Supporting Information for

Computational Study of the Ni-Catalyzed C−H Oxidative Cycloaddition of Aromatic Amides with Alkynes

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Amide N−H Oxidative Addition with Different Ligands on the Ni Catalyst

As discussed in the main text, the catalytic cycle begins with the coordination of the 2-pyridinylmethylamine directing group to the Ni center followed by the oxidative addition of the amide N−H bond. Under the experimental conditions of 10 mol% $Ni(cod)_2$, 40 mol% PPh_3 ligand, and 3 or more equivalents of internal alkyne, either cod, PPh_3, or the alkyne (2-butyne) can potentially bind to the Ni center and promote the amide N−H oxidative addition (**TS1**). These different mechanisms were considered computationally (Figure S1). Our calculations indicate that the most favorable amide N−H oxidative addition pathway involves binding of two PPh_3 ligand with an activation barrier of 28.0 kcal/mol with respect to **1** and $Ni(cod)_2$ to form the phosphine-bound Ni(II)-hydride complex **5**. The amide N−H oxidative addition with cod, one PPh_3, and alkyne ligands have slightly higher barriers.

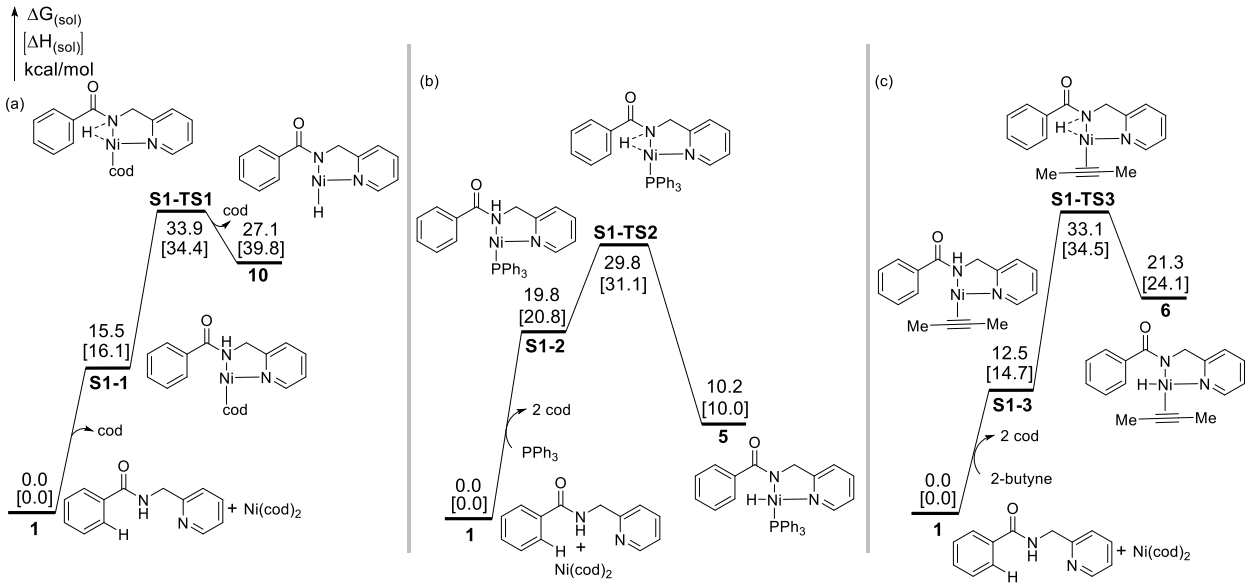

Figure S1. Reaction energy profiles of amide N−H oxidative addition of **1** and $Ni(cod)_2$ with (a) a cod ligand, (b) a PPh_3 ligand, and (c) an alkyne ligand.

Other Mechanisms of the Ni-Catalyzed *ortho* C(sp^2)−H Metalation

Several different mechanisms of the Ni-catalyzed *ortho* C(sp^2)−H metalation of **1** were considered computationally. These alternative mechanisms include: (a) σ-bond metathesis with an alkyl-Ni(II) complex (Figure S2); (b) σ-bond metathesis with phosphine-bound Ni(II)-hydride (Figure S3); (c) C−H oxidative addition and subsequent N−H σ-bond metathesis (Figure S4); and (d) deprotonation by the amide N (Figure S5). These alternative mechanisms were ruled out because of the high activation barriers.

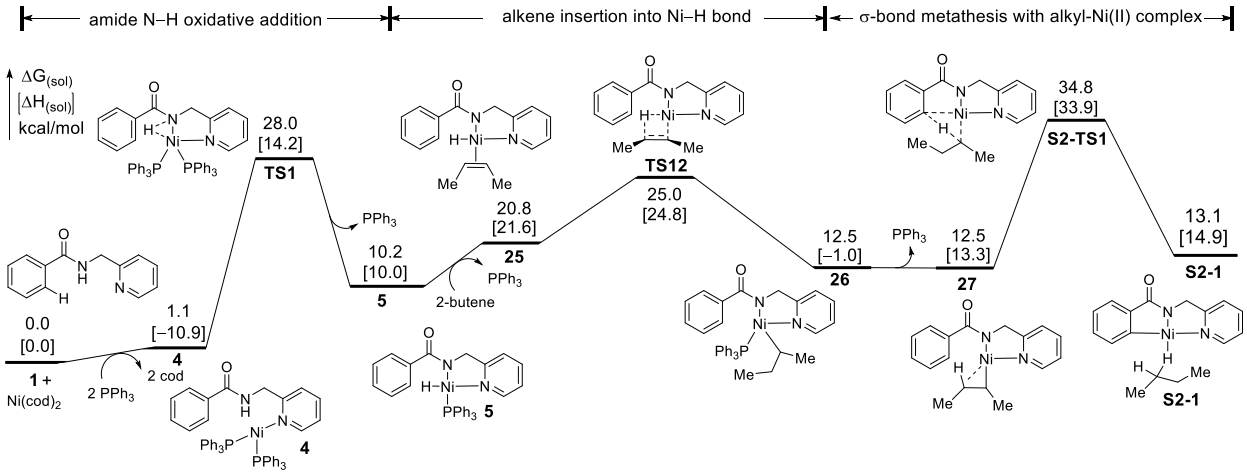

Figure S2. Reaction energy profile of Ni-catalyzed *ortho* C(sp^2)−H metalation of amide **1** with *cis*-2-butene acting as the hydrogen acceptor.

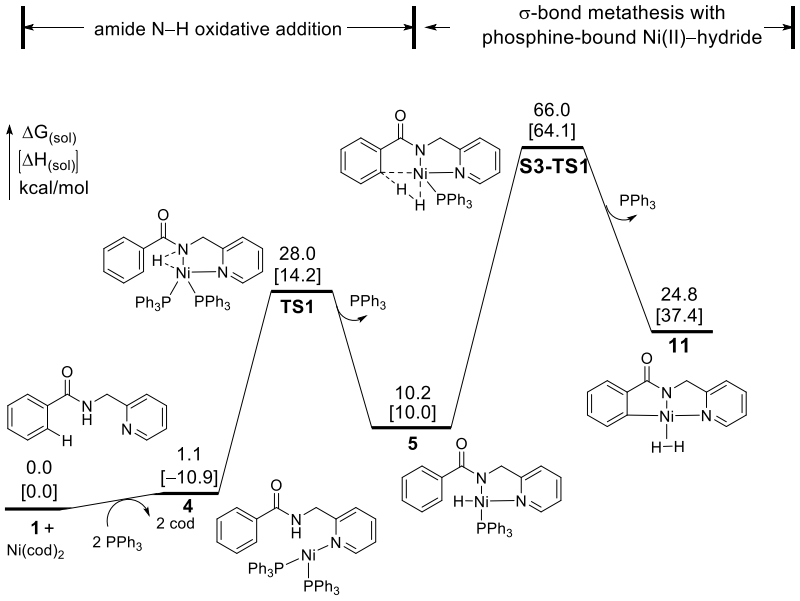

Figure S3. Reaction energy profile of *ortho* C−H metalation mechanism of amide **1** with 2-butyne via σ-bond metathesis with phosphine-bound Ni(II)-hydride complex **5**. All energies are with respect to the separate reactant **1** and $Ni(cod)_2$.

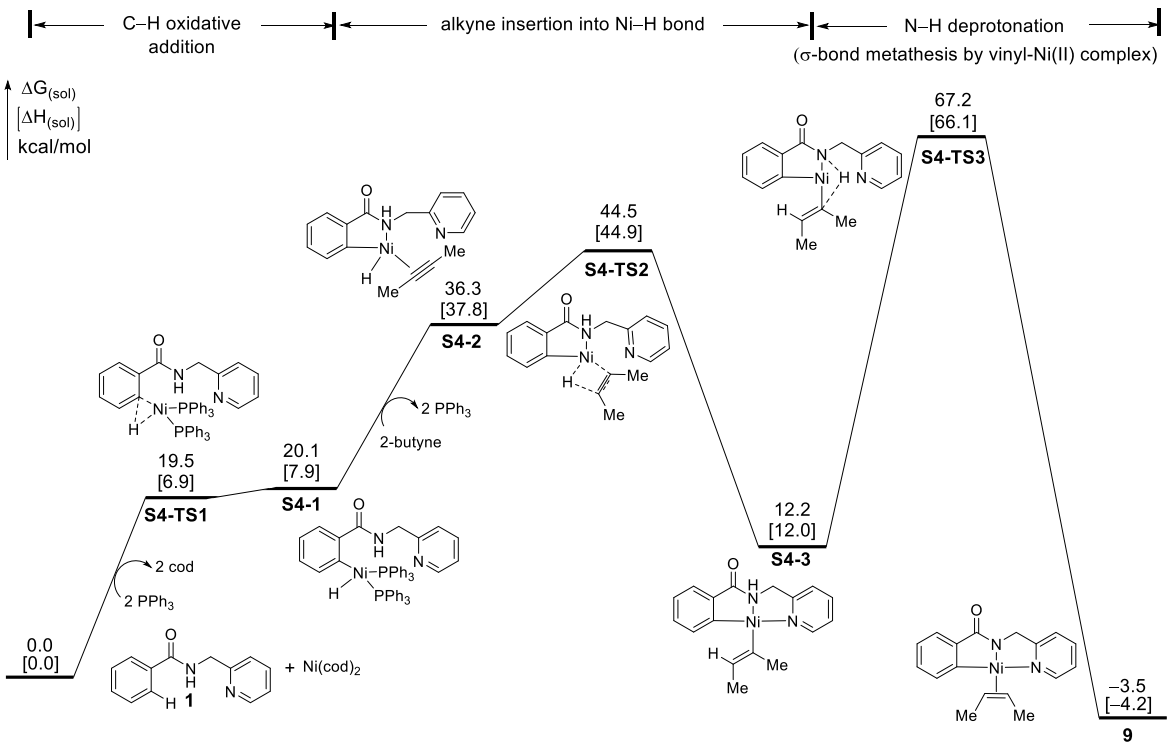

Figure S4. Reaction energy profile of phenyl *ortho* C(sp^2)−H metalation mechanism of amide **1** with 2-butyne via C−H bond oxidative addition by Ni(0) catalyst and subsequent N−H σ-bond metathesis with an alkenyl-Ni(II) complex. All energies are with respect to the separate reactant **1** and $Ni(cod)_2$.

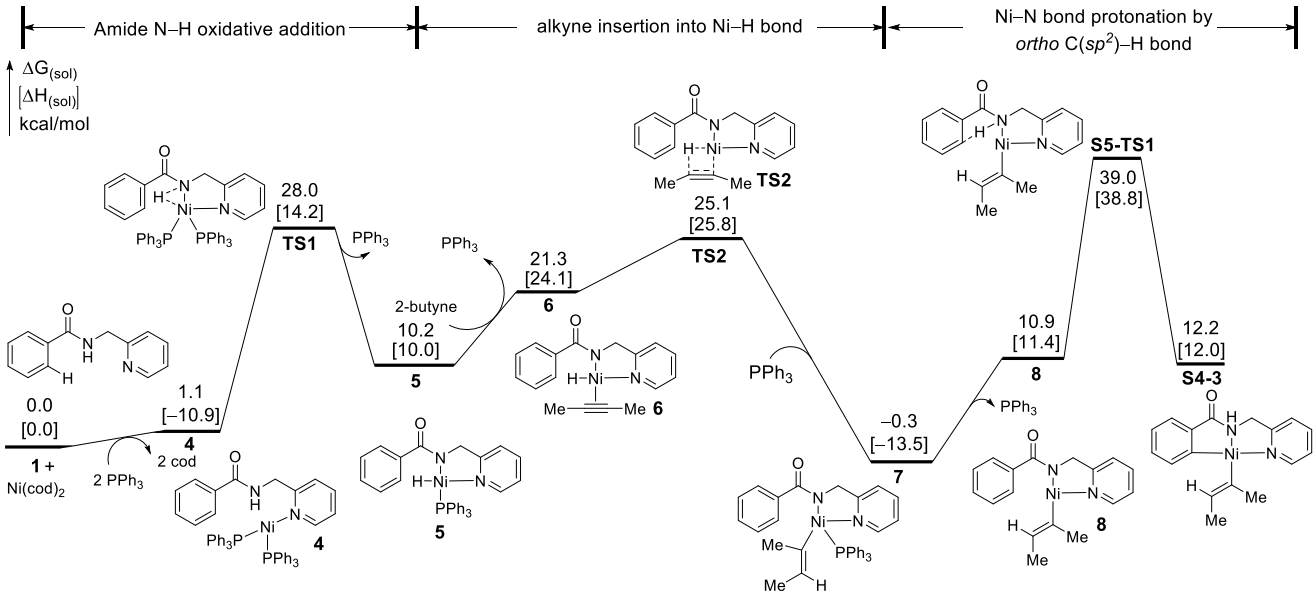

Figure S5. Reaction energy profile of *ortho* C−H metalation of amide **1** with 2-butyne via deprotonation of the *ortho* C(sp^2)−H bond by the amide N. All energies are with respect to the separate reactant **1** and $Ni(cod)_2$.

C−N Reductive Elimination with a Model Substrate Containing 8-Aminoquinoline Directing Group

Amide with 8-aminoquinoline moiety (**19**) has a much higher C−N bond reductive elimination barrier than amide **1** with the 2-pyridinylmethylamine directing group.

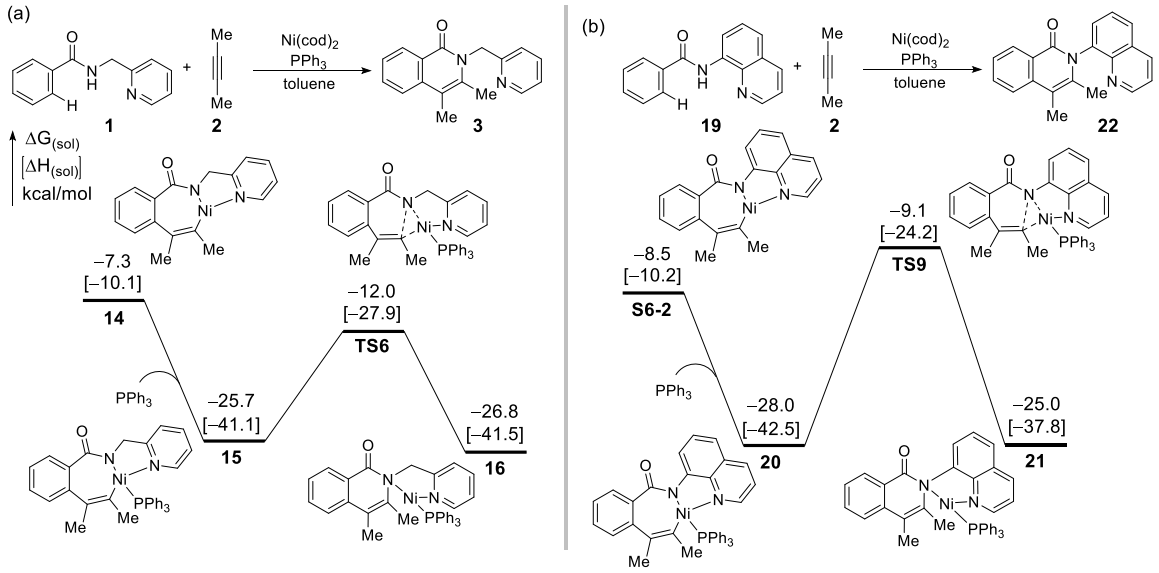

Figure S6. Reaction energy profile of C−N reductive elimination of (a) amide **1** with 2-pyridinylmethylamine directing group (b) amide **19** with 8-aminoquinoline directing group. Energies are with respect to the separate reactants (amide and alkyne), PPh_3, and $Ni(cod)_2$.

Cartesian Coordinates

1
B3LYP electronic energy: -687.34244057 a.u.
B3LYP enthalpy: -687.102154 a.u.
B3LYP free energy: -687.158779 a.u.
M06 SCF energy in solution: -687.05295399 a.u.
M06 enthalpy in solution: -686.812667 a.u.
M06 free energy in solution: -686.869292 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-2.308068	1.091401	-0.443391
C	-2.324438	-0.256903	-0.058424
C	-3.526123	-0.826795	0.382929
C	-4.685702	-0.058610	0.460704
C	-4.660436	1.287562	0.086049
C	-3.471193	1.858905	-0.371388
H	-1.399060	1.543367	-0.830920
H	-3.523642	-1.876749	0.656517
H	-5.610774	-0.508941	0.810772
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H	-3.449505	2.900901	-0.679260
C	-1.115944	-1.151978	-0.107903
O	-1.215237	-2.378831	-0.077973
N	0.096365	-0.533808	-0.187660
H	0.213629	0.457282	-0.014104
C	1.318258	-1.304953	-0.169908
H	1.401024	-1.908952	-1.084161
H	1.299827	-2.026751	0.659945
C	2.527226	-0.396444	-0.042064
C	3.822123	-0.930035	-0.095853
C	3.353686	1.731529	0.255029
C	4.908998	-0.072300	0.036443
H	3.965675	-1.997704	-0.238733
C	4.674297	1.293312	0.216676
H	3.122396	2.786250	0.392089
H	5.923389	-0.460043	-0.001048
H	5.492017	1.999220	0.323416
N	2.300215	0.912041	0.129464

2
B3LYP electronic energy: -155.97565014 a.u.
B3LYP enthalpy: -155.884293 a.u.
B3LYP free energy: -155.917843 a.u.
M06 SCF energy in solution: -155.89629461 a.u.
M06 enthalpy in solution: -155.804937 a.u.
M06 free energy in solution: -155.838487 a.u.

Cartesian coordinates

ATOM	X	Y	Z
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C	0.000000	0.000000	-0.604618
C	0.000000	0.000000	2.066401
H	-0.510415	0.885024	2.466657
H	-0.511246	-0.884545	2.466657
H	1.021661	-0.000479	2.466657
C	0.000000	0.000000	-2.066401
H	0.511246	-0.884545	-2.466657
H	-1.021661	-0.000479	-2.466657
H	0.510415	0.885024	-2.466657

3
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B3LYP enthalpy: -841.874974 a.u.
B3LYP free energy: -841.937196 a.u.
M06 SCF energy in solution: -841.81451713 a.u.
M06 enthalpy in solution: -841.501009 a.u.
M06 free energy in solution: -841.563231 a.u.

Cartesian coordinates

ATOM	X	Y	Z
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H	4.991261	1.497705	1.021528
C	-3.970441	-1.972617	0.405679
C	-2.693720	-2.015608	-0.128814
C	-1.921755	-0.844284	-0.218564
C	-2.424354	0.398284	0.231780
C	-3.731390	0.414161	0.776311
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H	-4.568977	-2.876505	0.474282
H	-4.156238	1.344958	1.134630
H	-5.485744	-0.703949	1.282546
C	-0.576363	-0.945757	-0.784025
O	-0.081968	-2.009296	-1.175928
N	0.146986	0.250600	-0.860188
C	1.497723	0.115581	-1.454274
C	2.592416	-0.173357	-0.437428
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N	3.386664	0.857452	-0.104896
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H	-2.255512	-2.939956	-0.489711
H	1.425661	-0.711803	-2.160826
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C	-0.344969	1.489899	-0.415714
C	-1.603461	1.590188	0.120357
C	-2.206161	2.893720	0.595360
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H	-1.545857	3.750073	0.465155
H	-3.131643	3.119303	0.049742
C	0.587220	2.663810	-0.598643
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H	0.244915	3.532627	-0.039797

4
B3LYP electronic energy: -2929.25716193 a.u.
B3LYP enthalpy: -2928.427177 a.u.
B3LYP free energy: -2928.571265 a.u.
M06 SCF energy in solution: -2929.94195799 a.u.
M06 enthalpy in solution: -2929.111973 a.u.
M06 free energy in solution: -2929.256061 a.u.

Cartesian coordinates

ATOM	X	Y	Z
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5

B3LYP electronic energy: -1892.96291400 a.u.
B3LYP enthalpy: -1892.430254 a.u.
B3LYP free energy: -1892.529842 a.u.
M06 SCF energy in solution: -1893.98377719 a.u.
M06 enthalpy in solution: -1893.451117 a.u.
M06 free energy in solution: -1893.550705 a.u.

