-2.299991	-2.653347
H	3.060411	-0.783303	-2.900572
C	-2.291110	-0.272815	0.703198
C	-0.967305	-0.030541	0.344177
C	-0.629805	0.223103	-0.991049
C	-1.642327	0.234472	-1.963360
C	-2.963851	-0.001186	-1.600301
C	-3.314860	-0.260723	-0.261007
H	-2.543337	-0.470656	1.741414
H	-0.180436	-0.035409	1.094021
H	-1.363034	0.430633	-2.993982
H	-3.744106	0.012825	-2.356816
C	0.803115	0.459797	-1.404747
O	1.080537	0.519446	-2.602063
B	-4.792533	-0.524874	0.140875
O	-5.193080	-0.799376	1.427634
O	-5.837233	-0.510892	-0.753602
C	-6.647068	-0.763229	1.452374
C	-7.045347	0.632967	1.949235
H	-8.129870	0.729923	2.057482
H	-6.584615	0.806557	2.925547
H	-6.693228	1.412413	1.267816
C	-7.013737	-1.015858	-0.063290
C	-7.129257	-2.503517	-0.421928
H	-8.032801	-2.953386	0.000585
H	-7.171950	-2.602309	-1.510058
H	-6.261500	-3.065575	-0.065602
C	-8.236649	-0.255700	-0.573011
H	-8.385558	-0.470964	-1.635077
H	-9.139805	-0.563614	-0.035562
H	-8.115212	0.823180	-0.462597
C	-7.140265	-1.829292	2.428723
H	-6.800269	-1.584947	3.439202
H	-8.234516	-1.871280	2.441216
H	-6.755676	-2.818554	2.174744
O	3.584239	1.108955	1.235329
H	4.401549	0.601371	1.135374
F	4.366554	2.515503	-0.505775

Ar^{B}C(O)F

B3LYP/BSI SCF energy: -855.534968a.u.

M06/BSII SCF energy in solution: -855.233167a.u.

M06/BSII free energy in solution: -855.003439a.u.

C	-1.330587	1.169564	-0.122560
C	-2.722413	1.166551	-0.123912
C	-3.412060	-0.047767	0.005387
C	-2.701818	-1.251199	0.134818
C	-1.311680	-1.234269	0.133125
C	-0.601264	-0.025976	0.004848
H	-0.794245	2.108665	-0.221525
H	-3.279597	2.090822	-0.223207
H	-3.255863	-2.178773	0.233726
H	-0.760474	-2.164754	0.231843
C	-4.888459	-0.106310	0.009900
O	-5.584066	-1.074285	0.111434
F	-5.453166	1.127810	-0.121192
B	0.957949	-0.011627	0.002910
O	1.698527	1.128432	-0.177190
O	1.721522	-1.136661	0.180182
C	3.090321	0.793684	0.099618
C	3.364204	1.226078	1.545718
H	4.411170	1.070787	1.822511
H	3.136484	2.290735	1.646059
H	2.733619	0.678714	2.251876
C	3.105449	-0.774394	-0.102237
C	3.381503	-1.201528	-1.549439
H	4.424225	-1.026715	-1.830620
H	3.173316	-2.270249	-1.648809
H	2.737802	-0.666124	-2.252927
C	4.010383	-1.544876	0.856624
H	3.923867	-2.617267	0.660115
H	5.058164	-1.259078	0.717041
H	3.736998	-1.370692	1.898631
C	3.975721	1.582035	-0.862956
H	3.867456	2.652529	-0.666822
H	5.029719	1.318369	-0.726830
H	3.702444	1.401447	-1.903900

TS1^{ArB}

B3LYP/BSI SCF energy: -2726.635526a.u.

M06/BSII SCF energy in solution: -2725.78342a.u.

M06/BSII free energy in solution: -2725.098159a.u.

Ni	-1.898193	-0.152666	-0.036031

P	-2.623084	1.783625	0.666741	H	0.447232	0.561683	1.286520
C	-0.358004	-2.639939	-1.836666	H	1.310601	0.975940	-2.896982
C	1.014338	-2.806907	-1.982435	H	3.754796	0.925212	-2.394370
C	1.830270	-2.893603	-0.841917	C	-0.726781	0.710767	-1.192685
C	1.252736	-2.834412	0.434307	O	-1.146956	1.050929	-2.282057
C	-0.124817	-2.679621	0.561427	B	5.011878	0.609298	0.045867
C	-0.968513	-2.572935	-0.564820	O	5.525181	0.555628	1.316440
H	-0.982784	-2.548816	-2.719777	O	5.965315	0.513778	-0.934544
H	1.465583	-2.853867	-2.967087	C	6.919272	0.141428	1.200588
H	1.897531	-2.899412	1.304680	C	6.947400	-1.373949	1.438918
H	-0.565537	-2.633871	1.553153	H	7.969490	-1.764023	1.411992
C	-3.946214	2.409427	-0.444788	H	6.528265	-1.582340	2.427330
C	-4.397111	1.606631	-1.502878	H	6.342539	-1.910859	0.703701
C	-4.536000	3.666226	-0.227266	C	7.268829	0.552325	-0.285326
C	-5.430885	2.058097	-2.327273	C	7.780099	1.992830	-0.420138
H	-3.943531	0.637644	-1.685325	H	8.791934	2.102878	-0.018508
C	-5.567711	4.109058	-1.052366	H	7.800024	2.262986	-1.479554
H	-4.182806	4.305245	0.577403	H	7.123017	2.698733	0.095798
C	-6.016073	3.304017	-2.103751	C	8.198876	-0.409512	-1.021422
H	-5.772206	1.432509	-3.146503	H	8.355187	-0.057162	-2.045094
H	-6.018730	5.081724	-0.878184	H	9.175324	-0.461107	-0.528267
H	-6.818279	3.651992	-2.748285	H	7.777323	-1.414628	-1.070965
C	-1.446815	3.189202	0.826732	C	7.725804	0.862437	2.278568
C	-0.841612	3.485595	2.057929	H	7.384331	0.540311	3.266411
C	-1.092648	3.943042	-0.304456	H	8.790534	0.620534	2.194728
C	0.092244	4.517796	2.157878	H	7.608260	1.945972	2.218054
H	-1.091427	2.915314	2.947145	B	-2.592443	-2.481128	-0.425647
C	-0.160081	4.974245	-0.199522	O	-2.912583	-1.708297	0.832337
H	-1.541717	3.722115	-1.267186	O	-3.334226	-3.696846	-0.328666
C	0.434209	5.264657	1.030155	F	-3.043213	-1.650907	-1.541504
H	0.550286	4.736628	3.118019	C	3.296085	-3.003121	-0.940128
H	0.102940	5.549770	-1.082078	O	4.094832	-3.031243	-0.045367
H	1.161136	6.067649	1.108400	F	3.729091	-3.069561	-2.230075
C	-3.442365	1.723024	2.324271	C	-4.172063	-2.232883	1.336962
H	-2.772866	1.285233	3.067977	C	-4.057759	-3.750001	0.899650
H	-3.746306	2.722625	2.645263	C	-5.338907	-1.512278	0.647726
H	-4.324734	1.087534	2.241712	H	-5.316527	-1.676696	-0.430614
C	2.537596	0.650254	0.767263	H	-6.302137	-1.850870	1.041203
C	1.173848	0.654646	0.484754	H	-5.266139	-0.435108	0.824830
C	0.730056	0.766303	-0.839306	C	-4.232400	-2.022939	2.849550
C	1.670268	0.886900	-1.876956	H	-4.352323	-0.963088	3.090763
C	3.029709	0.861626	-1.587881	H	-5.088822	-2.555621	3.276358
C	3.489439	0.732941	-0.262917	H	-3.324530	-2.380880	3.338642
H	2.877396	0.553003	1.794300	C	-5.406404	-4.428788	0.635347

H	-5.231567	-5.465580	0.333369
H	-6.036836	-4.440741	1.531873
H	-5.948626	-3.935116	-0.172833
C	-3.253231	-4.599989	1.900534
H	-3.800684	-4.774830	2.832591
H	-3.044910	-5.568336	1.437451
H	-2.294745	-4.133796	2.141701

IM2^{ArB}

B3LYP/BSI SCF energy: -2726.639594a.u.

M06/BSII SCF energy in solution: -2725.79292a.u.

M06/BSII free energy in solution: -2725.110825a.u.

