Electronic Supplementary Information

Origins of Lewis Acid Accelerations in Nickel Catalysed C–H, C–C and C–O Bond Cleavages

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Comparison of the Barriers of Oxidative Additions Using Different Levels of Theories

The barriers of C–CN and C–O bond cleavages with Ni(0) catalysts in the absence (**TS1** and **TS3**) and presence (**TS2**, **TS4** and **TS7**) of Lewis acids were calculated using a few popular modern density functionals (Table S1). Although the barrier difference differs by a few kcal/mol among the methods tested, the trend of Lewis acid-assisted reactivity (**TS2** vs **TS1** for C–CN bond cleavages; **TS4** vs **TS3** and **TS7** vs **TS3** for C–O bond cleavages), *i.e.*, both the relative free energies in solvents ($\Delta\Delta G^{\ddagger}_{sol}$) and the relative electronic energy in gas-phase ($\Delta\Delta E^{\ddagger}$), is only minimally affected by the choice of the density functional and the basis set in both optimization and single-point energy calculations. Thus, a more commonly used combination of computational methods, M06 for single point calculations and B3LYP for geometry optimization, was chosen in the present study. Due to the better efficiency in the EDA calculations, the basis set of def2-SVP (for optimization) and def2-TZVP (for single-point energy calculation) is thus chosen in this study.

Table S1. Comparison of barriers (in kcal/mol) of C–CN (TS2 vsTS1) and C–O (TS4 vs TS3; TS7 vs TS3) oxidative addition on Ni(0) with and without $AlMe_3$ using different levels of theories.

Method for Single Point Energy Calculation	Method for Geometry Optimization	$\Delta\Delta G^{\ddagger}_{sol}$ ($\Delta\Delta E^{\ddagger}$) (TS2–TS1)	$\Delta\Delta G^{\ddagger}_{sol}$ ($\Delta\Delta E^{\ddagger}$) (TS4–TS3)	$\Delta\Delta G^{\ddagger}_{sol}$ ($\Delta\Delta E^{\ddagger}$) (TS7–TS3)
M06/def2-TZVP	B3LYP/def2-SVP	–9.2 (–6.1)	–7.8 (–9.7)	–9.3 (–9.2)
B3LYP-D3/def2-TZVP		–6.4 (–5.0)	–8.5 (–10.5)	–11.3 (–11.3)
ωB97xD/def2-TZVP		–5.7 (–4.3)	–6.3 (–8.3)	–7.9 (–7.9)
M06/SDD−6-311+G(d,p)		–8.3 (–5.5)	–7.7 (–9.70)	–9.9 (–9.7)
B3LYP-D3/SDD−6-311+G(d,p)		–5.4 (–4.0)	–8.1 (–10.1)	–10.3 (–10.1)
ωB97xD/SDD−6-311+G(d,p)		–5.0 (–3.5)	–6.5 (–8.5)	–8.7 (–8.5)
M06/def2-TZVP	B3LYP/LANL2DZ–6-31G(d)	–8.8 (–7.7)	–9.9 (–8.3)	–7.8 (–8.5)
B3LYP-D3/def2-TZVP		–7.6 (–6.6)	–9.4 (–7.8)	–9.4 (–10.2)
ωB97xD/def2-TZVP		–7.0 (–5.9)	–8.1 (–6.5)	–6.0 (–6.7)
M06/SDD−6-311+G(d,p)		–9.9 (–7.1)	–10.8 (–9.3)	–6.8 (–7.5)
B3LYP-D3/SDD−6-311+G(d,p)		–6.4 (–5.5)	–9.7 (–8.1)	–8.7 (–9.5)
ωB97xD/SDD−6-311+G(d,p)		–6.1 (–5.1)	–9.0 (–7.5)	–5.3 (–6.1)

Solvent Effects on the Results of EDA

To study whether the results of EDA could be affected by solvents, we preformed EDA calculations for the C–CN and C–O oxidative addition transition states in both gas-phase and solvents (Table S2). The solvents used in calculations were chosen according to the experimental conditions. The solvation energy term was included in the reported electrostatic interaction energies ($\Delta\Delta E_{elstat}$). The results show that solvents are not expected to have a significant impact on the difference of each energy term. The results based on gas-phase EDA calculations were reported in the main text.

Table S2. Comparison of the energy terms of EDA calculated in gas phase and solvent.

$\Delta\Delta E$ = ΔE(w/ $AlMe_3$) – ΔE(w/o $AlMe_3$)	**C–CN cleavage (TS2–TS1)**		**$C_{(benzyl)}$–O cleavage (TS4–TS3)**		**$C_{(benzyl)}$–O cleavage (TS7–TS3)**	
	gas	toluene	gas	m-xylene	gas	m-xylene
$\Delta\Delta E_{Pauli}$	3.0	2.7	**-46.0**	**-48.2**	23.8	21.1
$\Delta\Delta E_{elstat}$	-0.6	-0.3	23.9	22.9	**-17.0**	**-14.3**
$\Delta\Delta E_{pol}$	-2.9	-1.9	13.1	12.5	**-12.8**	**-12.5**
$\Delta\Delta E_{ct}$	**-17.1**	**-15.7**	12.1	11.9	-4.5	-8.5
$\Delta\Delta E_{disp}$	-1.2	-1.3	-5.8	-5.6	-4.7	-4.5

Interactions of Substrates with $AlMe_3$

The substrates investigated in this work can form stable Lewis acid/base adducts with $AlMe_3$. The computed free energies in solvents (ΔG_{sol}) and gas-phase electronic energies (ΔE_{gas}) are shown in Fig. S1.

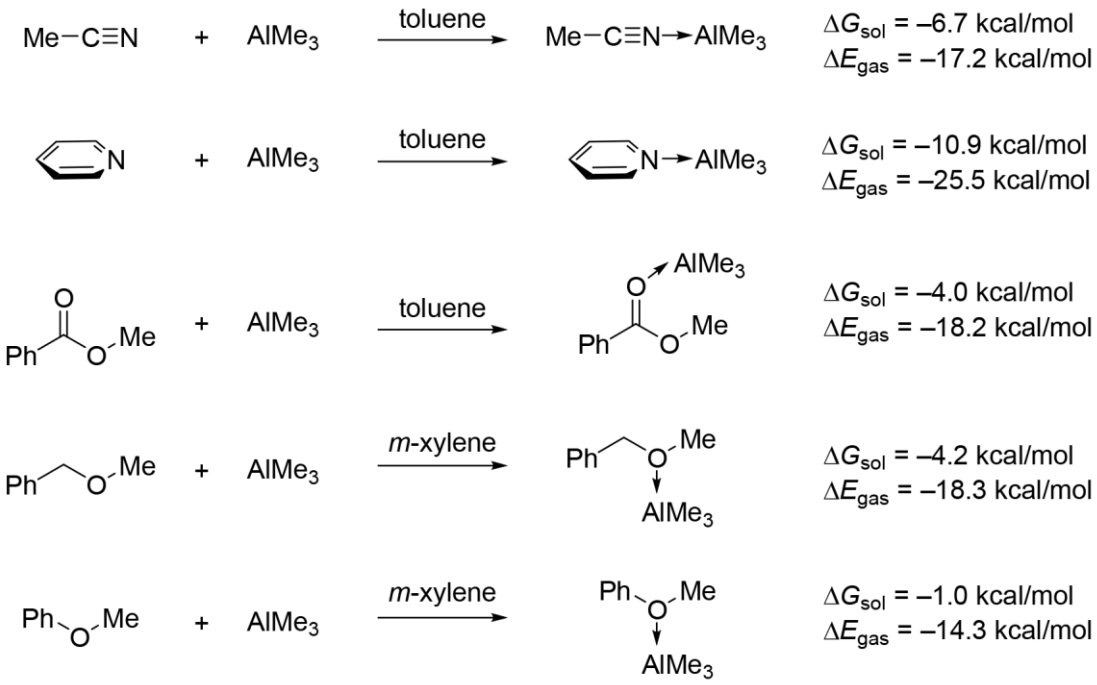

Fig. S1. Computed interaction energies of substrates with $AlMe_3$. Energies are with respect to the separated substrates and $AlMe_3$.

Energy Profiles of C–CN, C–H and C–O Bond Cleavages

The energy profiles for the oxidative additions of C–CN, C–H and C–O bonds with Ni(0) are shown in Fig. S2-S6. The general trend is that the transition state with $AlMe_3$ have a lower barrier than that without $AlMe_3$. The difference in the gas-phase activation electronic energies ($\Delta\Delta E^{\ddagger}$) is consistent with that of the activation free energies in solvents ($\Delta\Delta G^{\ddagger}$). Since the EDA calculation is performed in gas phase, the $\Delta\Delta E^{\ddagger}$ is discussed in the main text.

It should be noted that, because the complexes of Ni catalysts with substrate and substrate-LA may have different energetics relative to the pre-catalysts, the computed activation energies are with respect to the more stable species along the respective energy profile (e.g., for the C–CN cleavage in Fig. S2). In addition, for the Ni catalysts with NHC ligand (SIPr), the SIPr-Ni-SIPr is chosen as the resting state, and thus the computed barriers are relatively high due to the energy cost of the dissociation of one SIPr ligand from SIPr-Ni-SIPr. In fact, there is an equilibrium between SIPr-Ni-SIPr and SIPr-Ni-substrate due to the concentrations of ligand and Ni pre-catalyst in real experimental conditions. However, no matter what energy reference is chosen, the barrier of the transition state with Lewis acids is lower than that without Lewis acids.

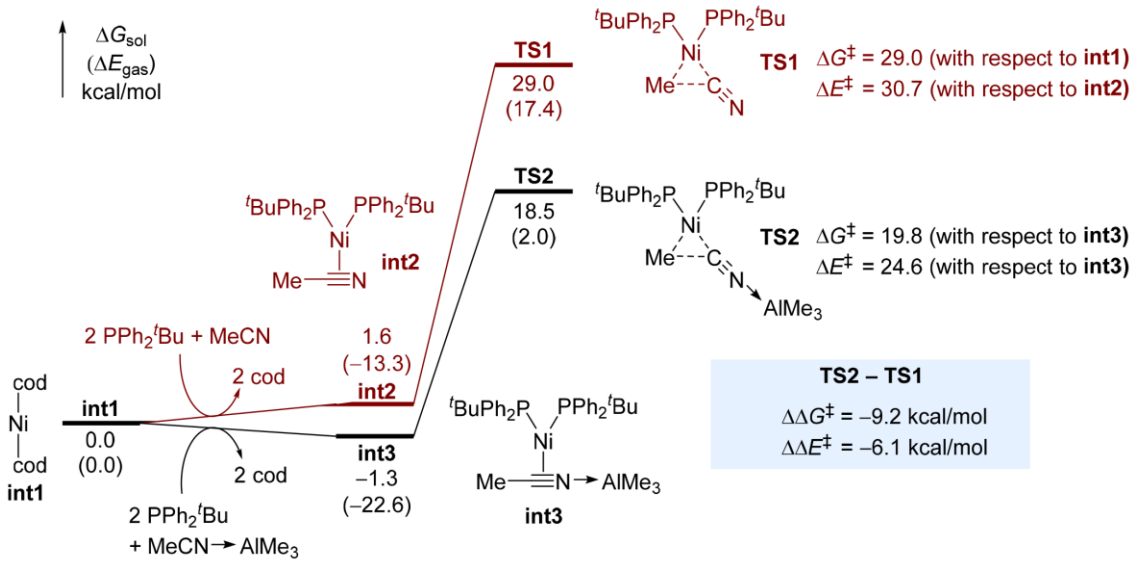

Fig. S2. Energy profiles for C–CN oxidative addition on Ni(0) with and without $AlMe_3$.

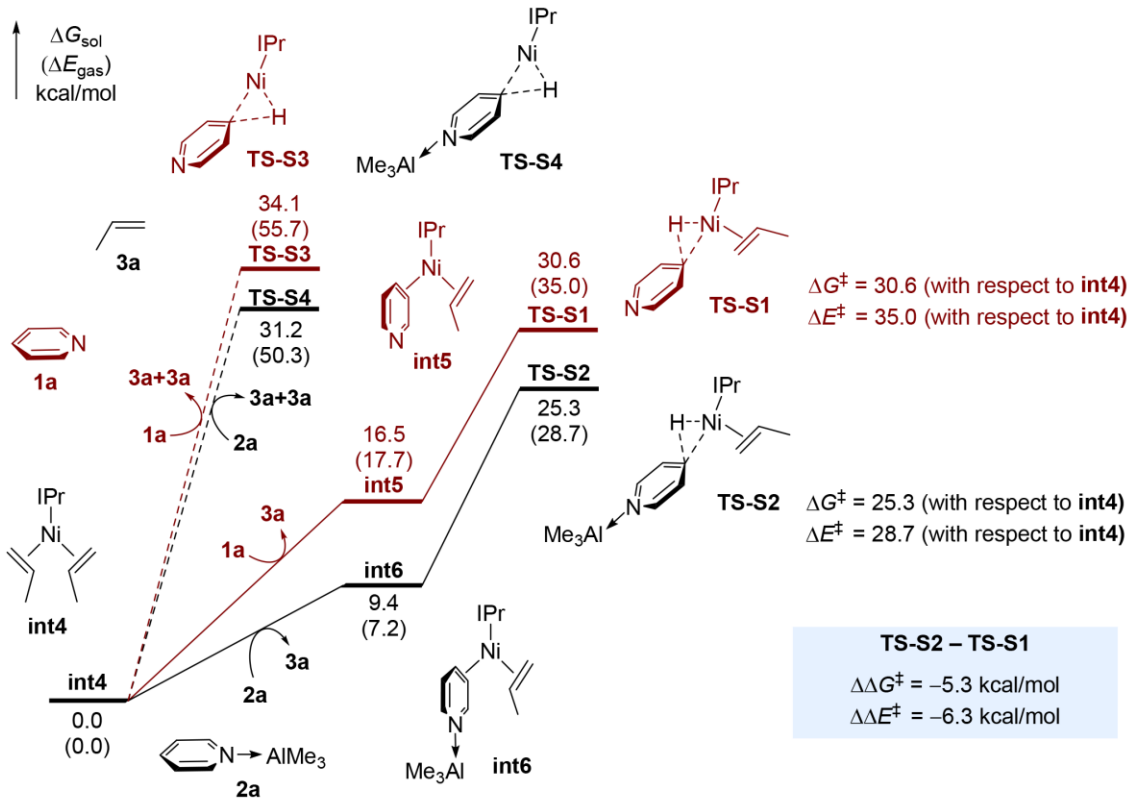

Fig. S3. Energy profiles for pyridine *para*-C–H oxidative additions on Ni(0) with and without $AlMe_3$.