Cartesian coordinates

ATOM	X	Y	Z
H	1.279412	-6.347923	0.917962
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H	2.076678	-2.133825	1.251859
Ni	-0.555821	-0.850620	0.034920
C	-5.462262	1.748893	-0.225537
C	-4.894635	0.573190	-0.715314
C	-3.943200	-0.128853	0.036463
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C	-4.191052	1.509197	1.814555
C	-5.113553	2.220555	1.043227
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H	-3.934793	1.854245	2.813850
H	-5.568573	3.127875	1.433182
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O	-4.194097	-2.139362	-1.189340
N	-2.170264	-1.830563	-0.160283
C	-1.896623	-3.210227	-0.536919
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C	0.994873	-5.308692	0.777964
C	1.851160	-4.275892	1.165433
C	1.442379	-2.963432	0.967367
N	0.253231	-2.642991	0.420248

H	-0.936297	-5.754478	-0.085235
H	-5.186698	0.171141	-1.680347
H	-2.701208	-3.880719	-0.204675
H	-1.856586	-3.342586	-1.633086
H	-2.888352	-0.211488	1.907633
H	-1.262629	0.363529	-0.380312
P	1.049258	0.672590	-0.064487
C	2.769947	0.201404	0.438231
C	3.708295	-0.254889	-0.500268
C	3.110992	0.161010	1.802550
C	4.957656	-0.724873	-0.087913
H	3.467999	-0.239255	-1.558609
C	4.360933	-0.305004	2.212458
H	2.399724	0.504073	2.549233
C	5.289186	-0.749800	1.267378
H	5.672705	-1.068494	-0.830737
H	4.608883	-0.319003	3.270533
H	6.262724	-1.112224	1.586107
C	1.263123	1.232648	-1.812990
C	0.553021	0.571483	-2.825571
C	2.116892	2.291698	-2.162141
C	0.698863	0.955203	-4.160881
H	-0.127788	-0.232928	-2.561514
C	2.258615	2.676187	-3.494821
H	2.667801	2.825233	-1.393792
C	1.550928	2.007123	-4.497342
H	0.139362	0.435209	-4.933611
H	2.918661	3.500860	-3.750451
H	1.660529	2.310037	-5.535272
C	0.758881	2.227866	0.894165
C	1.809637	3.092592	1.250295
C	-0.552920	2.582659	1.243309
C	1.551114	4.282465	1.930829
H	2.836221	2.833332	1.011201
C	-0.808277	3.775629	1.922465
H	-1.376802	1.926857	0.984711
C	0.240306	4.628395	2.267413
H	2.375380	4.938200	2.199026
H	-1.832636	4.029737	2.180421
H	0.040453	5.555339	2.798467

6

B3LYP electronic energy: -1012.64110188 a.u.
B3LYP enthalpy: -1012.309126 a.u.
B3LYP free energy: -1012.383729 a.u.
M06 SCF energy in solution: -1013.93806468 a.u.
M06 enthalpy in solution: -1013.606089 a.u.
M06 free energy in solution: -1013.680692 a.u.

Cartesian coordinates

ATOM	X	Y	Z
H	-5.340776	2.330389	-0.908825
H	-5.451362	-0.183763	-0.957133
H	-3.359939	-1.471778	-0.450487
Ni	-0.396323	-0.636769	0.277528
C	5.059054	0.335230	0.430657
C	3.886948	1.033235	0.718696
C	2.715453	0.795861	-0.012382
C	2.753441	-0.121712	-1.071280
C	3.932155	-0.803983	-1.376625
C	5.085387	-0.586656	-0.619164
H	5.955971	0.517843	1.017372

H	3.952467	-1.502876	-2.209701
H	6.001614	-1.123395	-0.852729
C	1.506028	1.639517	0.304738
O	1.680899	2.812202	0.668235
N	0.257886	1.111923	0.112445
C	-0.784773	2.127541	0.226620
C	-2.124522	1.552508	-0.130657
C	-3.248590	2.344125	-0.395830
C	-4.459665	1.731247	-0.696471
C	-4.526480	0.334454	-0.725670
C	-3.372175	-0.385605	-0.450577
N	-2.199640	0.206975	-0.162014
H	-3.159549	3.425789	-0.365914
H	3.860743	1.779511	1.506364
H	-0.836797	2.544424	1.247084
H	-0.561490	2.992433	-0.413759
C	-1.159928	-2.432832	1.012493
C	-0.853702	-2.622868	-0.167699
C	-1.578183	-2.516744	2.418289
H	-1.948097	-3.523570	2.648924
H	-0.734701	-2.297560	3.082058
H	-2.374357	-1.797805	2.641692
C	-0.532988	-3.149947	-1.501354
H	-1.056119	-2.596145	-2.288871
H	0.542405	-3.068818	-1.693465
H	-0.819174	-4.206621	-1.574703
H	0.928457	-1.072121	0.681445
H	1.858078	-0.286533	-1.661750

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B3LYP electronic energy: -2048.97236024 a.u.
B3LYP enthalpy: -2048.343272 a.u.
B3LYP free energy: -2048.455648 a.u.
M06 SCF energy in solution: -2049.92258781 a.u.
M06 enthalpy in solution: -2049.293500 a.u.
M06 free energy in solution: -2049.405876 a.u.

Cartesian coordinates

ATOM	X	Y	Z
H	-0.584681	6.261885	0.699177
H	-1.857257	4.582925	2.078581
H	-1.444567	2.163101	1.679339
Ni	0.563580	0.554236	-0.336559
C	5.982289	-1.341339	0.270766
C	5.271257	-0.484225	-0.568563
C	4.159302	0.221932	-0.091489
C	3.797682	0.085635	1.254914
C	4.519521	-0.756228	2.102707
C	5.608680	-1.479711	1.610973
H	6.836175	-1.892910	-0.115417
H	4.236500	-0.844430	3.149299
H	6.169954	-2.137984	2.269804
C	3.486989	1.210217	-1.011916
O	4.178696	1.775293	-1.876859
N	2.182374	1.511714	-0.773304
C	1.737874	2.745186	-1.412976
C	0.700988	3.355382	-0.504919
C	0.500916	4.730323	-0.363992
C	-0.427240	5.195187	0.564580
C	-1.135483	4.269443	1.331564
C	-0.901791	2.915404	1.117123
N	-0.013696	2.462624	0.216033

H	1.088428	5.418481	-0.963872
H	5.570216	-0.335803	-1.601309
H	2.578250	3.431281	-1.568776
H	1.298821	2.579111	-2.414593
H	2.953746	0.655665	1.631302
P	-1.413517	-0.520156	0.012979
C	-1.505741	-1.171552	1.735668
C	-2.445988	-2.131193	2.147957
C	-0.599969	-0.662371	2.679569
C	-2.486357	-2.556177	3.476469
H	-3.137786	-2.557211	1.427555
C	-0.642289	-1.087828	4.008870
H	0.151732	0.056655	2.363390
C	-1.587147	-2.033386	4.409551
H	-3.217415	-3.300094	3.781631
H	0.069739	-0.688171	4.725690
H	-1.617821	-2.369857	5.442330
C	-2.882310	0.602013	-0.148971
C	-3.979880	0.588824	0.723963
C	-2.885955	1.509458	-1.222392
C	-5.055804	1.457189	0.523890
H	-3.997673	-0.093800	1.567327
C	-3.967885	2.365459	-1.430675
H	-2.031916	1.550770	-1.893678
C	-5.055414	2.343083	-0.554704
H	-5.896428	1.437312	1.212537
H	-3.955233	3.056132	-2.269513
H	-5.894999	3.015322	-0.709559
C	-1.924359	-1.961691	-1.032349
C	-2.811322	-1.806046	-2.108135
C	-1.380208	-3.233947	-0.786423
C	-3.144483	-2.893584	-2.918985
H	-3.255084	-0.838727	-2.316972
C	-1.721899	-4.319312	-1.592735
H	-0.687062	-3.377106	0.033836
C	-2.601927	-4.152597	-2.664131
H	-3.833273	-2.751872	-3.747508
H	-1.294002	-5.296057	-1.383910
H	-2.863347	-4.998817	-3.293800
C	1.223324	-1.076115	-1.072998
C	1.710675	-2.060234	-0.303851
H	1.707228	-1.921646	0.778688
C	1.186146	-1.075051	-2.580543
H	1.826923	-0.277781	-2.977804
H	1.519616	-2.022861	-3.022627
H	0.170085	-0.884384	-2.954935
C	2.357164	-3.354708	-0.742561
H	1.886912	-4.221077	-0.254134
H	2.302859	-3.513483	-1.823267
H	3.417429	-3.368202	-0.455627

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B3LYP electronic energy: -1012.67485433 a.u.
B3LYP enthalpy: -1012.339776 a.u.
B3LYP free energy: -1012.410825 a.u.
M06 SCF energy in solution: -1013.96140538 a.u.
M06 enthalpy in solution: -1013.626327 a.u.
M06 free energy in solution: -1013.697376 a.u.

Cartesian coordinates

ATOM	X	Y	Z
H	5.617913	-1.393299	0.529183

H	5.009799	1.029807	0.852459
H	2.622565	1.710496	0.523368
Ni	0.104304	0.225375	-0.193142
C	-4.449275	-0.506630	0.796767
C	-3.504459	-1.498682	0.537568
C	-2.345342	-1.193779	-0.181437
C	-2.159627	0.122237	-0.653759
C	-3.105620	1.121038	-0.381487
C	-4.249761	0.806027	0.348050
H	-5.346847	-0.751588	1.359117
H	-2.941949	2.127788	-0.754027
H	-4.990401	1.572187	0.559748
C	-1.257413	-2.233927	-0.327609
O	-1.477957	-3.442017	-0.182800
N	-0.064966	-1.638823	-0.534794
C	1.134928	-2.428001	-0.435356
C	2.273739	-1.505560	-0.078328
C	3.589701	-1.953363	0.065934
C	4.593088	-1.054099	0.407776
C	4.260861	0.290245	0.589632
C	2.939709	0.680241	0.422878
N	1.963375	-0.194597	0.100467
H	3.807462	-3.005829	-0.088088
H	1.034348	-3.220437	0.324061
H	1.378701	-2.951392	-1.375524
C	0.186843	2.105622	0.141978
C	0.517076	2.961466	-0.840447
H	0.792491	2.543734	-1.814297
C	-0.190543	2.506361	1.551120
H	-0.186455	3.591802	1.720941
H	-1.191698	2.137021	1.810175
H	0.497844	2.059287	2.283277
C	0.564715	4.473774	-0.805539
H	-0.118855	4.906228	-1.549828
H	0.294001	4.886152	0.170694
H	1.569246	4.843463	-1.057352
H	-1.392843	0.333432	-1.420492
H	-3.632748	-2.517104	0.890797

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B3LYP electronic energy: -1012.69342946 a.u.
B3LYP enthalpy: -1012.356917 a.u.
B3LYP free energy: -1012.426001 a.u.
M06 SCF energy in solution: -1013.98777136 a.u.
M06 enthalpy in solution: -1013.651259 a.u.
M06 free energy in solution: -1013.720343 a.u.

Cartesian coordinates

ATOM	X	Y	Z
H	5.549404	1.738288	-0.001500
H	5.220618	-0.763601	-0.001490
H	2.913710	-1.649872	-0.000568
Ni	-0.038047	-0.336988	0.000275
C	-4.785144	0.225307	-0.000797
C	-3.870258	1.280186	-0.000569
C	-2.505807	1.001433	-0.000196
C	-1.998477	-0.309605	-0.000024
C	-2.932624	-1.352310	-0.000209
C	-4.311666	-1.086622	-0.000605
H	-5.854237	0.422121	-0.001094
H	-2.627109	-2.397320	-0.000022
H	-5.014364	-1.917534	-0.000758

C	-1.472815	2.073976	0.000163
O	-1.686529	3.289267	0.000370
N	-0.235656	1.504131	0.000347
C	0.909444	2.372140	0.001132
C	2.152255	1.535089	0.000190
C	3.427021	2.113975	-0.000399
C	4.553843	1.303791	-0.000998
C	4.376593	-0.081774	-0.001027
C	3.083476	-0.583906	-0.000471
N	1.979280	0.191474	0.000142
H	3.513125	3.196390	-0.000393
H	-4.189490	2.319416	-0.000654
H	0.917032	3.044729	-0.873328
H	0.917401	3.042730	0.877181
C	0.047790	-2.453000	-0.685300
C	0.047843	-2.452919	0.686165
H	-0.906989	-2.320563	-1.184977
H	-0.906895	-2.320473	1.185908
C	1.158016	-2.883775	1.610961
H	2.054394	-3.231593	1.091531
H	1.445913	-2.078788	2.297356
H	0.798659	-3.714320	2.232308
C	1.157740	-2.883975	-1.610345
H	1.445261	-2.079054	-2.296986
H	2.054314	-3.231719	-1.091237
H	0.798058	-3.714613	-2.231379

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B3LYP electronic energy: -856.64492133 a.u.
B3LYP enthalpy: -856.406682 a.u.
B3LYP free energy: -856.463590 a.u.
M06 SCF energy in solution: -858.01435687 a.u.
M06 enthalpy in solution: -857.776118 a.u.
M06 free energy in solution: -857.833026 a.u.

Cartesian coordinates

ATOM	X	Y	Z
H	5.671025	0.306412	-0.574297
H	4.879642	-2.077960	-0.730815
H	2.445030	-2.548829	-0.366782
Ni	0.092956	-0.842124	0.294336
C	-4.316298	-0.095727	-0.896954
C	-3.371511	0.903066	-0.661502
C	-2.242861	0.631448	0.114695
C	-2.085360	-0.660367	0.667627
C	-3.031975	-1.665267	0.416311
C	-4.145881	-1.382919	-0.370590
H	-5.191333	0.124347	-1.503425
H	-2.895502	-2.649585	0.853614
H	-4.884892	-2.154212	-0.568010
C	-1.133920	1.657155	0.211672
O	-1.312116	2.855124	-0.030717
N	0.032632	1.038383	0.489508
C	1.279142	1.742017	0.324483
C	2.351759	0.719540	0.032403
C	3.696183	1.053812	-0.147574
C	4.624260	0.056553	-0.426826
C	4.190547	-1.268442	-0.515292
C	2.844824	-1.544501	-0.318785
N	1.944442	-0.574873	-0.051035
H	3.996937	2.094222	-0.071146
H	-3.474696	1.898178	-1.082932

H	1.221586	2.478648	-0.493140
H	1.563589	2.316798	1.221921
H	0.142167	-2.342657	0.172087
H	-1.372348	-0.829679	1.499926

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B3LYP electronic energy: -856.63799857 a.u.
B3LYP enthalpy: -856.401976 a.u.
B3LYP free energy: -856.458673 a.u.
M06 SCF energy in solution: -858.01603405 a.u.
M06 enthalpy in solution: -857.780011 a.u.
M06 free energy in solution: -857.836708 a.u.

Cartesian coordinates

ATOM	X	Y	Z
H	-5.755299	0.469369	-0.000265
H	-5.097303	-1.961419	0.000540
H	-2.673691	-2.533440	0.000695
Ni	-0.043778	-0.827336	-0.000017
C	4.605333	-0.093464	0.000058
C	3.663355	0.940802	0.000207
C	2.309009	0.622445	0.000106
C	1.858986	-0.708445	-0.000111
C	2.806862	-1.733692	-0.000262
C	4.176768	-1.421971	-0.000192
H	5.668136	0.134855	0.000126
H	2.508028	-2.780848	-0.000442
H	4.909357	-2.226456	-0.000326
C	1.214847	1.641831	0.000130
O	1.348535	2.865478	0.000312
N	0.012071	0.992485	-0.000121
C	-1.226435	1.727594	-0.000216
C	-2.366930	0.744340	-0.000178
C	-3.708387	1.139916	-0.000374
C	-4.709477	0.176016	-0.000132
C	-4.350061	-1.175076	0.000300
C	-3.001345	-1.498422	0.000410
N	-2.025959	-0.567125	0.000156
H	-3.949813	2.198433	-0.000696
H	3.961701	1.986281	0.000377
H	-1.312155	2.390351	0.877053
H	-1.312071	2.390296	-0.877525
H	-0.023595	-2.487425	0.394354
H	-0.023708	-2.487201	-0.394649

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B3LYP electronic energy: -855.44423500 a.u.
B3LYP enthalpy: -855.225872 a.u.
B3LYP free energy: -855.281979 a.u.
M06 SCF energy in solution: -856.81731860 a.u.
M06 enthalpy in solution: -856.598956 a.u.
M06 free energy in solution: -856.655063 a.u.

Cartesian coordinates

ATOM	X	Y	Z
H	-5.751522	0.396166	0.000247
H	-5.073164	-2.028362	0.000088
H	-2.640604	-2.579049	-0.000121
Ni	-0.044244	-0.824532	-0.000063
C	4.595476	-0.169443	0.000079

C	3.671779	0.881130	0.000057
C	2.312541	0.582135	0.000018
C	1.840789	-0.742223	0.000003
C	2.772097	-1.783609	0.000030
C	4.146593	-1.492101	0.000067
H	5.661964	0.041081	0.000107
H	2.457194	-2.827224	0.000020
H	4.867957	-2.306770	0.000087
C	1.229638	1.613634	-0.000013
O	1.364903	2.836706	-0.000027
N	0.013944	0.984403	-0.000025
C	-1.234668	1.701826	-0.000087
C	-2.366535	0.703255	-0.000019
C	-3.710990	1.086219	0.000106
C	-4.703180	0.112091	0.000146
C	-4.332532	-1.235858	0.000063
C	-2.980626	-1.546955	-0.000051
N	-2.015945	-0.605511	-0.000087
H	-3.963448	2.142190	0.000173
H	3.990509	1.920509	0.000064
H	-1.328771	2.361015	0.878711
H	-1.328779	2.360856	-0.879009

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B3LYP electronic energy: -1011.46027935 a.u.
B3LYP enthalpy: -1011.148421 a.u.
B3LYP free energy: -1011.218805 a.u.
M06 SCF energy in solution: -1012.76132676 a.u.
M06 enthalpy in solution: -1012.449468 a.u.
M06 free energy in solution: -1012.519852 a.u.

Cartesian coordinates

ATOM	X	Y	Z
H	-5.754504	1.076019	-0.000363
H	-5.141540	-1.366801	-0.000084
H	-2.716282	-1.980156	0.000214
Ni	-0.022139	-0.357961	0.000389
C	4.634835	0.459573	0.000128
C	3.669595	1.471231	-0.000023
C	2.321174	1.125678	0.000139
C	1.893418	-0.214504	0.000401
C	2.868495	-1.215421	0.000542
C	4.232045	-0.876705	0.000429
H	5.692645	0.710899	0.000019
H	2.591142	-2.267241	0.000742
H	4.980448	-1.667025	0.000559
C	1.219840	2.137244	0.000067
O	1.358730	3.362737	-0.000395
N	0.022404	1.485368	0.000583
C	-1.201270	2.243447	0.000298
C	-2.360671	1.284561	0.000140
C	-3.694689	1.707318	-0.000098
C	-4.714246	0.762817	-0.000184
C	-4.379292	-0.594534	-0.000035
C	-3.035859	-0.942712	0.000167
N	-2.044569	-0.031029	0.000261
H	-3.915221	2.770557	-0.000212
H	3.942180	2.523838	-0.000248
H	-1.275113	2.910100	0.876249
H	-1.274710	2.910040	-0.875724
C	-0.092814	-2.378672	0.614884
C	-0.092411	-2.378084	-0.616448

C	-0.052043	-2.656302	2.056679
H	-0.126372	-3.735192	2.241414
H	0.888820	-2.293768	2.484799
H	-0.873389	-2.159126	2.584340
C	-0.050612	-2.653719	-2.058567
H	-0.872155	-2.156603	-2.585981
H	0.890157	-2.289754	-2.485674
H	-0.123855	-3.732431	-2.244794

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B3LYP electronic energy: -1011.46731376 a.u.
B3LYP enthalpy: -1011.154777 a.u.
B3LYP free energy: -1011.219936 a.u.
M06 SCF energy in solution: -1012.76088936 a.u.
M06 enthalpy in solution: -1012.448353 a.u.
M06 free energy in solution: -1012.513512 a.u.

Cartesian coordinates

ATOM	X	Y	Z
H	6.095805	-1.444901	-0.466737
H	5.872284	0.996823	-1.035072
H	3.622857	2.059535	-0.839386
Ni	0.792880	0.907458	-0.007856
C	-4.246895	-2.053333	-0.786209
C	-2.948815	-2.151865	-0.302023
C	-2.175347	-1.028714	0.053377
C	-2.766019	0.261851	-0.057695
C	-4.100898	0.327886	-0.521316
C	-4.831191	-0.793236	-0.893002
H	-4.796007	-2.949859	-1.061387
H	-4.578692	1.296318	-0.610333
H	-5.848827	-0.678705	-1.258015
C	-0.818409	-1.462959	0.586768
O	-0.781196	-2.510487	1.252206
N	0.342175	-0.860317	0.190253
C	1.518779	-1.640016	0.582932
C	2.780396	-0.975452	0.113664
C	4.006963	-1.641681	0.021906
C	5.136045	-0.942105	-0.388964
C	5.017873	0.414747	-0.706381
C	3.769943	1.010914	-0.597557
N	2.675572	0.334494	-0.195870
H	4.060672	-2.696830	0.271248
H	-2.496322	-3.126878	-0.165951
H	1.570651	-1.770831	1.676574
H	1.455038	-2.660408	0.181744
C	-0.786808	1.725900	0.242762
C	-2.114440	1.557032	0.257051
C	-3.009404	2.762794	0.515771
H	-2.441483	3.578614	0.971369
H	-3.460570	3.155391	-0.405974
H	-3.830900	2.509982	1.195778
C	0.027546	2.986298	0.338385
H	-0.242320	3.746739	-0.403786
H	0.070380	3.431849	1.339635
H	1.116221	2.760640	0.095137

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B3LYP electronic energy: -2047.78046699 a.u.
B3LYP enthalpy: -2047.173732 a.u.