Ni	1.725433	0.315957	-0.117227
P	1.964553	-1.627620	-1.176290
C	3.146524	3.055952	-0.862398
C	2.252320	3.996182	-1.346599
C	1.014727	4.194260	-0.698606
C	0.691424	3.438592	0.425252
C	1.605994	2.485154	0.907747
C	2.863997	2.281859	0.287967
H	4.103703	2.910570	-1.352626
H	2.491716	4.590757	-2.220952
H	-0.259901	3.605509	0.919771
H	1.386610	1.993478	1.851440
C	1.180012	-1.908906	-2.817911
C	0.210930	-2.901017	-3.024013
C	1.562912	-1.093470	-3.896551
C	-0.357766	-3.080315	-4.286572
H	-0.098390	-3.540179	-2.204318
C	0.996377	-1.279986	-5.155816
H	2.286674	-0.298511	-3.752196
C	0.034977	-2.273693	-5.354340
H	-1.105585	-3.854469	-4.432352
H	1.300835	-0.641848	-5.980030
H	-0.407068	-2.415221	-6.336335
C	1.528826	-3.122517	-0.199499
C	2.341364	-4.266544	-0.182887
C	0.335545	-3.126523	0.541521
C	1.970727	-5.386538	0.562745
H	3.269562	-4.290362	-0.743533
C	-0.037057	-4.251328	1.278946
H	-0.308212	-2.252019	0.538392
C	0.781838	-5.381923	1.294212
H	2.613136	-6.262216	0.571474
H	-0.963930	-4.239992	1.844907
H	0.496034	-6.254364	1.874465
C	3.764931	-1.773301	-1.550884
H	4.320584	-1.748088	-0.613570
H	3.986197	-2.676357	-2.124842
H	4.064830	-0.897430	-2.129591
C	-2.682522	0.089581	0.977083
C	-1.364629	0.262439	0.559583
C	-1.083052	0.630804	-0.764453
C	-2.142998	0.818819	-1.665198
C	-3.456324	0.635725	-1.244279
C	-3.752436	0.269945	0.082384
H	-2.893478	-0.181966	2.007739
H	-0.547213	0.129783	1.264515
H	-1.909884	1.110484	-2.684070
H	-4.272773	0.781384	-1.946139
C	0.332530	0.831261	-1.249514
O	0.549612	1.335210	-2.335811
B	-5.225805	0.085286	0.551119
O	-5.570552	-0.314569	1.818751
O	-6.309132	0.310696	-0.260256
C	-7.011707	-0.140899	1.952718
C	-7.227160	1.211298	2.644896
H	-8.286118	1.398504	2.845992
H	-6.691443	1.210448	3.598037
H	-6.837764	2.035135	2.040404
C	-7.492423	-0.159428	0.447898
C	-7.787361	-1.569008	-0.081577
H	-8.705484	-1.979476	0.349187
H	-7.908771	-1.520452	-1.167114
H	-6.964410	-2.255776	0.135708
C	-8.652799	0.778911	0.123614
H	-8.886774	0.716888	-0.942950
H	-9.550425	0.497011	0.683837
H	-8.408984	1.817288	0.353992
C	-7.554840	-1.270955	2.824348
H	-7.135952	-1.190149	3.831450
H	-8.645078	-1.210358	2.906560
H	-7.289078	-2.252053	2.427115
B	3.972828	1.259227	0.922920
O	3.279536	-0.089649	1.138610
O	4.402261	1.632027	2.243541
C	3.464796	-0.515564	2.518408

C	3.827751	-2.002002	2.541700
H	4.094812	-2.314579	3.557222
H	2.978445	-2.609658	2.218642
H	4.673797	-2.216899	1.886393
C	4.629339	0.446627	2.999463
C	4.568719	0.805215	4.487816
H	4.658938	-0.084711	5.120848
H	5.400141	1.474387	4.727292
H	3.642643	1.325557	4.739866
C	6.032603	-0.105072	2.673747
H	6.761287	0.685631	2.873265
H	6.290622	-0.973039	3.289874
H	6.119877	-0.372001	1.619083
C	2.157170	-0.307668	3.294022
H	1.341813	-0.824160	2.776020
H	2.223996	-0.722788	4.304418
H	1.904910	0.750931	3.384320
C	0.031314	5.187128	-1.176809
O	-1.044515	5.435864	-0.715587
F	0.474624	5.863250	-2.273930
F	5.008145	1.069542	-0.023631

TS2^{ArB}

B3LYP/BSI SCF energy: -2726.624186a.u.

M06/BSII SCF energy in solution: -2725.77544a.u.

M06/BSII free energy in solution: -2725.092984a.u.

Ni	-1.803145	0.050186	-0.576022
P	-1.796425	2.308454	-0.656203
C	-1.735196	-2.780024	-1.704282
C	-1.215064	-4.072037	-1.698561
C	-0.708339	-4.613373	-0.509688
C	-0.733016	-3.846045	0.665488
C	-1.269958	-2.565650	0.640603
C	-1.797599	-1.984261	-0.538509
H	-2.113099	-2.372930	-2.635600
H	-1.192633	-4.660609	-2.608894
H	-0.328992	-4.271609	1.578677
H	-1.271500	-2.002619	1.568990
C	-0.539858	3.267055	-1.610116
C	0.305246	4.209762	-1.007071
C	-0.433803	3.045159	-2.994628
C	1.233383	4.919343	-1.771636
H	0.242207	4.397807	0.059026
C	0.490747	3.761025	-3.753809
H	-1.051017	2.296122	-3.478646
C	1.326665	4.699690	-3.145567
H	1.880689	5.646044	-1.289073
H	0.561494	3.577126	-4.821876
H	2.048507	5.253063	-3.739314
C	-1.811393	3.109580	1.001118
C	-2.729016	4.108615	1.360022
C	-0.858440	2.694556	1.947616
C	-2.695789	4.676291	2.635936
H	-3.474778	4.450122	0.649934
C	-0.819160	3.271462	3.217368
H	-0.139584	1.923694	1.684477
C	-1.741407	4.260858	3.565448
H	-3.415327	5.445829	2.900287
H	-0.072493	2.944127	3.934957
H	-1.716398	4.705023	4.556206
C	-3.374884	2.825691	-1.466002
H	-4.214763	2.405434	-0.910306
H	-3.463981	3.912044	-1.545314
H	-3.388360	2.395156	-2.470153
C	2.656529	-0.253717	0.689217
C	1.344908	-0.221968	0.220579
C	1.085319	-0.139656	-1.153595
C	2.161663	-0.090648	-2.053623
C	3.469043	-0.118119	-1.580703
C	3.742910	-0.199651	-0.201817
H	2.850081	-0.327715	1.755870
H	0.509661	-0.281055	0.912590
H	1.942998	-0.029470	-3.114761
H	4.298336	-0.076882	-2.281623
C	-0.320726	-0.082755	-1.691715
O	-0.522392	-0.079452	-2.896963
B	5.208477	-0.234378	0.319087
O	5.540892	-0.262921	1.652126
O	6.303500	-0.237811	-0.510067
C	6.972316	-0.517530	1.740535
C	7.138124	-2.023839	1.981908
H	8.188563	-2.296982	2.119855
H	6.588429	-2.301604	2.885337
H	6.734469	-2.607039	1.149602
C	7.483856	-0.050722	0.320786
C	7.830660	1.442865	0.258569
H	8.750531	1.667987	0.806467

H	7.973582	1.729521	-0.786871
H	7.022765	2.055293	0.668930
C	8.623679	-0.880262	-0.266779
H	8.877448	-0.501006	-1.260760
H	9.519248	-0.812473	0.359789
H	8.347048	-1.930910	-0.368645
C	7.529890	0.269480	2.924766
H	7.089131	-0.105242	3.852994
H	8.616220	0.151010	2.995179
H	7.299163	1.333492	2.848302
B	-3.792681	-1.264122	-0.501506
O	-3.759026	-0.008637	0.206132
O	-4.458472	-2.218336	0.264644
C	-4.430734	-0.189307	1.501432
C	-5.289741	1.050921	1.750685
H	-5.904020	0.915965	2.647190
H	-4.649084	1.922252	1.913619
H	-5.951363	1.260159	0.908440
C	-5.251244	-1.521420	1.247706
C	-5.401422	-2.420030	2.475038
H	-5.953212	-1.911432	3.272794
H	-5.960562	-3.317630	2.196717
H	-4.432770	-2.738224	2.863293
C	-6.632284	-1.266118	0.620334
H	-7.053435	-2.226291	0.311350
H	-7.324873	-0.796647	1.325904
H	-6.555360	-0.634907	-0.269210
C	-3.387469	-0.314306	2.613130
H	-2.717205	0.548868	2.585952
H	-3.872789	-0.332304	3.593726
H	-2.795367	-1.223308	2.514239
C	-0.139011	-5.971458	-0.445325
O	0.322346	-6.532577	0.507047
F	-0.174346	-6.605970	-1.652965
F	-4.032685	-1.164660	-1.841298

TS^{con}-Me

B3LYP/BSI SCF energy: -1985.289875a.u.