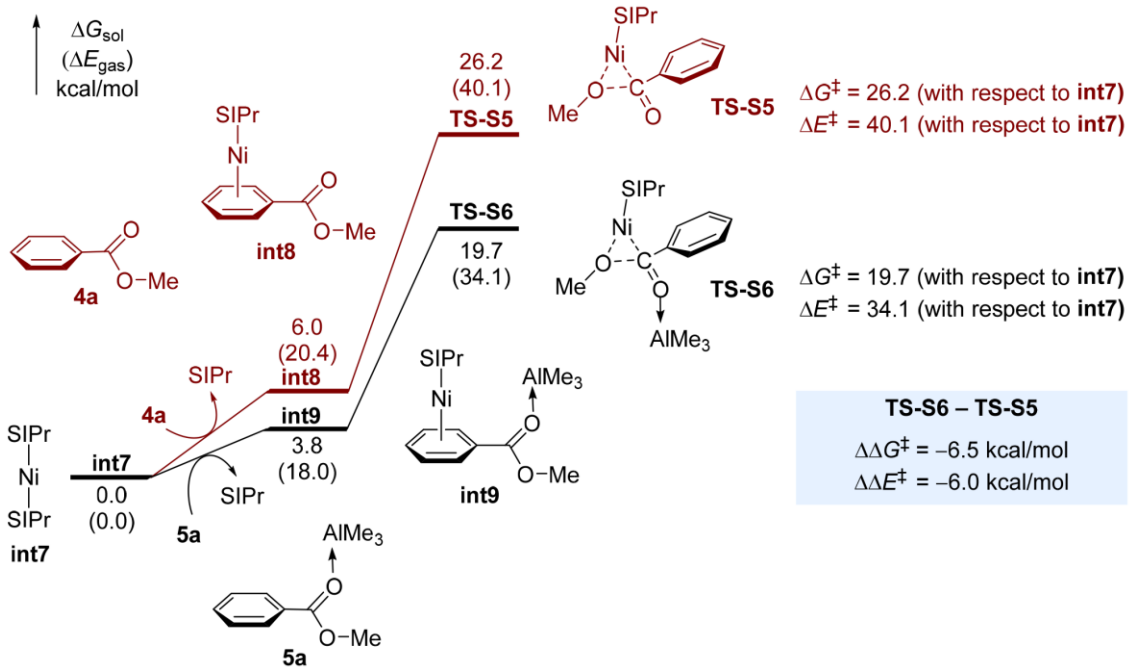

Fig. S4. Energy profiles for C(acyl)–O oxidative additions on Ni(0) with and without $AlMe_3$.

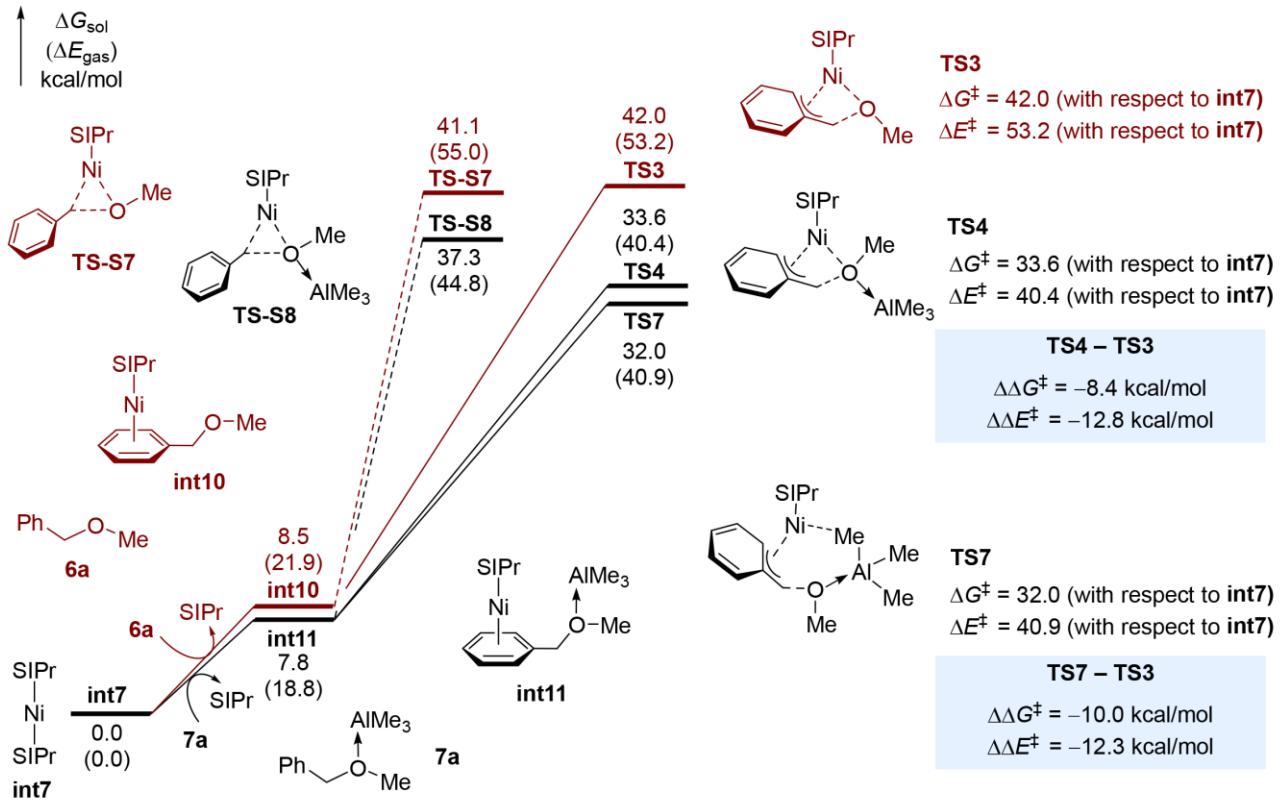

Fig. S5. Energy profiles for C(benzyl)–O oxidative additions on Ni(0) with and without $AlMe_3$.

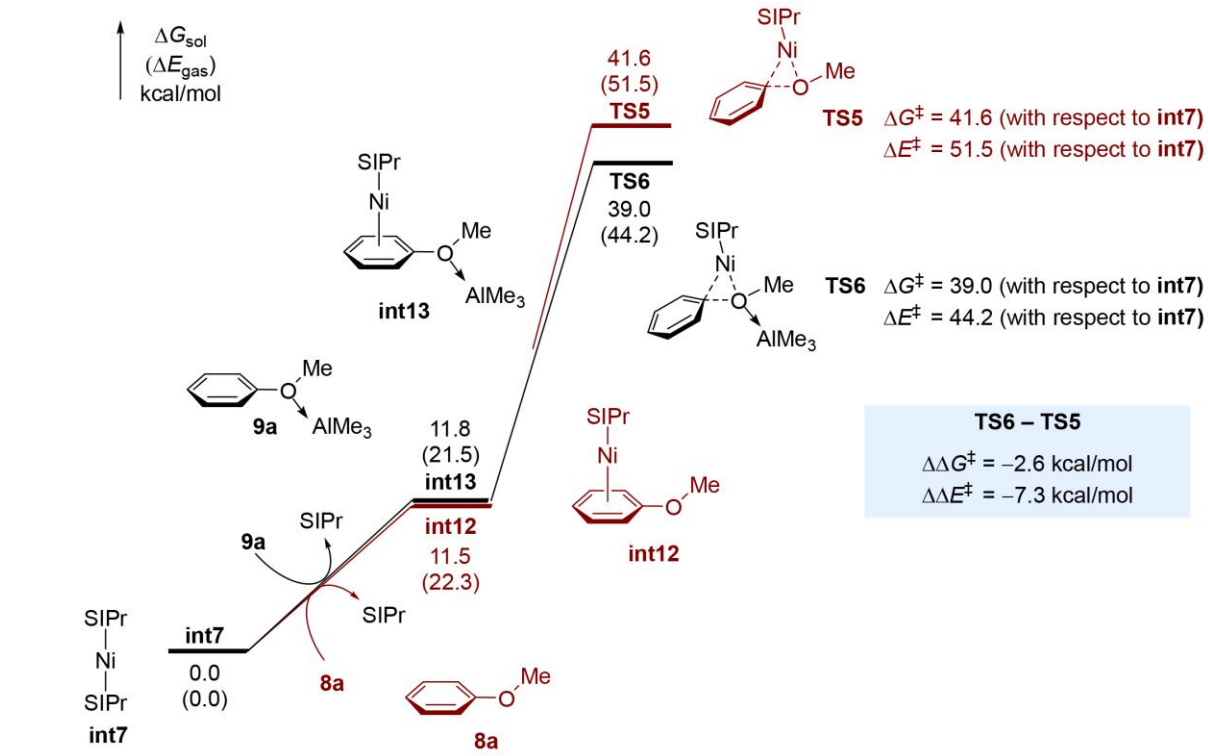

Fig. S6. Energy profiles for the C(phenyl)–O oxidative additions on Ni(0) with and without $AlMe_3$.

Oxidative Additions of Pyridine C–H and C(acyl)–O Bonds with Ni(0)

The computed barriers and EDA results for Ni-catalyzed C–H and C(acyl)–O cleavages are shown in Fig. S7 and S9. The barrier differences indicate that $AlMe_3$ can promote the cleavages of both C–H (**TS-S1** vs **TS-S2**) and C(acyl)–O (**TS-S5** vs **TS-S6**) bonds. The EDA results along IRC and the bar charts show that the difference in charge transfer (ΔE_{ct}) is the most significant effect on favoring C–H and C(acyl)–O oxidative additions in the presence of $AlMe_3$ (Fig. S7b-c and S7b-c). The COVPs results clearly demonstrate that the stronger charge transfer in **TS-S2** than that in **TS-S1** is mainly due to the larger electron donation from the occupied Ni d orbital to the σ*(C–H) antibonding orbital ($\Delta E_{ct(d\rightarrow\sigma^*)}$ = –63.4 kcal/mol of **TS-S2** vs $\Delta E_{ct(d\rightarrow\sigma^*)}$ = –57.9 kcal/mol of **TS-S1**, Fig. S7d). Also, the stronger electron donation from the occupied Ni d orbital to the σ*(C–O) and π*(C=O) antibonding orbitals in **TS-S6** ($\Delta E_{ct(d\rightarrow\sigma^*+\pi^*)}$ = –121.8 kcal/mol) than that in **TS-S5** ($\Delta E_{ct(d\rightarrow\sigma^*+\pi^*)}$ = –88.6 kcal/mol) leads to the lower barrier of C(acyl)–O cleavage with $AlMe_3$.

In addition, we also performed EDA for the transition states of pyridine C-H cleavage without olefin coordination (**TS-S3** and **TS-S4**, Fig. S8). The results show that the charge transfer effect is also the dominant factor the Lewis acid acceleration.

Together with the C–CN bond cleavage reported in the main text, the dominant role of Lewis acids in lowering the barriers of **TS-I** type oxidative addition transition states is to increase the stabilizing charger transfer effect.

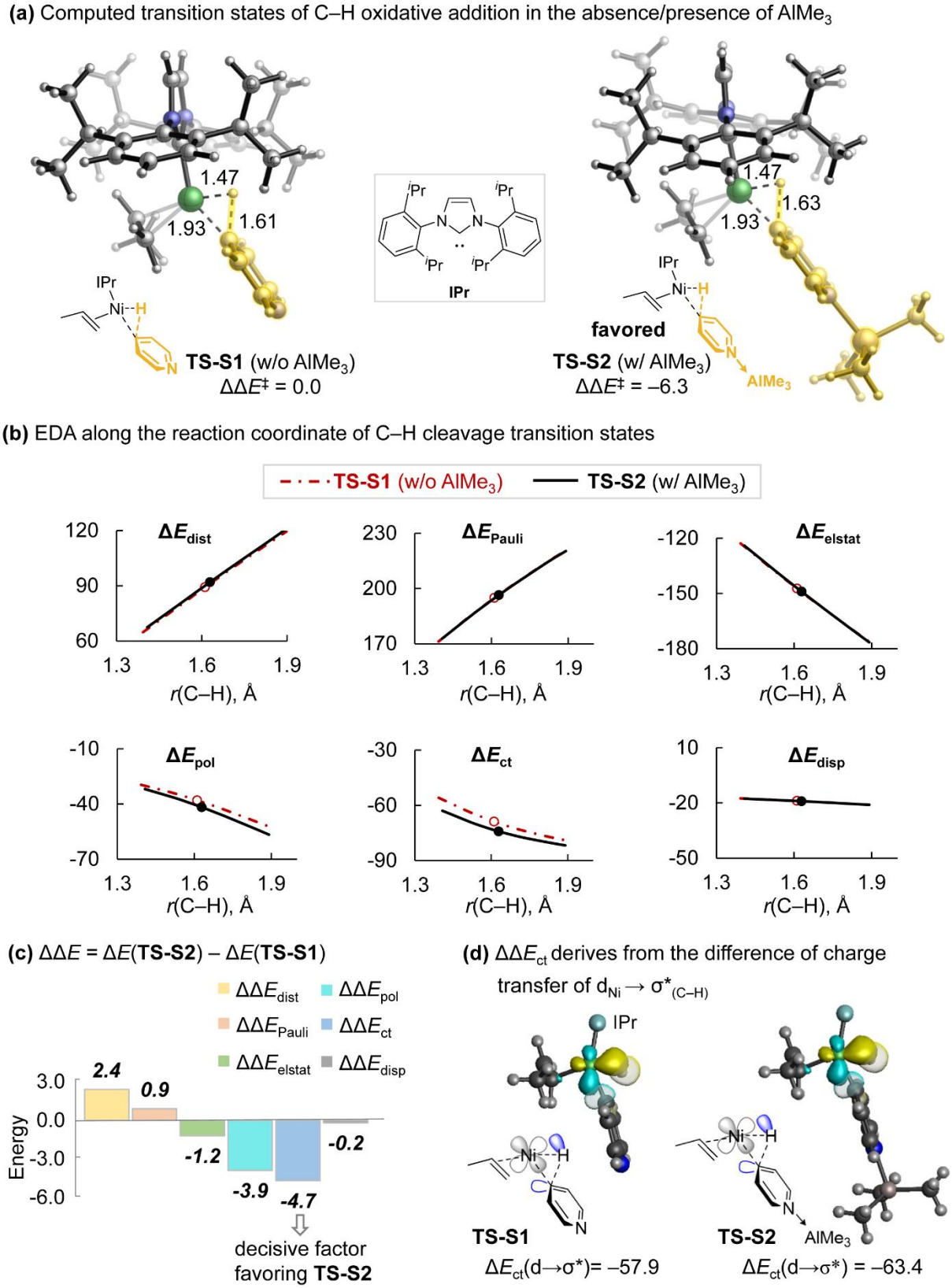

Fig. S7. Lewis acid-assisted C–H bond oxidative addition with Ni(0) in the presence of olefin coordination. Energies and key bond distances are shown in kcal/mol and Å, respectively.