B3LYP free energy: -2047.282009 a.u.
M06 SCF energy in solution: -2048.73200194 a.u.
M06 enthalpy in solution: -2048.125267 a.u.
M06 free energy in solution: -2048.233544 a.u.

Cartesian coordinates

ATOM	X	Y	Z
H	-0.933836	6.461968	-0.334151
H	-2.456559	4.705462	-1.306666
H	-1.875990	2.313149	-0.965878
Ni	0.490901	0.793715	0.738469
C	4.395558	-1.114486	-2.097897
C	4.187714	0.041462	-1.350995
C	3.440025	0.027245	-0.161157
C	2.926293	-1.201976	0.319700
C	3.172778	-2.363400	-0.438099
C	3.877872	-2.327317	-1.638298
H	4.967748	-1.072188	-3.021463
H	2.785301	-3.313381	-0.080628
H	4.031229	-3.242825	-2.205019
C	3.311904	1.382075	0.510733
O	4.283398	2.156442	0.479061
N	2.095819	1.717824	1.006606
C	1.896600	3.105963	1.357132
C	0.675418	3.625976	0.632953
C	0.410469	4.991937	0.491398
C	-0.720671	5.404335	-0.204810
C	-1.567819	4.435065	-0.745782
C	-1.247286	3.096211	-0.557004
N	-0.156752	2.689693	0.120726
H	1.101669	5.713560	0.916558
H	4.617554	0.987661	-1.663439
H	1.742759	3.238214	2.442745
H	2.786087	3.690222	1.090371
C	1.168259	-0.528606	1.911738
C	2.215720	-1.319940	1.628022
C	2.802761	-2.357317	2.573140
H	2.285528	-2.389527	3.534966
H	2.757792	-3.367539	2.145633
H	3.862552	-2.146606	2.769955
C	0.471479	-0.421017	3.247736
H	-0.622716	-0.446962	3.152451
H	0.756224	-1.208788	3.957312
H	0.714935	0.541289	3.720642
P	-1.171427	-0.555814	-0.044449
C	-1.373488	-0.179778	-1.844191
C	-2.611011	-0.148375	-2.504334
C	-0.203495	0.099948	-2.573355
C	-2.677160	0.153233	-3.866617
H	-3.525758	-0.352391	-1.956893
C	-0.273200	0.388785	-3.936942
H	0.761836	0.092120	-2.072569
C	-1.510084	0.419049	-4.585293
H	-3.642598	0.178568	-4.365224
H	0.639609	0.597252	-4.487963
H	-1.564272	0.652526	-5.645252
C	-0.921800	-2.386748	-0.013750
C	-0.991736	-3.060932	1.217290
C	-0.621324	-3.119716	-1.169399
C	-0.776508	-4.436126	1.285754
H	-1.221698	-2.513982	2.126098
C	-0.401371	-4.498068	-1.097288
H	-0.555259	-2.621226	-2.130378
C	-0.478728	-5.159599	0.127659

H	-0.837800	-4.942228	2.245468
H	-0.170773	-5.051076	-2.003920
H	-0.308866	-6.231575	0.182269
C	-2.857882	-0.373373	0.687485
C	-3.876570	-1.322183	0.492063
C	-3.126638	0.752959	1.480915
C	-5.136385	-1.136480	1.061964
H	-3.679628	-2.213876	-0.095869
C	-4.387980	0.937079	2.051690
H	-2.340896	1.481411	1.659449
C	-5.395091	-0.005592	1.840943
H	-5.914418	-1.878352	0.902826
H	-4.578641	1.812187	2.667069
H	-6.375320	0.134241	2.288690

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B3LYP electronic energy: -2047.78815697 a.u.
B3LYP enthalpy: -2047.180333 a.u.
B3LYP free energy: -2047.289682 a.u.
M06 SCF energy in solution: -2048.73372173 a.u.
M06 enthalpy in solution: -2048.125898 a.u.
M06 free energy in solution: -2048.235247 a.u.

Cartesian coordinates

ATOM	X	Y	Z
N	2.072412	1.777850	-0.239662
C	2.043447	0.739900	-1.254270
C	2.813433	-0.469000	-0.950894
C	3.526267	-0.600994	0.268483
C	2.885503	-1.474634	-1.931683
C	3.625042	-2.625544	-1.707685
H	2.343205	-1.321568	-2.858023
C	4.320684	-2.779202	-0.497954
H	3.668427	-3.402412	-2.466039
H	4.904089	-3.678018	-0.315696
O	1.615944	1.034976	-2.392241
C	2.722978	1.583322	1.012930
C	3.443883	0.451368	1.269209
C	4.151405	0.231033	2.587226
H	3.761477	-0.653868	3.107578
H	5.224529	0.062778	2.430732
H	4.061894	1.078705	3.266721
C	2.538450	2.712684	2.002219
H	2.539256	2.340706	3.027919
H	3.331075	3.470138	1.928068
H	1.580517	3.214532	1.848184
C	4.274578	-1.782745	0.468658
H	4.826734	-1.919614	1.392220
C	1.932297	3.152534	-0.767021
H	2.071313	3.060506	-1.849091
H	2.725328	3.791813	-0.368027
C	0.569060	3.761500	-0.514163
C	0.335343	5.124413	-0.707465
C	-0.950777	5.626687	-0.521274
H	1.152081	5.776740	-1.004206
C	-1.652554	3.402889	0.036967
C	-1.965662	4.746188	-0.142493
H	-1.156240	6.683301	-0.667855
H	-2.405148	2.682824	0.339269
H	-2.982874	5.089755	0.016531
N	-0.410628	2.909942	-0.143268
Ni	0.159669	0.956920	-0.109847

P	-1.128177	-0.724304	0.084766
C	-1.432899	-1.715093	-1.454831
C	-2.102351	-2.950034	-1.450189
C	-0.959168	-1.204686	-2.673741
C	-2.305803	-3.651829	-2.638699
H	-2.458930	-3.369956	-0.514030
C	-1.166725	-1.908639	-3.863356
H	-0.404403	-0.270345	-2.687746
C	-1.841042	-3.130299	-3.849176
H	-2.823833	-4.607556	-2.619517
H	-0.791757	-1.502068	-4.799208
H	-1.998180	-3.679086	-4.774466
C	-2.843203	-0.187300	0.579887
C	-3.000873	0.451214	1.824764
C	-3.961364	-0.284333	-0.260963
C	-4.238109	0.957217	2.222229
H	-2.144131	0.550402	2.487647
C	-5.199349	0.235545	0.131136
H	-3.870345	-0.769239	-1.227617
C	-5.344467	0.853862	1.372918
H	-4.338389	1.435659	3.193528
H	-6.052179	0.150009	-0.537842
H	-6.308443	1.252471	1.678223
C	-0.788651	-2.057323	1.339561
C	-1.777373	-2.674426	2.122402
C	0.542813	-2.476144	1.488620
C	-1.441340	-3.684048	3.028096
H	-2.813854	-2.363869	2.033160
C	0.876535	-3.491634	2.385048
H	1.319789	-2.002946	0.897638
C	-0.114653	-4.097091	3.160855
H	-2.219699	-4.148354	3.628875
H	1.913598	-3.804042	2.478072
H	0.144833	-4.883115	3.865563

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B3LYP electronic energy: -1011.48456289 a.u.
B3LYP enthalpy: -1011.169746 a.u.
B3LYP free energy: -1011.234462 a.u.
M06 SCF energy in solution: -1012.78216964 a.u.
M06 enthalpy in solution: -1012.467353 a.u.
M06 free energy in solution: -1012.532069 a.u.

Cartesian coordinates

ATOM	X	Y	Z
N	0.046435	-0.316211	1.361314
C	-0.690215	-1.415083	0.916464
C	-1.949774	-1.117752	0.206186
C	-2.278841	0.204732	-0.186931
C	-2.772020	-2.201785	-0.131433
C	-3.943128	-2.006008	-0.850866
H	-2.457960	-3.190884	0.185396
C	-4.288144	-0.705736	-1.242220
H	-4.580908	-2.847192	-1.106960
H	-5.202968	-0.533559	-1.804567
O	-0.271077	-2.562076	1.087860
C	-0.298099	1.060374	1.071442
C	-1.419612	1.335146	0.199520
C	-2.056842	2.718099	0.163811
H	-2.436369	2.944969	-0.837930
H	-2.905992	2.810008	0.859594
H	-1.341639	3.509015	0.398636

C	0.171934	2.035617	2.140025
H	-0.201019	3.040948	1.947442
H	-0.201850	1.721303	3.125483
H	1.262451	2.109291	2.202512
Ni	0.417039	1.181738	-0.655169
C	-3.477135	0.375388	-0.916938
H	-3.779486	1.368388	-1.230066
C	1.454188	-0.588497	1.640786
H	1.508416	-1.597904	2.047882
H	1.812187	0.103107	2.408909
C	2.399563	-0.507950	0.433358
C	3.540974	-1.312855	0.433143
C	4.462297	-1.228479	-0.607994
H	3.694013	-2.008925	1.252303
C	3.062198	0.443157	-1.589240
C	4.216896	-0.326350	-1.642554
H	5.348194	-1.856641	-0.613584
H	2.834296	1.159536	-2.372094
H	4.900468	-0.217763	-2.478338
N	2.158460	0.362231	-0.584475

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B3LYP electronic energy: -1012.69417319 a.u.
B3LYP enthalpy: -1012.358004 a.u.
B3LYP free energy: -1012.423398 a.u.
M06 SCF energy in solution: -1013.98985502 a.u.
M06 enthalpy in solution: -1013.653686 a.u.
M06 free energy in solution: -1013.719080 a.u.

Cartesian coordinates

ATOM	X	Y	Z
H	-6.031777	-1.595633	0.078312
H	-5.955289	0.868700	-0.436784
H	-3.728321	1.978489	-0.590487
Ni	-0.786345	0.900139	-0.299277
C	4.591965	-1.522536	-0.754754
C	3.259666	-1.835260	-0.509267
C	2.328547	-0.879672	-0.056583
C	2.786625	0.439842	0.171136
C	4.142630	0.729055	-0.055563
C	5.044246	-0.226097	-0.515741
H	5.271896	-2.289568	-1.116396
H	4.493774	1.741639	0.132139
H	6.084213	0.041965	-0.684651
C	0.960638	-1.499313	0.220596
O	0.965204	-2.690981	0.580114
N	-0.220950	-0.845524	0.034971
C	-1.350093	-1.737678	0.300624
C	-2.673300	-1.061196	0.092984
C	-3.887074	-1.753503	0.192614
C	-5.082746	-1.072213	0.004763
C	-5.046399	0.296939	-0.281958
C	-3.810636	0.918928	-0.367780
N	-2.647795	0.258184	-0.185246
H	-3.875587	-2.816104	0.415339
H	2.904053	-2.850031	-0.643095
H	-1.297776	-2.635721	-0.332856
H	-1.309999	-2.131027	1.329076
C	0.838341	1.809755	-0.461296
C	1.902770	1.601399	0.606494
C	1.372001	1.458553	2.046678
H	0.767333	0.555166	2.160341

H	2.208478	1.407256	2.752625
H	0.752932	2.319901	2.329363
C	-0.105561	2.979088	-0.395932
H	-0.074044	3.637169	-1.269938
H	-1.207189	2.614849	-0.422508
H	-0.055545	3.563804	0.526676
H	2.552205	2.492835	0.605347
H	1.248168	1.655099	-1.463815

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B3LYP electronic energy: -801.67770518 a.u.
B3LYP enthalpy: -801.417445 a.u.
B3LYP free energy: -801.475207 a.u.
M06 SCF energy in solution: -801.32637643 a.u.
M06 enthalpy in solution: -801.066116 a.u.
M06 free energy in solution: -801.123878 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-2.760070	1.134315	0.397010
C	-2.693085	-0.218998	0.031965
C	-3.870398	-0.884915	-0.337589
C	-5.086921	-0.207559	-0.365762
C	-5.144755	1.143118	-0.011868
C	-3.980595	1.809813	0.375065
H	-1.873922	1.666529	0.732446
H	-3.804640	-1.936117	-0.597352
H	-5.991196	-0.732441	-0.661639
H	-6.093833	1.672151	-0.030672
H	-4.021915	2.855551	0.667154
C	-1.425774	-1.029378	0.033289
O	-1.451725	-2.257373	0.039653
N	-0.260718	-0.297628	0.010925
H	-0.306559	0.711857	-0.085414
C	1.056393	-0.759636	0.032681
C	2.059742	0.268718	-0.026579
C	1.444498	-2.088013	0.108557
C	3.440880	-0.092437	-0.006805
C	2.818804	-2.422867	0.128570
H	0.686578	-2.857390	0.147953
C	2.546844	2.515874	-0.158911
C	4.380564	0.967934	-0.069822
C	3.803591	-1.461951	0.072757
H	3.091980	-3.472873	0.188712
C	3.940219	2.269845	-0.146041
H	2.175257	3.537928	-0.218618
H	5.443102	0.736494	-0.057364
H	4.855504	-1.734595	0.087578
H	4.636777	3.101115	-0.195668
N	1.637437	1.561571	-0.101416

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B3LYP electronic energy: -2162.11711390 a.u.
B3LYP enthalpy: -2161.490898 a.u.
B3LYP free energy: -2161.601629 a.u.
M06 SCF energy in solution: -2163.00729417 a.u.
M06 enthalpy in solution: -2162.381078 a.u.
M06 free energy in solution: -2162.491809 a.u.

Cartesian coordinates

ATOM	X	Y	Z
H	4.747126	-4.095845	0.534989
H	2.389961	-4.633375	1.184085
H	0.657619	-2.851509	1.025569
Ni	0.730914	0.089710	-0.424244
C	1.214893	3.139561	0.348580
C	-0.028659	3.188565	-0.318732
C	2.459815	2.436889	-0.157215
O	3.518570	3.071892	-0.189806
N	2.348478	1.087565	-0.389928
C	3.230089	-1.085471	-0.031427
C	4.292283	-2.037483	0.038961
C	3.963645	-3.343927	0.475626
C	2.667027	-3.645158	0.831002
C	1.681998	-2.641633	0.736734
N	1.940421	-1.411431	0.307856
C	0.087038	1.232356	-1.797782
C	-0.214591	2.531922	-1.645089
P	-1.347029	-0.731497	0.010801
C	-1.365068	-1.225909	1.792097
C	-2.031549	-2.357906	2.284836
C	-0.654613	-0.408596	2.689642
C	-1.990629	-2.664069	3.647155
H	-2.578837	-3.006552	1.608115
C	-0.626109	-0.711455	4.051377
H	-0.120242	0.463630	2.320659
C	-1.291510	-1.841490	4.532291
H	-2.507157	-3.546711	4.015049
H	-0.076253	-0.068348	4.732835
H	-1.261630	-2.081996	5.591587
C	-2.796134	0.404180	-0.137479
C	-3.224804	0.790049	-1.419262
C	-3.464711	0.916635	0.982261
C	-4.303104	1.659830	-1.573487
H	-2.723122	0.404771	-2.300902
C	-4.541931	1.793009	0.824682
H	-3.150003	0.637164	1.981855
C	-4.964178	2.166147	-0.450721
H	-4.625474	1.943653	-2.571669
H	-5.049574	2.180301	1.703990
H	-5.803588	2.845609	-0.571963
C	-1.914308	-2.222470	-0.919611
C	-3.258561	-2.632914	-0.938175
C	-0.968747	-2.968106	-1.640859
C	-3.640533	-3.772928	-1.645894
H	-4.008906	-2.053238	-0.408693
C	-1.353173	-4.108002	-2.350306
H	0.068806	-2.647925	-1.653346
C	-2.688427	-4.513395	-2.351542
H	-4.683191	-4.079190	-1.651832
H	-0.610002	-4.671811	-2.907521
H	-2.989306	-5.397506	-2.907118
C	3.472608	0.273272	-0.430168
C	4.782545	0.626771	-0.759682
H	4.991530	1.648553	-1.039002
C	5.821615	-0.328009	-0.706139
C	5.602963	-1.633810	-0.319484
H	6.824941	-0.011879	-0.980885
H	6.413414	-2.356494	-0.281984
C	-0.715032	3.454651	-2.744693
H	-1.716688	3.841716	-2.513674
H	-0.057056	4.327060	-2.851352
H	-0.775640	2.958937	-3.716612
C	0.117144	0.477151	-3.106391

H	-0.539916	-0.403428	-3.099342
H	-0.169092	1.092830	-3.968724
H	1.131374	0.102321	-3.303792
C	1.385522	3.850494	1.547517
C	0.336909	4.566521	2.119326
H	0.487671	5.099657	3.054664
C	-0.899021	4.609517	1.470253
H	-1.726634	5.168996	1.899784
C	-1.065896	3.942999	0.258304
H	2.365701	3.844305	2.014510
H	-2.025702	3.992086	-0.248522

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B3LYP electronic energy: -2162.11360825 a.u.
B3LYP enthalpy: -2161.486780 a.u.
B3LYP free energy: -2161.600345 a.u.
M06 SCF energy in solution: -2163.00031973 a.u.
M06 enthalpy in solution: -2162.373491 a.u.
M06 free energy in solution: -2162.487056 a.u.

Cartesian coordinates

ATOM	X	Y	Z
N	-2.275328	-0.922447	-0.205906
C	-1.577339	-1.309858	0.999000
C	-0.842775	-2.576259	0.918653
C	-0.842753	-3.352343	-0.268594
C	-0.201207	-3.042200	2.079846
C	0.468901	-4.255681	2.074467
H	-0.246041	-2.423323	2.969006
C	0.490365	-5.029282	0.903322
H	0.970919	-4.606676	2.971673
H	1.011139	-5.983295	0.891406
O	-1.801307	-0.684448	2.047859
C	-2.177429	-1.662045	-1.418824
C	-1.504066	-2.849108	-1.463666
C	-1.378809	-3.658208	-2.734562
H	-0.329842	-3.753548	-3.044877
H	-1.764710	-4.675245	-2.589354
H	-1.932528	-3.227930	-3.569065
C	-2.837410	-0.995099	-2.603601
H	-2.372912	-1.305385	-3.540182
H	-3.909766	-1.217268	-2.669315
H	-2.730973	0.091244	-2.530621
C	-0.156202	-4.587166	-0.243877
H	-0.129206	-5.205749	-1.134434
C	-3.286276	1.301604	0.105770
C	-4.425166	2.122267	0.359102
C	-4.211156	3.520767	0.470577
C	-1.870476	3.135009	0.050140
C	-2.936528	4.019760	0.321354
H	-5.053907	4.177087	0.671535
H	-0.862731	3.510610	-0.096089
H	-2.734436	5.083497	0.398684
N	-2.022545	1.817043	-0.055879
Ni	-0.579257	0.450562	-0.068064
P	1.530051	0.632610	-0.063059
C	2.363388	0.351005	1.570753
C	3.742470	0.118456	1.701802
C	1.566177	0.360114	2.726697
C	4.313211	-0.080585	2.960131
H	4.371852	0.085008	0.816865
C	2.139511	0.163572	3.985276

H	0.491304	0.493315	2.635411
C	3.513353	-0.053713	4.105257
H	5.382132	-0.260236	3.045565
H	1.508303	0.171381	4.870303
H	3.958572	-0.210960	5.084537
C	2.058598	2.361393	-0.521778
C	1.445593	2.942379	-1.647123
C	2.983059	3.129503	0.200943
C	1.761485	4.240234	-2.049106
H	0.709133	2.367255	-2.204496
C	3.287708	4.436878	-0.191106
H	3.468152	2.710830	1.076640
C	2.683574	4.994955	-1.317888
H	1.282651	4.665210	-2.928012
H	4.002750	5.017180	0.386976
H	2.924440	6.010126	-1.622657
C	2.592038	-0.389115	-1.202035
C	3.571318	0.138611	-2.056466
C	2.378355	-1.777836	-1.203363
C	4.316263	-0.700898	-2.890615
H	3.757047	1.207868	-2.075879
C	3.130278	-2.615723	-2.025643
H	1.619188	-2.202219	-0.553971
C	4.100402	-2.079029	-2.876967
H	5.068798	-0.273242	-3.548782
H	2.953818	-3.688339	-2.002902
H	4.681674	-2.730357	-3.524773
C	-3.450453	-0.103624	0.007857
C	-4.700552	-0.670306	0.135191
H	-4.806974	-1.749018	0.067807
C	-5.832783	0.143817	0.369892
C	-5.699338	1.510172	0.485808
H	-6.809289	-0.320442	0.472041
H	-6.566546	2.136633	0.678517

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B3LYP electronic energy: -1203.19644595 a.u.
B3LYP enthalpy: -1202.828356 a.u.
B3LYP free energy: -1202.907213 a.u.
M06 SCF energy in solution: -1204.39931281 a.u.
M06 enthalpy in solution: -1204.031223 a.u.
M06 free energy in solution: -1204.110080 a.u.