M06/BSII SCF energy in solution: -1984.60463a.u.

M06/BSII free energy in solution: -1983.938541a.u.

C	1.154946	1.631986	-0.445981
C	1.044067	2.097123	-1.769504
H	0.865721	1.394735	-2.580602
C	1.162581	3.457039	-2.079840
H	1.074498	3.782292	-3.114350
C	1.395797	4.392843	-1.070937
H	1.488534	5.448875	-1.309431
C	1.523027	3.950429	0.247986
C	1.412885	2.589500	0.551821
C	-2.181771	1.510449	0.063784
H	-1.562037	2.086620	-0.636449
C	-2.011305	2.173069	1.449217
H	-2.619198	1.636769	2.189024
H	-0.968960	2.109743	1.774302
C	-2.458023	3.644078	1.419586
H	-1.789420	4.205460	0.753686
H	-2.346559	4.082861	2.418542
C	-3.908116	3.779225	0.935768
H	-4.580673	3.316269	1.672508
H	-4.194583	4.835864	0.874090
C	-4.103612	3.096837	-0.424408
H	-3.524252	3.637071	-1.186120
H	-5.154429	3.152444	-0.733837
C	-3.649153	1.625034	-0.403923
H	-3.778678	1.201164	-1.404195
H	-4.303681	1.053951	0.266255
C	-2.148742	-0.994731	-1.536035
H	-3.235905	-0.879535	-1.429419
C	-1.712333	-0.266173	-2.827107
H	-1.929075	0.805728	-2.766383
H	-0.622880	-0.353892	-2.929346
C	-2.383233	-0.865717	-4.073563
H	-3.468833	-0.700666	-4.018307
H	-2.033777	-0.339211	-4.969656
C	-2.101477	-2.369387	-4.190278
H	-2.624177	-2.791079	-5.056956
H	-1.027483	-2.522219	-4.367289
C	-2.513086	-3.107346	-2.909289
H	-2.257899	-4.171320	-2.982199
H	-3.605813	-3.056696	-2.798570
C	-1.851557	-2.505417	-1.656417
H	-0.767624	-2.663406	-1.699381
H	-2.210376	-3.042690	-0.772698
C	-1.945458	-1.269323	1.406799
H	-1.593019	-2.258761	1.084828
C	-3.467510	-1.369707	1.635775
H	-3.987756	-1.613932	0.702448

H	-3.854407	-0.397258	1.965117
C	-3.797158	-2.426556	2.705845
H	-4.880372	-2.458458	2.874337
H	-3.510142	-3.419167	2.330733
C	-3.057488	-2.149679	4.022829
H	-3.432338	-1.211424	4.456364
H	-3.274356	-2.938426	4.752850
C	-1.543111	-2.032047	3.797048
H	-1.146545	-3.005046	3.474252
H	-1.035760	-1.785302	4.737308
C	-1.208386	-0.972501	2.733318
H	-1.494637	0.015110	3.111868
H	-0.127006	-0.941412	2.560873
F	0.937140	-2.239052	0.232359
Ni	0.955334	-0.194268	-0.053736
P	-1.361256	-0.186373	-0.020902
H	1.722067	4.664427	1.044185
H	1.548054	2.272166	1.583312
C	3.854464	-0.029889	-0.885220
C	5.196941	0.239821	-0.618610
C	5.615011	0.268887	0.707246
C	4.737670	0.032621	1.760744
C	3.405155	-0.247589	1.459878
C	2.914300	-0.300062	0.133382
H	3.530089	-0.028518	-1.922337
H	5.912655	0.437790	-1.410323
H	5.104747	0.065789	2.781820
H	2.730100	-0.445215	2.291140
F	6.911671	0.531320	0.981114
B	2.262297	-2.486993	-0.257541
C	2.342466	-2.672840	-1.826057
H	1.773607	-1.932166	-2.396862
H	3.374398	-2.665200	-2.188934
H	1.926015	-3.661941	-2.071564
C	3.179975	-3.295210	0.738238
H	4.243248	-3.116656	0.551744
H	2.976788	-3.084875	1.791567
H	3.004209	-4.369593	0.574057

TS1^{sw}-Me

B3LYP/BSI SCF energy: -1985.283107a.u.

M06/BSII SCF energy in solution: -1984.60739a.u.

M06/BSII free energy in solution: -1983.937919a.u.

C	1.437265	1.258033	-0.070817
C	1.765156	2.213683	-1.047622
H	1.569652	2.004825	-2.094588
C	2.381951	3.415735	-0.688033
H	2.633930	4.140421	-1.458729
C	2.681788	3.683930	0.650318
H	3.160231	4.618890	0.928520
C	2.373633	2.734023	1.623687
C	1.752585	1.530435	1.266183
C	-1.424801	0.289507	1.879727
H	-0.867735	1.226986	2.009522
C	-0.687050	-0.775870	2.722946
H	-1.207264	-1.737195	2.653182
H	0.323329	-0.941616	2.334993
C	-0.633922	-0.351493	4.200629
H	-0.030517	0.562315	4.293402
H	-0.123611	-1.123175	4.788777
C	-2.039957	-0.094214	4.763134
H	-2.598340	-1.041019	4.785057
H	-1.977329	0.253277	5.800932
C	-2.808064	0.924789	3.909053
H	-2.323930	1.907877	3.992369
H	-3.829783	1.047927	4.287609
C	-2.851221	0.512418	2.425770
H	-3.380866	1.276876	1.846974
H	-3.430391	-0.414522	2.329403
C	-2.080246	1.557100	-0.735852
H	-3.151831	1.450313	-0.524194
C	-1.644652	2.913933	-0.141543
H	-1.829631	2.941106	0.937494
H	-0.570663	3.057366	-0.284607
C	-2.407040	4.069261	-0.815801
H	-3.478255	3.989336	-0.579266
H	-2.066136	5.022456	-0.394944
C	-2.221957	4.061256	-2.339536
H	-2.798744	4.873387	-2.797643
H	-1.166208	4.252900	-2.575421
C	-2.635563	2.710456	-2.938781
H	-2.446122	2.694681	-4.018370
H	-3.718981	2.572205	-2.809801
C	-1.890161	1.543710	-2.269534
H	-0.819825	1.612427	-2.496125
H	-2.233376	0.594114	-2.696834
C	-2.436790	-1.371241	-0.531387

H	-2.063333	-1.581524	-1.542909
C	-3.942189	-1.047382	-0.670687
H	-4.100237	-0.162605	-1.292992
H	-4.372008	-0.824388	0.313463
C	-4.700318	-2.230028	-1.304331
H	-5.767278	-1.985054	-1.367062
H	-4.350468	-2.362008	-2.337790
C	-4.494721	-3.538210	-0.530068
H	-4.963005	-3.451706	0.460950
H	-5.000086	-4.365243	-1.042121
C	-3.001809	-3.846678	-0.357158
H	-2.551654	-4.059310	-1.336283
H	-2.864781	-4.747605	0.252359
C	-2.260505	-2.666904	0.293622
H	-2.668198	-2.511450	1.299977
H	-1.201753	-2.916000	0.416799
Ni	0.796721	-0.383617	-0.703360
P	-1.276712	0.032710	0.025517
H	2.620447	2.920836	2.666107
H	1.549986	0.798355	2.041366
C	4.016280	-0.493371	-0.897864
C	4.851061	-0.292161	0.194164
C	4.624642	-1.038943	1.349394
C	3.608665	-1.979700	1.429054
C	2.790547	-2.168119	0.308442
C	2.957964	-1.435539	-0.888049
H	4.174158	0.098690	-1.794746
H	5.659620	0.431420	0.176380
H	3.477220	-2.553147	2.341239
H	2.019867	-2.932918	0.365409
F	5.424876	-0.844146	2.420974
B	2.109816	-1.723597	-2.274496
F	1.662279	-0.345416	-2.735855
C	0.709192	-2.513629	-1.949286
H	0.892317	-3.536956	-1.601238
H	0.044429	-2.101024	-1.149918
H	0.074423	-2.553468	-2.841426
C	2.984357	-2.421585	-3.435609
H	2.404905	-2.537992	-4.361857
H	3.876839	-1.832642	-3.684722
H	3.335274	-3.420977	-3.145932

TS2^{sw}-Me

B3LYP/BSI SCF energy: -1985.277335a.u.