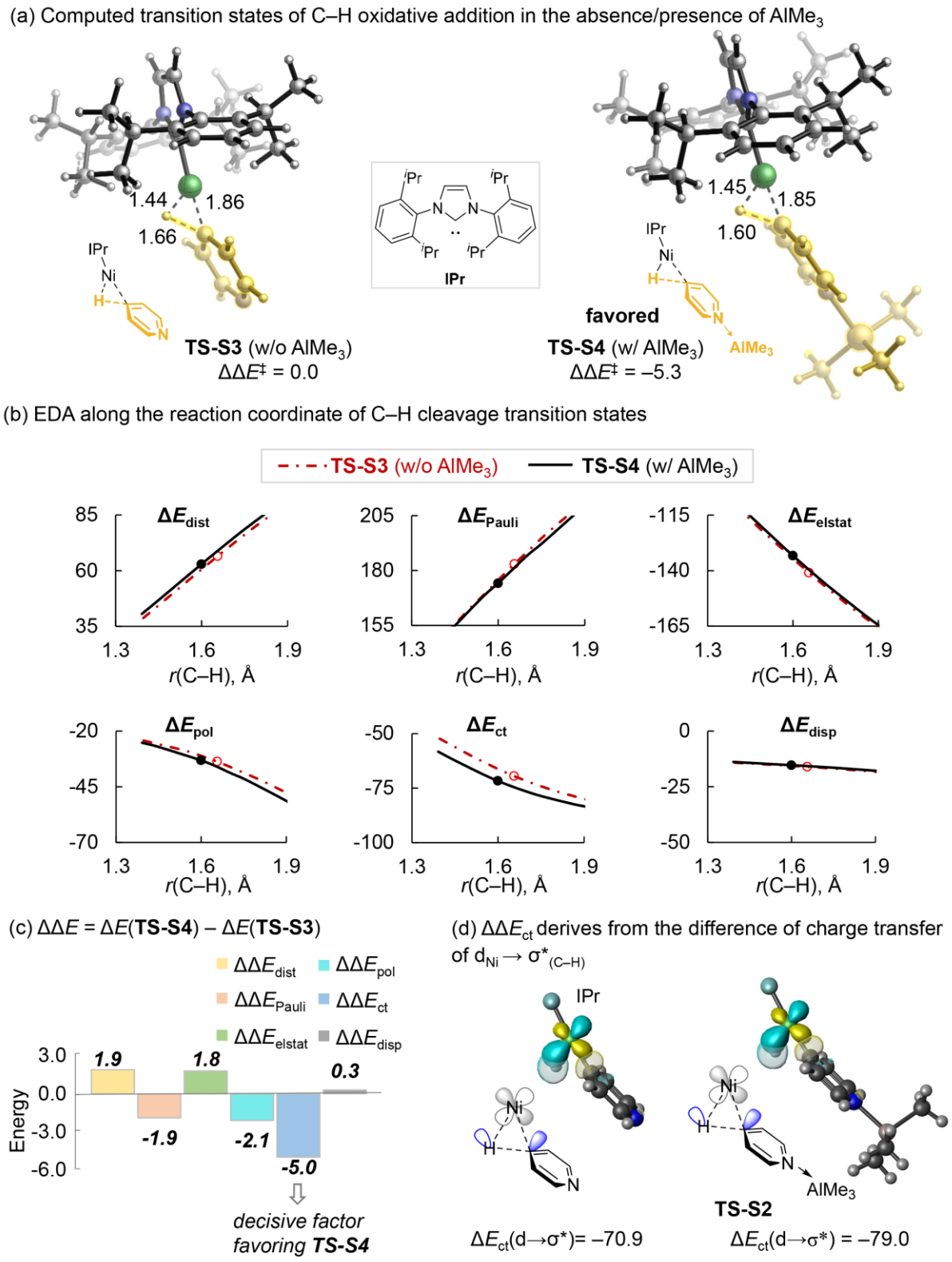

Fig. S8. Lewis acid-assisted C–H bond oxidative addition with Ni(0) in the absence of olefin coordination. Energies and key bond distances are shown in kcal/mol and Å, respectively.

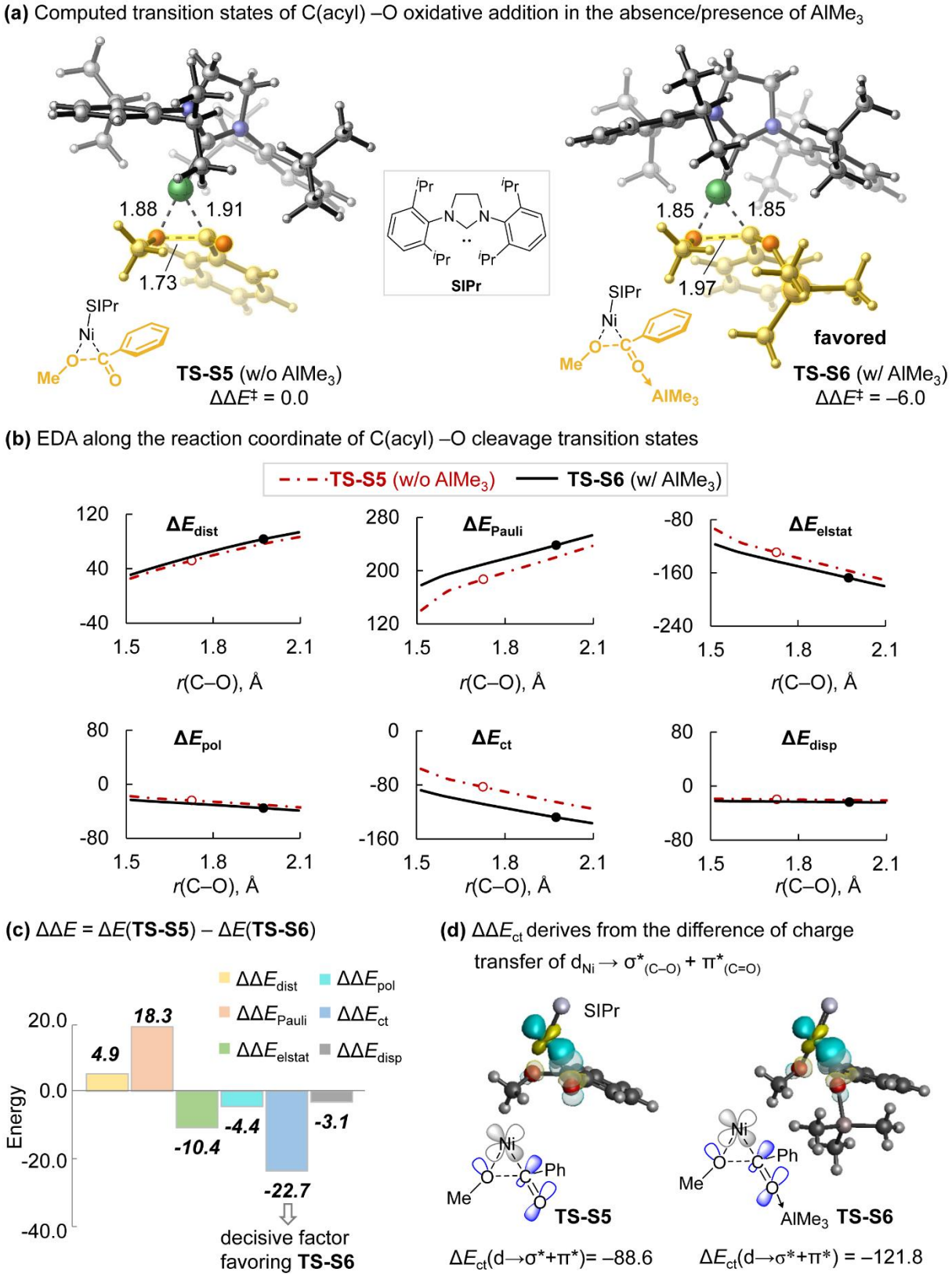

Fig. S9. Lewis acid-assisted C(acyl)–O bond oxidative addition with Ni(0). Energies and key bond distances are shown in kcal/mol and Å, respectively.

EDA Results along IRC for C(benzyl)–O and C(phenyl)–O Oxidative Additions

The EDA results along IRC for C(benzyl)–O and C(phenyl)–O oxidative additions with Ni(0) are shown in Fig. S10-S12. As described in the bar charts of the main text, the reduced Pauli repulsion is the decisive factor for the increased reactivity of **TS4** and **TS6** (belonging to the **TS-II** type transition state), and the strengthened electrostatics and polarization are the most significant factors for **TS7** (belonging to the **TS-III** type). Here, these energy terms along IRC shows the consistent results.

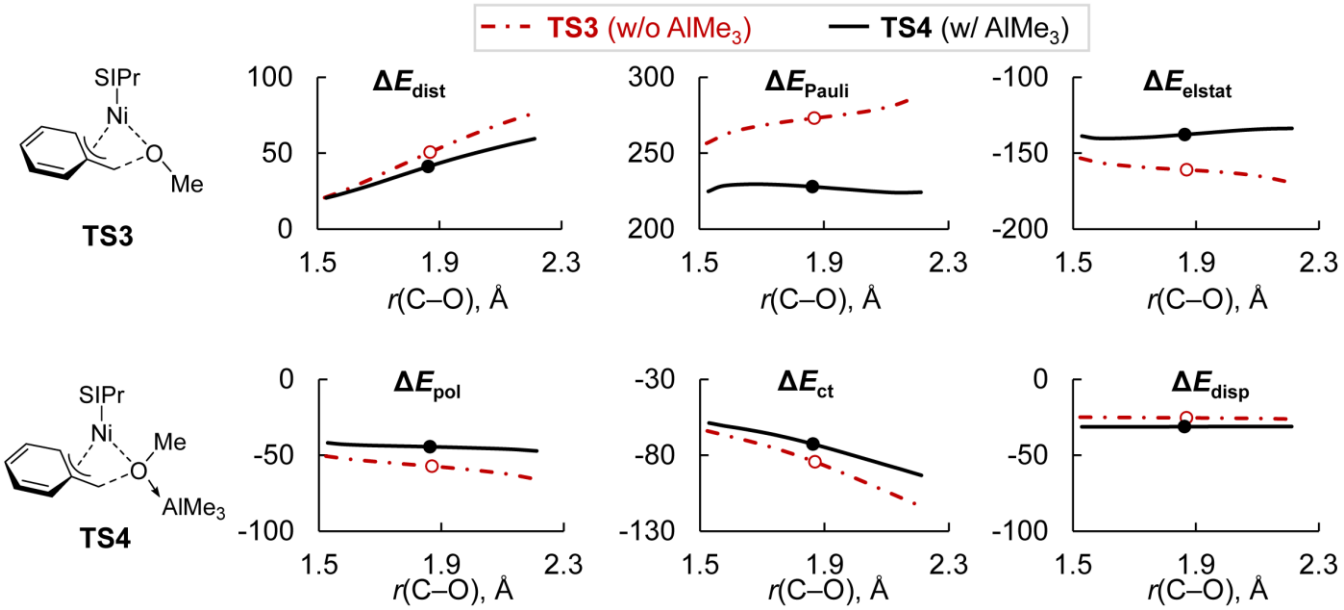

Fig. S10. EDA results along IRC of C(benzyl)–O oxidative addition transition states (**TS-II** type). Energies are shown in kcal/mol.

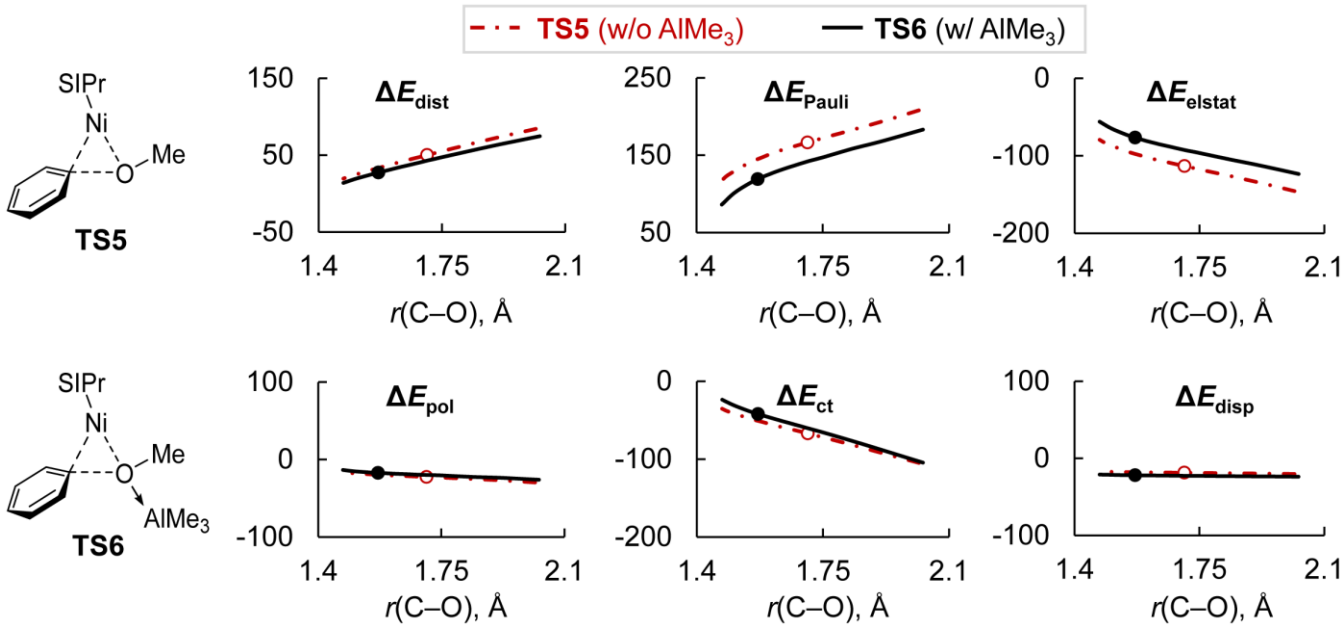

Fig. S11. EDA results along IRC of C(phenyl)–O oxidative addition transition states (**TS-II** type). Energies are shown in kcal/mol.

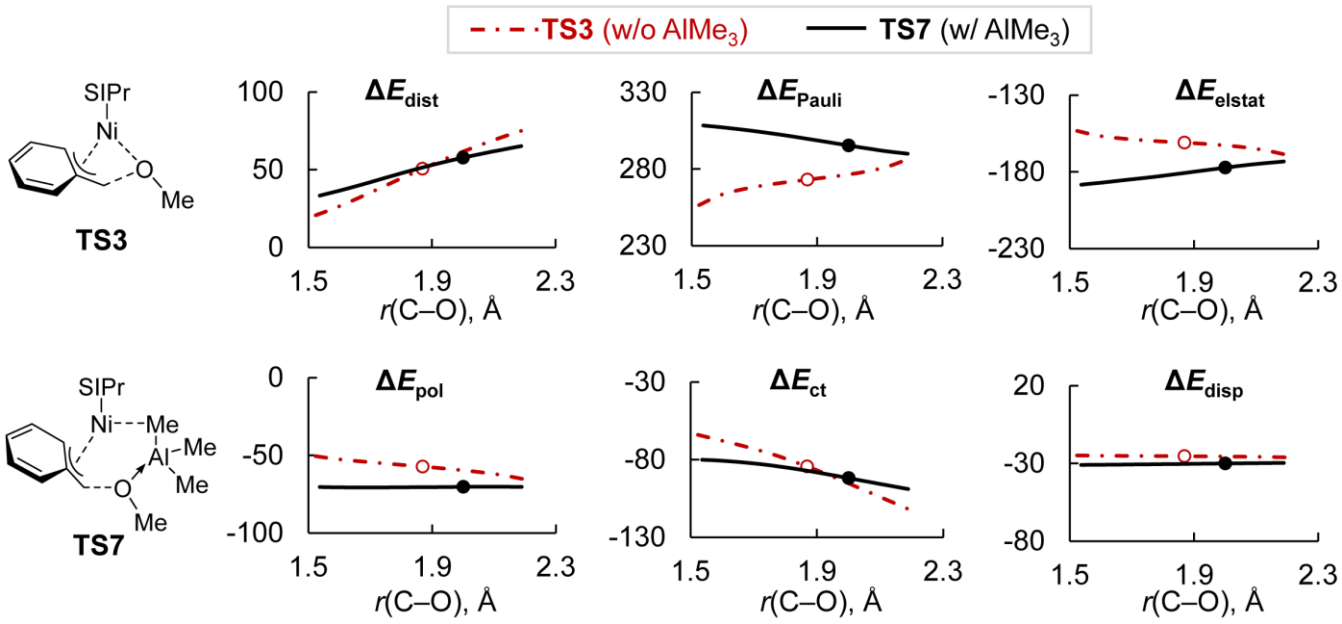

Fig. S12. EDA results along IRC of C(benzyl)–O oxidative addition transition states (**TS-III** type). Energies are shown in kcal/mol.