Cartesian coordinates

ATOM	X	Y	Z
H	-3.922241	4.451198	-0.327043
H	-4.505367	2.367298	0.961135
H	-2.733084	0.632247	1.274042
Ni	0.274966	0.356811	0.399299
C	4.592509	-1.526324	-0.030457
C	4.236071	-0.278432	-0.550823
C	2.935612	0.185948	-0.374857
C	1.962741	-0.560963	0.313933
C	2.330949	-1.808178	0.825729
C	3.641127	-2.285129	0.653053
H	5.603626	-1.905050	-0.158147
H	1.614044	-2.429148	1.357623
H	3.913777	-3.258628	1.056103
C	2.460650	1.502944	-0.899632
O	3.136912	2.321500	-1.526879
N	1.145909	1.659439	-0.573370
C	0.455415	2.862639	-0.960227

C	-0.958293	2.790321	-0.450845
C	-1.895304	3.806281	-0.669276
C	-3.183513	3.671169	-0.165544
C	-3.512147	2.516490	0.550530
C	-2.533522	1.548653	0.728588
N	-1.284286	1.675548	0.242566
H	-1.602035	4.688336	-1.230618
H	4.946698	0.342233	-1.091169
H	0.946153	3.766003	-0.560294
H	0.445875	2.999875	-2.054660
C	-0.465486	-0.754456	2.015896
C	-0.887233	-1.306987	0.993094
C	-0.032116	-0.377175	3.366847
C	-1.549409	-2.134775	0.018881
C	-2.775171	-2.747670	0.347097
C	-0.990541	-2.352620	-1.254377
C	-3.422910	-3.560109	-0.580083
H	-3.206661	-2.584086	1.330409
C	-1.647033	-3.167570	-2.174223
H	-0.041968	-1.887074	-1.501270
C	-2.862538	-3.771188	-1.842903
H	-4.366719	-4.029548	-0.316390
H	-1.205780	-3.331923	-3.153197
H	-3.371070	-4.404487	-2.564557
H	-0.495338	-1.033627	4.114107
H	1.056643	-0.467030	3.449585
H	-0.301402	0.658576	3.602233

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B3LYP electronic energy: -1321.13470004 a.u.
B3LYP enthalpy: -1320.677555 a.u.
B3LYP free energy: -1320.764756 a.u.
M06 SCF energy in solution: -1322.27854586 a.u.
M06 enthalpy in solution: -1321.821401 a.u.
M06 free energy in solution: -1321.908602 a.u.

Cartesian coordinates

ATOM	X	Y	Z
H	3.800481	-4.586488	-0.720560
H	4.524021	-2.374760	0.242303
H	2.790175	-0.608722	0.587988
Ni	-0.305064	-0.393183	0.040054
C	-4.561099	1.599365	-0.517849
C	-4.275335	0.273325	-0.855828
C	-2.989680	-0.220015	-0.650282
C	-1.963479	0.572085	-0.105339
C	-2.260112	1.898719	0.220043
C	-3.553721	2.406347	0.013770
H	-5.559217	2.001939	-0.671860
H	-1.500028	2.555883	0.634510
H	-3.769740	3.441232	0.272336
C	-2.585182	-1.613311	-1.009758
O	-3.315343	-2.476828	-1.501783
N	-1.263690	-1.778798	-0.716472
C	-0.627664	-3.038698	-1.004420
C	0.832787	-2.928750	-0.662172
C	1.742160	-3.969948	-0.878924
C	3.081541	-3.789004	-0.554998
C	3.488009	-2.563673	-0.019093
C	2.531024	-1.577339	0.174777
N	1.231559	-1.750044	-0.132255

H	1.388684	-4.905140	-1.302744
H	-5.028368	-0.385925	-1.280747
H	-1.078366	-3.870190	-0.435803
H	-0.738403	-3.320903	-2.064430
C	0.545669	0.813813	1.536341
C	0.903424	1.277708	0.443283
C	0.331258	0.599133	2.996369
C	1.170714	-0.610637	3.469933
H	2.239599	-0.449534	3.290388
H	1.025125	-0.760500	4.545943
H	0.867720	-1.525787	2.951809
C	-1.157848	0.344510	3.316672
H	-1.277366	0.223674	4.399767
H	-1.785436	1.175712	2.984923
H	-1.519795	-0.561507	2.822056
C	0.808973	1.878999	3.725347
H	1.865252	2.083230	3.517998
H	0.222886	2.749587	3.413960
H	0.690943	1.753683	4.808124
C	1.524495	2.026352	-0.619858
C	2.759889	2.663286	-0.384383
C	0.926152	2.139971	-1.888735
C	3.377240	3.395277	-1.395433
H	3.223255	2.581435	0.594694
C	1.551989	2.875617	-2.893210
H	-0.029275	1.657926	-2.067933
C	2.776895	3.502688	-2.652884
H	4.328495	3.883325	-1.201134
H	1.078941	2.959046	-3.867633
H	3.261260	4.073493	-3.440313

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B3LYP electronic energy: -1013.88643269 a.u.
B3LYP enthalpy: -1013.530110 a.u.
B3LYP free energy: -1013.602178 a.u.
M06 SCF energy in solution: -1015.17871973 a.u.
M06 enthalpy in solution: -1014.822397 a.u.
M06 free energy in solution: -1014.894465 a.u.

Cartesian coordinates

ATOM	X	Y	Z
H	5.602196	-2.098754	-0.720923
H	5.559354	0.407112	-0.976976
H	3.409922	1.599098	-0.600705
Ni	0.454810	0.630127	0.197159
C	-4.921200	-0.716890	0.350323
C	-3.708934	-1.304566	0.709516
C	-2.544250	-1.045960	-0.025344
C	-2.626284	-0.223282	-1.157188
C	-3.843895	0.347031	-1.532080
C	-4.992487	0.111578	-0.772850
H	-5.813688	-0.913475	0.939253
H	-3.897422	0.972585	-2.420037
H	-5.939474	0.561246	-1.061150
C	-1.283921	-1.770178	0.375909
O	-1.379300	-2.915514	0.840677
N	-0.073653	-1.171339	0.148260
C	1.036600	-2.091135	0.367233
C	2.335781	-1.453542	-0.027734
C	3.508768	-2.193828	-0.220511
C	4.684919	-1.538430	-0.563553
C	4.666784	-0.147887	-0.707844

C	3.468058	0.519180	-0.500223
N	2.325318	-0.111208	-0.168720
H	3.481847	-3.272653	-0.102079
H	-3.644689	-1.979470	1.557106
H	1.102225	-2.407291	1.422744
H	0.889943	-3.025481	-0.192542
C	1.034858	2.518200	0.927582
C	0.713889	2.632033	-0.413298
H	-0.907462	0.965625	0.549146
H	-1.733895	-0.044777	-1.748205
H	2.074456	2.298596	1.171458
H	1.521555	2.492447	-1.132741
C	0.214022	2.997845	2.096837
H	0.265490	2.286033	2.927596
H	0.613168	3.955838	2.461735
H	-0.837889	3.139412	1.841670
C	-0.524474	3.263227	-0.996046
H	-0.296290	4.286631	-1.328831
H	-0.872314	2.705704	-1.871756
H	-1.348371	3.309598	-0.281773

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B3LYP electronic energy: -2050.19052546 a.u.
B3LYP enthalpy: -2049.537110 a.u.
B3LYP free energy: -2049.649670 a.u.
M06 SCF energy in solution: -2051.13928256 a.u.
M06 enthalpy in solution: -2050.485867 a.u.
M06 free energy in solution: -2050.598427 a.u.

Cartesian coordinates

ATOM	X	Y	Z
H	6.578979	-1.711209	1.196328
H	6.288224	-0.847889	-1.153867
H	4.007911	-0.249952	-1.921829
Ni	1.081232	-0.207360	-0.432810
C	-2.590087	-4.437646	-1.041297
C	-1.776954	-4.024255	0.012629
C	-0.657634	-3.211838	-0.221294
C	-0.343168	-2.864929	-1.541693
C	-1.143207	-3.296472	-2.602971
C	-2.275458	-4.074477	-2.354471
H	-3.462440	-5.055573	-0.842827
H	-0.874803	-3.035572	-3.624236
H	-2.900496	-4.409165	-3.178667
C	0.214738	-2.838332	0.957165
O	0.276640	-3.632803	1.913531
N	0.879464	-1.663983	0.872897
C	1.921697	-1.464204	1.859903
C	3.210528	-1.250159	1.098497
C	4.464948	-1.585817	1.612576
C	5.597753	-1.439201	0.817091
C	5.442598	-0.960274	-0.483215
C	4.165082	-0.624929	-0.919637
N	3.068540	-0.747543	-0.152363
H	4.533800	-1.981727	2.621144
H	-1.979009	-4.332163	1.033898
H	1.717968	-0.581058	2.491179
H	2.001800	-2.326890	2.530870
C	1.328901	1.072644	-1.939037
C	1.526053	0.195645	-3.188403
H	0.553348	-2.282494	-1.738429

P	-0.770244	0.894840	0.245409
C	-2.298017	0.837788	-0.789752
C	-3.531973	1.288212	-0.287247
C	-2.243024	0.329666	-2.094113
C	-4.677595	1.243122	-1.080480
H	-3.597783	1.665676	0.728854
C	-3.392510	0.282158	-2.886321
H	-1.304777	-0.043577	-2.486035
C	-4.609548	0.740517	-2.382906
H	-5.624746	1.593530	-0.679052
H	-3.334654	-0.122517	-3.892907
H	-5.504670	0.699572	-2.997820
C	-1.430206	0.432137	1.914367
C	-1.297108	1.244400	3.049631
C	-2.085499	-0.804195	2.043272
C	-1.796207	0.823499	4.285940
H	-0.815672	2.213022	2.980049
C	-2.582491	-1.220209	3.276056
H	-2.210514	-1.447221	1.178905
C	-2.435828	-0.409201	4.404124
H	-1.684392	1.467843	5.154168
H	-3.075934	-2.184585	3.355319
H	-2.819172	-0.737023	5.366676
C	-0.395678	2.697605	0.424664
C	-1.160381	3.707188	-0.175629
C	0.730964	3.066511	1.180994
C	-0.815728	5.051783	-0.011272
H	-2.027899	3.449725	-0.773466
C	1.063929	4.409199	1.358801
H	1.352574	2.296782	1.631810
C	0.290871	5.406919	0.759827
H	-1.418180	5.820837	-0.487419
H	1.933386	4.674431	1.954303
H	0.554200	6.453131	0.889464
H	0.387044	1.618892	-2.086107
C	2.419112	2.145570	-1.771145
H	3.419463	1.707168	-1.872123
H	2.377492	2.561243	-0.757858
H	1.716598	0.800572	-4.089591
H	2.367421	-0.503226	-3.096860
H	0.640086	-0.413649	-3.405551
C	2.299871	3.315954	-2.765464
H	3.100947	4.050401	-2.612611
H	2.358923	2.977140	-3.806902
H	1.342516	3.835837	-2.638384

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B3LYP electronic energy: -1013.90307810 a.u.
B3LYP enthalpy: -1013.544772 a.u.
B3LYP free energy: -1013.616736 a.u.
M06 SCF energy in solution: -1015.19393082 a.u.
M06 enthalpy in solution: -1014.835625 a.u.
M06 free energy in solution: -1014.907589 a.u.

Cartesian coordinates

ATOM	X	Y	Z
H	5.773207	-1.755303	-0.310434
H	5.572531	0.754124	-0.417631
H	3.304956	1.770558	-0.245047
Ni	0.524559	0.604426	0.099905
C	-4.799879	-0.697080	0.307340
C	-3.607317	-1.358009	0.597242

C	-2.450986	-1.109116	-0.155623
C	-2.526868	-0.219839	-1.237335
C	-3.726647	0.429038	-1.541668
C	-4.863052	0.200600	-0.763126
H	-5.685362	-0.888967	0.908297
H	-3.776422	1.103179	-2.393571
H	-5.796202	0.706877	-0.997166
C	-1.199386	-1.887362	0.176042
O	-1.309468	-3.066432	0.550797
N	-0.010901	-1.251089	0.015193
C	1.122405	-2.135270	0.213633
C	2.406690	-1.385409	0.009256
C	3.648353	-2.024453	-0.080493
C	4.804084	-1.270112	-0.237364
C	4.698368	0.122627	-0.299443
C	3.440179	0.697538	-0.206460
N	2.315921	-0.035909	-0.061765
H	3.687605	-3.107990	-0.025682
H	1.127264	-2.575093	1.226529
H	1.087325	-3.003454	-0.462372
C	0.713078	2.508349	0.229019
C	-0.722102	2.326464	0.610496
H	-1.036029	1.208633	0.430981
C	1.002659	3.266314	-1.056846
H	0.820221	4.347011	-0.944870
H	2.046581	3.155054	-1.375243
H	0.373407	2.915299	-1.884070
C	-1.105132	2.610021	2.066467
H	-0.412793	2.115227	2.755722
H	-1.064222	3.687960	2.259136
H	-2.117583	2.259486	2.292063
H	-1.646670	-0.058788	-1.853764
H	-3.550776	-2.085397	1.401115
H	1.352591	2.815001	1.064076
H	-1.413354	2.807292	-0.092591

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B3LYP electronic energy: -1013.88520129 a.u.
B3LYP enthalpy: -1013.528902 a.u.
B3LYP free energy: -1013.600892 a.u.
M06 SCF energy in solution: -1015.17745386 a.u.
M06 enthalpy in solution: -1014.821155 a.u.
M06 free energy in solution: -1014.893145 a.u.

Cartesian coordinates

ATOM	X	Y	Z
H	5.330240	-2.381303	-1.006464
H	5.416295	0.119107	-1.314862
H	3.386026	1.444667	-0.804861
Ni	0.398559	0.652096	0.241550
C	-5.035247	-0.470876	0.387845
C	-3.849691	-1.118158	0.733301
C	-2.672798	-0.889173	0.007866
C	-2.717148	-0.032990	-1.101204
C	-3.908442	0.598928	-1.461889
C	-5.068238	0.390909	-0.711836
H	-5.936981	-0.645980	0.969420
H	-3.932642	1.250710	-2.332068
H	-5.994568	0.888011	-0.989154
C	-1.443712	-1.671173	0.398740
O	-1.586870	-2.812757	0.860781
N	-0.210462	-1.124029	0.166804

C	0.863753	-2.082242	0.389681
C	2.169129	-1.519787	-0.090831
C	3.276907	-2.334914	-0.353377
C	4.463528	-1.762077	-0.793133
C	4.516518	-0.376548	-0.965707
C	3.379759	0.367240	-0.681593
N	2.227239	-0.179153	-0.248081
H	3.189342	-3.408147	-0.215379
H	-3.815542	-1.817379	1.562667
H	0.960969	-2.350581	1.456535
H	0.653049	-3.033279	-0.117809
C	0.806633	2.519301	1.170027
C	0.832664	2.669311	-0.201715
H	-0.946819	0.998355	0.638067
H	-1.816950	0.123988	-1.686272
H	-0.115406	2.773708	1.688634
H	1.800357	2.646703	-0.701860
C	2.015516	2.380518	2.060059
H	2.915848	2.102135	1.505721
H	2.211641	3.338273	2.563680
H	1.851429	1.634070	2.845406
C	-0.294967	3.244422	-1.022538
H	-0.432409	2.695385	-1.960724
H	-1.241711	3.223091	-0.476349
H	-0.069269	4.287970	-1.287227

cis-butene

B3LYP electronic energy: -157.22172609 a.u.
B3LYP enthalpy: -157.106612 a.u.
B3LYP free energy: -157.140812 a.u.
M06 SCF energy in solution: -157.13228102 a.u.
M06 enthalpy in solution: -157.017167 a.u.
M06 free energy in solution: -157.051367 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	0.669537	0.664357	0.000123
H	1.169853	1.633540	-0.000127
C	-0.669243	0.664309	0.000039
H	-1.169538	1.633529	-0.000234
C	1.593282	-0.521993	-0.000033
H	2.250856	-0.505519	-0.880032
H	2.250602	-0.506256	0.880205
H	1.060095	-1.476754	-0.000453
C	-1.593449	-0.521804	0.000005
H	-2.251152	-0.505307	0.879890
H	-2.250540	-0.505499	-0.880382
H	-1.060936	-1.476952	0.000333

trans-butene

B3LYP electronic energy: -157.22387050 a.u.
B3LYP enthalpy: -157.108916 a.u.
B3LYP free energy: -157.142690 a.u.
M06 SCF energy in solution: -157.13401404 a.u.
M06 enthalpy in solution: -157.019060 a.u.
M06 free energy in solution: -157.052834 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	0.538159	0.395577	-0.000039

C	-0.538138	-0.395547	-0.000008
H	-0.392393	-1.477879	-0.000072
C	-1.963781	0.079247	0.000018
H	-2.508479	-0.290062	-0.879875
H	-2.507879	-0.288084	0.881102
H	-2.022879	1.173243	-0.001168
C	1.963779	-0.079251	0.000047
H	2.508127	0.288738	0.880647
H	2.022745	-1.173270	-0.000330
H	2.508220	0.289237	-0.880371
H	0.392424	1.477926	-0.000044

cod

B3LYP electronic energy: -312.02446496 a.u.
B3LYP enthalpy: -311.834900 a.u.
B3LYP free energy: -311.874794 a.u.
M06 SCF energy in solution: -311.86167603 a.u.
M06 enthalpy in solution: -311.672111 a.u.
M06 free energy in solution: -311.712005 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	0.008110	-1.704646	-0.218327
C	1.083058	-1.107451	0.665571
C	1.923422	-0.010896	-0.024155
C	1.215178	1.236011	-0.495444
H	0.291642	-2.634803	-0.711991
H	1.771464	-1.909771	0.959658
H	2.741191	0.283647	0.653636
H	1.821932	1.841492	-1.171141
C	-1.215201	-1.236052	-0.495388
C	-1.923414	0.010885	-0.024175
C	-1.083040	1.107501	0.665572
C	-0.008103	1.704610	-0.218337
H	-1.821999	-1.841574	-1.171014
H	-2.741289	-0.283542	0.653558
H	-1.771498	1.909816	0.959532
H	-0.291585	2.634840	-0.711897
H	2.425435	-0.455887	-0.896261
H	0.665797	-0.724098	1.600149
H	-0.665858	0.724206	1.600210
H	-2.425295	0.455902	-0.896344

Ni(cod)2

B3LYP electronic energy: -793.39808640 a.u.
B3LYP enthalpy: -793.015649 a.u.
B3LYP free energy: -793.075395 a.u.
M06 SCF energy in solution: -794.75361191 a.u.
M06 enthalpy in solution: -794.371175 a.u.
M06 free energy in solution: -794.430921 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	1.537926	0.470607	1.481211
C	2.636584	-0.583207	1.420138
C	2.245574	-1.837050	0.602206
C	1.394386	-1.538005	-0.615237
H	1.004176	0.534137	2.426473
H	2.886554	-0.894887	2.441858
H	3.154458	-2.393615	0.317668

H	0.780744	-2.369788	-0.957744
C	1.394541	1.538311	0.615105
C	2.245001	1.837395	-0.602808
C	2.635669	0.583687	-1.421076
C	1.537278	-0.470451	-1.481579
H	0.780830	2.369860	0.958059
H	3.153993	2.394028	-0.318777
H	2.884838	0.895531	-2.442946
H	1.003055	-0.534152	-2.426557
H	1.673467	-2.514249	1.249344
H	3.553423	-0.140761	1.016951
H	3.552911	0.141418	-1.018603
H	1.672508	2.514614	-1.249596
C	-1.537362	-0.470438	1.481372
C	-2.635631	0.583842	1.421032
C	-2.245276	1.837339	0.602269
C	-1.394987	1.538166	-0.615733
H	-1.003673	-0.534562	2.426645
H	-2.884216	0.896004	2.442943
H	-3.154434	2.393717	0.318272
H	-0.780697	2.369420	-0.958299
C	-1.394564	-1.538235	0.615237
C	-2.245031	-1.837310	-0.602674
C	-2.636582	-0.583518	-1.420289
C	-1.538285	0.470534	-1.481702
H	-0.781405	-2.370106	0.958399
H	-3.153611	-2.394705	-0.318817
H	-2.886848	-0.895184	-2.441949
H	-1.003782	0.533502	-2.426559
H	-1.672727	2.514799	1.248735
H	-3.553180	0.141625	1.019152
H	-3.553358	-0.141271	-1.016742
H	-1.672127	-2.513784	-1.249902
Ni	0.000131	-0.000414	0.000612

pph3

B3LYP electronic energy: -1036.28167341 a.u.
B3LYP enthalpy: -1035.990465 a.u.
B3LYP free energy: -1036.053750 a.u.
M06 SCF energy in solution: -1035.91870448 a.u.
M06 enthalpy in solution: -1035.627496 a.u.
M06 free energy in solution: -1035.690781 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	-0.000292	-0.000205	-1.207261
C	-1.651129	-0.252142	-0.403091
C	-2.760887	0.334847	-1.035175
C	-1.864490	-1.006304	0.761282
C	-4.044384	0.191016	-0.507993
H	-2.616572	0.905051	-1.950174
C	-3.151204	-1.160145	1.283050
H	-1.023296	-1.478066	1.260285
C	-4.242948	-0.560021	0.652940
H	-4.889911	0.655575	-1.008843
H	-3.299353	-1.749757	2.184400
H	-5.243284	-0.682075	1.060130
C	1.043483	-1.303970	-0.403035
C	1.807372	-1.110071	0.758391
C	1.086387	-2.560144	-1.032079
C	2.584250	-2.147202	1.280270
H	1.799325	-0.144674	1.255489

C	1.853008	-3.599513	-0.504862
H	0.517436	-2.721508	-1.944962
C	2.606574	-3.394331	0.653241
H	3.172149	-1.979093	2.179212
H	1.870543	-4.565119	-1.003692
H	3.212451	-4.199615	1.060333
C	0.607441	1.555594	-0.403981
C	1.676961	2.218056	-1.030901
C	0.054739	2.123319	0.754681
C	2.193938	3.401684	-0.503895
H	2.103777	1.804103	-1.941747
C	0.564673	3.314745	1.276152
H	-0.779624	1.635588	1.249725
C	1.636616	3.954745	0.651396
H	3.023930	3.897495	-1.000775
H	0.122966	3.742104	2.172957
H	2.031442	4.882066	1.058227