M06/BSII SCF energy in solution: -1984.60214a.u.

M06/BSII free energy in solution: -1983.933992a.u.

C	1.216460	1.489540	-0.384293
C	1.231342	1.822829	-1.750043
H	1.131720	1.043295	-2.501209
C	1.379325	3.148784	-2.173549
H	1.387079	3.375272	-3.237553
C	1.522499	4.176352	-1.239487
H	1.640765	5.205684	-1.566656
C	1.528829	3.861061	0.121468
C	1.384049	2.534418	0.541290
C	-2.085919	1.518765	-0.259811
H	-1.339924	1.964750	-0.929577
C	-2.102826	2.382603	1.021128
H	-2.854691	1.990267	1.717914
H	-1.133503	2.336756	1.525335
C	-2.450340	3.845333	0.697039
H	-1.650117	4.271304	0.077701
H	-2.474918	4.430957	1.624131
C	-3.793560	3.953654	-0.037882
H	-4.602907	3.641095	0.638019
H	-3.999217	4.996345	-0.307697
C	-3.811973	3.067765	-1.290118
H	-3.088602	3.457388	-2.019817
H	-4.795607	3.108168	-1.773704
C	-3.456318	1.603537	-0.969092
H	-3.457411	1.029809	-1.900350
H	-4.240551	1.173457	-0.333483
C	-1.970258	-1.199274	-1.447883
H	-3.053623	-1.028612	-1.507013
C	-1.325153	-0.698119	-2.760409
H	-1.469656	0.380362	-2.885161
H	-0.243653	-0.868066	-2.700671
C	-1.887524	-1.443128	-3.982724
H	-2.956549	-1.209586	-4.092729
H	-1.394761	-1.080008	-4.892470
C	-1.707721	-2.961041	-3.846992
H	-2.162272	-3.477641	-4.700771
H	-0.635703	-3.199857	-3.867512
C	-2.311691	-3.472285	-2.532047
H	-2.124827	-4.546874	-2.418934
H	-3.403864	-3.346488	-2.558865
C	-1.744673	-2.721511	-1.313247

H	-0.670372	-2.920067	-1.237268
H	-2.216186	-3.110691	-0.404252
C	-2.208916	-1.018758	1.496047
H	-1.867324	-2.059027	1.395220
C	-3.751637	-1.046350	1.478441
H	-4.124960	-1.415629	0.517007
H	-4.137312	-0.026117	1.595284
C	-4.301881	-1.921677	2.619174
H	-5.398214	-1.902452	2.604578
H	-4.006283	-2.966200	2.445765
C	-3.776392	-1.465233	3.987609
H	-4.176147	-0.466091	4.212190
H	-4.142950	-2.131879	4.776988
C	-2.241591	-1.410164	4.005988
H	-1.840208	-2.428217	3.901509
H	-1.885197	-1.032369	4.971602
C	-1.692239	-0.530650	2.869476
H	-2.002105	0.505878	3.039846
H	-0.596477	-0.531447	2.888345
Ni	0.972311	-0.282956	0.204967
P	-1.351374	-0.197543	0.027929
H	1.657816	4.647592	0.861664
H	1.417886	2.316184	1.606173
C	3.848753	-0.037783	-0.679786
C	5.180888	0.283750	-0.432234
C	5.623551	0.301319	0.886864
C	4.781922	-0.005190	1.950830
C	3.458013	-0.343386	1.669595
C	2.944563	-0.377089	0.351716
H	3.500843	-0.042231	-1.708735
H	5.872454	0.527571	-1.232382
H	5.168715	0.020154	2.964726
H	2.812343	-0.596273	2.508353
F	6.910610	0.619552	1.141956
B	2.249907	-2.363214	-0.175800
C	3.587473	-3.218763	-0.163165
H	4.256804	-2.957641	-0.988379
H	4.149062	-3.129930	0.771267
H	3.323864	-4.280759	-0.284502
C	1.197035	-2.566601	1.026399
H	0.554524	-3.426121	0.799052
H	1.734768	-2.762145	1.958462
H	0.476906	-1.759622	1.289790
F	1.675210	-2.212276	-1.439962

Ph[Ni]F

M06/BSII SCF energy in solution: -2596.04645 a.u.

M06/BSII free energy in solution: -2595.066297 a.u

C	-0.008509	1.675112	-0.674033
C	-0.045142	1.911119	-2.054134
H	-0.109374	1.071250	-2.745768
C	0.003962	3.201043	-2.578632
H	-0.021402	3.345628	-3.656753
C	0.084533	4.301972	-1.733575
H	0.124803	5.308608	-2.140749
C	0.106205	4.094059	-0.358248
C	0.058459	2.802668	0.155784
C	2.836018	-0.904942	1.655389
H	2.270730	-1.849367	1.666393
C	2.379319	-0.131841	2.894581
H	2.914958	0.824470	2.963840
H	1.310560	0.105868	2.819648
C	2.660297	-0.945435	4.151186
H	2.059687	-1.867740	4.121185
H	2.338860	-0.390004	5.040938
C	4.137399	-1.302409	4.251714
H	4.721655	-0.376615	4.373657
H	4.326394	-1.909491	5.145312
C	4.618138	-2.031526	3.004521
H	4.106406	-3.003913	2.932730
H	5.691608	-2.246395	3.075246
C	4.325518	-1.229489	1.740560
H	4.657559	-1.789763	0.857328
H	4.907097	-0.295159	1.760246
C	2.711045	-1.420385	-1.226807
H	3.812004	-1.454149	-1.241490
C	2.209288	-2.834728	-0.935697
H	2.575399	-3.186318	0.036873
H	1.112067	-2.823469	-0.861819
C	2.652013	-3.799120	-2.029478
H	3.750959	-3.872536	-2.022873
H	2.271299	-4.804989	-1.814261
C	2.193710	-3.338609	-3.404566
H	2.543559	-4.031950	-4.179102
H	1.092575	-3.354287	-3.442701
C	2.674639	-1.924432	-3.693387
H	2.310716	-1.583504	-4.670432

H	3.775002	-1.914850	-3.746969
C	2.221795	-0.963839	-2.603033
H	1.120905	-0.925771	-2.585822
H	2.563043	0.054758	-2.828090
C	3.247314	1.324160	-0.389103
H	2.617652	1.809745	-1.153077
C	4.622253	1.090806	-1.019645
H	5.302312	0.639837	-0.282211
H	4.564085	0.391901	-1.861778
C	5.207278	2.413638	-1.505652
H	6.194600	2.243737	-1.952622
H	4.563868	2.810218	-2.306685
C	5.298304	3.438025	-0.384026
H	5.686147	4.390300	-0.765490
H	6.020329	3.083764	0.368208
C	3.945912	3.638423	0.283842
H	3.240735	4.085114	-0.434709
H	4.030748	4.342702	1.120745
C	3.377870	2.312558	0.771025
H	2.410449	2.469312	1.260606
H	4.054912	1.890810	1.528728
C	-3.274779	1.274543	-0.508726
H	-2.669042	1.668022	-1.342027
C	-3.354005	2.379514	0.547170
H	-3.989762	2.040816	1.378857
H	-2.362566	2.587611	0.964745
C	-3.951275	3.649792	-0.042320
H	-3.285722	4.022524	-0.836700
H	-3.996413	4.434241	0.723111
C	-5.333649	3.383761	-0.618502
H	-6.015875	3.105141	0.199925
H	-5.745727	4.293260	-1.072193
C	-5.289870	2.255489	-1.637627
H	-4.690234	2.575169	-2.504155
H	-6.296237	2.039938	-2.017195
C	-4.672653	0.985035	-1.059631
H	-4.642605	0.218107	-1.841732
H	-5.316819	0.594370	-0.258133
C	-2.766431	-1.548587	-1.070140
H	-3.867242	-1.548667	-1.098467
C	-2.247513	-1.253160	-2.480095
H	-2.572492	-0.261658	-2.820577
H	-1.145750	-1.225171	-2.447873
C	-2.696174	-2.319090	-3.469894
H	-3.794241	-2.292017	-3.553880
H	-2.300406	-2.095143	-4.468057
C	-2.260546	-3.703715	-3.017214
H	-2.608072	-4.467608	-3.723408
H	-1.159706	-3.752505	-3.016711
C	-2.768162	-3.999885	-1.613842
H	-2.426008	-4.987709	-1.281414
H	-3.868943	-4.038313	-1.628851
C	-2.314836	-2.936834	-0.620968
H	-1.221395	-2.946735	-0.523594
H	-2.711398	-3.167535	0.375722
C	-2.824899	-0.728104	1.749194
H	-2.286951	-1.685342	1.825624
C	-4.314381	-1.003275	1.938768
H	-4.708694	-1.623581	1.123683
H	-4.875157	-0.056384	1.916344
C	-4.544746	-1.693536	3.279964
H	-5.615481	-1.877581	3.432002
H	-4.055751	-2.679935	3.257437
C	-3.977580	-0.876704	4.433888
H	-4.539658	0.067244	4.513387
H	-4.123296	-1.406613	5.383091
C	-2.503577	-0.555456	4.222478
H	-1.915409	-1.486267	4.238263
H	-2.127100	0.068240	5.042655
C	-2.285019	0.141813	2.886502
H	-2.800690	1.111615	2.900074
H	-1.218883	0.350733	2.728487
F	-0.013222	-1.703450	1.043330
Ni	-0.016725	-0.027998	0.127327
P	2.229402	-0.173391	0.064233
P	-2.258639	-0.175724	0.076724
H	0.163410	4.943739	0.319355
H	0.078129	2.671388	1.238888

[B1]

M06/BSII SCF energy in solution: -507.369782 a.u.