EDA Results for the Disfavored C(benzyl)–O Oxidative Addition

Even for the less favorable transition state of C(benzyl)–O oxidative addition on Ni(0) without the η^3-benzyl coordination (**TS-S8**, Fig. S13), the EDA results also reveal that the reduced Pauli repulsion is the key factor for the lower barrier of **TS-S8** than **TS-S7**. This emphasizes that the important role of Pauli repulsion in affecting the reactivity of **TS-II** type transition state with Lewis acids.

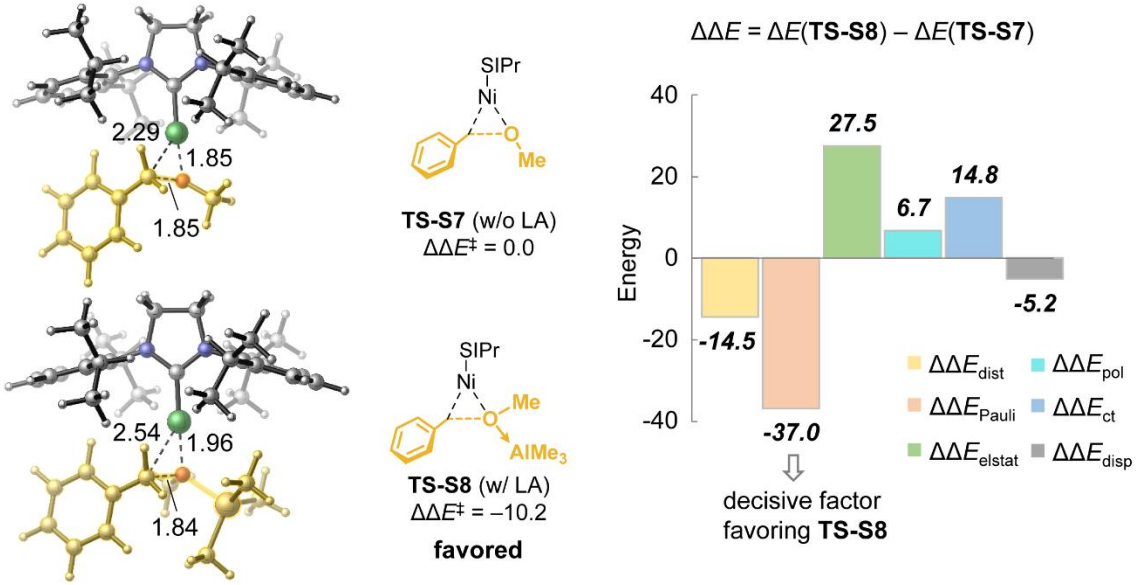

Fig. S13. Less favorable Lewis acid-assisted C(benzyl)–O bond oxidative addition with Ni(0). Energies and key bond distances are shown in kcal/mol and Å, respectively.

Effects of Distortion and Dispersion on $AlMe_3$-Assisted C(benzyl)–O Oxidative Addition

Compared to the nearly planar geometry of BnOMe ($D(C_1C_2C_3O)$ = 5.8°), the substrates in **TS3** ($D(C_1C_2C_3O)$ = 88.0°) and **TS4** ($D(C_1C_2C_3O)$ = 94.2°) are highly distorted. Because the $AlMe_3$ coordination to BnOMe can pre-distort the geometry ($D(C_1C_2C_3O)$ = 57.4°), the computed distortion energy of **TS4** with $AlMe_3$ is smaller than that of **TS3**.

In addition, The NCI plot clearly shows that there are stronger no-covalent interactions between $AlMe_3$ and the NHC ligand in **TS4**, which accounts for the computed larger dispersion energy.

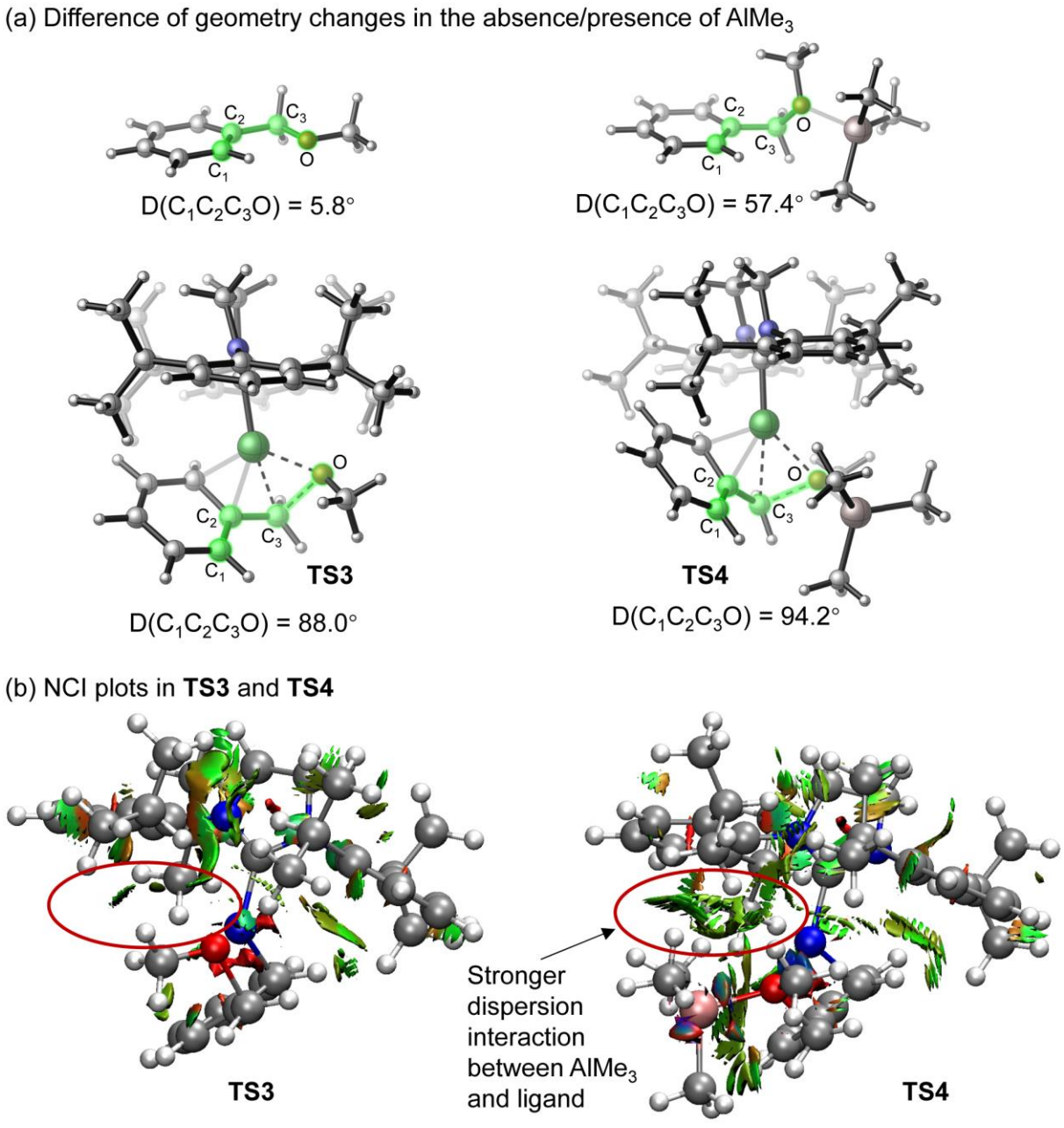

Fig. S14. (a) Comparison of substrate geometry. (b) Non-covalent interactions in the absence /presence of $AlMe_3$.

Cartesian Coordinates (Å) and Energies of the Optimized Structures

TS1

B3LYP SCF energy: -3564.75283054 a.u.
B3LYP enthalpy: -3564.054816 a.u.
B3LYP free energy: -3564.171542 a.u.
M06 SCF energy in solution: -3565.49396591 a.u.
M06 enthalpy in solution: -3564.795951 a.u.
M06 free energy in solution: -3564.912677 a.u.
Three lowest frequencies (cm-1): -405.4491 11.7807 13.0283
Imaginary frequency: -405.4491 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	0.126769	-2.667173	-1.634436
N	0.118790	-3.823644	-1.394901
C	0.852562	-1.731293	-3.040448
H	1.913849	-2.002055	-3.096386
H	0.289288	-2.307539	-3.783405
H	0.716269	-0.655718	-3.284753
P	-1.900289	-0.547599	-0.385293
C	-3.383224	-1.409499	-1.286587
C	-3.373137	-2.898017	-0.888823
C	-3.136405	-1.286763	-2.801297
C	-4.747397	-0.786879	-0.951298
C	-2.346618	1.253917	-0.443546
C	-2.819866	2.019492	0.634645
C	-3.105190	3.380522	0.479692
C	-2.919771	4.008581	-0.753755
C	-2.423670	3.267137	-1.831091
C	-2.130586	1.910955	-1.671931
C	-2.070190	-1.100737	1.373483
C	-3.181639	-0.869813	2.207190
C	-3.222556	-1.383419	3.506261
C	-2.159690	-2.149146	3.995386
C	-1.056458	-2.398071	3.176255
C	-1.011592	-1.875701	1.880171
H	-3.624059	-3.038188	0.172981
H	-4.135522	-3.430975	-1.483245
H	-3.205634	-0.244522	-3.148592
H	-2.151137	-1.685072	-3.080897
H	-4.791381	0.284130	-1.200400
H	-5.014182	-0.908739	0.108186
H	-5.530804	-1.297795	-1.538122
H	-2.953454	1.565279	1.615604
H	-3.472312	3.952248	1.336150
H	-3.149211	5.070532	-0.873639
H	-2.255885	3.747322	-2.798845
H	-1.713732	1.355655	-2.515818
H	-4.032215	-0.289451	1.849534
H	-4.094256	-1.188773	4.136730
H	-2.196477	-2.555215	5.009688
H	-0.225004	-3.006347	3.541327
H	-0.153934	-2.091412	1.239903
P	1.804185	0.459617	-0.435745
C	2.779603	1.614343	-1.649606

C	1.759288	2.316838	-2.568120
H	1.118458	1.590672	-3.090634
H	1.098861	3.012087	-2.031006
C	3.663457	0.701352	-2.522050
H	4.156188	1.311728	-3.298081
H	4.450028	0.205057	-1.935957
C	3.675202	2.656946	-0.962332
H	4.477350	2.183667	-0.378298
H	3.118056	3.330072	-0.296131
H	4.161857	3.279881	-1.733445
C	3.149002	-0.586443	0.310170
C	4.142167	-0.063530	1.161714
C	5.157274	-0.881039	1.662802
C	5.195209	-2.240087	1.330863
C	4.206435	-2.774761	0.503502
C	3.189635	-1.955942	-0.001897
H	2.414890	-2.400682	-0.627528
H	4.212706	-3.837866	0.250175
H	5.988691	-2.879763	1.726194
H	5.919361	-0.455342	2.321086
H	4.114460	0.986891	1.455919
C	1.311139	1.514390	1.014593
C	1.307745	0.957234	2.308345
C	0.860284	1.689281	3.410906
C	0.401556	2.999307	3.250558
C	0.375403	3.559062	1.971356
C	0.813219	2.822116	0.867296
H	0.749849	3.284165	-0.117310
H	0.003691	4.575927	1.822522
H	0.059155	3.575240	4.114088
H	0.872145	1.227915	4.401796
H	1.661146	-0.063009	2.464293
Ni	0.124158	-0.906439	-1.307445
H	-3.904113	-1.863110	-3.345166
H	-2.401327	-3.377010	-1.077755
H	3.078373	-0.074708	-3.035146
H	2.295811	2.901389	-3.335086

TS2

B3LYP SCF energy: -3926.84607986 a.u.
B3LYP enthalpy: -3926.030590 a.u.
B3LYP free energy: -3926.168610 a.u.
M06 SCF energy in solution: -3927.67149538 a.u.
M06 enthalpy in solution: -3926.856006 a.u.
M06 free energy in solution: -3926.994026 a.u.
Three lowest frequencies (cm-1): -359.5377 13.7820 16.5142
Imaginary frequency: -359.5377 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	2.161625	-0.248061	-1.303823
N	3.269726	-0.406342	-0.920015
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H	2.063568	1.690366	-2.691186

H	2.195458	0.072530	-3.451754
H	0.584304	0.761070	-3.165332
P	-0.369161	-1.898552	-0.303255
C	0.328256	-3.518602	-1.096997
C	1.750138	-3.737286	-0.548348
C	0.392987	-3.310272	-2.621483
C	-0.539247	-4.751350	-0.796154
C	-2.195756	-2.018443	-0.598923
C	-3.161351	-2.333844	0.370566
C	-4.517322	-2.407014	0.034434
C	-4.938731	-2.158872	-1.273565
C	-3.993257	-1.811596	-2.243700
C	-2.640442	-1.732554	-1.905702
C	-0.057916	-2.104677	1.504218
C	0.857896	-1.207726	2.083237
C	1.225776	-1.319695	3.427373
C	0.673631	-2.326406	4.222075
C	-0.236264	-3.228533	3.661546
C	-0.592758	-3.125465	2.314535
H	1.746193	-3.939475	0.532504
H	2.195630	-4.613332	-1.049290
H	-0.607798	-3.250551	-3.075193
H	0.951602	-2.400446	-2.885771
H	-1.577226	-4.630607	-1.140703
H	-0.552329	-5.000156	0.274559
H	-0.113917	-5.624235	-1.320761
H	-2.867475	-2.507361	1.404855
H	-5.248406	-2.656150	0.807814
H	-5.998129	-2.223494	-1.534466
H	-4.308881	-1.596408	-3.267949
H	-1.921011	-1.436248	-2.672943
H	1.313523	-0.427789	1.470370
H	1.959339	-0.624174	3.841423
H	0.959631	-2.417107	5.273083
H	-0.665547	-4.026341	4.273237
H	-1.287902	-3.856329	1.901852
P	-0.859982	1.899179	-0.488029
C	-1.622305	3.060180	-1.831974
C	-2.328443	2.181558	-2.884691
H	-1.642784	1.438125	-3.319772
H	-3.194258	1.635711	-2.483957
C	-0.447967	3.788747	-2.515811
H	-0.839639	4.392664	-3.351757
H	0.073230	4.468707	-1.827156
C	-2.593124	4.116423	-1.279665
H	-2.089193	4.809219	-0.590963
H	-3.454974	3.681018	-0.756205
H	-2.982675	4.719110	-2.118432
C	0.244550	3.034161	0.480488
C	-0.257967	4.048220	1.319697
C	0.610360	4.903577	2.001128
C	1.995699	4.757879	1.865504
C	2.507376	3.747311	1.049767
C	1.637416	2.892451	0.363802
H	2.058442	2.099750	-0.253740
H	3.586093	3.607449	0.946773