TS1

B3LYP electronic energy: -2929.20985284 a.u.
B3LYP enthalpy: -2928.386361 a.u.
B3LYP free energy: -2928.527456 a.u.
M06 SCF energy in solution: -2929.89551772 a.u.
M06 enthalpy in solution: -2929.072026 a.u.
M06 free energy in solution: -2929.213121 a.u.
Imaginary frequency: -1121.0759 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ni	-0.203715	0.043557	-0.626059
N	0.356118	-1.112507	-2.312515
H	0.008816	-1.411280	-0.858719
C	-0.393706	-0.405325	-3.350355
H	-0.035792	-0.718014	-4.337100
H	-1.450149	-0.691573	-3.260533
C	-0.329833	1.105812	-3.244911
C	-0.272681	1.934714	-4.367173
C	-0.295751	3.318620	-4.199567
H	-0.205263	1.492130	-5.355989
C	-0.416506	2.951391	-1.835213
C	-0.375847	3.838505	-2.907796
H	-0.248518	3.978508	-5.061631
H	-0.468201	3.306653	-0.811430
H	-0.395841	4.908465	-2.726391
N	-0.389449	1.616540	-1.993137
C	1.612385	-1.515720	-2.667357
O	2.180651	-1.159763	-3.709467
C	2.295239	-2.518957	-1.768429
C	1.592294	-3.520805	-1.083841
C	3.696672	-2.520311	-1.717529
C	2.275056	-4.493278	-0.349307
H	0.509251	-3.553686	-1.145170
C	4.378602	-3.477529	-0.967979
H	4.235359	-1.763016	-2.276652
C	3.669965	-4.469094	-0.282531
H	1.716559	-5.272248	0.163606
H	5.464550	-3.456843	-0.925225
H	4.202763	-5.224649	0.289662
P	1.542925	0.747369	0.721115
C	2.011533	-0.192263	2.252973
C	1.954671	0.345546	3.547018

C	2.415347	-1.530687	2.097895
C	2.289574	-0.434687	4.657710
H	1.650830	1.376700	3.695193
C	2.759796	-2.303620	3.206295
H	2.461448	-1.972601	1.107350
C	2.695073	-1.759302	4.492518
H	2.237664	0.000082	5.652821
H	3.077262	-3.332618	3.059589
H	2.960609	-2.362483	5.356950
C	3.202586	0.951060	-0.087533
C	3.244893	1.162559	-1.473499
C	4.412435	0.921669	0.626685
C	4.463181	1.346649	-2.131162
H	2.325073	1.155308	-2.046772
C	5.629928	1.105092	-0.030510
H	4.404221	0.750202	1.698767
C	5.658250	1.319881	-1.411019
H	4.472675	1.489454	-3.207969
H	6.557209	1.076893	0.536397
H	6.607857	1.455973	-1.922273
C	1.231690	2.456651	1.387024
C	2.189990	3.482494	1.388320
C	-0.050014	2.739937	1.889971
C	1.874050	4.751983	1.879515
H	3.186650	3.295253	1.002944
C	-0.362331	4.004509	2.391716
H	-0.813258	1.968308	1.878086
C	0.599964	5.017176	2.384213
H	2.629052	5.534174	1.867291
H	-1.361830	4.195775	2.772784
H	0.357383	6.005989	2.764975
P	-2.239483	-0.464562	0.152828
C	-3.421011	-1.254756	-1.051867
C	-4.763802	-0.876169	-1.204450
C	-2.935686	-2.324259	-1.825002
C	-5.596674	-1.548418	-2.103547
H	-5.166521	-0.053509	-0.622361
C	-3.770658	-3.001296	-2.714146
H	-1.892095	-2.615820	-1.743354
C	-5.105369	-2.614448	-2.857469
H	-6.633267	-1.237950	-2.208931
H	-3.374926	-3.826204	-3.300988
H	-5.754988	-3.137389	-3.554346
C	-3.197854	1.016006	0.729613
C	-3.567966	1.212685	2.068954
C	-3.479101	2.036901	-0.197200
C	-4.205334	2.391554	2.468517
H	-3.363024	0.443227	2.806066
C	-4.126674	3.206223	0.199373
H	-3.193202	1.910973	-1.237365
C	-4.490318	3.390054	1.536648
H	-4.486282	2.521219	3.510713
H	-4.344289	3.976708	-0.535976
H	-4.992639	4.302516	1.846870
C	-2.403488	-1.644270	1.576181
C	-1.253302	-2.000089	2.291541
C	-3.636880	-2.200690	1.958217
C	-1.329391	-2.882462	3.372883
H	-0.294632	-1.591137	1.994497
C	-3.713168	-3.082114	3.035928
H	-4.539270	-1.952079	1.407259
C	-2.558765	-3.423945	3.747372
H	-0.423343	-3.141900	3.913522
H	-4.673302	-3.506831	3.318046

H	-2.620466	-4.113569	4.585455

TS2

B3LYP electronic energy: -1012.63427171 a.u.
B3LYP enthalpy: -1012.303376 a.u.
B3LYP free energy: -1012.374601 a.u.
M06 SCF energy in solution: -1013.93428652 a.u.
M06 enthalpy in solution: -1013.603391 a.u.
M06 free energy in solution: -1013.674616 a.u.
Imaginary frequency: -92.9440 cm-1

Cartesian coordinates

ATOM	X	Y	Z
H	-5.373841	-2.246692	1.047822
H	-5.291096	0.214531	1.573681
H	-3.223458	1.480514	0.995650
Ni	-0.466310	0.655316	-0.311805
C	4.939483	-0.523813	-0.233506
C	3.771278	-1.135950	-0.687157
C	2.560617	-0.958859	-0.004900
C	2.551259	-0.192144	1.169056
C	3.725067	0.401289	1.638554
C	4.920518	0.247172	0.931938
H	5.868779	-0.658130	-0.781666
H	3.708990	0.976064	2.561951
H	5.833581	0.713133	1.294259
C	1.345387	-1.701711	-0.507230
O	1.500233	-2.812282	-1.038182
N	0.121690	-1.145812	-0.284957
C	-0.978698	-2.042965	-0.615130
C	-2.247563	-1.477704	-0.044514
C	-3.375928	-2.253663	0.238768
C	-4.492684	-1.656181	0.813083
C	-4.453687	-0.290154	1.103315
C	-3.305374	0.421255	0.781547
N	-2.231036	-0.149053	0.204582
H	-3.358108	-3.316915	0.020832
H	-1.095095	-2.178694	-1.705503
H	-0.797338	-3.051537	-0.221339
C	-1.138721	2.550090	-0.598066
C	0.055333	2.652870	-0.252984
H	0.870750	0.967293	-0.788973
C	-2.453069	3.047277	-1.064926
H	-2.300111	3.771236	-1.874376
H	-3.092394	2.247200	-1.448169
H	-2.995381	3.563756	-0.263072
C	1.345824	3.284433	0.086952
H	2.034416	3.230753	-0.764141
H	1.184414	4.338288	0.344026
H	1.832167	2.783812	0.928287
H	1.622122	-0.079025	1.719010
H	3.777596	-1.769583	-1.568456

TS3

B3LYP electronic energy: -1012.64500659 a.u.
B3LYP enthalpy: -1012.314419 a.u.
B3LYP free energy: -1012.383966 a.u.
M06 SCF energy in solution: -1013.94111571 a.u.
M06 enthalpy in solution: -1013.610528 a.u.
M06 free energy in solution: -1013.680075 a.u.

Imaginary frequency: -1229.2779 cm-1

Cartesian coordinates

ATOM	X	Y	Z
H	5.661997	-1.455104	-0.255343
H	5.121621	1.003972	-0.237729
H	2.717092	1.690344	-0.123927
Ni	0.090691	0.172675	0.015896
C	-4.712936	-0.491783	-0.176842
C	-3.720363	-1.461804	-0.027029
C	-2.376632	-1.100513	0.054853
C	-1.999388	0.262079	0.000259
C	-3.004921	1.222841	-0.173210
C	-4.352078	0.851068	-0.262270
H	-5.758067	-0.784064	-0.237610
H	-2.744747	2.277718	-0.226649
H	-5.112363	1.617347	-0.391863
C	-1.331936	-2.188254	0.090097
O	-1.596570	-3.385451	0.239951
N	-0.102188	-1.662511	-0.099484
C	1.073999	-2.487759	-0.056867
C	2.268236	-1.567856	-0.091394
C	3.586897	-2.026415	-0.156490
C	4.632771	-1.111470	-0.204050
C	4.338492	0.254540	-0.192626
C	3.008957	0.646213	-0.125151
N	1.994454	-0.239100	-0.067997
H	3.775378	-3.095514	-0.173387
H	1.109600	-3.118034	0.847815
H	1.129419	-3.189733	-0.905587
C	0.163258	2.131468	0.388040
C	0.093371	2.998633	-0.640362
H	-0.296537	2.622093	-1.588731
C	0.591564	2.473065	1.797087
H	0.768854	3.544322	1.951305
H	-0.174629	2.159125	2.517480
H	1.509601	1.939700	2.078259
C	0.488203	4.453181	-0.672892
H	-0.368766	5.082384	-0.949865
H	0.876431	4.813308	0.283428
H	1.258371	4.626874	-1.437088
H	-3.955130	-2.522102	0.011287
H	-1.015747	1.203947	0.338973

TS4

B3LYP electronic energy: -856.61535223 a.u.
B3LYP enthalpy: -856.382052 a.u.
B3LYP free energy: -856.438216 a.u.
M06 SCF energy in solution: -857.99555580 a.u.
M06 enthalpy in solution: -857.762256 a.u.
M06 free energy in solution: -857.818420 a.u.
Imaginary frequency: -1224.9880 cm-1

Cartesian coordinates

ATOM	X	Y	Z
H	5.772271	0.409564	-0.069370
H	5.068460	-2.004833	0.041198
H	2.626379	-2.529153	0.088575
Ni	0.124094	-0.829117	0.041322
C	-4.626095	0.021668	-0.069798
C	-3.596391	0.960802	0.013755
C	-2.265530	0.551920	0.065485

C	-1.937032	-0.823833	0.043778
C	-2.979899	-1.754161	-0.061813
C	-4.315304	-1.335533	-0.117448
H	-5.661979	0.348379	-0.107517
H	-2.765062	-2.820929	-0.095810
H	-5.106373	-2.077171	-0.194608
C	-1.173302	1.591262	0.054751
O	-1.375045	2.805360	0.139545
N	0.033189	0.996055	-0.088214
C	1.258257	1.748446	-0.082394
C	2.391107	0.753578	-0.050924
C	3.738816	1.120420	-0.080632
C	4.721068	0.136974	-0.047501
C	4.336213	-1.205087	0.013907
C	2.982492	-1.507106	0.040262
N	2.027391	-0.553690	0.008132
H	4.000536	2.172909	-0.129446
H	-3.793579	2.029388	0.024544
H	1.360556	2.394714	-0.970191
H	1.328251	2.425054	0.785507
H	-0.952301	-1.848737	0.322026
H	0.018099	-2.379443	0.263720

TS5

B3LYP electronic energy: -1011.42443657 a.u.
B3LYP enthalpy: -1011.114184 a.u.
B3LYP free energy: -1011.181129 a.u.
M06 SCF energy in solution: -1012.72479346 a.u.
M06 enthalpy in solution: -1012.414541 a.u.
M06 free energy in solution: -1012.481486 a.u.
Imaginary frequency: -256.4272 cm-1

Cartesian coordinates

ATOM	X	Y	Z
H	5.831588	-0.934674	-0.483834
H	5.103207	1.385474	-1.137399
H	2.680241	1.960456	-0.962871
Ni	0.173672	0.422273	-0.077378
C	-4.279585	-0.791727	-1.070823
C	-3.383755	-1.573188	-0.332541
C	-2.146740	-1.060351	0.044327
C	-1.796967	0.276075	-0.277111
C	-2.675943	1.026265	-1.069667
C	-3.909084	0.492487	-1.468144
H	-5.245901	-1.196174	-1.361050
H	-2.420183	2.046140	-1.340370
H	-4.582506	1.093869	-2.073873
C	-1.059788	-1.995713	0.524737
O	-1.262375	-3.117392	1.001338
N	0.130903	-1.430191	0.239982
C	1.378004	-2.090146	0.509160
C	2.483242	-1.158228	0.067602
C	3.824295	-1.547534	0.005460
C	4.787252	-0.641402	-0.425363
C	4.388753	0.647226	-0.788689
C	3.042843	0.974784	-0.695768
N	2.107607	0.100281	-0.275656
H	4.095140	-2.560337	0.287935
H	-3.599741	-2.609066	-0.083258
H	1.511510	-2.331157	1.579508
H	1.470114	-3.051470	-0.021643
C	-0.052005	2.279021	0.337275

C	-1.069319	1.703211	0.885187
C	-2.061092	1.795383	1.994623
H	-1.802499	2.652403	2.629523
H	-3.083112	1.925508	1.623142
H	-2.044873	0.891396	2.613000
C	0.690598	3.566758	0.405874
H	0.771875	4.033254	-0.584739
H	0.203124	4.289282	1.074531
H	1.714366	3.412438	0.770132

TS6

B3LYP electronic energy: -2047.75970320 a.u.
B3LYP enthalpy: -2047.154604 a.u.
B3LYP free energy: -2047.261985 a.u.
M06 SCF energy in solution: -2048.70940455 a.u.
M06 enthalpy in solution: -2048.104305 a.u.
M06 free energy in solution: -2048.211686 a.u.
Imaginary frequency: -308.3586 cm-1

Cartesian coordinates

ATOM	X	Y	Z
N	-2.126993	1.415105	-1.068062
C	-3.038538	1.294729	-0.020329
C	-3.370735	-0.075916	0.435567
C	-3.138306	-1.253181	-0.341805
C	-4.089547	-0.162715	1.643400
C	-4.576011	-1.372204	2.113034
H	-4.267945	0.761256	2.183783
C	-4.380815	-2.531427	1.344300
H	-5.116868	-1.419987	3.054344
H	-4.767067	-3.487055	1.691930
O	-3.560693	2.303507	0.478663
C	-1.535053	-0.182432	-1.841986
C	-2.426040	-1.207432	-1.598733
C	-2.694537	-2.284333	-2.634211
H	-2.137960	-3.213285	-2.437575
H	-3.758891	-2.549624	-2.669442
H	-2.408431	-1.959122	-3.638396
C	-0.936846	0.068048	-3.210639
H	-0.253622	-0.750851	-3.467392
H	-1.694765	0.134981	-4.004058
H	-0.345396	0.989544	-3.238177
Ni	-0.431588	0.739032	-0.572314
C	-3.695443	-2.466588	0.142106
H	-3.556393	-3.374583	-0.437311
C	-1.923379	2.782441	-1.542989
H	-2.876284	3.319208	-1.566057
H	-1.526026	2.739327	-2.565049
C	-0.927467	3.517475	-0.661500
C	-0.931868	4.904229	-0.502329
C	0.040816	5.500979	0.296353
H	-1.698857	5.499259	-0.988406
C	0.940051	3.320190	0.702139
C	0.999734	4.694204	0.910953
H	0.047652	6.577692	0.442227
H	1.666545	2.651411	1.153602
H	1.775601	5.115292	1.542263
N	-0.000575	2.738654	-0.061097
P	1.260816	-0.550361	0.055662
C	1.231999	-0.910519	1.868184
C	1.927171	-1.989899	2.438869
C	0.476096	-0.073731	2.703982

C	1.878621	-2.214790	3.815142
H	2.497997	-2.662542	1.805218
C	0.429516	-0.299482	4.081129
H	-0.094139	0.743322	2.270484
C	1.132161	-1.368557	4.638974
H	2.418627	-3.055386	4.243113
H	-0.167235	0.352418	4.713217
H	1.090065	-1.549489	5.709749
C	2.919941	0.222525	-0.231377
C	3.966007	0.210570	0.703596
C	3.120308	0.882695	-1.456615
C	5.181753	0.837313	0.417458
H	3.833262	-0.284941	1.660034
C	4.338983	1.495987	-1.747278
H	2.313460	0.917257	-2.184416
C	5.372997	1.477343	-0.807921
H	5.980159	0.822150	1.154874
H	4.477641	1.995818	-2.702360
H	6.319955	1.962612	-1.028802
C	1.433054	-2.235585	-0.680733
C	2.582751	-2.676468	-1.350782
C	0.332994	-3.104325	-0.569084
C	2.634286	-3.962154	-1.897055
H	3.442604	-2.021302	-1.446990
C	0.393833	-4.390556	-1.104707
H	-0.570288	-2.772961	-0.065703
C	1.542968	-4.822034	-1.773297
H	3.532463	-4.290170	-2.414010
H	-0.459537	-5.055627	-1.002054
H	1.585683	-5.822844	-2.194868

TS7

B3LYP electronic energy: -1011.42933525 a.u.
B3LYP enthalpy: -1011.117711 a.u.
B3LYP free energy: -1011.182773 a.u.
M06 SCF energy in solution: -1012.72151978 a.u.
M06 enthalpy in solution: -1012.409896 a.u.
M06 free energy in solution: -1012.474958 a.u.
Imaginary frequency: -331.7593 cm-1

Cartesian coordinates

ATOM	X	Y	Z
N	0.165869	0.315969	0.949524
C	-0.407278	-0.954272	1.005959
C	-1.712798	-1.130825	0.330980
C	-2.530697	-0.058859	-0.140432
C	-2.166118	-2.458826	0.224207
C	-3.394925	-2.761886	-0.339633
H	-1.516335	-3.236745	0.610601
C	-4.216383	-1.716682	-0.790923
H	-3.721841	-3.794687	-0.423009
H	-5.185505	-1.936274	-1.232570
O	0.168725	-1.880021	1.594011
C	-0.823386	1.694060	0.227261
C	-2.147714	1.330897	0.017104
C	-3.248205	2.376350	0.037033
H	-3.680001	2.536776	-0.960708
H	-4.074927	2.076282	0.694679
H	-2.884264	3.345595	0.383946
C	-0.415970	3.032084	0.814585
H	-0.682136	3.844490	0.128956
H	-0.899779	3.234964	1.779859

H	0.666288	3.096814	0.960090
Ni	0.503232	0.925242	-0.806748
C	-3.798053	-0.401094	-0.679725
H	-4.450250	0.389022	-1.037136
C	1.505646	0.402028	1.544635
H	1.541924	-0.193691	2.460902
H	1.707197	1.448325	1.802005
C	2.577731	-0.080220	0.568943
C	3.764950	-0.670387	0.999081
C	4.721071	-1.052884	0.059573
H	3.926111	-0.836770	2.059539
C	3.253218	-0.249232	-1.652568
C	4.461742	-0.837170	-1.294049
H	5.648705	-1.519718	0.378300
H	3.001583	-0.068991	-2.693138
H	5.173777	-1.125022	-2.060661
N	2.327297	0.126106	-0.750520

TS8

B3LYP electronic energy: -1012.65217490 a.u.
B3LYP enthalpy: -1012.317919 a.u.
B3LYP free energy: -1012.384019 a.u.
M06 SCF energy in solution: -1013.95263027 a.u.
M06 enthalpy in solution: -1013.618374 a.u.
M06 free energy in solution: -1013.684474 a.u.
Imaginary frequency: -276.9975 cm-1

Cartesian coordinates

ATOM	X	Y	Z
H	5.678537	-1.220915	-0.702974
H	5.043345	1.082443	-1.500111
H	2.667308	1.806951	-1.256913
Ni	0.141233	0.470216	-0.204043
C	-4.314231	-0.720531	-1.152015
C	-3.472635	-1.425662	-0.289812
C	-2.259953	-0.876621	0.128290
C	-1.902358	0.441587	-0.253058
C	-2.729400	1.106493	-1.172833
C	-3.917391	0.531092	-1.628987
H	-5.254793	-1.157063	-1.477831
H	-2.475647	2.114795	-1.495397
H	-4.544587	1.075056	-2.330714
C	-1.201310	-1.806505	0.683487
O	-1.437355	-2.834381	1.327640
N	-0.005995	-1.368052	0.237543
C	1.216235	-2.062983	0.534943
C	2.351111	-1.216473	0.003074
C	3.665646	-1.682802	-0.086650
C	4.655328	-0.865289	-0.621670
C	4.309097	0.413767	-1.063383
C	2.989351	0.824364	-0.934204
N	2.029509	0.038358	-0.407217
H	3.893352	-2.688368	0.253767
H	-3.701700	-2.440138	0.026262
H	1.357470	-2.235811	1.617170
H	1.261227	-3.062049	0.071602
C	0.048965	2.371792	0.190387
C	-1.143664	1.813236	0.861920
H	-0.212235	3.014370	-0.657077
H	-2.050434	2.386690	0.696380
C	1.182873	2.949581	1.022967

H	2.042942	3.211716	0.396622
H	0.877536	3.875977	1.535244
H	1.539599	2.257115	1.792665
C	-1.070895	1.369243	2.315816
H	-0.196526	0.750507	2.532170
H	-1.023702	2.260240	2.956850
H	-1.962584	0.799621	2.592461

TS9

B3LYP electronic energy: -2162.08635190 a.u.
B3LYP enthalpy: -2161.462036 a.u.
B3LYP free energy: -2161.571927 a.u.
M06 SCF energy in solution: -2162.97609107 a.u.
M06 enthalpy in solution: -2162.351775 a.u.
M06 free energy in solution: -2162.461666 a.u.
Imaginary frequency: -323.7549 cm-1