M06/BSII free energy in solution: -507.28688 a.u

C	-0.110385	-1.198881	0.000015
C	-1.497178	-1.212080	0.000004
C	-2.157988	0.000000	-0.000004
C	-1.497177	1.212079	0.000000
C	-0.110385	1.198881	0.000010

C	0.610200	0.000000	0.000019
H	0.424445	-2.144776	0.000023
H	-2.065234	-2.136820	0.000000
H	-2.065235	2.136819	-0.000006
H	0.424445	2.144776	0.000013
F	-3.504585	0.000000	-0.000017
B	2.170415	0.000000	0.000029
O	2.812560	-1.205273	-0.000015
H	3.773646	-1.165704	-0.000062
O	2.812559	1.205273	-0.000002
H	3.773646	1.165705	-0.000087

PCy_3

M06/BSII SCF energy in solution: -1046.79708 a.u.

M06/BSII free energy in solution: -1046.361576 a.u

C	0.549289	1.553544	-0.464261
H	-0.061035	2.295286	-1.010076
C	1.977773	1.707917	-0.985045
H	2.633358	1.006415	-0.448100
H	2.030080	1.435728	-2.048116
C	2.494375	3.124311	-0.769330
H	1.892165	3.822958	-1.370216
H	3.526716	3.210548	-1.130188
C	2.408845	3.518105	0.697981
H	3.090004	2.878481	1.280947
H	2.752185	4.550000	0.840326
C	0.992943	3.349760	1.231995
H	0.323448	4.054253	0.713830
H	0.952220	3.607334	2.297699
C	0.481631	1.927907	1.016522
H	-0.543276	1.836625	1.398009
H	1.098651	1.236582	1.606996
C	-1.796173	-0.109978	-0.063006
H	-1.560615	-0.006618	1.008414
C	-2.695395	1.056711	-0.477726
H	-2.194535	2.015920	-0.296261
H	-2.870392	0.998491	-1.564908
C	-4.034950	1.028758	0.246709
H	-3.865569	1.173735	1.325311
H	-4.658994	1.867442	-0.086034
C	-4.751063	-0.293760	0.024291
H	-5.705166	-0.312147	0.564872
H	-4.993175	-0.396223	-1.045022
C	-3.872905	-1.459079	0.451371
H	-4.380232	-2.413877	0.265275
H	-3.702207	-1.402603	1.537787
C	-2.527678	-1.437282	-0.264737
H	-2.685697	-1.599004	-1.344141
H	-1.913482	-2.274851	0.088856
C	0.757303	-1.487668	-0.354091
H	0.064565	-2.325065	-0.549650
C	1.082503	-1.501511	1.136304
H	0.187118	-1.293627	1.736446
H	1.802830	-0.699560	1.354446
C	1.697026	-2.835880	1.547538
H	1.940304	-2.826661	2.617309
H	0.952968	-3.634869	1.402362
C	2.937561	-3.146712	0.722441
H	3.712290	-2.395806	0.943450
H	3.355651	-4.119172	1.009552
C	2.629729	-3.118410	-0.768097
H	1.925810	-3.930498	-1.007645
H	3.538779	-3.310508	-1.351383
C	2.011550	-1.787310	-1.179031
H	2.755600	-0.990416	-1.032574
H	1.766027	-1.792354	-2.249081
P	-0.214705	-0.053498	-1.063830

TS^{con}-F

M06/BSII SCF energy in solution: -2056.56218 a.u.

M06/BSII free energy in solution: -2055.938783 a.u

C	-1.183807	1.383315	0.669071
C	-1.074824	1.690073	2.027134
H	-0.768671	0.924991	2.739765
C	-1.353395	2.971235	2.498589
H	-1.266181	3.184078	3.561749
C	-1.744027	3.973145	1.619432
H	-1.962373	4.972472	1.985527
C	-1.860315	3.679153	0.264941
C	-1.589864	2.397603	-0.203002
C	2.075054	1.562402	0.176193
H	1.473684	1.973628	1.004211
C	1.809345	2.442473	-1.045629
H	2.433622	2.094836	-1.881669
H	0.764783	2.355919	-1.366002
C	2.152443	3.894144	-0.741293

H	1.488885	4.257383	0.059305
H	1.956452	4.519576	-1.620473
C	3.602523	4.028571	-0.300221
H	4.259877	3.754192	-1.140106
H	3.834414	5.070787	-0.050204
C	3.902143	3.120335	0.883128
H	3.319065	3.456184	1.754496
H	4.959145	3.193511	1.166370
C	3.545580	1.667210	0.585715
H	3.758618	1.054438	1.468571
H	4.187912	1.292674	-0.224509
C	2.201919	-1.151019	1.288259
H	3.282464	-0.964876	1.185779
C	1.755566	-0.676501	2.673022
H	1.936842	0.398673	2.798061
H	0.665339	-0.817609	2.758448
C	2.450847	-1.455034	3.780835
H	3.531607	-1.245960	3.742548
H	2.099357	-1.106425	4.759315
C	2.220668	-2.950131	3.625849
H	2.743192	-3.504459	4.414401
H	1.147378	-3.165390	3.749591
C	2.669263	-3.425324	2.252941
H	2.479913	-4.498766	2.134955
H	3.757509	-3.286136	2.160430
C	1.972077	-2.655463	1.137775
H	0.893523	-2.870877	1.163003
H	2.336912	-3.009160	0.165935
C	1.899818	-0.903983	-1.623175
H	1.600757	-1.955315	-1.480925
C	3.400521	-0.888957	-1.902616
H	3.959425	-1.267914	-1.037550
H	3.731694	0.147012	-2.067241
C	3.718138	-1.720350	-3.139947
H	4.794419	-1.688713	-3.347974
H	3.467849	-2.773209	-2.936357
C	2.925838	-1.238611	-4.347059
H	3.244362	-0.215089	-4.599992
H	3.147711	-1.859656	-5.222987
C	1.430062	-1.236931	-4.062072
H	1.090080	-2.270419	-3.895416
H	0.874888	-0.859949	-4.929253
C	1.105827	-0.400149	-2.831070
H	1.354718	0.649542	-3.036980
H	0.028463	-0.430477	-2.612469
F	-0.906341	-2.363208	-0.447842
Ni	-0.880799	-0.346533	0.052242
P	1.355024	-0.140506	-0.022334
H	-2.174141	4.451486	-0.433669
H	-1.711329	2.186377	-1.265055
C	-3.807496	-0.192783	0.840809
C	-5.075575	0.238497	0.480526
C	-5.374203	0.319269	-0.866367
C	-4.475477	-0.028601	-1.855606
C	-3.220817	-0.469989	-1.460462
C	-2.843524	-0.557729	-0.110308
H	-3.560371	-0.234251	1.900482
H	-5.822931	0.520680	1.216032
H	-4.765127	0.042123	-2.899757
H	-2.513931	-0.766034	-2.236117
F	-6.599504	0.750509	-1.229776
B	-2.104923	-2.525063	0.303314
O	-1.985028	-2.630425	1.676785
H	-1.395409	-1.976680	2.065965
O	-3.003742	-3.333879	-0.343160
H	-3.745864	-3.563868	0.222658

TS1^{sw}-F

M06/BSII SCF energy in solution: -2056.57828 a.u.