H	2.673238	5.425164	2.404221
H	0.201858	5.684838	2.647496
H	-1.334158	4.161882	1.462010
C	-2.194068	1.529591	0.748857
C	-1.829963	1.324643	2.094035
C	-2.782486	0.980711	3.056031
C	-4.125161	0.831211	2.698313
C	-4.498673	1.007795	1.364557
C	-3.543257	1.341945	0.400074
H	-3.871213	1.447666	-0.633041
H	-5.541185	0.879859	1.063004
H	-4.872649	0.572298	3.452439
H	-2.468258	0.832028	4.092190
H	-0.790177	1.439579	2.403381
Ni	0.421500	0.023665	-1.186632
Al	5.116649	-0.426673	-0.203778
C	4.827831	-0.273579	1.776089
H	4.303083	-1.150077	2.199074
H	5.790386	-0.193170	2.315813
H	4.240761	0.623186	2.052830
C	5.866432	-2.171366	-0.827690
H	5.869110	-2.266710	-1.929504
H	6.916758	-2.294295	-0.502347
H	5.313915	-3.042947	-0.429862
C	5.936213	1.204752	-1.032520
H	6.981577	1.340538	-0.695916
H	5.968603	1.155889	-2.136950
H	5.403045	2.138548	-0.769347
H	0.292142	3.092317	-2.933614
H	-2.694061	2.817368	-3.708895
H	0.909420	-4.168070	-3.083817
H	2.410185	-2.878883	-0.732578

TS3

B3LYP SCF energy: -3054.36975020 a.u.
B3LYP enthalpy: -3053.575185 a.u.
B3LYP free energy: -3053.690416 a.u.
M06 SCF energy in solution: -3055.00680610 a.u.
M06 enthalpy in solution: -3054.212241 a.u.
M06 free energy in solution: -3054.327472 a.u.
Three lowest frequencies (cm-1): -389.6580 18.0413 29.3978
Imaginary frequency: -389.6580 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	0.050013	0.137443	-0.556318
C	0.913614	0.430413	-2.746195
C	-0.603326	0.263661	-2.830996
H	1.237059	1.461544	-2.975954
H	1.455640	-0.248283	-3.419304
H	-1.098566	1.060118	-3.405111
H	-0.882064	-0.700381	-3.287482
N	-1.001040	0.303352	-1.409153
N	1.175934	0.114575	-1.332005

C	-2.385468	0.440510	-1.051040
C	-3.271571	-0.641265	-1.269440
C	-2.858747	1.692408	-0.571232
C	-4.639340	-0.445479	-1.021017
C	-4.232242	1.825955	-0.326564
C	-5.118758	0.774108	-0.557270
H	-5.338141	-1.268413	-1.187809
H	-4.624591	2.772418	0.046124
H	-6.186816	0.908098	-0.366655
C	2.520162	0.075242	-0.827674
C	3.133644	1.268871	-0.370214
C	3.233973	-1.150650	-0.857863
C	4.448483	1.193635	0.113512
C	4.548132	-1.166942	-0.368655
C	5.149020	-0.010117	0.124270
H	4.935554	2.099813	0.480566
H	5.113341	-2.101286	-0.375033
H	6.172437	-0.045182	0.507047
C	-1.913347	2.872347	-0.333209
H	-1.004847	2.456181	0.131065
C	-2.802491	-2.006885	-1.766534
H	-1.702660	-2.007518	-1.745971
C	2.636984	-2.423492	-1.455200
H	1.546864	-2.279502	-1.498630
C	2.452543	2.633440	-0.456872
H	1.398536	2.465587	-0.719366
Ni	0.070738	-0.057917	1.320374
O	0.297984	1.572727	2.531870
C	0.535553	-1.919288	1.840476
H	1.582902	-1.914233	1.510359
C	0.185611	-1.153225	3.040507
C	0.920908	0.028046	3.380846
H	0.736850	0.459888	4.372324
H	1.962772	0.105109	3.058682
C	-0.208957	-3.122980	1.581528
C	-1.296327	-3.478109	2.340696
H	0.112611	-3.770678	0.760473
H	-1.845351	-4.396900	2.118058
C	-0.992238	-1.540651	3.778084
C	-1.701394	-2.667562	3.448381
H	-1.285079	-0.941138	4.645775
H	-2.564551	-2.966806	4.048961
C	-1.511438	3.566268	-1.649415
H	-2.397391	3.983241	-2.156723
H	-0.816129	4.397835	-1.449360
H	-1.015476	2.883459	-2.351706
C	-2.473506	3.925262	0.634055
H	-2.830605	3.477282	1.572341
H	-1.687107	4.653864	0.886201
H	-3.306983	4.492681	0.188152
C	3.087248	3.477802	-1.580967
H	3.078058	2.952174	-2.549285
H	2.543942	4.429129	-1.704340
H	4.137595	3.721495	-1.350807
C	2.458579	3.402531	0.875029
H	3.483285	3.620345	1.218982

H	1.950188	4.372950	0.746497
H	1.923953	2.842124	1.656402
C	-3.260369	-2.269674	-3.214543
H	-2.937621	-1.473699	-3.903820
H	-2.855935	-3.226158	-3.585004
H	-4.359490	-2.328022	-3.276380
C	-3.259213	-3.147934	-0.842035
H	-4.354967	-3.265204	-0.846159
H	-2.827423	-4.105284	-1.177718
H	-2.933844	-2.974341	0.193045
C	3.146576	-2.645554	-2.894456
H	4.235432	-2.818460	-2.901126
H	2.663901	-3.526674	-3.348704
H	2.950887	-1.779124	-3.544356
C	2.904061	-3.682936	-0.613786
H	2.600411	-3.551486	0.434594
H	2.343661	-4.538390	-1.024414
H	3.969491	-3.964340	-0.622605
C	-0.750136	2.106491	3.279919
H	-0.924928	3.153065	2.971236
H	-1.707801	1.558901	3.166803
H	-0.513221	2.128415	4.367944

TS4

B3LYP SCF energy: -3416.44120043 a.u.
B3LYP enthalpy: -3415.528701 a.u.
B3LYP free energy: -3415.662360 a.u.
M06 SCF energy in solution: -3417.18005626 a.u.
M06 enthalpy in solution: -3416.267557 a.u.
M06 free energy in solution: -3416.401216 a.u.
Three lowest frequencies (cm-1): -334.9564 20.4060 29.9002
Imaginary frequency: -334.9564 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-0.584847	0.627436	-0.545279
C	-2.249042	1.890203	-1.665858
C	-0.875340	2.349368	-2.147554
H	-2.942803	1.646915	-2.483272
H	-2.727761	2.657035	-1.035540
H	-0.667462	2.054408	-3.192244
H	-0.739119	3.436753	-2.074183
N	0.029656	1.634959	-1.229359
N	-1.916565	0.691744	-0.869589
C	1.447720	1.832662	-1.379399
C	2.094605	2.863697	-0.654844
C	2.148403	1.065202	-2.342093
C	3.461883	3.074491	-0.883886
C	3.516317	1.310859	-2.523724
C	4.171363	2.304306	-1.801839
H	3.983618	3.856510	-0.329182
H	4.078469	0.713027	-3.244476
H	5.238988	2.480481	-1.955566
C	-2.930291	-0.272435	-0.533935

C	-2.956389	-1.520072	-1.221552
C	-3.948376	0.058578	0.396930
C	-3.976185	-2.429448	-0.909746
C	-4.954273	-0.886305	0.656261
C	-4.966932	-2.122570	0.021619
H	-4.009278	-3.394045	-1.416565
H	-5.741915	-0.645417	1.372715
H	-5.754831	-2.847071	0.242974
C	1.475292	-0.025910	-3.168970
H	0.390501	0.057181	-3.018098
C	1.354200	3.765790	0.328588
H	0.410197	3.263511	0.588738
C	-4.031078	1.415575	1.094539
H	-3.050282	1.902374	0.985384
C	-1.952152	-1.860915	-2.324498
H	-0.970432	-1.491030	-1.993189
Ni	0.164653	-0.432647	0.823407
O	1.081898	-2.599793	0.967879
C	0.353487	-3.681120	0.407362
H	0.659276	-3.828948	-0.638792
H	0.538376	-4.620966	0.958639
H	-0.727800	-3.465690	0.431304
C	-0.718182	0.108849	2.476036
H	-1.700932	-0.353931	2.305664
C	0.392613	-0.756700	2.877482
C	0.349701	-2.157846	2.623240
H	1.048967	-2.798272	3.164335
H	-0.629484	-2.609950	2.442203
C	-0.729819	1.450858	3.007810
C	0.310097	1.938723	3.755031
H	-1.603741	2.080878	2.828284
H	0.267377	2.957318	4.149007
C	1.490756	-0.178966	3.617491
C	1.447081	1.119400	4.050052
H	2.342565	-0.816047	3.866638
H	2.268448	1.527033	4.644376
Al	3.064697	-2.821595	1.037179
C	3.716659	-0.945149	0.845901
H	4.077736	-0.512959	1.795674
H	4.553240	-0.879471	0.126614
H	2.934757	-0.258355	0.470920
C	3.418869	-3.714685	2.797659
H	2.801701	-4.617037	2.970859
H	4.467163	-4.070384	2.793764
H	3.323051	-3.079976	3.697630
C	3.468402	-4.066997	-0.474713
H	3.079837	-5.089777	-0.315727
H	3.126283	-3.740573	-1.472119
H	4.568337	-4.169719	-0.548162
C	1.729761	0.133087	-4.677704
H	1.150184	-0.614354	-5.243853
H	1.437333	1.133125	-5.036283
H	2.790199	-0.015833	-4.936351
C	1.888488	-1.419137	-2.670301
H	2.974074	-1.576113	-2.765483
H	1.630118	-1.542533	-1.609373

H	1.381999	-2.211129	-3.246072
C	-1.802606	-3.364953	-2.598034
H	-2.694913	-3.785517	-3.089515
H	-0.952609	-3.536864	-3.276589
H	-1.619889	-3.941609	-1.680719
C	-2.310349	-1.149459	-3.645249
H	-3.295556	-1.483051	-4.010817
H	-2.348269	-0.057361	-3.538986
H	-1.566280	-1.382613	-4.423942
C	-5.095790	2.312959	0.429131
H	-6.102139	1.882617	0.559618
H	-5.099924	3.317192	0.883964
H	-4.929642	2.429650	-0.652130
C	-4.321011	1.306970	2.602338
H	-4.246781	2.299526	3.075022
H	-5.339195	0.934801	2.797880
H	-3.614244	0.637059	3.112412
C	1.013461	5.127555	-0.310341
H	1.931564	5.679976	-0.570095
H	0.425419	5.021157	-1.235093
H	0.433164	5.752024	0.388959
C	2.133731	3.979104	1.635680
H	3.043316	4.580789	1.477074
H	1.510742	4.521891	2.363917
H	2.428749	3.021606	2.086947

TS5

B3LYP SCF energy:	-1677.29132126 a.u.		
B3LYP enthalpy:	-1676.520421 a.u.		
B3LYP free energy:	-1676.637932 a.u.		
M06 SCF energy in solution:	-3015.72491454 a.u.		
M06 enthalpy in solution:	-3014.954014 a.u.		
M06 free energy in solution:	-3015.071525 a.u.		
Three lowest frequencies (cm-1):	-347.8824	12.7666	21.2449
Imaginary frequency:	-347.8824 cm-1		

Cartesian coordinates

ATOM	X	Y	Z
N	-1.626882	0.250631	-1.125737
N	0.496174	0.633156	-1.455774
C	-0.405002	0.224322	-0.525088
C	-1.589505	0.640645	-2.547685
C	-0.117531	1.042669	-2.736267
C	-2.862370	-0.158211	-0.516598
C	-3.271539	-1.506387	-0.616114
C	-4.498720	-1.866614	-0.046853
C	-5.299684	-0.925846	0.594450
C	-4.885161	0.400764	0.673168
C	-3.668553	0.813558	0.116905
C	-2.416919	-2.571316	-1.295257
C	-3.248753	2.275670	0.225580
C	1.892470	0.882805	-1.229446
C	2.292230	2.105052	-0.645110
C	3.662295	2.330428	-0.463807

C	4.606820	1.392720	-0.871237
C	4.194144	0.209644	-1.476950
C	2.836192	-0.069702	-1.671179
C	1.296626	3.188676	-0.239362
C	2.424218	-1.357692	-2.377607
H	-1.880278	-0.205531	-3.183173
H	0.360217	0.530306	-3.576880
H	-4.828719	-2.900330	-0.103279
H	-5.515704	1.128720	1.176238
H	-1.525428	-2.081498	-1.698705
H	-2.311067	2.394239	-0.326063
H	3.993768	3.257947	-0.004312
H	4.938136	-0.512253	-1.801523
H	0.293197	2.842723	-0.504355
H	1.332460	-1.425871	-2.331964
C	2.834989	-1.325977	-3.864921
H	3.925486	-1.285787	-3.972616
H	2.482232	-2.227149	-4.380932
H	2.422215	-0.452767	-4.384236
C	2.982877	-2.614205	-1.685705
H	2.617495	-3.515083	-2.194330
H	4.078557	-2.640586	-1.718528
H	2.676199	-2.658954	-0.637338
C	-4.284299	3.222970	-0.410673
H	-5.242971	3.190229	0.119873
H	-3.924694	4.258383	-0.377339
H	-4.476758	2.962996	-1.458157
C	-2.963505	2.665111	1.689367
H	-2.625212	3.706809	1.750967
H	-3.861459	2.566095	2.310973
H	-2.184496	2.022802	2.114559
C	1.550631	4.503007	-1.005046
H	0.785609	5.246764	-0.751535
H	2.526752	4.933495	-0.753639
H	1.528170	4.347109	-2.089984
C	1.294663	3.427369	1.281697
H	0.566285	4.203467	1.547117
H	1.022013	2.507692	1.809152
H	2.277954	3.754033	1.640477
C	-1.926687	-3.619790	-0.278029
H	-2.764464	-4.168879	0.167936
H	-1.268109	-4.348472	-0.765938
H	-1.368128	-3.136005	0.529198
C	-3.155988	-3.238130	-2.471782
H	-3.485710	-2.498958	-3.211420
H	-2.498974	-3.955991	-2.976935
H	-4.043428	-3.784781	-2.132339
H	5.665890	1.587587	-0.723240
H	-6.247917	-1.226598	1.032341
H	0.008384	2.122721	-2.885061
H	-2.286323	1.462828	-2.743536
Ni	-0.209847	-0.237621	1.287629
C	1.320645	-1.103181	2.164718
C	1.417304	-2.511960	2.045848
C	2.659196	-3.137422	2.078901
C	3.836220	-2.396689	2.260348

C	3.741654	-1.012225	2.412398
C	2.504490	-0.364339	2.385567
H	4.642722	-0.417840	2.549870
H	2.465026	0.714841	2.492253
O	-0.070342	-0.709170	3.074414
C	0.155226	0.230566	4.117899
H	1.089229	-0.011060	4.643867
H	0.206305	1.268876	3.767211
H	-0.685928	0.139704	4.813841
H	0.511214	-3.100835	1.943864
H	2.709662	-4.219570	1.973884
H	4.801956	-2.893100	2.292606

TS6

B3LYP SCF energy: -2039.49364138 a.u.
B3LYP enthalpy: -2038.603277 a.u.
B3LYP free energy: -2038.740657 a.u.
M06 SCF energy in solution: -3377.88185508 a.u.
M06 enthalpy in solution: -3376.991491 a.u.
M06 free energy in solution: -3377.128871 a.u.
Three lowest frequencies (cm-1): -228.0861 11.4537 22.8370
Imaginary frequency: -228.0861 cm-1