Cartesian coordinates

ATOM	X	Y	Z
N	2.264530	0.953882	-0.210088
C	2.377242	1.975559	0.750807
C	0.544974	3.345322	-0.417247
O	3.305206	1.983809	1.563069
C	0.983178	1.208713	-1.517834
C	0.583230	2.524410	-1.606318
Ni	0.645016	-0.038769	-0.084759
C	3.116162	-1.303511	0.128523
C	4.168252	-2.266567	0.066221
C	3.867750	-3.585342	0.494201
C	1.625843	-2.864923	0.979850
C	2.602975	-3.884412	0.948612
H	4.643005	-4.346831	0.456407
H	0.622769	-3.075850	1.340006
H	2.343843	-4.882951	1.286019
N	1.860270	-1.620658	0.587080
P	-1.484443	-0.635505	0.003898
C	-2.132496	-0.507939	1.730083
C	-3.495056	-0.337215	2.023429
C	-1.213601	-0.580412	2.789642
C	-3.927918	-0.253251	3.347880
H	-4.216953	-0.259168	1.215739
C	-1.648865	-0.498548	4.113379
H	-0.153300	-0.684418	2.573242
C	-3.006669	-0.335830	4.394616
H	-4.984925	-0.117368	3.561452
H	-0.925058	-0.549024	4.922300
H	-3.345208	-0.263966	5.424799
C	-1.793298	-2.402475	-0.460281
C	-2.638205	-3.261833	0.258286
C	-1.121773	-2.906358	-1.587893
C	-2.809436	-4.589208	-0.143541
H	-3.163108	-2.897607	1.135879
C	-1.303801	-4.227740	-1.996391
H	-0.450178	-2.259226	-2.146189
C	-2.146625	-5.074338	-1.271986
H	-3.464457	-5.242732	0.426846
H	-0.780730	-4.598051	-2.874178
H	-2.282592	-6.106567	-1.583525
C	-2.740905	0.291644	-0.980044
C	-3.674353	-0.326131	-1.824651
C	-2.738831	1.693223	-0.875791
C	-4.589836	0.441951	-2.549478

H	-3.692222	-1.407233	-1.918665
C	-3.662145	2.455220	-1.591339
H	-2.014774	2.190214	-0.237697
C	-4.587720	1.832218	-2.433122
H	-5.306797	-0.050593	-3.201336
H	-3.653505	3.537470	-1.493023
H	-5.301909	2.428096	-2.995351
C	3.346564	0.038548	-0.297827
C	4.599795	0.389470	-0.769205
H	4.778283	1.414818	-1.075691
C	5.639574	-0.563607	-0.831848
C	5.436509	-1.866960	-0.427075
H	6.612871	-0.258823	-1.206186
H	6.236310	-2.600378	-0.486724
C	0.176029	3.135767	-2.933621
H	0.569168	4.154580	-3.045137
H	0.543886	2.550325	-3.780356
H	-0.916828	3.198130	-3.044942
C	1.300556	0.365139	-2.735360
H	0.376257	0.128686	-3.276975
H	1.979658	0.872325	-3.434827
H	1.766880	-0.585783	-2.460058
C	1.341247	3.036978	0.726966
C	1.297536	3.871969	1.859524
C	0.481823	4.991733	1.902650
H	0.448589	5.614239	2.792566
C	-0.282560	5.323675	0.772499
H	-0.915106	6.208499	0.783602
C	-0.237265	4.528709	-0.361932
H	1.943824	3.616855	2.692863
H	-0.834017	4.805529	-1.225858

TS10A

B3LYP electronic energy: -1203.16320932 a.u.
B3LYP enthalpy: -1202.796526 a.u.
B3LYP free energy: -1202.871715 a.u.
M06 SCF energy in solution: -1204.36529071 a.u.
M06 enthalpy in solution: -1203.998607 a.u.
M06 free energy in solution: -1204.073796 a.u.
Imaginary frequency: -237.8356 cm-1

Cartesian coordinates

ATOM	X	Y	Z
H	-2.529588	5.273066	-0.425132
H	-3.727502	3.163136	-1.100836
H	-2.488998	1.001918	-0.975695
Ni	0.363494	0.216588	-0.147611
C	4.316256	-2.219710	-0.977448
C	4.246348	-1.040182	-0.227456
C	3.013330	-0.486829	0.101104
C	1.811837	-1.136377	-0.282158
C	1.895749	-2.280479	-1.087943
C	3.142623	-2.816301	-1.436931
H	5.282312	-2.649714	-1.229092
H	0.987407	-2.784075	-1.404337
H	3.187686	-3.711238	-2.052452
C	2.939269	0.942929	0.588477
O	3.877106	1.550033	1.115365
N	1.732984	1.439285	0.245754
C	1.365410	2.803785	0.505530
C	-0.068078	2.978473	0.060586
C	-0.703485	4.222637	0.028517

C	-2.026456	4.310829	-0.391118
C	-2.694928	3.144229	-0.768608
C	-2.010964	1.937312	-0.708797
N	-0.727006	1.850374	-0.307969
H	-0.150753	5.107676	0.328860
H	5.140302	-0.496638	0.067656
H	1.451654	3.071385	1.573809
H	2.008981	3.521095	-0.029327
C	-0.853390	-1.238080	0.176903
C	0.237965	-1.568532	0.792855
C	0.778487	-2.378794	1.923226
C	-2.274505	-1.548525	0.149967
C	-2.954424	-1.667867	-1.078051
C	-3.010853	-1.724805	1.338798
C	-4.314646	-1.973971	-1.116377
H	-2.396636	-1.531585	-2.000986
C	-4.372249	-2.021251	1.296473
H	-2.506463	-1.618309	2.294993
C	-5.030020	-2.150462	0.070253
H	-4.816666	-2.073510	-2.075337
H	-4.921617	-2.153226	2.225149
H	-6.090806	-2.383792	0.040564
H	1.382824	-1.759753	2.595713
H	-0.059537	-2.796577	2.494131
H	1.411205	-3.200382	1.571213

TS10B

B3LYP electronic energy: -1203.15837362 a.u.
B3LYP enthalpy: -1202.791891 a.u.
B3LYP free energy: -1202.866893 a.u.
M06 SCF energy in solution: -1204.36260487 a.u.
M06 enthalpy in solution: -1203.996122 a.u.
M06 free energy in solution: -1204.071124 a.u.
Imaginary frequency: -244.9127 cm-1

Cartesian coordinates

ATOM	X	Y	Z
H	-6.441282	-0.893005	0.729714
H	-5.343948	-2.415596	-0.948984
H	-2.921634	-2.078435	-1.449146
Ni	-0.779333	-0.123505	-0.440888
C	2.572812	2.938780	-1.717745
C	1.774722	3.056042	-0.574727
C	0.935323	2.015477	-0.190374
C	0.912633	0.806067	-0.930824
C	1.667761	0.724635	-2.107851
C	2.490290	1.788513	-2.500786
H	3.229862	3.753583	-2.010588
H	1.653409	-0.186082	-2.697565
H	3.079707	1.700975	-3.409987
C	-0.153912	2.271818	0.826903
O	-0.136648	3.193272	1.650151
N	-1.152026	1.396134	0.598844
C	-2.386578	1.421160	1.331854
C	-3.276449	0.350872	0.741833
C	-4.625760	0.214107	1.079259
C	-5.389751	-0.782014	0.480733
C	-4.785980	-1.629822	-0.450778
C	-3.439186	-1.448798	-0.735120
N	-2.695014	-0.487396	-0.153925
H	-5.063195	0.897568	1.800683
H	1.744226	3.971877	0.010105

H	-2.248530	1.224603	2.410719
H	-2.891255	2.398780	1.272971
C	0.059762	-1.774083	-0.896031
C	0.997197	-1.075591	-0.330322
C	-0.236142	-3.197472	-1.210889
C	2.253173	-1.227065	0.404639
C	3.155462	-2.226905	-0.003228
C	2.563272	-0.455637	1.536779
C	4.328579	-2.457852	0.713904
H	2.934922	-2.813934	-0.890135
C	3.737926	-0.690146	2.248546
H	1.881266	0.325679	1.856113
C	4.624719	-1.690881	1.842439
H	5.015655	-3.232825	0.384028
H	3.961747	-0.086064	3.123667
H	5.541896	-1.866937	2.397867
H	-0.348788	-3.347558	-2.293107
H	0.557448	-3.870634	-0.860000
H	-1.176960	-3.518440	-0.746434

TS11A

B3LYP electronic energy: -1321.09886709 a.u.
B3LYP enthalpy: -1320.643225 a.u.
B3LYP free energy: -1320.726153 a.u.
M06 SCF energy in solution: -1322.24610984 a.u.
M06 enthalpy in solution: -1321.790468 a.u.
M06 free energy in solution: -1321.873396 a.u.
Imaginary frequency: -227.0653 cm-1

Cartesian coordinates

ATOM	X	Y	Z
H	-2.863804	5.518467	-0.136996
H	-3.957446	3.454336	-1.077973
H	-2.663330	1.319474	-1.075291
Ni	0.197359	0.540837	-0.233858
C	4.166084	-1.347404	-1.872660
C	4.113339	-0.327011	-0.915457
C	2.897211	0.050609	-0.355452
C	1.703111	-0.632174	-0.705725
C	1.760615	-1.603941	-1.713929
C	2.985618	-1.954532	-2.298316
H	5.118475	-1.638089	-2.308405
H	0.856432	-2.121581	-2.016615
H	3.010868	-2.719769	-3.070067
C	2.784680	1.375053	0.368915
O	3.741149	1.987506	0.854988
N	1.505654	1.787812	0.279323
C	1.067991	3.079044	0.730728
C	-0.359224	3.254068	0.260885
C	-1.031475	4.477686	0.315040
C	-2.334539	4.570107	-0.163695
C	-2.945839	3.428681	-0.686778
C	-2.229309	2.238797	-0.698342
N	-0.968420	2.146623	-0.233620
H	-0.520624	5.346316	0.719377
H	4.997932	0.238246	-0.632885
H	1.101301	3.183014	1.830977
H	1.695569	3.893890	0.337448
C	-0.895850	-1.044321	-0.068448
C	0.252286	-1.360146	0.443610
C	0.854456	-2.195801	1.563617
C	1.891898	-3.224648	1.068868

H	1.468559	-3.878614	0.298742
H	2.781953	-2.742676	0.657967
H	2.204853	-3.852854	1.911426
C	-0.324150	-2.954685	2.218763
H	-1.077321	-2.262092	2.607648
H	-0.816034	-3.623654	1.505022
H	0.049338	-3.559826	3.053005
C	1.506080	-1.272767	2.615388
H	0.782374	-0.551316	3.009854
H	1.880133	-1.875863	3.451520
H	2.349273	-0.716811	2.197086
C	-2.274482	-1.482701	-0.179411
C	-2.610787	-2.588370	-0.987423
C	-3.314600	-0.817283	0.501313
C	-3.933191	-3.011392	-1.104769
H	-1.822273	-3.110094	-1.522319
C	-4.635119	-1.250294	0.386223
H	-3.073017	0.028331	1.138836
C	-4.953112	-2.346008	-0.419388
H	-4.167585	-3.867380	-1.732418
H	-5.418512	-0.730325	0.931964
H	-5.983165	-2.679043	-0.511028

TS11B

B3LYP electronic energy: -1321.09317788 a.u.
B3LYP enthalpy: -1320.637882 a.u.
B3LYP free energy: -1320.721839 a.u.
M06 SCF energy in solution: -1322.23867978 a.u.
M06 enthalpy in solution: -1321.783384 a.u.
M06 free energy in solution: -1321.867341 a.u.
Imaginary frequency: -246.5845 cm-1

Cartesian coordinates

ATOM	X	Y	Z
H	-6.479805	-0.290346	-0.872264
H	-5.605637	1.586170	0.564079
H	-3.163625	1.667425	1.048255
Ni	-0.737461	-0.113342	0.290353
C	2.554768	-2.684926	2.469297
C	1.864987	-3.083476	1.319189
C	1.049784	-2.187148	0.636317
C	0.940426	-0.844915	1.079998
C	1.584455	-0.473457	2.267692
C	2.384406	-1.391730	2.960466
H	3.194775	-3.389642	2.993734
H	1.500576	0.545530	2.630153
H	2.888042	-1.080384	3.872247
C	0.059004	-2.710721	-0.377341
O	0.122079	-3.830259	-0.896310
N	-0.931514	-1.806816	-0.507944
C	-2.148115	-2.092485	-1.213265
C	-3.170352	-1.069266	-0.772341
C	-4.525081	-1.169317	-1.101625
C	-5.422983	-0.217107	-0.631834
C	-4.943690	0.825469	0.163885
C	-3.583845	0.876465	0.439781
N	-2.707525	-0.038575	-0.019476
H	-4.860920	-2.002859	-1.711093
H	1.895872	-4.108629	0.958987
H	-2.034603	-2.035157	-2.311836
H	-2.517151	-3.109191	-1.007145
C	0.090769	1.622664	0.427047

C	1.021786	0.792639	0.045316
C	-0.163467	3.109547	0.452951
C	1.152222	3.901329	0.287530
H	1.648689	3.656355	-0.656436
H	0.950716	4.979932	0.298030
H	1.849350	3.681416	1.103727
C	-1.115889	3.481035	-0.707669
H	-2.065044	2.940988	-0.641258
H	-1.332534	4.556529	-0.689439
H	-0.660801	3.240290	-1.674474
C	-0.807701	3.501436	1.802222
H	-1.747015	2.964817	1.972841
H	-0.139115	3.267446	2.638355
H	-1.019097	4.577712	1.826886
C	2.249555	0.677451	-0.757343
C	3.454382	1.252971	-0.322857
C	2.224362	0.000575	-1.988208
C	4.600691	1.174801	-1.113765
H	3.488217	1.757669	0.637674
C	3.373582	-0.079968	-2.772835
H	1.300476	-0.465634	-2.317636
C	4.564376	0.509278	-2.340737
H	5.525082	1.628632	-0.766149
H	3.338869	-0.606643	-3.722730
H	5.459642	0.444100	-2.953193

TS12

B3LYP electronic energy: -1013.87919699 a.u.
B3LYP enthalpy: -1013.524021 a.u.
B3LYP free energy: -1013.594470 a.u.
M06 SCF energy in solution: -1015.17240822 a.u.
M06 enthalpy in solution: -1014.817232 a.u.
M06 free energy in solution: -1014.887681 a.u.
Imaginary frequency: -70.6604 cm-1

Cartesian coordinates

ATOM	X	Y	Z
H	-5.614033	-2.117114	0.672731
H	-5.510799	0.321493	1.304403
H	-3.371875	1.530954	1.010859
Ni	-0.459963	0.651576	-0.091781
C	4.885672	-0.771054	-0.307011
C	3.674121	-1.314781	-0.732642
C	2.496364	-1.093330	-0.006630
C	2.564281	-0.353667	1.182579
C	3.780218	0.174067	1.621786
C	4.942821	-0.023489	0.872240
H	5.788460	-0.938843	-0.889114
H	3.822136	0.732537	2.554128
H	5.888658	0.391700	1.211447
C	1.232592	-1.759830	-0.494874
O	1.321674	-2.854435	-1.071492
N	0.033836	-1.164979	-0.222847
C	-1.096084	-2.009869	-0.577314
C	-2.368188	-1.407815	-0.058554
C	-3.544144	-2.155456	0.073037
C	-4.695126	-1.548867	0.559507
C	-4.643425	-0.197531	0.910126
C	-3.444542	0.481905	0.746931

N	-2.324975	-0.096155	0.269037
H	-3.536296	-3.205644	-0.201913
H	-1.183598	-2.147846	-1.669827
H	-0.968774	-3.025412	-0.178213
C	-1.069254	2.664863	-0.192376
C	0.196180	2.679030	0.364937
H	0.887418	0.903451	-0.539769
C	-1.407385	3.071075	-1.606037
H	-1.616115	4.149336	-1.665708
H	-0.593043	2.850423	-2.302112
H	-2.301638	2.546226	-1.959659
C	1.448006	3.250435	-0.257213
H	1.426425	3.220715	-1.348907
H	1.544140	4.301973	0.051496
H	2.338758	2.716714	0.084584
H	1.661395	-0.205684	1.766388
H	3.619222	-1.927492	-1.626816
H	0.252034	2.556637	1.447480
H	-1.901591	2.651057	0.506040

TS13

B3LYP electronic energy: -1013.88312428 a.u.
B3LYP enthalpy: -1013.527926 a.u.
B3LYP free energy: -1013.598368 a.u.
M06 SCF energy in solution: -1015.17582113 a.u.
M06 enthalpy in solution: -1014.820623 a.u.
M06 free energy in solution: -1014.891065 a.u.
Imaginary frequency: -39.9876 cm-1

Cartesian coordinates

ATOM	X	Y	Z
H	5.310133	-2.433601	-0.934765
H	5.357350	0.026721	-1.479611
H	3.337609	1.382949	-1.008820
Ni	0.422394	0.668007	0.230206
C	-5.019015	-0.467353	0.173856
C	-3.854336	-1.096846	0.611105
C	-2.638455	-0.893972	-0.055487
C	-2.620879	-0.081698	-1.198256
C	-3.790437	0.532351	-1.650045
C	-4.990610	0.350578	-0.959035
H	-5.952127	-0.622318	0.709942
H	-3.765911	1.148800	-2.545654
H	-5.900263	0.833421	-1.307639
C	-1.430981	-1.652732	0.437964
O	-1.597416	-2.765540	0.960702
N	-0.193442	-1.113797	0.230753
C	0.882869	-2.033139	0.572384
C	2.178732	-1.512037	0.021360
C	3.282479	-2.340438	-0.208591
C	4.446968	-1.802361	-0.743351
C	4.478938	-0.439158	-1.045378
C	3.349398	0.323323	-0.780343
N	2.222561	-0.187445	-0.247449
H	3.208261	-3.398239	0.023744
H	0.983494	-2.168760	1.664355
H	0.679794	-3.038421	0.181214
C	1.090370	2.650686	-0.010696
C	0.379116	2.606715	1.170826
H	-0.933774	1.015509	0.595319

C	0.545086	3.203270	-1.305172
H	0.875104	4.242040	-1.452113
H	0.893354	2.628098	-2.171205
H	-0.549370	3.192050	-1.310640
C	1.002546	2.432029	2.532166
H	2.017497	2.026422	2.468153
H	1.056013	3.405414	3.041150
H	0.403409	1.767565	3.163176
H	-1.689535	0.053317	-1.738550
H	-3.865907	-1.762975	1.467903
H	2.173006	2.570946	0.065893
H	-0.640403	2.984578	1.173800

S1-1

B3LYP electronic energy: -1168.69512914 a.u.
B3LYP enthalpy: -1168.262121 a.u.
B3LYP free energy: -1168.339576 a.u.
M06 SCF energy in solution: -1169.91908215 a.u.
M06 enthalpy in solution: -1169.486074 a.u.
M06 free energy in solution: -1169.563529 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	0.004448	1.752700	1.563808
C	0.873608	2.857712	0.982655
C	1.317914	2.584438	-0.478647
C	0.290283	1.820023	-1.294229
H	0.501462	1.048552	2.231199
H	1.767033	2.978490	1.608476
H	1.590283	3.538725	-0.962896
H	0.700621	1.282324	-2.151362
C	-1.378191	1.758178	1.573776
C	-2.261590	2.781187	0.883020
C	-1.776602	3.194416	-0.538584
C	-1.089693	2.068943	-1.310806
H	-1.888404	1.097062	2.273551
H	-2.380150	3.686273	1.502139
H	-2.643618	3.551550	-1.109459
H	-1.646092	1.679366	-2.165482
H	2.238557	1.988510	-0.461119
H	0.341775	3.813761	1.041247
H	-1.102205	4.054983	-0.464009
H	-3.267110	2.347237	0.801658
Ni	-0.748956	0.505972	-0.051861
N	0.353193	-1.494356	0.241248
H	0.461737	-1.735581	-0.737527
C	-0.723602	-2.237034	0.912300
H	-0.479542	-3.304961	0.997689
H	-0.787084	-1.834037	1.928109
C	-2.030217	-2.041453	0.188098
C	-2.963350	-3.064795	0.053062
C	-4.194062	-2.799199	-0.552989
H	-2.729316	-4.056311	0.430469
C	-3.442978	-0.538599	-0.863909
C	-4.433171	-1.503632	-1.013358
H	-4.939507	-3.580827	-0.662849
H	-3.586576	0.473618	-1.226713
H	-5.370858	-1.239205	-1.492752
N	-2.249983	-0.783319	-0.275968
C	1.555467	-1.337755	0.944259
O	1.585331	-1.442370	2.164504
C	2.791030	-1.059826	0.140924

C	2.799313	-0.827460	-1.243721
C	4.009012	-1.070154	0.837380
C	4.003365	-0.619015	-1.915695
H	1.871118	-0.764313	-1.803381
C	5.210534	-0.861067	0.164770
H	3.985885	-1.247504	1.907153
C	5.211231	-0.638054	-1.214472
H	3.996170	-0.432243	-2.985900
H	6.147041	-0.872683	0.715563
H	6.147921	-0.474647	-1.740551

S1-2

B3LYP electronic energy: -1892.94583430 a.u.
B3LYP enthalpy: -1892.410276 a.u.
B3LYP free energy: -1892.511756 a.u.
M06 SCF energy in solution: -1893.96946606 a.u.
M06 enthalpy in solution: -1893.433908 a.u.
M06 free energy in solution: -1893.535388 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ni	0.653431	-0.922718	0.421263
N	0.469209	-2.918176	0.377302
H	0.174036	-3.313666	1.263389
C	1.704961	-3.486863	-0.167833
H	1.837949	-4.525327	0.160874
H	1.571005	-3.489064	-1.256784
C	2.914359	-2.647832	0.192028
C	4.212096	-3.155145	0.109465
C	5.290834	-2.315544	0.380672
H	4.369702	-4.193769	-0.168150
C	3.713918	-0.559868	0.794560
C	5.035867	-0.987864	0.727367
H	6.309029	-2.689494	0.321470
H	3.468052	0.463882	1.058194
H	5.842080	-0.294403	0.944814
N	2.664935	-1.365499	0.540089
C	-0.596298	-2.576452	-0.527695
O	-0.374405	-2.545715	-1.753834
C	-1.983023	-2.654529	0.035173
C	-2.287380	-2.688525	1.408058
C	-3.037431	-2.735288	-0.887187
C	-3.605151	-2.820286	1.840905
H	-1.503619	-2.563749	2.151567
C	-4.356411	-2.856423	-0.452365
H	-2.792810	-2.706949	-1.943302
C	-4.647548	-2.906167	0.912175
H	-3.820096	-2.845630	2.906286
H	-5.159393	-2.916152	-1.182607
H	-5.675202	-3.005147	1.251743
P	-0.094170	1.035921	0.046401
C	0.707660	1.640866	-1.515483
C	1.350735	2.879069	-1.655179
C	0.701232	0.753307	-2.608736
C	1.965528	3.229068	-2.861315
H	1.377256	3.576581	-0.823716
C	1.304545	1.112189	-3.814168
H	0.231920	-0.223762	-2.510788
C	1.940384	2.350237	-3.944362
H	2.461889	4.192375	-2.951490
H	1.284381	0.418150	-4.650659
H	2.416377	2.624932	-4.882332

C	-1.889115	1.404502	-0.272863
C	-2.832596	0.867640	0.617248
C	-2.345873	2.186002	-1.344831
C	-4.194184	1.117859	0.451862
H	-2.497919	0.236155	1.435220
C	-3.711354	2.430827	-1.515076
H	-1.636268	2.601260	-2.053725
C	-4.638176	1.901082	-0.616458
H	-4.908646	0.686576	1.147985
H	-4.048562	3.035915	-2.353214
H	-5.700150	2.089749	-0.751964
C	0.296841	2.343570	1.309194
C	-0.261126	3.632651	1.286995
C	1.179143	2.015222	2.349747
C	0.073706	4.570728	2.264806
H	-0.968770	3.901261	0.507926
C	1.514164	2.951672	3.330516
H	1.583586	1.006932	2.394557
C	0.964426	4.233816	3.287354
H	-0.366603	5.564185	2.232116
H	2.195652	2.676629	4.131756
H	1.219442	4.964158	4.050966

S1-3

B3LYP electronic energy: -1012.66114652 a.u.
B3LYP enthalpy: -1012.324671 a.u.
B3LYP free energy: -1012.398358 a.u.
M06 SCF energy in solution: -1013.95756440 a.u.
M06 enthalpy in solution: -1013.621089 a.u.
M06 free energy in solution: -1013.694776 a.u.