M06/BSII free energy in solution: -2055.951255 a.u

C	1.012258	1.712265	-0.142335
C	1.056999	2.808830	-1.010307
H	0.669733	2.719011	-2.024295
C	1.602283	4.020655	-0.600477
H	1.632104	4.860223	-1.290788
C	2.105433	4.159661	0.688050
H	2.524730	5.107970	1.012554
C	2.071649	3.075909	1.556836
C	1.525396	1.862915	1.145842
C	-1.120376	-0.229123	1.910188
H	-0.780264	0.777025	2.204749
C	-0.030249	-1.204936	2.356347
H	-0.322305	-2.234009	2.110754
H	0.903157	-1.006485	1.814167
C	0.181162	-1.100070	3.860888
H	0.551222	-0.092711	4.106562
H	0.956722	-1.806204	4.180825

C	-1.117859	-1.356300	4.612851
H	-1.435129	-2.395834	4.435862
H	-0.961686	-1.257302	5.693398
C	-2.220344	-0.414778	4.148892
H	-1.948670	0.620584	4.407445
H	-3.158533	-0.632729	4.673080
C	-2.434543	-0.504723	2.642026
H	-3.215648	0.200225	2.331048
H	-2.792851	-1.511349	2.382895
C	-2.443459	1.354117	-0.185654
H	-3.424937	0.964633	0.126808
C	-2.171104	2.598322	0.661047
H	-2.173425	2.346089	1.728430
H	-1.176681	3.001365	0.430407
C	-3.221112	3.667847	0.382347
H	-4.208238	3.302569	0.706179
H	-3.004768	4.559664	0.982262
C	-3.277945	4.017886	-1.097069
H	-4.037890	4.786706	-1.280397
H	-2.311715	4.449016	-1.402931
C	-3.557665	2.779597	-1.935340
H	-3.576126	3.029006	-3.002676
H	-4.556529	2.388473	-1.685319
C	-2.517912	1.698378	-1.674990
H	-1.532466	2.052903	-2.010313
H	-2.743285	0.803952	-2.269657
C	-2.143569	-1.528428	-0.671864
H	-1.871928	-1.431558	-1.735503
C	-3.672271	-1.556769	-0.593929
H	-4.106606	-0.625016	-0.972190
H	-3.992202	-1.657851	0.453270
C	-4.216546	-2.722764	-1.414353
H	-5.310470	-2.744770	-1.342561
H	-3.975789	-2.550125	-2.474410
C	-3.625824	-4.054142	-0.977176
H	-3.953331	-4.275133	0.050496
H	-4.005459	-4.866203	-1.608228
C	-2.105583	-4.015443	-1.013381
H	-1.763697	-3.892978	-2.053002
H	-1.687157	-4.962546	-0.652857
C	-1.578134	-2.860347	-0.172973
H	-1.886972	-3.012588	0.871258
H	-0.480315	-2.856309	-0.164033
Ni	0.610117	0.104425	-0.964244
P	-1.270926	-0.055204	0.077176
H	2.474390	3.172453	2.562240
H	1.522605	1.028467	1.844293
C	3.976888	0.005228	-1.007034
C	4.794337	0.080047	0.113462
C	4.678769	-0.907490	1.069609
C	3.795891	-1.961350	0.946888
C	2.994704	-2.010323	-0.186747
C	3.055781	-1.033832	-1.189192
H	4.046973	0.793495	-1.752811
H	5.499935	0.892724	0.256814
H	3.742522	-2.716372	1.725510
H	2.295274	-2.840755	-0.282831
F	5.459753	-0.842287	2.170224
B	2.116703	-1.122040	-2.516629
O	2.575967	-1.977037	-3.551186
H	3.527001	-2.091035	-3.519348
O	0.697747	-1.472417	-2.149288
H	0.617081	-2.365466	-1.801316
F	1.902100	0.263814	-2.956050

TS2^{sw}-F

M06/BSII SCF energy in solution: -2056.57249 a.u.

M06/BSII free energy in solution: -2055.94754 a.u.

C	1.235469	1.478012	0.132966
C	1.435370	2.406021	-0.897234
H	1.356972	2.089660	-1.937553
C	1.730766	3.737448	-0.628596
H	1.875037	4.435072	-1.450949
C	1.838618	4.179532	0.685793
H	2.067088	5.219676	0.901201
C	1.668926	3.267193	1.719848
C	1.379649	1.932096	1.445731
C	-1.705820	0.313812	1.756439
H	-1.319171	1.343999	1.838773
C	-0.887894	-0.525653	2.739744
H	-1.247037	-1.563355	2.738639
H	0.165489	-0.557962	2.431624
C	-1.020704	0.041689	4.147505
H	-0.586515	1.053454	4.168538
H	-0.441629	-0.564159	4.854829
C	-2.480478	0.109869	4.575933
H	-2.880953	-0.913598	4.645712

H	-2.565650	0.547098	5.577948
C	-3.316130	0.900708	3.578718
H	-2.985563	1.951145	3.576226
H	-4.370588	0.904738	3.880014
C	-3.176557	0.336857	2.169021
H	-3.776892	0.925836	1.464394
H	-3.579723	-0.686726	2.150197
C	-2.262112	1.242657	-0.973788
H	-3.330944	0.992085	-0.895996
C	-2.097375	2.662660	-0.430503
H	-2.455962	2.720489	0.604512
H	-1.035311	2.939382	-0.414257
C	-2.864836	3.656773	-1.293688
H	-3.942591	3.440233	-1.225082
H	-2.724101	4.671557	-0.902856
C	-2.433982	3.579133	-2.750366
H	-2.997395	4.298806	-3.356383
H	-1.372902	3.863855	-2.829129
C	-2.614000	2.169240	-3.293622
H	-2.280785	2.109439	-4.336543
H	-3.685379	1.913379	-3.290418
C	-1.856213	1.155969	-2.447144
H	-0.774857	1.344659	-2.529940
H	-2.022116	0.140501	-2.831023
C	-2.197021	-1.645425	-0.534126
H	-1.733865	-1.837788	-1.515712
C	-3.711785	-1.624113	-0.749631
H	-4.005508	-0.810634	-1.422486
H	-4.224647	-1.447585	0.207049
C	-4.181329	-2.950539	-1.340183
H	-5.269407	-2.931033	-1.476064
H	-3.743361	-3.066613	-2.343459
C	-3.773111	-4.135440	-0.478112
H	-4.294993	-4.076280	0.489705
H	-4.088512	-5.075469	-0.946073
C	-2.271825	-4.139322	-0.229243
H	-1.742159	-4.297203	-1.182230
H	-1.992551	-4.970831	0.428738
C	-1.825846	-2.816534	0.379028
H	-2.328767	-2.688307	1.348864
H	-0.749465	-2.832231	0.601109
Ni	0.856048	-0.270965	-0.416040
P	-1.348013	-0.062722	-0.020796
H	1.768809	3.593201	2.753017
H	1.269553	1.240864	2.280055
C	3.888680	0.144302	-0.734980
C	5.153340	0.026320	-0.173007
C	5.319684	-0.854901	0.876658
C	4.287486	-1.625344	1.373910
C	3.041560	-1.502601	0.773678
C	2.801136	-0.618831	-0.291334
H	3.751621	0.856256	-1.546611
H	5.998271	0.610132	-0.526081
H	4.468805	-2.305519	2.200780
H	2.233382	-2.134924	1.146063
F	6.542002	-0.969407	1.439498
B	2.031119	-1.705338	-2.005635
O	2.907742	-2.758772	-2.067473
H	3.763495	-2.515764	-2.433384
O	0.735916	-1.987712	-1.516620
H	0.707394	-2.826034	-1.037860
F	2.063263	-0.751327	-2.978655

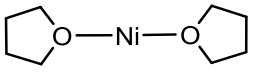
THF

B3LYP/BSI SCF energy: -232.456281a.u.

M06/BSII SCF energy in solution: -232.354902a.u.

M06/BSII free energy in solution: -232.266504a.u.

C	-1.165455	-0.430603	-0.132011
O	-0.000139	-1.251514	-0.000047
C	1.165343	-0.430855	0.132061
C	0.733619	0.996334	-0.227362
C	-0.733374	0.996507	0.227332
H	-1.535935	-0.481037	-1.167647
H	-1.950335	-0.821637	0.525775
H	1.535634	-0.481307	1.167764
H	1.950251	-0.822104	-0.525565
H	1.343972	1.760778	0.261754
H	0.795928	1.153911	-1.310164
H	-0.795642	1.154135	1.310135
H	-1.343556	1.761072	-0.26180

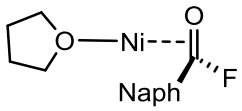


B3LYP/BSI SCF energy: -635.847283a.u.

M06/BSII SCF energy in solution: -635.660307a.u.

M06/BSII free energy in solution: -635.465766a.u.