Cartesian coordinates

ATOM	X	Y	Z
O	-0.650350	2.439347	-1.022983
Ni	-0.222428	0.630712	-0.422342
C	0.394186	2.509312	0.146975
C	1.731289	2.868251	-0.146481
C	-0.164851	2.890372	1.390408
C	2.497248	3.515801	0.820942
H	2.190171	2.592741	-1.088042
C	0.626264	3.532533	2.337406
H	-1.203886	2.674320	1.603229
C	1.959747	3.860895	2.064370
H	3.535141	3.746889	0.593432
C	-0.115664	2.844975	-2.315233
H	-0.932368	2.745773	-3.026942
H	0.217690	3.883980	-2.243000
H	0.709311	2.197196	-2.605853
C	-2.228428	5.179775	-0.644210
Al	-2.711103	3.261334	-0.853126
C	-3.554107	2.305076	0.674160
C	-3.431125	2.707722	-2.631941
H	-3.143578	5.785750	-0.559801
H	-1.635582	5.380922	0.257240
H	-3.432813	2.799543	1.647619
H	-4.637518	2.242708	0.489684
H	-4.526940	2.809921	-2.595592
H	-3.237372	1.656601	-2.885762
H	-3.205852	1.269650	0.783059
H	-3.098787	3.319696	-3.482010
H	-1.669921	5.589694	-1.497466
N	1.514198	-1.670848	0.052590

N	-0.594373	-2.094561	0.418816
C	0.272992	-1.106875	0.064388
C	1.516329	-3.121766	0.325313
C	0.048010	-3.394789	0.689408
C	2.730251	-1.004900	-0.316088
C	3.071198	-0.884442	-1.682171
C	4.259101	-0.217241	-2.007308
C	5.099882	0.282421	-1.015623
C	4.774670	0.102925	0.325940
C	3.593172	-0.546734	0.704073
C	2.237269	-1.519923	-2.791732
C	3.304345	-0.790411	2.182829
C	-2.012509	-1.950775	0.591872
C	-2.525767	-1.666359	1.876734
C	-3.915041	-1.571632	2.023778
C	-4.768938	-1.761328	0.940982
C	-4.245194	-2.065668	-0.312393
C	-2.864053	-2.178299	-0.511779
C	-1.626051	-1.479276	3.095287
C	-2.328930	-2.546623	-1.891946
H	1.838952	-3.674357	-0.566213
H	-0.404174	-4.182059	0.076262
H	4.538886	-0.102894	-3.051283
H	5.449191	0.471719	1.093748
H	1.335669	-1.939413	-2.335898
H	2.297194	-1.212082	2.258614
H	-4.333696	-1.341608	2.999746
H	-4.919839	-2.220783	-1.149992
H	-0.586776	-1.559013	2.761722
H	-1.241036	-2.637746	-1.814066
C	-2.874118	-3.906418	-2.371418
H	-3.960603	-3.878833	-2.513733
H	-2.422399	-4.180189	-3.332449
H	-2.654757	-4.704636	-1.652449
C	-2.614057	-1.439177	-2.923329
H	-2.194064	-1.707577	-3.900831
H	-3.690588	-1.278269	-3.053614
H	-2.166357	-0.492559	-2.602875
C	4.295117	-1.820047	2.767065
H	5.320767	-1.432284	2.752426
H	4.040626	-2.049775	3.808767
H	4.291939	-2.758243	2.199828
C	3.313169	0.500956	3.018688
H	3.057581	0.273633	4.060936
H	4.301683	0.975709	3.020605
H	2.592041	1.228002	2.637990
C	-1.868252	-2.584577	4.143727
H	-1.171467	-2.475216	4.983417
H	-2.885960	-2.534615	4.548212
H	-1.732862	-3.585149	3.716207
C	-1.785626	-0.083095	3.725131
H	-1.109830	0.024645	4.582287
H	-1.546106	0.700791	3.001304
H	-2.808044	0.084670	4.082825
C	1.767761	-0.501976	-3.845242
H	2.610386	-0.002703	-4.337836

H	1.177701	-1.001965	-4.622626
H	1.135124	0.260351	-3.381686
C	3.010413	-2.677683	-3.457620
H	3.332634	-3.422456	-2.720708
H	2.380873	-3.182363	-4.200308
H	3.907531	-2.314048	-3.972445
H	-5.843979	-1.675615	1.075008
H	6.018849	0.794599	-1.289214
H	-0.080690	-3.673651	1.742301
H	2.207245	-3.365637	1.138405
H	0.185304	3.796020	3.295790
H	2.563509	4.380041	2.802498

TS7

B3LYP SCF energy: -3416.44495307 a.u.
B3LYP enthalpy: -3415.533819 a.u.
B3LYP free energy: -3415.669620 a.u.
M06 SCF energy in solution: -3417.17900408 a.u.
M06 enthalpy in solution: -3416.267870 a.u.
M06 free energy in solution: -3416.403671 a.u.
Three lowest frequencies (cm-1): -221.8581 19.5412 21.6266
Imaginary frequency: -221.8581 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-0.367383	-0.956544	0.350879
C	-1.660799	-2.346843	1.762469
C	-0.345447	-3.052913	1.442409
H	-1.715815	-2.007728	2.812279
H	-2.540997	-2.972550	1.566047
H	0.189789	-3.401979	2.335930
H	-0.487817	-3.918939	0.773002
N	0.412900	-1.996149	0.746305
N	-1.616222	-1.180394	0.857797
C	1.843109	-2.111241	0.624263
C	2.417280	-2.707003	-0.524004
C	2.645472	-1.703501	1.720954
C	3.812563	-2.847002	-0.566739
C	4.033957	-1.868302	1.624363
C	4.616515	-2.428887	0.490639
H	4.279588	-3.296108	-1.445070
H	4.671109	-1.551684	2.453247
H	5.701755	-2.545534	0.432734
C	-2.706342	-0.240102	0.889651
C	-2.636803	0.885891	1.749664
C	-3.874191	-0.504059	0.127540
C	-3.722195	1.775116	1.767575
C	-4.934434	0.411002	0.195768
C	-4.858230	1.549099	0.995256
H	-3.680630	2.654157	2.414277
H	-5.837444	0.230081	-0.390732
H	-5.692810	2.254289	1.026687
C	2.059258	-1.135924	3.012598
H	0.981335	-0.991769	2.853026

C	1.574707	-3.244230	-1.677411
H	0.581735	-2.774554	-1.613307
C	-4.036679	-1.761336	-0.724710
H	-3.035196	-2.201512	-0.850256
C	-1.477539	1.128653	2.713546
H	-0.675474	0.422605	2.460555
Ni	0.152209	0.497474	-0.756062
O	0.475571	3.701198	-0.436104
C	-0.083879	4.966703	-0.207612
H	0.401936	5.457951	0.653537
H	0.025242	5.643107	-1.080478
H	-1.164097	4.886072	0.022251
C	-1.165406	0.515041	-2.152559
H	-2.126732	0.751115	-1.677497
C	-0.306244	1.658919	-2.528833
C	-0.559675	2.949054	-2.026461
H	-0.170505	3.808558	-2.574063
H	-1.478382	3.115438	-1.461272
C	-1.170851	-0.615897	-3.067341
C	-0.323783	-0.695980	-4.134439
H	-1.881591	-1.425168	-2.885339
H	-0.355380	-1.565987	-4.795126
C	0.616351	1.493837	-3.646956
C	0.603722	0.370933	-4.418407
H	1.289288	2.322016	-3.884781
H	1.277011	0.285581	-5.275147
Al	2.342113	3.423584	-0.294674
C	2.279597	1.411187	-0.277324
H	2.163779	0.994620	-1.296106
H	3.113952	0.858577	0.181686
H	1.402297	1.159960	0.388381
C	3.224217	4.236181	-1.894401
H	3.081069	5.331711	-1.950054
H	4.318226	4.073743	-1.862664
H	2.880468	3.821101	-2.859942
C	2.922348	4.204815	1.453600
H	2.870891	5.309155	1.484218
H	2.344571	3.834090	2.320623
H	3.980289	3.946071	1.650429
C	2.228112	-2.126687	4.181598
H	1.734942	-1.744124	5.090199
H	1.798499	-3.115101	3.952419
H	3.292534	-2.281754	4.421631
C	2.641272	0.239459	3.383419
H	3.718575	0.180657	3.607263
H	2.507340	0.971479	2.575018
H	2.143263	0.632282	4.284849
C	-0.880575	2.539414	2.596387
H	-1.605101	3.315667	2.892687
H	-0.009588	2.638890	3.263530
H	-0.541312	2.755090	1.572823
C	-1.910418	0.834655	4.164232
H	-2.692559	1.536196	4.497540
H	-2.314269	-0.184429	4.276190
H	-1.054710	0.939853	4.851035
C	-4.931284	-2.800081	-0.016777

H	-5.957991	-2.416189	0.099163
H	-4.986391	-3.731878	-0.603307
H	-4.565198	-3.053467	0.989793
C	-4.598193	-1.472375	-2.128458
H	-4.560623	-2.383065	-2.747885
H	-5.652619	-1.155313	-2.087930
H	-4.031882	-0.686125	-2.647305
C	1.388344	-4.770270	-1.553840
H	2.355792	-5.292962	-1.634073
H	0.942111	-5.056125	-0.588552
H	0.733909	-5.149473	-2.355976
C	2.153436	-2.886839	-3.054877
H	3.114939	-3.391720	-3.242397
H	1.461184	-3.205276	-3.849281
H	2.307598	-1.802927	-3.157859

TS-S1

B3LYP SCF energy: -3033.33151218 a.u.
B3LYP enthalpy: -3032.552586 a.u.
B3LYP free energy: -3032.671391 a.u.
M06 SCF energy in solution: -3033.94526801 a.u.
M06 enthalpy in solution: -3033.166342 a.u.
M06 free energy in solution: -3033.285147 a.u.
Three lowest frequencies (cm-1): -504.5236 18.9907 24.6515
Imaginary frequency: -504.5236 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ni	-0.229079	0.897354	-0.854496
N	-0.725441	5.569935	-1.746077
C	-1.798012	4.801100	-1.525340
C	-1.738016	3.449803	-1.178988
C	-0.491721	2.795198	-1.044547
C	0.630456	3.628614	-1.263832
C	0.462397	4.970871	-1.615113
N	1.196203	-1.074357	0.967165
N	-0.938457	-1.349426	0.915595
C	0.895830	-2.057167	1.909230
C	-0.448726	-2.232006	1.874751
C	2.537980	-0.616878	0.701192
C	2.999933	0.555495	1.343447
C	3.358893	-1.377904	-0.162992
C	4.308555	0.975483	1.064922
C	4.661399	-0.913363	-0.399469
C	5.129889	0.254312	0.199722
C	2.148536	1.302154	2.367875
C	2.894417	-2.695742	-0.781970
C	3.261038	-2.836032	-2.268406
C	3.440677	-3.895645	0.017474
C	2.283121	2.829596	2.286920
C	2.462835	0.800697	3.791521
C	-2.335116	-1.227717	0.578802
C	-3.127413	-0.292290	1.282770
C	-2.871030	-2.072628	-0.420418

C	-4.483811	-0.201509	0.937980
C	-5.031739	-1.010500	-0.055889
C	-4.234173	-1.939481	-0.722187
C	-2.566006	0.550795	2.424906
C	-3.005522	2.021662	2.367759
C	-2.924761	-0.077388	3.786074
C	-2.032294	-3.142238	-1.117218
C	-2.255908	-3.198730	-2.637152
C	-2.277623	-4.525169	-0.481951
C	0.065493	-0.608193	0.343315
C	-0.928001	0.586030	-2.780862
C	0.284447	-0.065744	-2.682696
C	1.566520	0.514506	-3.223408
H	-2.776276	5.289644	-1.631925
H	-2.674390	2.903430	-1.029631
H	1.346504	5.597155	-1.797703
H	-0.354101	1.855442	0.256963
H	1.661028	-2.534436	2.513544
H	-1.098443	-2.894026	2.439097
H	5.320509	-1.475217	-1.064389
H	4.693817	1.880014	1.538737
H	1.796496	-2.725174	-0.714040
H	1.097676	1.066561	2.150316
H	4.542278	-3.920331	-0.014525
H	3.069397	-4.844820	-0.402382
H	3.141078	-3.855514	1.075513
H	2.808995	-3.750922	-2.683972
H	4.349480	-2.918595	-2.418777
H	2.903183	-1.981223	-2.859504
H	3.510332	1.012899	4.063100
H	2.306440	-0.284868	3.888121
H	1.815117	1.300917	4.529958
H	1.570381	3.304514	2.979589
H	2.061654	3.202302	1.276371
H	3.289246	3.177082	2.572849
H	6.146127	0.601694	-0.003675
H	-5.123141	0.513914	1.458876
H	-6.091059	-0.920213	-0.309852
H	-1.471180	0.542826	2.330888
H	-2.743430	2.482527	1.404483
H	-2.501659	2.595436	3.161964
H	-4.090258	2.138420	2.524332
H	-2.480641	0.504393	4.610238
H	-2.558393	-1.112604	3.868905
H	-4.016588	-0.097496	3.938250
H	-0.973956	-2.889307	-0.955069
H	-2.092398	-2.219241	-3.110392
H	-3.273706	-3.534281	-2.893113
H	-1.556025	-3.915844	-3.095473
H	-2.057908	-4.523380	0.596675
H	-1.639991	-5.289752	-0.955203
H	-3.327612	-4.836448	-0.607694
H	-4.680228	-2.574373	-1.490430
H	-1.012958	1.540644	-3.304619
H	0.296582	-1.139003	-2.469578
H	-1.869249	0.052930	-2.609467

H	2.412071	0.366156	-2.531904
H	1.469018	1.594431	-3.409200
H	1.647092	3.234888	-1.165850
H	1.841924	0.029898	-4.178623

TS-S2

B3LYP SCF energy: -3395.42304282 a.u.
B3LYP enthalpy: -3394.526499 a.u.
B3LYP free energy: -3394.667048 a.u.
M06 SCF energy in solution: -3396.12090969 a.u.
M06 enthalpy in solution: -3395.224366 a.u.
M06 free energy in solution: -3395.364915 a.u.
Three lowest frequencies (cm-1): -467.9135 8.0275 16.2094
Imaginary frequency: -467.9135 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ni	0.128575	-0.025021	-0.626256
Al	6.915779	-0.666734	-0.480008
N	4.867221	-0.419951	-0.479585
C	4.284779	0.795928	-0.512712
C	2.909242	0.976331	-0.481846
C	2.024234	-0.129871	-0.426772
C	2.669878	-1.391646	-0.374209
C	4.053126	-1.492351	-0.411850
C	7.181589	-2.129669	-1.818087
C	7.589930	1.131100	-1.042260
C	7.299233	-1.172213	1.415824
N	-2.500378	-0.717258	0.777003
N	-2.032892	1.385132	0.736026
C	-3.477380	-0.071559	1.534443
C	-3.184645	1.251899	1.505002
C	-2.528022	-2.140833	0.535845
C	-1.666080	-2.984961	1.276449
C	-3.461219	-2.646307	-0.398688
C	-1.750168	-4.363971	1.037927
C	-3.507567	-4.036332	-0.586395
C	-2.660316	-4.886417	0.119288
C	-0.713973	-2.431935	2.335703
C	-4.426806	-1.749143	-1.172750
C	-4.431328	-2.037107	-2.684016
C	-5.855677	-1.852913	-0.604393
C	0.554032	-3.276421	2.526508
C	-1.438072	-2.247889	3.684444
C	-1.383027	2.646141	0.473873
C	-0.419218	3.120308	1.392947
C	-1.757025	3.378464	-0.676608
C	0.195357	4.349296	1.110932
C	-0.138604	5.078847	-0.028773
C	-1.108876	4.600216	-0.907798
C	-0.087790	2.376098	2.684383
C	1.419610	2.304542	2.974956
C	-0.843409	2.999438	3.874883
C	-2.874157	2.913696	-1.609008