Cartesian coordinates

ATOM	X	Y	Z
H	-5.029636	-2.810724	0.426348
H	-5.063644	-0.672139	1.753567
H	-3.178093	0.943016	1.463423
Ni	-0.647764	0.992603	-0.198257
C	4.490777	-1.644006	1.106044
C	3.141736	-1.919108	0.897895
C	2.361044	-1.075246	0.093039
C	2.951398	0.054905	-0.492405
C	4.303185	0.326135	-0.284339
C	5.075729	-0.522413	0.512073
H	5.086907	-2.303860	1.730308
H	4.749400	1.207664	-0.736017
H	6.128494	-0.306837	0.673914
C	0.937622	-1.479365	-0.119387
O	0.419015	-2.407869	0.482266
N	0.190066	-0.776658	-1.099975
C	-1.001663	-1.486967	-1.603883
C	-2.160609	-1.348667	-0.642870
C	-3.165083	-2.306946	-0.539241
C	-4.234629	-2.077677	0.325758
C	-4.255582	-0.893417	1.063623
C	-3.210411	0.011216	0.910436
N	-2.177085	-0.202972	0.071397
H	-3.102543	-3.220657	-1.122782
H	2.668529	-2.785908	1.346521
H	-1.265317	-1.014071	-2.556944
H	-0.782926	-2.545378	-1.783310
C	0.304616	2.623700	-0.228153
C	-0.873482	2.773911	0.279559

C	1.549696	3.376762	-0.562587
H	1.449174	4.450961	-0.349269
H	2.409621	3.007108	0.012235
H	1.815270	3.278189	-1.624691
C	-1.863489	3.719206	0.865226
H	-2.817505	3.693063	0.321838
H	-2.087323	3.470988	1.911985
H	-1.499122	4.756947	0.846006
H	2.353586	0.752033	-1.069264
H	0.754402	-0.365059	-1.835484

S2-1

B3LYP electronic energy: -1013.90665166 a.u.
B3LYP enthalpy: -1013.546788 a.u.
B3LYP free energy: -1013.620479 a.u.
M06 SCF energy in solution: -1015.19293111 a.u.
M06 enthalpy in solution: -1014.833067 a.u.
M06 free energy in solution: -1014.906758 a.u.

Cartesian coordinates

ATOM	X	Y	Z
H	5.865990	-0.970984	-0.008461
H	5.116976	1.378106	-0.529671
H	2.681710	1.858777	-0.590559
Ni	0.084708	0.086342	-0.179250
C	-4.512319	-0.979847	-0.389390
C	-3.511686	-1.912585	-0.100478
C	-2.185344	-1.492619	-0.059772
C	-1.810949	-0.156199	-0.289873
C	-2.823502	0.761829	-0.587680
C	-4.165402	0.349324	-0.636851
H	-5.554379	-1.287275	-0.427025
H	-2.598006	1.807457	-0.790445
H	-4.941049	1.076232	-0.869828
C	-1.041512	-2.415155	0.204998
O	-1.106722	-3.620164	0.454084
N	0.125105	-1.711846	0.119854
C	1.393627	-2.353093	0.342458
C	2.488341	-1.342918	0.129013
C	3.842903	-1.687354	0.183939
C	4.810556	-0.717042	-0.045439
C	4.400528	0.587601	-0.332868
C	3.040829	0.860755	-0.366007
N	2.095539	-0.072703	-0.132954
H	4.119457	-2.714739	0.400467
H	-3.741098	-2.958298	0.088692
H	1.472844	-2.770726	1.361002
H	1.544819	-3.206889	-0.337758
C	-1.121170	2.793949	2.205371
H	-1.557333	1.812111	1.992028
H	-1.812410	3.335261	2.860681
H	-0.188654	2.636599	2.761994
C	-0.868130	3.573994	0.912296
H	-0.456916	4.565914	1.148559
H	-1.817988	3.752946	0.391754
C	0.109799	2.878213	-0.044124
H	-0.354370	1.906967	-0.346223
H	1.036745	2.661927	0.498183
C	0.402737	3.670263	-1.321756
H	0.846800	4.642530	-1.077255
H	1.095675	3.138703	-1.983997
H	-0.517198	3.856266	-1.887115

S4-1

B3LYP electronic energy: -2929.22069242 a.u.
B3LYP enthalpy: -2928.394966 a.u.
B3LYP free energy: -2928.538585 a.u.
M06 SCF energy in solution: -2929.90780630 a.u.
M06 enthalpy in solution: -2929.082080 a.u.
M06 free energy in solution: -2929.225699 a.u.

Cartesian coordinates

ATOM	X	Y	Z
H	-7.111855	-1.941537	0.294014
H	-6.781688	-2.404380	2.747043
H	-4.514986	-3.091406	3.529373
C	-2.240185	1.584078	-4.772309
C	-2.670245	0.435415	-4.120612
C	-1.972432	-0.079941	-3.012046
C	-0.807878	0.563228	-2.528403
C	-0.384884	1.712566	-3.226984
C	-1.084569	2.226090	-4.318476
H	-2.790687	1.971463	-5.625774
H	-0.725687	3.124548	-4.817152
C	-2.569977	-1.327325	-2.425648
O	-3.427582	-1.989145	-3.022486
N	-2.151538	-1.697164	-1.174877
C	-2.601126	-2.929990	-0.541576
C	-3.814750	-2.762271	0.358357
C	-5.052309	-2.373102	-0.178143
C	-6.139530	-2.237681	0.679666
C	-5.961324	-2.495555	2.040994
C	-4.694805	-2.879974	2.476024
N	-3.636808	-3.014003	1.663946
H	-5.133067	-2.194486	-1.245901
H	-3.552875	-0.101000	-4.454183
H	-2.837269	-3.631838	-1.347876
H	-1.786408	-3.339782	0.061762
Ni	0.335447	0.066885	-1.053844
P	2.186227	-0.993957	-0.231230
P	-0.439999	1.592930	0.514177
H	-1.464567	-1.113353	-0.704739
H	0.672384	-0.745201	-2.240157
C	2.333551	-2.756489	-0.782331
C	3.534694	-3.471578	-0.642331
C	1.223936	-3.399681	-1.347882
C	3.620427	-4.800241	-1.055599
H	4.408449	-2.988831	-0.214807
C	1.309136	-4.734026	-1.755219
H	0.300230	-2.847903	-1.490817
C	2.505798	-5.435498	-1.610790
H	4.558236	-5.338981	-0.948014
H	0.440154	-5.217438	-2.193107
H	2.574320	-6.470876	-1.933971
C	3.692603	-0.201056	-0.964032
C	3.567346	0.398517	-2.229111
C	4.948932	-0.197411	-0.337497
C	4.671556	0.984031	-2.850402
H	2.600683	0.400432	-2.724393
C	6.050930	0.392685	-0.959752
H	5.069155	-0.644108	0.644353
C	5.915862	0.984346	-2.216956
H	4.556658	1.440275	-3.830116
H	7.015932	0.388229	-0.459489

H	6.775005	1.442787	-2.699528
C	2.583625	-1.117179	1.575826
C	2.370976	-2.305833	2.292905
C	2.986165	0.029194	2.283689
C	2.566758	-2.349521	3.675568
H	2.056281	-3.205138	1.773624
C	3.189124	-0.019540	3.662753
H	3.147488	0.964196	1.757016
C	2.979814	-1.208876	4.364488
H	2.400325	-3.280947	4.210500
H	3.506068	0.877579	4.187674
H	3.135041	-1.244602	5.439443
C	-1.213583	0.951094	2.063405
C	-2.108586	1.718209	2.829779
C	-0.899315	-0.346710	2.489311
C	-2.658765	1.199654	4.001797
H	-2.382761	2.716862	2.503547
C	-1.453288	-0.866411	3.660509
H	-0.217256	-0.953785	1.904039
C	-2.330941	-0.092941	4.419966
H	-3.349918	1.803005	4.584619
H	-1.206294	-1.878434	3.966114
H	-2.766802	-0.496988	5.329945
C	-1.727698	2.774946	-0.085619
C	-1.526810	4.159671	-0.154563
C	-2.958574	2.245197	-0.508716
C	-2.536296	4.998663	-0.635470
H	-0.584945	4.591714	0.167321
C	-3.964652	3.084216	-0.982733
H	-3.131413	1.173758	-0.472409
C	-3.755819	4.464410	-1.049323
H	-2.364600	6.070933	-0.683347
H	-4.908866	2.657642	-1.309659
H	-4.539221	5.117227	-1.425093
C	0.914383	2.710795	1.098473
C	1.911877	3.062532	0.173592
C	1.001707	3.209849	2.406403
C	2.966450	3.898813	0.543623
H	1.871538	2.669410	-0.838428
C	2.060726	4.041273	2.778095
H	0.249034	2.942295	3.140901
C	3.044307	4.388475	1.849499
H	3.730151	4.156233	-0.185113
H	2.116018	4.417032	3.796594
H	3.868127	5.033921	2.142332
H	0.518964	2.230743	-2.909500

S4-2

B3LYP electronic energy: -1012.63066483 a.u.
B3LYP enthalpy: -1012.295685 a.u.
B3LYP free energy: -1012.368353 a.u.
M06 SCF energy in solution: -1013.91923014 a.u.
M06 enthalpy in solution: -1013.584250 a.u.
M06 free energy in solution: -1013.656918 a.u.

Cartesian coordinates

ATOM	X	Y	Z
H	3.013581	-1.560670	2.916149
H	5.402339	-1.278891	2.230337
H	5.900145	-0.804099	-0.189743
Ni	-0.680289	0.956500	-0.072073
C	-4.561366	-1.770269	0.454586

C	-3.393316	-2.185561	-0.171270
C	-2.298170	-1.305717	-0.208171
C	-2.323539	-0.000922	0.331401
C	-3.530279	0.383805	0.945235
C	-4.622180	-0.484987	1.015457
H	-5.422003	-2.431629	0.508796
H	-3.630324	1.376739	1.381510
H	-5.538049	-0.161786	1.506935
C	-1.046719	-1.697060	-0.862059
O	-0.851737	-2.600502	-1.647647
N	0.066185	-0.795670	-0.446316
C	1.320474	-0.983285	-1.203893
C	2.513473	-1.023176	-0.268169
C	3.276286	-1.359140	1.879893
C	4.606059	-1.201504	1.496852
C	4.877564	-0.938121	0.152292
H	1.245963	-1.933122	-1.748206
H	1.428628	-0.182651	-1.938115
C	0.628220	2.288436	-0.407593
C	-0.346383	3.068320	0.030609
C	1.991018	2.637357	-0.903039
H	2.122105	2.318953	-1.946012
H	2.199985	3.716671	-0.859544
H	2.765116	2.122354	-0.320823
C	-0.536835	4.553037	0.201949
H	-0.748741	4.816575	1.245969
H	0.370133	5.083722	-0.106135
H	-1.372442	4.924725	-0.404737
H	-3.312627	-3.169067	-0.626833
H	0.298165	-1.034000	0.533778
N	2.252625	-1.274538	1.020206
C	3.817624	-0.844164	-0.745384
H	3.991323	-0.637022	-1.797617
H	-1.314556	2.524384	0.364091

S4-3

B3LYP electronic energy: -1012.67171505 a.u.
B3LYP enthalpy: -1012.335704 a.u.
B3LYP free energy: -1012.405549 a.u.
M06 SCF energy in solution: -1013.96138094 a.u.
M06 enthalpy in solution: -1013.625370 a.u.
M06 free energy in solution: -1013.695215 a.u.

Cartesian coordinates

ATOM	X	Y	Z
H	5.716877	-1.165517	-0.163769
H	5.036604	1.257096	-0.230170
H	2.588603	1.810522	-0.092923
Ni	0.017059	0.214629	0.219257
C	-4.634543	-0.587373	-0.112841
C	-3.658053	-1.560843	-0.277670
C	-2.310760	-1.210934	-0.086206
C	-1.885423	0.108975	0.222848
C	-2.904987	1.066590	0.357335
C	-4.250499	0.723120	0.210346
H	-5.685229	-0.834987	-0.238459
H	-2.645971	2.101486	0.561324
H	-5.016029	1.486994	0.333230
C	-1.245612	-2.210396	-0.270654
O	-1.246018	-3.209944	-0.961462
N	-0.048033	-1.803284	0.465045
C	1.219628	-2.469913	0.159909

C	2.341882	-1.451140	0.085736
C	3.678257	-1.846877	0.008579
C	4.671410	-0.876883	-0.103052
C	4.298516	0.467108	-0.138036
C	2.948423	0.787869	-0.052564
N	1.985484	-0.146390	0.065533
H	3.928614	-2.903540	0.032664
H	1.457868	-3.251757	0.891324
H	1.093309	-2.975065	-0.804211
C	0.057447	2.108564	0.158581
C	0.117732	2.782230	-1.003739
H	0.062553	2.208175	-1.932150
C	0.084182	2.755117	1.527725
H	0.156589	3.851246	1.503867
H	-0.820523	2.496895	2.094053
H	0.930784	2.385864	2.125493
C	0.227033	4.275478	-1.227300
H	-0.643158	4.653355	-1.783493
H	0.294116	4.845000	-0.295661
H	1.111026	4.524595	-1.832512
H	-3.915586	-2.581807	-0.547700
H	-0.249913	-1.755055	1.463574

S6-2

B3LYP electronic energy: -1125.80168765 a.u.
B3LYP enthalpy: -1125.469527 a.u.
B3LYP free energy: -1125.537568 a.u.
M06 SCF energy in solution: -1127.03407735 a.u.
M06 enthalpy in solution: -1126.701917 a.u.
M06 free energy in solution: -1126.769958 a.u.

Cartesian coordinates

ATOM	X	Y	Z
H	5.898436	0.009044	0.637785
H	5.220257	2.388530	0.996313
H	2.812238	3.010084	0.736390
Ni	0.269766	1.298034	-0.018084
C	-3.098999	0.063899	0.079171
C	-0.906689	-1.268714	-0.662677
O	-0.781273	-2.190428	-1.469147
N	0.178050	-0.553186	-0.172403
C	2.534124	-0.214294	0.091657
C	4.859214	0.313689	0.540683
C	4.491042	1.627836	0.737991
C	3.136167	1.982673	0.593838
N	2.196957	1.097128	0.282034
C	-1.424452	1.823037	-0.343345
C	-2.704053	1.435896	-0.318775
C	1.459900	-1.108093	-0.230609
C	1.808723	-2.439440	-0.477440
H	1.042969	-3.141739	-0.770379
C	3.145869	-2.874925	-0.363623
C	3.885825	-0.659121	0.205211
C	4.178701	-2.023841	-0.027306
H	3.358004	-3.923414	-0.556789
H	5.203248	-2.376001	0.049366
C	-3.806479	2.443707	-0.610570
H	-4.302305	2.794644	0.304985
H	-3.405521	3.323794	-1.120842
H	-4.581675	2.009255	-1.252147
C	-0.821617	3.186514	-0.514601
H	0.284653	3.154648	-0.243754

H	-0.825380	3.564941	-1.543814
H	-1.223702	3.941052	0.171307
C	-2.279722	-1.090007	-0.034349
C	-2.795032	-2.327955	0.395777
C	-4.057123	-2.457304	0.963888
H	-4.407008	-3.430282	1.297734
C	-4.866759	-1.328737	1.072686
H	-5.864300	-1.398645	1.498765
C	-4.391995	-0.102794	0.622175
H	-2.177292	-3.208627	0.259641
H	-5.040816	0.761442	0.708870

S1-TS1

B3LYP electronic energy: -1168.65949502 a.u.
B3LYP enthalpy: -1168.231667 a.u.
B3LYP free energy: -1168.308813 a.u.
M06 SCF energy in solution: -1169.88480544 a.u.
M06 enthalpy in solution: -1169.456977 a.u.
M06 free energy in solution: -1169.534123 a.u.
Imaginary frequency: -1027.4139 cm-1

Cartesian coordinates

ATOM	X	Y	Z
H	3.967981	-4.403329	-0.209825
H	4.258149	-2.818862	-2.142066
H	2.760340	-0.822020	-2.276542
Ni	0.397197	0.240500	-0.373147
C	-5.320628	-0.143533	0.034949
C	-4.257475	-0.737549	0.711850
C	-2.979953	-0.781993	0.134670
C	-2.796744	-0.257152	-1.152012
C	-3.866238	0.322823	-1.837827
C	-5.127356	0.389987	-1.242703
H	-6.302754	-0.103413	0.498947
H	-3.715158	0.715231	-2.840421
H	-5.958231	0.845749	-1.775275
C	-1.891083	-1.466428	0.916434
O	-2.178793	-2.390444	1.685501
N	-0.603463	-1.021996	0.730688
C	0.442157	-1.749924	1.449228
C	1.543724	-2.126559	0.481088
C	2.346099	-3.258025	0.634770
C	3.339318	-3.522631	-0.306983
C	3.504332	-2.646779	-1.380677
C	2.670804	-1.535612	-1.463100
N	1.715798	-1.276211	-0.555599
H	2.181888	-3.922870	1.477157
H	-4.395871	-1.181600	1.692357
H	0.872612	-1.121224	2.244109
H	0.005225	-2.631107	1.927676
H	-0.673724	0.463258	0.637362
H	-1.818864	-0.319420	-1.620079
C	-0.004782	2.185819	-0.801670
C	-0.155889	3.244738	0.294522
C	0.169179	2.855459	1.753532
C	1.484488	2.183228	2.070675
H	-0.895911	2.103937	-1.423210
H	-1.205765	3.562671	0.293921
H	0.072321	3.759606	2.376971
H	1.464932	1.600717	2.993213
C	1.183979	1.740061	-1.416459
C	2.622895	2.171462	-1.168245

C	2.941542	2.956904	0.122716
C	2.643762	2.214609	1.401250
H	1.052233	1.359897	-2.435066
H	2.935974	2.798771	-2.018625
H	4.012327	3.197978	0.100373
H	3.470720	1.632125	1.809211
H	-0.627031	2.184587	2.103774
H	0.412504	4.138623	0.011444
H	2.421630	3.917986	0.103167
H	3.274190	1.286295	-1.206141

S1-TS2

B3LYP electronic energy: -1892.92471338 a.u.
B3LYP enthalpy: -1892.394781 a.u.
B3LYP free energy: -1892.496547 a.u.
M06 SCF energy in solution: -1893.94755887 a.u.
M06 enthalpy in solution: -1893.417626 a.u.
M06 free energy in solution: -1893.519392 a.u.
Imaginary frequency: -1107.4239 cm-1