Ni	-0.000009	-0.105211	0.000162
C	-2.735656	-0.873451	-0.769130
O	-1.892849	-0.120143	0.135236
C	-2.643635	0.959141	0.758551
C	-4.075688	0.828136	0.217506
C	-4.147786	-0.638379	-0.238892
H	-2.609497	-0.489744	-1.788778
H	-2.398318	-1.910397	-0.734374
H	-2.581426	0.810018	1.840799
H	-2.166476	1.907541	0.503567
H	-4.823359	1.080700	0.974036
H	-4.223671	1.496237	-0.637629
H	-4.349365	-1.299440	0.610853
H	-4.912413	-0.814204	-1.000412
C	2.643424	0.959194	-0.758499
O	1.892813	-0.120075	-0.134934
C	2.735915	-0.873509	0.769041
C	4.147880	-0.638336	0.238410
C	4.075605	0.828224	-0.217811
H	2.580951	0.810026	-1.840727
H	2.166301	1.907589	-0.503433
H	2.610063	-0.489962	1.788788
H	2.398593	-1.910459	0.734231
H	4.912735	-0.814226	0.999686
H	4.349230	-1.299296	-0.611469
H	4.223751	1.496239	0.637364
H	4.823084	1.080909	-0.974490

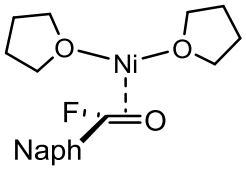


B3LYP/BSI SCF energy: -1001.890708a.u.

M06/BSII SCF energy in solution: -1001.57584a.u.

M06/BSII free energy in solution: -1001.355214a.u.

F	-0.364188	2.749841	0.608986
Ni	-1.318188	0.736851	-0.960507
O	0.036804	1.868173	-1.446028
C	0.111648	1.689404	-0.170919
C	4.006348	-1.707178	-1.252741
C	3.964730	-1.559080	0.113955
C	3.034029	-0.678474	0.729390
C	2.114715	0.064812	-0.089613
C	2.197432	-0.103980	-1.501308
C	3.115297	-0.966720	-2.062509
H	3.721524	-1.091249	2.739390
H	4.724210	-2.382246	-1.710175
H	4.651079	-2.111859	0.750785
C	3.015324	-0.521481	2.140675
C	1.178855	0.948001	0.562770
H	1.534264	0.472653	-2.131035
H	3.158166	-1.071785	-3.143131
C	1.215177	1.074063	1.945761
C	2.128371	0.345125	2.734431
H	0.521550	1.754699	2.423696
H	2.124334	0.475565	3.812897
C	-2.419331	-1.862614	-0.112586
O	-2.694207	-0.460400	-0.414464
C	-3.902830	-0.012278	0.280913
C	-4.309149	-1.186176	1.173303
C	-3.742335	-2.401958	0.421386
H	-2.074145	-2.331372	-1.035383
H	-1.621183	-1.903393	0.635715
H	-3.657360	0.899697	0.827356
H	-4.651946	0.213246	-0.484276
H	-3.840800	-1.096825	2.159004
H	-5.391539	-1.235360	1.315295
H	-3.599803	-3.274043	1.064263
H	-4.401862	-2.689114	-0.404590



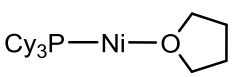
B3LYP/BSI SCF energy: -1234.368118a.u.

M06/BSII SCF energy in solution: -1233.95356a.u.

M06/BSII free energy in solution: -1233.624462a.u.

F	-0.287546	0.489783	2.811153
Ni	1.008813	0.003867	0.463438
O	0.236525	-1.306336	1.497326
C	-0.463559	-0.204566	1.587193
C	-3.729993	-2.378562	-1.946548
C	-4.385091	-1.297758	-1.403651
C	-3.789595	-0.514195	-0.377598
C	-2.473824	-0.851968	0.095118
C	-1.835645	-1.988885	-0.478565

C	-2.445021	-2.726928	-1.471194
H	-5.482436	0.822182	-0.180773
H	-4.199433	-2.968286	-2.729256
H	-5.379628	-1.025308	-1.749013
C	-4.486787	0.587108	0.187089
C	-1.878285	-0.037231	1.127248
H	-0.864464	-2.273135	-0.097933
H	-1.935289	-3.592603	-1.886031
C	-2.614677	1.017230	1.653614
C	-3.911282	1.327831	1.191525
H	-2.173882	1.608892	2.446127
H	-4.449893	2.159388	1.638276
C	0.624248	2.910625	0.144027
O	1.237048	1.738621	-0.451866
C	0.897287	1.789016	-1.858607
C	1.066085	3.267648	-2.233264
C	0.821903	4.026128	-0.897206
H	-0.435027	2.696367	0.325800
H	1.123437	3.080863	1.098324
H	1.569559	1.104321	-2.376697
H	-0.137596	1.447869	-1.986257
H	2.076888	3.457415	-2.604022
H	0.363479	3.560921	-3.017209
H	1.681652	4.652176	-0.645546
H	-0.056817	4.674272	-0.943584
C	4.031729	-0.207457	0.093909
O	2.769986	-0.760011	-0.359113
C	2.854883	-2.216325	-0.411797
C	4.252641	-2.572294	0.105019
C	5.060367	-1.297953	-0.190944
H	4.196087	0.725642	-0.449974
H	3.963155	0.011973	1.166700
H	2.045990	-2.623141	0.197830
H	2.710715	-2.511944	-1.456907
H	4.222956	-2.759051	1.183552
H	4.658363	-3.463223	-0.381339
H	5.954436	-1.199780	0.430567
H	5.368111	-1.269127	-1.242242



B3LYP/BSI SCF energy: -1001.890708a.u.

M06/BSII SCF energy in solution: -1001.57584a.u.

M06/BSII free energy in solution: -1001.355214a.u.

F	-0.364188	2.749841	0.608986
Ni	-1.318188	0.736851	-0.960507
O	0.036804	1.868173	-1.446028
C	0.111648	1.689404	-0.170919
C	4.006348	-1.707178	-1.252741
C	3.964730	-1.559080	0.113955
C	3.034029	-0.678474	0.729390
C	2.114715	0.064812	-0.089613
C	2.197432	-0.103980	-1.501308
C	3.115297	-0.966720	-2.062509
H	3.721524	-1.091249	2.739390
H	4.724210	-2.382246	-1.710175
H	4.651079	-2.111859	0.750785
C	3.015324	-0.521481	2.140675
C	1.178855	0.948001	0.562770
H	1.534264	0.472653	-2.131035
H	3.158166	-1.071785	-3.143131
C	1.215177	1.074063	1.945761
C	2.128371	0.345125	2.734431
H	0.521550	1.754699	2.423696
H	2.124334	0.475565	3.812897
C	-2.419331	-1.862614	-0.112586
O	-2.694207	-0.460400	-0.414464
C	-3.902830	-0.012278	0.280913
C	-4.309149	-1.186176	1.173303
C	-3.742335	-2.401958	0.421386
H	-2.074145	-2.331372	-1.035383
H	-1.621183	-1.903393	0.635715
H	-3.657360	0.899697	0.827356
H	-4.651946	0.213246	-0.484276
H	-3.840800	-1.096825	2.159004
H	-5.391539	-1.235360	1.315295
H	-3.599803	-3.274043	1.064263
H	-4.401862	-2.689114	-0.404590

TS3-dim

B3LYP/BSI SCF energy: -2586.162753a.u.

M06/BSII SCF energy in solution: -2585.32751a.u.

M06/BSII free energy in solution: -2584.625965a.u.