C	-2.542705	3.088517	-3.099647
C	-4.197083	3.625715	-1.262556
C	-1.583997	0.172530	0.278124
C	0.420764	0.366308	-2.640449
C	-0.652362	-0.497611	-2.547167
C	-0.523325	-1.975324	-2.820603
H	4.965820	1.648413	-0.572237
H	2.522055	1.997736	-0.517531
H	4.547542	-2.467645	-0.391380
H	6.786315	-1.875622	-2.819182
H	6.727811	-3.096317	-1.528879
H	8.260838	-2.332467	-1.953473
H	7.192578	1.465683	-2.018836
H	8.689875	1.097421	-1.156676
H	7.388733	1.938912	-0.313628
H	7.005292	-0.387769	2.137847
H	8.381366	-1.345209	1.568110
H	6.791571	-2.103530	1.729859
H	0.827933	0.048120	0.664101
H	-4.282785	-0.613983	2.019430
H	-3.682702	2.103865	1.957649
H	-4.217397	-4.459070	-1.300563
H	-1.096630	-5.044732	1.584828
H	-4.093216	-0.708696	-1.044309
H	-0.384981	-1.442930	1.984666
H	-6.250286	-2.876357	-0.712320
H	-6.537261	-1.171851	-1.139424
H	-5.893488	-1.595646	0.465060
H	-5.065171	-1.303227	-3.207229
H	-4.837470	-3.035629	-2.911656
H	-3.420678	-1.980908	-3.113264
H	-1.791361	-3.216854	4.074473
H	-2.309486	-1.581561	3.600034
H	-0.755028	-1.812524	4.431860
H	1.263716	-2.743015	3.177671
H	1.062429	-3.474021	1.570948
H	0.341933	-4.245710	3.006385
H	-2.708845	-5.965826	-0.045395
H	0.947286	4.743690	1.797192
H	0.356206	6.032392	-0.230049
H	-0.441391	1.341190	2.570447
H	1.975730	1.875607	2.128660
H	1.603308	1.669710	3.856312
H	1.846776	3.295456	3.198003
H	-0.641230	2.435812	4.800125
H	-1.932599	3.002920	3.713391
H	-0.528609	4.042917	4.040296
H	-3.024080	1.837517	-1.435225
H	-1.598575	2.592830	-3.370264
H	-2.461656	4.149546	-3.384598
H	-3.342043	2.649781	-3.717979
H	-4.487592	3.460456	-0.213737
H	-5.016321	3.258731	-1.902230
H	-4.110107	4.713815	-1.416221
H	-1.369908	5.191006	-1.788061
H	1.400566	0.009094	-2.965622

H	-1.667234	-0.089655	-2.573505
H	0.271432	1.449837	-2.698330
H	-1.119376	-2.582704	-2.122403
H	0.524528	-2.304491	-2.750103
H	2.088582	-2.315060	-0.311201
H	-0.879250	-2.212194	-3.840337

TS-S3

B3LYP SCF energy: -2915.48830668 a.u.
B3LYP enthalpy: -2914.796092 a.u.
B3LYP free energy: -2914.906154 a.u.
M06 SCF energy in solution: -2916.06623016 a.u.
M06 enthalpy in solution: -2915.374015 a.u.
M06 free energy in solution: -2915.484077 a.u.
Three lowest frequencies (cm-1): -566.5133 11.8194 23.4537
Imaginary frequency: -566.5133 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ni	0.001360	0.959081	0.724784
C	0.004926	2.583708	1.620407
C	-1.186639	3.310827	1.844819
C	-1.127088	4.662956	2.191704
H	-2.164027	2.829569	1.744834
C	1.148918	4.656647	2.190836
H	-2.056665	5.227816	2.344573
H	2.081736	5.216342	2.342966
H	0.000389	1.020722	2.167719
C	1.200681	3.304181	1.844018
H	2.175314	2.817475	1.743472
N	0.012873	5.341044	2.363280
N	1.073699	-1.350552	-0.830378
N	-1.078684	-1.347750	-0.829997
C	2.455792	-1.016689	-0.582100
C	-2.459738	-1.010274	-0.580957
C	-0.001506	-0.662551	-0.331186
C	0.675734	-2.430520	-1.609518
C	-0.683821	-2.428729	-1.609295
C	3.102845	-0.105999	-1.446748
C	3.121112	-1.638788	0.497407
C	-3.126228	-1.631016	0.498568
C	-3.104610	-0.097096	-1.444617
C	4.452609	0.180005	-1.196904
C	4.471148	-1.317219	0.699215
C	-4.475103	-1.305355	0.701599
C	-4.453290	0.192954	-1.193607
C	5.131444	-0.419188	-0.137202
C	-5.133221	-0.404756	-0.133761
C	2.360719	0.606014	-2.574156
C	2.401462	-2.572136	1.466735
C	-2.409144	-2.567727	1.466512
C	-2.361119	0.613503	-2.572012
H	1.390278	-3.094428	-2.087663
H	-1.400280	-3.090778	-2.087149

H	4.981054	0.886237	-1.840092
H	5.013288	-1.772944	1.530186
H	-5.018043	-1.760005	1.532654
H	-4.979998	0.901220	-1.835996
H	1.455167	0.021511	-2.798600
H	1.467798	-2.899690	0.985217
H	-1.475425	-2.895610	0.985377
H	-1.456855	0.027108	-2.796700
C	-3.171962	0.700791	-3.874574
H	-4.050247	1.358071	-3.773361
H	-2.548758	1.119117	-4.681035
H	-3.528079	-0.289784	-4.199204
C	-1.898149	2.006386	-2.105482
H	-1.330586	2.519905	-2.898064
H	-2.756526	2.641154	-1.832788
H	-1.250669	1.930327	-1.216588
C	3.204781	-3.840498	1.794199
H	3.503340	-4.381759	0.882130
H	4.119170	-3.616592	2.366787
H	2.598557	-4.523091	2.411075
C	2.006685	-1.802563	2.741587
H	1.438993	-2.451298	3.428766
H	2.899952	-1.440158	3.276838
H	1.381790	-0.932043	2.489820
C	3.171466	0.691336	-3.876909
H	4.051323	1.346550	-3.775947
H	3.525150	-0.300087	-4.201600
H	2.549052	1.111112	-4.683224
C	1.900968	2.000041	-2.107841
H	1.253547	1.925799	-1.218760
H	2.760868	2.632890	-1.835489
H	1.334426	2.514684	-2.900424
C	-3.215131	-3.835504	1.789794
H	-3.514350	-4.373402	0.875957
H	-2.610619	-4.521197	2.404922
H	-4.129383	-3.611388	2.362528
C	-2.014438	-1.802043	2.743679
H	-1.387409	-0.932261	2.494685
H	-2.907500	-1.439117	3.278896
H	-1.448780	-2.453561	3.429907
H	-6.184548	-0.164243	0.044079
H	6.183641	-0.181832	0.039731

TS-S4

B3LYP SCF energy: -3277.57837627 a.u.
B3LYP enthalpy: -3276.768438 a.u.
B3LYP free energy: -3276.898143 a.u.
M06 SCF energy in solution: -3278.24035629 a.u.
M06 enthalpy in solution: -3277.430418 a.u.
M06 free energy in solution: -3277.560123 a.u.
Three lowest frequencies (cm-1): -578.7366 12.5379 16.2340
Imaginary frequency: -578.7366 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ni	-0.120205	-0.027586	-0.335125
C	-1.932921	-0.074017	-0.685163
C	-2.714545	1.108884	-0.710470
C	-4.098748	1.043215	-0.638020
H	-2.240836	2.091212	-0.777593
C	-4.059702	-1.264460	-0.593809
H	-4.709022	1.950699	-0.633396
H	-4.639431	-2.189611	-0.552283
H	-0.674811	-0.071218	-1.672792
C	-2.672365	-1.282503	-0.665176
H	-2.164436	-2.249495	-0.694960
N	-4.774230	-0.122033	-0.572276
N	2.520726	1.132646	0.443666
N	2.595053	-1.018921	0.433096
C	2.074603	2.500555	0.314180
C	2.245801	-2.413043	0.287635
C	1.755654	0.030261	0.174913
C	3.800164	0.778416	0.852426
C	3.847132	-0.581050	0.845727
C	2.306185	3.176647	-0.904147
C	1.449762	3.120447	1.419160
C	1.657814	-3.085438	1.381962
C	2.534772	-3.059801	-0.934410
C	1.887625	4.512140	-0.993144
C	1.051640	4.456998	1.273296
C	1.353187	-4.444584	1.220012
C	2.210312	-4.420154	-1.039240
C	1.269475	5.147483	0.082133
C	1.627209	-5.106484	0.024269
C	2.916448	2.481699	-2.117517
C	1.141484	2.361326	2.706623
C	1.294534	-2.362951	2.676397
C	3.108230	-2.312310	-2.134771
H	4.552535	1.518970	1.108365
H	4.648913	-1.270465	1.094373
H	2.043359	5.062969	-1.922912
H	0.559768	4.965897	2.104339
H	0.891849	-4.994578	2.042333
H	2.412449	-4.950372	-1.971953
H	3.405965	1.561000	-1.765933
H	1.800258	1.479746	2.742154
H	1.896166	-1.442042	2.725382
H	3.539189	-1.368607	-1.767679
Al	-6.837990	-0.097262	-0.413889
C	-7.105673	0.775457	1.365182
H	-6.678905	1.794457	1.422162
H	-8.182792	0.880968	1.594602
H	-6.665167	0.195957	2.197649
C	-7.329940	-2.032553	-0.505813
H	-8.429799	-2.137977	-0.448507
H	-7.027693	-2.525019	-1.449007
H	-6.925859	-2.640331	0.325533
C	-7.379686	1.003553	-1.991734
H	-7.063146	0.559014	-2.953400
H	-8.481022	1.097391	-2.039941

H	-6.987480	2.037694	-1.971762
H	1.381796	-6.166409	-0.080092
H	0.951193	6.189031	-0.009731
C	1.419938	3.178635	3.977653
H	0.731698	4.032539	4.081440
H	1.285641	2.547312	4.870339
H	2.448841	3.571576	3.990859
C	-0.309734	1.846002	2.678974
H	-0.541451	1.266367	3.586685
H	-1.027832	2.679039	2.612622
H	-0.480061	1.194045	1.805943
C	1.803293	2.057310	-3.094367
H	1.267230	2.935944	-3.489345
H	2.224354	1.503998	-3.949651
H	1.071485	1.409101	-2.588580
C	3.995617	3.322603	-2.817661
H	3.577325	4.227202	-3.287363
H	4.783372	3.641414	-2.116566
H	4.471595	2.735158	-3.618971
C	4.239742	-3.076173	-2.840341
H	3.879027	-3.997304	-3.325347
H	4.682606	-2.449130	-3.630496
H	5.042103	-3.356851	-2.139550
C	1.976985	-1.941897	-3.112711
H	2.369664	-1.354312	-3.958602
H	1.495893	-2.845564	-3.521714
H	1.205173	-1.344829	-2.603568
C	1.618311	-3.176602	3.939145
H	2.669020	-3.506827	3.951995
H	1.443165	-2.565029	4.838472
H	0.982245	-4.071373	4.030135
C	-0.186421	-1.940870	2.648181
H	-0.395040	-1.290075	1.782584
H	-0.849088	-2.817523	2.567959
H	-0.458349	-1.389248	3.562188

TS-S5

B3LYP SCF energy: -3128.39031533 a.u.
B3LYP enthalpy: -3127.612241 a.u.
B3LYP free energy: -3127.731120 a.u.
M06 SCF energy in solution: -3129.08853493 a.u.
M06 enthalpy in solution: -3128.310461 a.u.
M06 free energy in solution: -3128.429340 a.u.
Three lowest frequencies (cm-1): -173.0521 16.1029 25.3149
Imaginary frequency: -173.0521 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-0.966833	-0.217922	-2.211112
O	0.172409	-1.447039	-2.623677
O	-0.836035	0.855345	-2.781900
C	1.070525	-1.094793	-3.654615
H	0.881331	-1.737798	-4.532969
H	0.925476	-0.040708	-3.952075

H	2.118898	-1.235271	-3.337565
C	-2.286954	-0.933339	-2.106142
C	-2.405301	-2.308460	-1.845012
C	-3.452432	-0.174782	-2.300270
C	-3.664289	-2.907473	-1.779304
H	-1.502264	-2.905561	-1.721011
C	-4.711824	-0.774232	-2.223883
C	-4.822559	-2.142942	-1.962997
Ni	0.365852	-0.672577	-0.921416
C	0.579893	0.266639	0.680819
N	1.847963	0.437946	1.145187
N	-0.253358	0.839275	1.580565
C	1.920085	1.098566	2.456812
C	3.024814	0.022675	0.437298
C	0.450665	1.474391	2.711781
C	-1.684781	0.908929	1.495186
H	2.321536	0.407370	3.218448
H	2.587174	1.974744	2.421889
C	3.531331	-1.284822	0.631846
C	3.676654	0.951958	-0.411272
H	0.069507	1.086518	3.669812
H	0.285114	2.564039	2.706721
C	-2.292232	2.051352	0.923204
C	-2.452126	-0.142787	2.051773
C	4.686633	-1.656772	-0.071206
C	2.831797	-2.298985	1.532382
C	4.829237	0.529741	-1.087682
C	3.125709	2.356174	-0.642627
C	-3.693608	2.096565	0.881716
C	-1.484996	3.239427	0.403240
C	-3.848237	-0.050791	1.974977
C	-1.793042	-1.358087	2.700724
C	5.330173	-0.761323	-0.923064
H	5.088847	-2.665285	0.049182
C	3.790024	-2.964919	2.533789
C	2.078511	-3.344506	0.690215
H	2.075526	-1.755094	2.118187
H	5.341924	1.220987	-1.759998
C	2.358853	2.430982	-1.976287
C	4.207138	3.444922	-0.551412
H	2.394696	2.558995	0.154192
C	-4.464817	1.055040	1.391664
H	-4.189006	2.963703	0.438862
C	-1.650148	4.460406	1.330075
C	-1.822715	3.604802	-1.052062
H	-0.423932	2.948854	0.415093
H	-4.465745	-0.855928	2.377641
C	-1.658055	-2.515805	1.696588
C	-2.500771	-1.815161	3.986262
H	-0.770915	-1.061697	2.984662
H	6.229124	-1.070889	-1.462556
H	4.330997	-2.217651	3.136088
H	4.541397	-3.594692	2.030642
H	3.229536	-3.616863	3.223247
H	1.342074	-2.853431	0.031994
H	1.536500	-4.054087	1.336224