Cartesian coordinates

ATOM	X	Y	Z
H	-1.328372	6.548337	0.618169
H	0.520036	5.453837	1.928247
H	0.897545	3.000015	1.627470
Ni	-0.609416	0.748278	-0.235276
C	-5.085044	-2.919640	0.119638
C	-4.928657	-1.625128	-0.369422
C	-3.775277	-0.882922	-0.070771
C	-2.797681	-1.453483	0.755665
C	-2.959153	-2.747330	1.256360
C	-4.098759	-3.485527	0.933941
H	-5.978217	-3.487430	-0.128476
H	-2.194368	-3.170605	1.902379
H	-4.223777	-4.493619	1.321547
C	-3.696654	0.509940	-0.631736
O	-4.734901	1.115730	-0.919841
N	-2.442776	1.054280	-0.819461
C	-2.401893	2.412746	-1.364554
C	-1.634356	3.333007	-0.434448
C	-1.902006	4.699284	-0.335238
C	-1.129882	5.484616	0.519771
C	-0.104656	4.881845	1.249589
C	0.104424	3.514447	1.093260
N	-0.641470	2.753000	0.276014
H	-2.710151	5.133456	-0.916130
H	-5.692051	-1.161358	-0.985428
H	-1.894269	2.404389	-2.341421
H	-3.424603	2.765891	-1.522768
H	-1.557516	0.068822	-1.230598
H	-1.913992	-0.879602	1.019242
P	1.217900	-0.372764	-0.129660
C	1.662023	-1.479351	-1.551188
C	0.624667	-2.134245	-2.233982
C	2.985875	-1.702211	-1.961698
C	0.904196	-2.999527	-3.292052
H	-0.404105	-1.956379	-1.933114
C	3.263647	-2.560548	-3.028247
H	3.804366	-1.201851	-1.453581
C	2.224667	-3.212648	-3.694206
H	0.088589	-3.499585	-3.807747
H	4.293737	-2.716961	-3.338278

H	2.442093	-3.878820	-4.525031
C	2.761554	0.639158	0.081099
C	3.814257	0.294295	0.942441
C	2.862393	1.827330	-0.662161
C	4.940498	1.114443	1.052576
H	3.756151	-0.616065	1.531426
C	3.992029	2.639785	-0.561323
H	2.044464	2.116276	-1.317465
C	5.034110	2.285868	0.299416
H	5.745568	0.834632	1.727337
H	4.055153	3.552272	-1.148650
H	5.911335	2.921688	0.385616
C	1.275362	-1.514588	1.329718
C	0.683910	-1.075458	2.526753
C	1.857482	-2.790386	1.295790
C	0.685314	-1.884298	3.663409
H	0.210432	-0.097085	2.560965
C	1.853105	-3.602926	2.432518
H	2.310226	-3.154968	0.379058
C	1.270010	-3.152573	3.618081
H	0.222596	-1.528061	4.580024
H	2.304612	-4.590722	2.388567
H	1.265551	-3.787460	4.500108

S1-TS3

B3LYP electronic energy: -1012.61930616 a.u.
B3LYP enthalpy: -1012.289527 a.u.
B3LYP free energy: -1012.361897 a.u.
M06 SCF energy in solution: -1013.91937047 a.u.
M06 enthalpy in solution: -1013.589591 a.u.
M06 free energy in solution: -1013.661961 a.u.
Imaginary frequency: -962.3250 cm-1

Cartesian coordinates

ATOM	X	Y	Z
H	-5.362782	-2.386912	0.808675
H	-5.312100	-0.034706	1.700063
H	-3.280512	1.354335	1.272181
Ni	-0.564166	0.777478	-0.299794
C	4.889112	-0.923292	0.235779
C	3.726352	-1.514088	-0.254012
C	2.464992	-1.040106	0.136417
C	2.389858	0.013265	1.057942
C	3.555995	0.594026	1.562760
C	4.807006	0.134011	1.146628
H	5.860088	-1.291810	-0.084929
H	3.485136	1.401521	2.287191
H	5.713320	0.589918	1.537130
C	1.260762	-1.760404	-0.407320
O	1.348964	-2.958295	-0.700183
N	0.094047	-1.045404	-0.542852
C	-1.061512	-1.804762	-1.015244
C	-2.294380	-1.383554	-0.248950
C	-3.394888	-2.221153	-0.059248
C	-4.500120	-1.747368	0.644281
C	-4.476516	-0.443646	1.141513
C	-3.347010	0.334264	0.909801
N	-2.279609	-0.119674	0.231015
H	-3.374092	-3.232108	-0.454370
H	-1.238279	-1.626828	-2.089002
H	-0.861655	-2.874150	-0.902425
C	-0.832628	2.681101	-0.283346

C	0.345081	2.454486	-0.692138
H	0.491788	0.294063	-1.214496
C	-1.931841	3.616061	0.060063
H	-1.667438	4.651582	-0.190648
H	-2.853705	3.364594	-0.478362
H	-2.163064	3.585290	1.132675
C	1.669548	2.885750	-1.199348
H	1.809751	2.578759	-2.242694
H	1.764889	3.978277	-1.149927
H	2.483155	2.439667	-0.617691
H	1.419586	0.368726	1.389880
H	3.770900	-2.355247	-0.938152

S2-TS1

B3LYP electronic energy: -1013.86025271 a.u.
B3LYP enthalpy: -1013.505305 a.u.
B3LYP free energy: -1013.574659 a.u.
M06 SCF energy in solution: -1015.15771146 a.u.
M06 enthalpy in solution: -1014.802764 a.u.
M06 free energy in solution: -1014.872118 a.u.
Imaginary frequency: -1276.7079 cm-1

Cartesian coordinates

ATOM	X	Y	Z
H	-5.910033	-0.800905	-0.136731
H	-5.119539	1.560969	-0.520859
H	-2.676027	2.009975	-0.508671
Ni	-0.159292	0.241976	-0.159208
C	4.487921	-1.053741	-0.431441
C	3.409356	-1.835828	-0.013758
C	2.125452	-1.298907	0.051782
C	1.893768	0.058854	-0.275688
C	2.981291	0.817122	-0.734045
C	4.267545	0.267834	-0.811859
H	5.486807	-1.479440	-0.479395
H	2.843936	1.854211	-1.026358
H	5.091416	0.882730	-1.165248
C	0.962748	-2.218730	0.323167
O	1.084546	-3.374781	0.740747
N	-0.197027	-1.607288	-0.007233
C	-1.456012	-2.260605	0.221599
C	-2.540916	-1.231132	0.040801
C	-3.900645	-1.556001	0.053259
C	-4.850708	-0.560723	-0.141998
C	-4.418021	0.750693	-0.352935
C	-3.054342	1.006629	-0.347236
N	-2.128394	0.047779	-0.149271
H	-4.194934	-2.589147	0.210867
H	-1.630767	-3.097917	-0.474260
H	-1.518527	-2.700528	1.231545
C	0.025771	2.325701	0.002524
C	0.945140	3.112789	0.960551
C	-0.034079	2.938678	-1.399057
H	-0.291070	4.008652	-1.354606
H	0.929020	2.862058	-1.917251
H	-0.777207	2.444885	-2.036369
H	3.527142	-2.884973	0.243577
H	1.057013	1.138134	0.016318
H	1.974461	3.144331	0.579701
H	-0.963801	2.350032	0.472099
H	0.601995	4.159807	0.971351
C	0.951703	2.569039	2.392848

H	-0.060474	2.560062	2.816815
H	1.335089	1.542781	2.427826
H	1.581425	3.183738	3.045943

S3-TS1

B3LYP electronic energy: -1892.85990968 a.u.
B3LYP enthalpy: -1892.334593 a.u.
B3LYP free energy: -1892.431418 a.u.
M06 SCF energy in solution: -1893.89030460 a.u.
M06 enthalpy in solution: -1893.364988 a.u.
M06 free energy in solution: -1893.461813 a.u.
Imaginary frequency: -2066.3011 cm-1

Cartesian coordinates

ATOM	X	Y	Z
H	-1.903996	-5.845354	1.044487
H	0.130052	-4.631583	1.909167
H	0.481315	-2.277042	1.250274
Ni	-1.091316	-0.288953	-0.580536
C	-3.632082	3.883252	0.567545
C	-4.157858	2.665559	0.137015
C	-3.294313	1.641904	-0.259816
C	-1.893988	1.802043	-0.251124
C	-1.389879	3.042224	0.173084
C	-2.246640	4.070245	0.583282
H	-4.295538	4.685621	0.881631
H	-0.320034	3.232232	0.171905
H	-1.831612	5.020563	0.914189
C	-3.858982	0.328340	-0.694412
O	-5.071558	0.087601	-0.767550
N	-2.884325	-0.568529	-1.004481
C	-3.235837	-1.946903	-1.238218
C	-2.333936	-2.787142	-0.379447
C	-2.592273	-4.117926	-0.050730
C	-1.710665	-4.811672	0.772576
C	-0.583291	-4.144434	1.252791
C	-0.377940	-2.821984	0.883290
N	-1.222207	-2.146768	0.074235
H	-3.491603	-4.588936	-0.435138
H	-5.228712	2.484049	0.101541
H	-4.292867	-2.113556	-0.997042
H	-3.095376	-2.232133	-2.296287
H	-1.180657	1.161000	-1.382691
H	-0.711678	0.535048	-2.170016
P	1.123216	0.155248	-0.105188
C	1.473210	-0.010246	1.703674
C	2.584118	-0.677274	2.243043
C	0.526372	0.553453	2.579022
C	2.749125	-0.770157	3.627632
H	3.319688	-1.132650	1.588112
C	0.703010	0.470074	3.960131
H	-0.349885	1.052758	2.172978
C	1.813320	-0.193973	4.487876
H	3.612101	-1.293339	4.031101
H	-0.033997	0.915243	4.622802
H	1.944821	-0.266704	5.564099
C	2.314157	-0.964829	-0.964046
C	1.830379	-2.058165	-1.696556
C	3.698192	-0.717590	-0.946920
C	2.712385	-2.905593	-2.370778
H	0.760718	-2.228096	-1.759790
C	4.577560	-1.566741	-1.618482

H	4.088074	0.151172	-0.424111
C	4.086080	-2.665672	-2.327934
H	2.322365	-3.746006	-2.938544
H	5.644849	-1.363342	-1.597536
H	4.771411	-3.322539	-2.856864
C	1.795536	1.818578	-0.536260
C	2.442027	2.628460	0.409482
C	1.682847	2.272481	-1.861792
C	2.962654	3.870494	0.037342
H	2.537069	2.298835	1.438522
C	2.205697	3.512318	-2.226828
H	1.167177	1.662892	-2.597201
C	2.846104	4.315142	-1.279734
H	3.457621	4.488565	0.781683
H	2.105646	3.853429	-3.253571
H	3.249304	5.282504	-1.566981

S4_TS1

B3LYP electronic energy: -2929.22012527 a.u.
B3LYP enthalpy: -2928.395962 a.u.
B3LYP free energy: -2928.539055 a.u.
M06 SCF energy in solution: -2929.90771640 a.u.
M06 enthalpy in solution: -2929.083553 a.u.
M06 free energy in solution: -2929.226646 a.u.
Imaginary frequency: -380.4939 cm-1

Cartesian coordinates

ATOM	X	Y	Z
H	-7.029226	-1.965467	0.362201
H	-6.679458	-2.356733	2.824860
H	-4.410081	-3.035538	3.606856
C	-2.156270	1.359132	-4.861073
C	-2.600521	0.244150	-4.162680
C	-1.904856	-0.241311	-3.040011
C	-0.725052	0.401986	-2.589305
C	-0.277844	1.507693	-3.345465
C	-0.980903	1.993006	-4.445795
H	-2.706818	1.723398	-5.724424
H	-0.607875	2.861889	-4.984498
C	-2.510268	-1.462490	-2.409253
O	-3.380644	-2.130857	-2.979937
N	-2.074789	-1.806371	-1.157676
C	-2.533484	-3.014508	-0.483868
C	-3.737609	-2.808266	0.421009
C	-4.977376	-2.426419	-0.115655
C	-6.055474	-2.257036	0.747722
C	-5.866431	-2.475205	2.114412
C	-4.598514	-2.855273	2.549292
N	-3.549248	-3.021391	1.731948
H	-5.067493	-2.279849	-1.187508
H	-3.494296	-0.289891	-4.468983
H	-2.783378	-3.736783	-1.267451
H	-1.717297	-3.414733	0.123806
Ni	0.333534	0.054203	-1.002192
P	2.183310	-0.976131	-0.174571
P	-0.488301	1.613341	0.472158
H	-1.397888	-1.201882	-0.696596
H	0.550009	-0.706378	-2.257718
C	2.387294	-2.736210	-0.718923
C	3.601911	-3.422543	-0.552299

C	1.308666	-3.403506	-1.315376
C	3.730850	-4.746255	-0.969914
H	4.451864	-2.919864	-0.100235
C	1.437134	-4.732704	-1.728554
H	0.373225	-2.875807	-1.473847
C	2.646806	-5.405244	-1.557504
H	4.678343	-5.262893	-0.840637
H	0.591600	-5.235082	-2.190450
H	2.749190	-6.436693	-1.884322
C	3.692322	-0.163783	-0.882705
C	3.587293	0.386352	-2.171863
C	4.928626	-0.098516	-0.221522
C	4.690670	0.982828	-2.783605
H	2.635744	0.342216	-2.694326
C	6.029976	0.504243	-0.833332
H	5.034121	-0.507919	0.778172
C	5.914909	1.045773	-2.114764
H	4.591216	1.399525	-3.782476
H	6.979327	0.548358	-0.305726
H	6.773630	1.513666	-2.588913
C	2.545387	-1.080029	1.640444
C	2.364947	-2.272196	2.359954
C	2.882851	0.086312	2.350438
C	2.529579	-2.299956	3.747310
H	2.099426	-3.186394	1.839187
C	3.056285	0.053510	3.733816
H	3.013595	1.025658	1.822469
C	2.879829	-1.139799	4.438248
H	2.388042	-3.234300	4.284366
H	3.322587	0.966097	4.260272
H	3.010885	-1.163151	5.516767
C	-1.286558	1.030109	2.032335
C	-2.211074	1.813144	2.745489
C	-0.953687	-0.239517	2.524515
C	-2.772002	1.338788	3.931210
H	-2.498543	2.789722	2.367723
C	-1.516917	-0.714262	3.710313
H	-0.250262	-0.859076	1.978584
C	-2.424090	0.075291	4.416856
H	-3.486201	1.953850	4.472600
H	-1.253063	-1.704488	4.068917
H	-2.867043	-0.293821	5.338238
C	-1.775207	2.753992	-0.207806
C	-1.598298	4.139960	-0.314323
C	-2.978479	2.187102	-0.661265
C	-2.603515	4.942800	-0.861234
H	-0.678179	4.600619	0.030133
C	-3.981380	2.990348	-1.200248
H	-3.132724	1.114154	-0.595956
C	-3.795953	4.371511	-1.304000
H	-2.450264	6.016268	-0.937431
H	-4.904130	2.534809	-1.548829
H	-4.576094	4.996287	-1.730813
C	0.837922	2.773475	1.041580
C	1.844741	3.111442	0.121421
C	0.899739	3.312633	2.335011
C	2.882144	3.973095	0.481111
H	1.824357	2.688120	-0.878999
C	1.942320	4.169029	2.697067
H	0.139690	3.057323	3.066274
C	2.934585	4.502275	1.772813
H	3.652982	4.219264	-0.244044
H	1.977582	4.575420	3.704667
H	3.745513	5.167191	2.058016

H	0.646575	2.008540	-3.062903

S4-TS2

B3LYP electronic energy: -1012.60588878 a.u.
B3LYP enthalpy: -1012.274552 a.u.
B3LYP free energy: -1012.345258 a.u.
M06 SCF energy in solution: -1013.90432039 a.u.
M06 enthalpy in solution: -1013.572984 a.u.
M06 free energy in solution: -1013.643690 a.u.
Imaginary frequency: -49.0271 cm-1

Cartesian coordinates

ATOM	X	Y	Z
H	2.778405	-1.093007	3.099583
H	5.217009	-1.065015	2.545151
H	5.887865	-1.019623	0.120364
Ni	-0.782728	1.119717	-0.199677
C	-4.431163	-1.820798	0.598494
C	-3.303313	-2.162700	-0.137449
C	-2.256748	-1.234000	-0.250120
C	-2.306475	0.061163	0.311659
C	-3.469864	0.373745	1.039212
C	-4.502914	-0.553696	1.194028
H	-5.249143	-2.527280	0.712075
H	-3.577474	1.356159	1.491484
H	-5.383398	-0.284851	1.774411
C	-1.025730	-1.589185	-0.971475
O	-0.885098	-2.448297	-1.820955
N	0.088449	-0.745813	-0.547647
C	1.376460	-1.088373	-1.170850
C	2.502927	-1.046269	-0.156121
C	3.114541	-1.075944	2.065015
C	4.472601	-1.060058	1.755277
C	4.840218	-1.034218	0.408281
H	1.293811	-2.098522	-1.592605
H	1.583801	-0.416596	-2.006442
C	0.742495	2.354646	-0.792261
C	0.017475	3.012378	-0.018913
H	-1.776281	2.135971	0.086599
C	1.909707	2.219518	-1.691802
H	1.630844	1.782121	-2.657204
H	2.353904	3.203581	-1.887092
H	2.685883	1.585888	-1.248988
C	-0.444741	4.164352	0.781703
H	-0.635286	3.878504	1.821165
H	0.320071	4.951283	0.773986
H	-1.374678	4.577947	0.375876
H	-3.211030	-3.133088	-0.617930
H	0.214665	-0.853377	0.470100
N	2.150503	-1.070989	1.135218
C	3.843295	-1.024290	-0.563649
H	4.092917	-1.005817	-1.621097

S4-TS3

B3LYP electronic energy: -1012.57477425 a.u.
B3LYP enthalpy: -1012.245256 a.u.
B3LYP free energy: -1012.313534 a.u.
M06 SCF energy in solution: -1013.86880593 a.u.
M06 enthalpy in solution: -1013.539288 a.u.
M06 free energy in solution: -1013.607566 a.u.

Imaginary frequency: -658.6480 cm-1

Cartesian coordinates

ATOM	X	Y	Z
H	-5.425811	-1.498326	-0.913648
H	-4.796643	0.678660	-2.011203
H	-2.460491	1.518439	-1.721271
Ni	0.076806	0.463235	-0.402705
C	4.688028	-0.380484	-0.505685
C	3.760449	-1.285027	0.009151
C	2.411309	-0.922484	0.077788
C	1.960136	0.336990	-0.377254
C	2.906064	1.230703	-0.891976
C	4.258317	0.870623	-0.959587
H	5.740146	-0.647331	-0.558922
H	2.600880	2.212519	-1.246932
H	4.981642	1.574183	-1.366230
C	1.376032	-1.893046	0.535864
O	1.514008	-3.105879	0.605905
N	0.156591	-1.233944	0.783459
C	-1.083363	-1.987182	0.804234
C	-2.162823	-1.259933	0.014479
C	-3.455999	-1.781590	-0.087844
C	-4.420190	-1.098166	-0.821568
C	-4.076210	0.108706	-1.434290
C	-2.778233	0.577634	-1.282778
N	-1.838399	-0.087555	-0.583692
H	-3.691780	-2.720046	0.405175
H	-0.904597	-2.982193	0.377849
H	-1.443769	-2.149955	1.830615
C	-0.292629	1.367316	1.593926
C	0.165077	2.397281	0.771243
H	1.240550	2.467692	0.614822
C	-1.692535	1.489081	2.159735
H	-2.403845	2.127289	1.610323
H	-2.170484	0.514597	2.323753
H	-1.584911	1.934947	3.161530
C	-0.579881	3.665784	0.378140
H	-0.134795	4.120541	-0.515101
H	-1.641955	3.490831	0.170806
H	-0.531497	4.420312	1.177789
H	4.059276	-2.274339	0.345126
H	0.176817	-0.278109	1.444201

S5-TS1

B3LYP electronic energy: -1012.61990838 a.u.
B3LYP enthalpy: -1012.289640 a.u.
B3LYP free energy: -1012.359332 a.u.
M06 SCF energy in solution: -1013.91305402 a.u.
M06 enthalpy in solution: -1013.582786 a.u.
M06 free energy in solution: -1013.652478 a.u.
Imaginary frequency: -1640.7856 cm-1

Cartesian coordinates

ATOM	X	Y	Z
H	5.615918	-1.316192	0.425135
H	4.967641	1.050811	0.981946
H	2.568524	1.732038	0.666550
Ni	0.056924	0.251845	-0.197513
C	-4.535990	-0.584901	0.411566
C	-3.546919	-1.560856	0.555667
C	-2.264313	-1.268605	0.100052

C	-1.929901	-0.018710	-0.465574
C	-2.938459	0.939055	-0.618074
C	-4.235781	0.648927	-0.182284
H	-5.549347	-0.786797	0.749099
H	-2.709614	1.911866	-1.043741
H	-5.021661	1.391898	-0.296104
C	-1.116639	-2.242607	0.076512
O	-1.083903	-3.345848	0.605650
N	-0.105606	-1.661085	-0.677058
C	1.187047	-2.293397	-0.819062
C	2.294693	-1.399672	-0.288435
C	3.610143	-1.849583	-0.155545
C	4.590391	-0.977232	0.308938
C	4.235113	0.336053	0.622065
C	2.910652	0.723433	0.463759
N	1.959236	-0.123498	0.025759
H	3.851022	-2.876795	-0.412115
H	1.166661	-3.248722	-0.277485
H	1.401285	-2.525435	-1.873301
C	0.015683	2.105732	0.224167
C	0.397926	3.019222	-0.684907
H	0.706989	2.665537	-1.672894
C	-0.451198	2.421634	1.627190
H	-0.404495	3.489703	1.879324
H	-1.488032	2.091618	1.771339
H	0.147889	1.882788	2.375377
C	0.453990	4.525532	-0.544575
H	-0.210968	5.013058	-1.271900
H	0.163376	4.872516	0.451115
H	1.465663	4.905593	-0.747828
H	-3.759769	-2.530521	0.996654
H	-0.867753	-0.659887	-1.245675