C	1.701647	-2.950903	-0.327196
H	0.790147	-3.272138	0.192943
C	1.384002	-3.069470	-1.835542

H	2.242262	-2.741268	-2.432480	H	5.374289	0.038895	-3.092129
H	0.549077	-2.410240	-2.092783	C	3.879928	-0.618409	-1.667288
C	1.041801	-4.523509	-2.202085	H	4.073446	-1.678696	-1.874222
H	0.109772	-4.810783	-1.695638	H	3.041666	-0.306735	-2.295423
H	0.847959	-4.597227	-3.278862	F	-1.122376	-1.647307	0.113289
C	2.162297	-5.491939	-1.795150	Ni	0.021639	-0.108624	-0.424223
H	3.061345	-5.275955	-2.390376	P	1.839672	-1.173712	0.265919
H	1.876764	-6.524990	-2.026884	O	1.327224	1.310885	-2.263462
C	2.501867	-5.358452	-0.303582	C	0.892829	1.382997	-1.120605
H	1.642334	-5.690535	0.295499	F	-1.693399	0.609814	-0.863196
H	3.338905	-6.016673	-0.040574	Ni	-2.758093	-0.952880	-0.453721
C	2.844591	-3.905366	0.072859	C	3.806875	5.799267	-0.910970
H	3.051053	-3.841241	1.147469	C	2.892482	5.872103	0.113904
H	3.767949	-3.613611	-0.443665	C	1.933680	4.842122	0.313978
C	1.869968	-1.310467	2.144291	C	1.922879	3.702580	-0.562955
H	2.796798	-1.839640	2.404626	C	2.875917	3.669263	-1.620468
C	0.689037	-2.124425	2.718971	C	3.791125	4.687575	-1.784629
H	0.692993	-3.142770	2.317422	H	0.995385	5.811225	2.004621
H	-0.258075	-1.675292	2.400206	H	4.534095	6.593271	-1.055064
C	0.751484	-2.190575	4.255037	H	2.886387	6.723921	0.789591
H	1.641473	-2.761135	4.558467	C	0.980795	4.933090	1.363506
H	-0.116031	-2.745944	4.630885	C	0.962606	2.656181	-0.311648
C	0.810034	-0.794793	4.889012	H	2.851409	2.837180	-2.310909
H	0.892835	-0.873888	5.979664	H	4.504993	4.638374	-2.602333
H	-0.130129	-0.263515	4.683303	C	0.062036	2.794884	0.733830
C	1.981964	0.016397	4.321047	C	0.053579	3.937104	1.562407
H	1.988034	1.029656	4.740173	H	-0.670138	2.010053	0.894840
H	2.929224	-0.452901	4.624136	H	-0.681721	4.019430	2.357547
C	1.919223	0.093927	2.786873	O	-4.626720	-3.011640	0.189289
H	1.022839	0.651259	2.488166	C	-4.089682	-2.029040	-0.216224
H	2.774150	0.666748	2.410992	C	-7.161919	1.947599	1.431411
C	3.527334	-0.447868	-0.170589	C	-7.052671	2.113405	0.068646
H	3.367179	0.626661	-0.001276	C	-6.253971	1.232130	-0.706252
C	4.726520	-0.874655	0.706883	C	-5.558008	0.163772	-0.054227
H	4.514240	-0.724267	1.769380	C	-5.694519	0.015305	1.349067
H	4.923783	-1.945534	0.574105	C	-6.478823	0.888897	2.073345
C	5.990499	-0.077376	0.334380	H	-6.650848	2.210072	-2.593557
H	6.831115	-0.414053	0.953335	H	-7.775304	2.626119	2.016536
H	5.827932	0.982011	0.578073	H	-7.577915	2.921297	-0.433854
C	6.334718	-0.205181	-1.155574	C	-6.125697	1.387066	-2.115311
H	6.618416	-1.244962	-1.373870	C	-4.758950	-0.719889	-0.862554
H	7.207684	0.413026	-1.397051	H	-5.185628	-0.802606	1.848349
C	5.138005	0.187721	-2.031681	H	-6.576781	0.760276	3.147198
H	4.927000	1.258264	-1.904603	C	-4.682061	-0.541192	-2.240288

C	-5.362113	0.525818	-2.869837
H	-4.099856	-1.234194	-2.841274
H	-5.276765	0.660143	-3.943269

IM4-dim

B3LYP/BSI SCF energy: -2586.179056a.u.

M06/BSII SCF energy in solution: -2585.33863a.u.

M06/BSII free energy in solution: -2584.638512a.u.

C	1.942831	-2.872471	-0.288174
H	1.072935	-3.248021	0.265612
C	1.590940	-3.046493	-1.783508
H	2.404325	-2.668454	-2.412480
H	0.701743	-2.457005	-2.028159
C	1.349414	-4.529301	-2.112898
H	0.457741	-4.876693	-1.572252
H	1.129100	-4.638785	-3.181399
C	2.551983	-5.401736	-1.724386
H	3.413403	-5.130342	-2.351436
H	2.339534	-6.457945	-1.928216
C	2.924137	-5.211957	-0.246856
H	2.110121	-5.595292	0.384533
H	3.816030	-5.799444	0.002733
C	3.166389	-3.729756	0.093422
H	3.399389	-3.630460	1.159810
H	4.049306	-3.379061	-0.456066
C	2.062216	-1.160809	2.142961
H	3.038209	-1.603706	2.383799
C	0.973569	-2.054792	2.777398
H	1.048564	-3.079048	2.398314
H	-0.017972	-1.691673	2.483811
C	1.092504	-2.075905	4.311453
H	2.036865	-2.562737	4.595185
H	0.288171	-2.691803	4.731092
C	1.054663	-0.664132	4.911163
H	1.182101	-0.708683	5.999324
H	0.066091	-0.219007	4.729306
C	2.132648	0.228380	4.282385
H	2.065343	1.249180	4.676775
H	3.126582	-0.149697	4.562148
C	2.012583	0.259801	2.749970
H	1.063070	0.731916	2.469056
H	2.803094	0.892506	2.331650
C	3.548234	-0.214140	-0.253889
H	3.300058	0.844891	-0.094655
C	4.814775	-0.518322	0.578325
H	4.634078	-0.366797	1.646537
H	5.098025	-1.570664	0.453086
C	5.987141	0.379305	0.140026
H	6.879511	0.127931	0.725996
H	5.742427	1.424342	0.376925
C	6.277689	0.257129	-1.361880
H	6.644424	-0.756633	-1.578466
H	7.080212	0.946742	-1.649494
C	5.014794	0.525127	-2.191330
H	4.712759	1.574714	-2.072197
H	5.219254	0.378194	-3.258513
C	3.851584	-0.383676	-1.760741
H	4.132466	-1.426396	-1.956614
H	2.961869	-0.162366	-2.355157
F	-0.992922	-1.847040	0.152931
Ni	0.016962	-0.215098	-0.383352
P	1.954239	-1.077185	0.265507
O	1.146649	1.308257	-2.244738
C	0.716434	1.357867	-1.099607
F	-1.790298	0.325313	-0.787559
Ni	-2.719459	-1.239054	-0.386898
C	3.041338	6.112868	-1.052447
C	2.131101	6.099525	-0.021416
C	1.321309	4.957867	0.224984
C	1.457592	3.797306	-0.612814
C	2.402971	3.852209	-1.675713
C	3.172379	4.977357	-1.884589
H	0.274507	5.852133	1.892708
H	3.653596	6.991843	-1.232600
H	2.013882	6.966815	0.623646
C	0.372990	4.957541	1.282611
C	0.642057	2.644411	-0.318031
H	2.487498	3.000222	-2.336299
H	3.883208	4.994194	-2.706162
C	-0.259108	2.697594	0.734817
C	-0.410591	3.854430	1.527939
H	-0.884222	1.831993	0.928102
H	-1.144437	3.865716	2.328303
O	-4.273756	-3.613671	0.157696
C	-3.656163	-2.673630	-0.054798
C	-6.938463	1.678869	1.620887
C	-7.222095	1.597021	0.276377

C	-6.382868	0.867096	-0.608217
C	-5.219259	0.208771	-0.079243
C	-4.956256	0.321157	1.314543
C	-5.792950	1.033098	2.145235
H	-7.544398	1.269887	-2.390047
H	-7.591232	2.240329	2.283184
H	-8.099657	2.093005	-0.131329
C	-6.663472	0.768234	-1.997617
C	-4.379168	-0.521208	-0.973449
H	-4.070541	-0.163109	1.718602
H	-5.573444	1.103966	3.206787
C	-4.695494	-0.611572	-2.313060
C	-5.840160	0.047708	-2.831032
H	-4.061522	-1.174793	-2.993391
H	-6.061210	-0.023651	-3.892507

CsF

B3LYP/BSI SCF energy: -119.98026a.u.

M06/BSII SCF energy in solution: -120.063439a.u.

M06/BSII free energy in solution: -120.087031a.u.

Cs	0.000000	0.000000	0.358882
F	0.000000	0.000000	-2.193170

CsCl

B3LYP/BSI SCF energy: -480.416533a.u.

M06/BSII SCF energy in solution: -480.440549a.u.

M06/BSII free energy in solution: -480.465528a.u.

Cl	0.000000	0.000000	-2.380619
Cs	0.000000	0.000000	0.735828

CsBr

B3LYP/BSI SCF energy: -33.618242a.u.

M06/BSII SCF energy in solution: -33.597733a.u.

M06/BSII free energy in solution: -33.624134a.u.

Cs	0.000000	0.000000	1.303893
Br	0.000000	0.000000	-2.048975