H	2.769846	-3.920598	0.053872
H	1.526701	1.711664	-2.003946
H	3.026131	2.217532	-2.827858
H	1.936065	3.438192	-2.124530
H	4.768073	3.386166	0.395281
H	3.745959	4.443753	-0.612757
H	4.934940	3.375916	-1.375973
H	-5.555412	1.106231	1.339389
H	-1.393991	4.224767	2.375751
H	-2.689747	4.827171	1.323835
H	-1.003727	5.289685	0.998692
H	-1.625959	2.762227	-1.730418
H	-1.201512	4.455215	-1.378910
H	-2.875850	3.912159	-1.161757
H	-1.068006	-2.201268	0.822382
H	-2.645559	-2.841289	1.333202
H	-1.158258	-3.381554	2.162434
H	-2.631429	-0.985234	4.698961
H	-1.911766	-2.602530	4.483917
H	-3.495966	-2.241137	3.781116
H	-5.807126	-2.615596	-1.909933
H	-3.743156	-3.981702	-1.590463
H	-3.352329	0.888116	-2.525574
H	-5.610740	-0.170995	-2.377868

TS-S6

B3LYP SCF energy: -3490.46451243 a.u.
B3LYP enthalpy: -3489.569725 a.u.
B3LYP free energy: -3489.711975 a.u.
M06 SCF energy in solution: -3491.25251461 a.u.
M06 enthalpy in solution: -3490.357727 a.u.
M06 free energy in solution: -3490.499977 a.u.
Three lowest frequencies (cm-1): -166.0476 10.9177 22.0050
Imaginary frequency: -166.0476 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	1.178697	-0.938902	-1.034799
O	-0.267441	-1.604590	-2.201200
O	1.701567	-1.840891	-0.359023
C	-0.518992	-2.980488	-2.065822
H	-0.237703	-3.496247	-3.001860
H	0.068854	-3.434285	-1.246108
H	-1.589713	-3.184015	-1.869432
C	1.987179	-0.054665	-1.928731
C	1.544229	0.358978	-3.198434
C	3.236732	0.387334	-1.459708
C	2.349614	1.182160	-3.986373
H	0.592174	-0.016803	-3.570928
C	4.031467	1.221877	-2.248952
C	3.593666	1.618341	-3.515429
Ni	-0.595553	-0.476960	-0.777736
C	-1.058407	0.670724	0.658350
N	-2.397595	0.707255	0.863628

N	-0.484583	1.503256	1.545275
C	-2.816780	1.637894	1.921481
C	-3.306752	-0.073584	0.072138
C	-1.462471	2.150023	2.447228
C	0.921467	1.736691	1.726814
H	-3.445554	2.442556	1.504443
H	-3.408527	1.118373	2.692247
C	-3.794458	0.457817	-1.147407
C	-3.692164	-1.357297	0.535575
H	-1.368058	3.245357	2.390993
H	-1.270217	1.852054	3.490361
C	1.641920	0.913840	2.624549
C	1.527148	2.828518	1.061745
C	-4.651551	-0.343918	-1.915665
C	-3.412433	1.850234	-1.644188
C	-4.555751	-2.111653	-0.269706
C	-3.152279	-1.941193	1.838797
C	3.010242	1.170761	2.792071
C	0.974471	-0.189911	3.442130
C	2.896218	3.045104	1.271986
C	0.734805	3.787118	0.176040
C	-5.027841	-1.613962	-1.484291
H	-5.031133	0.032968	-2.868003
C	-4.648281	2.723056	-1.923995
C	-2.486068	1.774201	-2.870882
H	-2.841260	2.343650	-0.843638
H	-4.859817	-3.109130	0.054124
C	-2.021407	-2.949686	1.561360
C	-4.252984	-2.558701	2.716492
H	-2.707062	-1.114194	2.412528
C	3.634276	2.219634	2.118705
H	3.597065	0.539362	3.462744
C	0.978770	0.159872	4.943191
C	1.595746	-1.572900	3.193066
H	-0.076219	-0.252887	3.121806
H	3.393997	3.873324	0.762373
C	1.296681	3.878673	-1.251530
C	0.637254	5.183180	0.821458
H	-0.288122	3.390400	0.091891
H	-5.694983	-2.222956	-2.099603
H	-5.305881	2.790572	-1.042666
H	-5.249282	2.327388	-2.758290
H	-4.340609	3.744966	-2.198553
H	-1.571853	1.206210	-2.636744
H	-2.187259	2.783907	-3.195967
H	-2.981202	1.276893	-3.720598
H	-1.204961	-2.483787	0.987645
H	-2.389686	-3.812216	0.982727
H	-1.597587	-3.331201	2.504019
H	-5.068972	-1.844441	2.911005
H	-3.833818	-2.870021	3.686548
H	-4.695697	-3.455550	2.254446
H	4.702916	2.399024	2.261624
H	0.510081	1.137855	5.140973
H	2.005520	0.201945	5.341291
H	0.431642	-0.604043	5.519446

H	1.552952	-1.843941	2.129758
H	1.054032	-2.342671	3.766465
H	2.650488	-1.610918	3.508416
H	1.343247	2.891024	-1.731156
H	2.312820	4.304106	-1.262530
H	0.660475	4.532147	-1.870912
H	0.208030	5.137848	1.835444
H	0.004299	5.849556	0.212634
H	1.629735	5.654584	0.906937
Al	3.159283	-3.205363	-0.384132
H	4.221783	2.261190	-4.137758
H	2.008402	1.476650	-4.982318
H	3.586787	0.070973	-0.476521
H	5.002646	1.554128	-1.873520
C	3.477554	-3.512256	-2.327770
H	2.572947	-3.836729	-2.873207
H	3.872308	-2.624296	-2.852819
H	4.227495	-4.315009	-2.463266
C	4.670498	-2.356392	0.614661
H	4.357899	-1.836356	1.538377
H	5.390060	-3.135832	0.930414
H	5.246493	-1.632389	0.010569
C	2.277169	-4.704532	0.594899
H	1.385671	-5.104385	0.077436
H	2.977323	-5.554675	0.703935
H	1.960938	-4.431104	1.618251

TS-S7

B3LYP SCF energy: -3054.36613425 a.u.
B3LYP enthalpy: -3053.571412 a.u.
B3LYP free energy: -3053.690538 a.u.
M06 SCF energy in solution: -3055.00439820 a.u.
M06 enthalpy in solution: -3054.209676 a.u.
M06 free energy in solution: -3054.328802 a.u.
Three lowest frequencies (cm-1): -480.3802 19.1589 23.7176
Imaginary frequency: -480.3802 cm-1

Cartesian coordinates

ATOM	X	Y	Z
N	0.054043	1.882609	-0.161231
N	2.055675	1.005556	-0.166501
C	0.726135	0.695583	-0.051983
C	0.922517	3.056105	-0.336139
C	2.331395	2.437185	-0.349411
C	-1.366976	2.039452	-0.103751
C	-2.109532	2.081694	-1.309390
C	-3.493227	2.298721	-1.232639
C	-4.127615	2.470803	-0.004180
C	-3.383968	2.428826	1.175005
C	-1.996931	2.223374	1.152586
C	-1.452196	1.902372	-2.675176
C	-1.212534	2.157112	2.460291
C	3.131952	0.061805	-0.107183
C	3.748108	-0.216133	1.136936

C	4.833571	-1.104092	1.155628
C	5.308576	-1.687429	-0.017479
C	4.700350	-1.394333	-1.237442
C	3.610861	-0.515400	-1.309190
C	3.217016	0.366765	2.443263
C	2.915516	-0.257624	-2.642611
H	0.686142	3.588419	-1.272810
H	2.866042	2.618845	-1.297972
H	-4.084573	2.331628	-2.150932
H	-3.892446	2.561944	2.132134
H	-0.389738	1.679758	-2.499609
H	-0.150732	2.304615	2.210235
H	5.315579	-1.345457	2.105528
H	5.079742	-1.859946	-2.149523
H	2.576876	1.223463	2.183657
H	2.349689	0.680927	-2.539655
C	3.883148	-0.078844	-3.821700
H	4.420878	-1.010174	-4.062412
H	3.328256	0.213938	-4.727761
H	4.635881	0.699475	-3.617578
C	1.884523	-1.368266	-2.917245
H	1.301898	-1.153839	-3.828752
H	2.381541	-2.343806	-3.050028
H	1.190730	-1.445538	-2.063699
C	-1.602871	3.261913	3.455233
H	-2.625865	3.129055	3.843022
H	-0.926251	3.244559	4.324876
H	-1.544814	4.263393	2.999006
C	-1.329698	0.758292	3.093375
H	-0.758165	0.707519	4.034745
H	-2.379575	0.507714	3.317154
H	-0.929431	-0.006285	2.406572
C	4.324787	0.888824	3.371264
H	3.882451	1.398301	4.242679
H	4.955811	0.074356	3.761965
H	4.984632	1.605922	2.856738
C	2.315138	-0.659113	3.154485
H	1.892868	-0.236441	4.081149
H	1.481190	-0.949786	2.493922
H	2.880852	-1.567577	3.420681
C	-2.036661	0.707032	-3.448826
H	-3.099652	0.859576	-3.696664
H	-1.494096	0.559598	-4.397057
H	-1.960842	-0.223742	-2.866914
C	-1.529739	3.190001	-3.516635
H	-1.089878	4.050190	-2.987256
H	-0.990393	3.065229	-4.470055
H	-2.573340	3.450958	-3.757695
H	6.158134	-2.374648	0.018645
H	-5.207171	2.638547	0.035565
H	2.970956	2.822870	0.463066
H	0.782718	3.773729	0.490905
Ni	0.093894	-0.978821	0.287809
C	-3.406530	-3.817820	-0.257358
C	-2.808331	-2.540775	-0.267023
C	-3.579742	-1.441216	0.162053

C	-4.900796	-1.612543	0.572153
C	-5.483665	-2.886077	0.570858
C	-4.729649	-3.987427	0.152303
H	-2.824387	-4.684256	-0.583484
H	-5.175410	-4.985850	0.147301
O	-0.443674	-2.663128	0.819936
C	0.391667	-3.790213	0.699701
H	0.890591	-3.953475	1.670355
H	-0.202141	-4.698035	0.470024
H	1.179872	-3.683231	-0.067895
C	-1.425193	-2.369585	-0.719169
H	-1.006644	-3.211654	-1.277864
H	-1.222545	-1.410239	-1.220124
H	-5.479991	-0.744407	0.897609
H	-3.130441	-0.446019	0.174916
H	-6.518883	-3.019095	0.895655

TS-S8

B3LYP SCF energy: -3416.43768852 a.u.
B3LYP enthalpy: -3415.524741 a.u.
B3LYP free energy: -3415.660415 a.u.
M06 SCF energy in solution: -3417.17257019 a.u.
M06 enthalpy in solution: -3416.259623 a.u.
M06 free energy in solution: -3416.395297 a.u.
Three lowest frequencies (cm-1): -411.9314 12.8752 29.0559
Imaginary frequency: -411.9314 cm-1

Cartesian coordinates

ATOM	X	Y	Z
N	-1.994453	-1.609804	0.058717
N	0.052144	-2.361208	-0.083298
C	-0.691816	-1.210256	-0.048384
C	-2.184739	-3.066492	0.018653
C	-0.742683	-3.591495	0.062302
C	-3.126488	-0.733952	0.134778
C	-3.623229	-0.375494	1.411338
C	-4.738859	0.470311	1.469989
C	-5.352239	0.931976	0.305507
C	-4.869910	0.542152	-0.942616
C	-3.758434	-0.305342	-1.055695
C	-2.937801	-0.860884	2.687154
C	-3.230588	-0.709306	-2.430321
C	1.481032	-2.447194	-0.108016
C	2.139271	-2.578736	-1.357241
C	3.532434	-2.736142	-1.360418
C	4.255267	-2.784879	-0.167843
C	3.593154	-2.671656	1.052588
C	2.201217	-2.503894	1.110758
C	1.361939	-2.513551	-2.669619
C	1.512857	-2.410518	2.470348
H	-2.791863	-3.411326	0.871182
H	-0.508569	-4.097962	1.014500
H	-5.134072	0.779368	2.439420
H	-5.366622	0.905225	-1.844884

H	-2.414223	-1.796181	2.434682
H	-2.585391	-1.589461	-2.286893
H	4.062741	-2.831657	-2.309761
H	4.168480	-2.715882	1.980379
H	0.329971	-2.827604	-2.448510
H	0.455184	-2.173410	2.287234
C	1.576065	-3.752069	3.225566
H	2.615892	-4.024054	3.470672
H	1.015801	-3.692126	4.173024
H	1.152110	-4.577592	2.632213
C	2.077643	-1.274150	3.340563
H	1.506569	-1.191797	4.279351
H	3.132048	-1.446822	3.610267
H	2.019437	-0.303700	2.826290
C	-4.342753	-1.119353	-3.408240
H	-4.984118	-0.267711	-3.686610
H	-3.904249	-1.509530	-4.341083
H	-4.991384	-1.902042	-2.983018
C	-2.339346	0.397309	-3.019843
H	-1.911242	0.084278	-3.986606
H	-2.909120	1.326025	-3.181586
H	-1.511400	0.617263	-2.324621
C	1.903252	-3.456856	-3.753957
H	1.222509	-3.465599	-4.620185
H	2.890079	-3.138286	-4.127037
H	1.999834	-4.491248	-3.387100
C	1.281629	-1.062671	-3.176929
H	0.687356	-1.001482	-4.103295
H	0.803289	-0.424105	-2.415271
H	2.287655	-0.663510	-3.388649
C	-1.861726	0.137842	3.151765
H	-2.315912	1.091950	3.460689
H	-1.297277	-0.268371	4.007943
H	-1.156367	0.355760	2.333881
C	-3.917783	-1.187821	3.823677
H	-4.705286	-1.885929	3.497529
H	-3.379387	-1.650851	4.666429
H	-4.410459	-0.284280	4.217113
H	5.340073	-2.918529	-0.191263
H	-6.216464	1.597885	0.372232
H	-0.521208	-4.302784	-0.750143
H	-2.715164	-3.365133	-0.903066
Ni	-0.118299	0.511772	-0.190506
C	3.703086	1.031823	0.056882
C	2.982498	2.124681	0.593210
C	3.671241	3.340923	0.811245
C	5.030444	3.450254	0.523611
C	5.730812	2.357632	-0.002314
C	5.060463	1.149445	-0.233212
H	3.188255	0.085963	-0.126308
H	5.599455	0.290992	-0.641299
O	0.480171	2.361744	-0.466981
C	1.186338	2.523726	-1.713340
H	0.443254	2.539886	-2.521344
H	1.746597	3.470613	-1.707648
H	1.880838	1.690650	-1.877686

Al	-0.726692	3.971597	-0.069068
C	-1.802261	3.461354	1.519084
H	-2.390569	4.348358	1.824845
H	-2.528089	2.655015	1.320794
H	-1.213257	3.167115	2.405680
C	-1.729855	4.211071	-1.771161
H	-2.481407	5.009812	-1.623088
H	-1.110149	4.530173	-2.628373
H	-2.290830	3.313199	-2.081572
C	0.602450	5.422453	0.300008
H	1.067742	5.372824	1.301738
H	1.419997	5.520102	-0.436860
H	0.058738	6.386387	0.272600
C	1.581518	1.999213	0.960301
H	1.241560	0.988794	1.238983
H	1.169041	2.793747	1.582324
H	3.126667	4.199441	1.209483
H	5.547415	4.395929	0.705240
H	6.795065	2.448256	-0.234049

int1

B3LYP SCF energy: -2131.83973655 a.u.
B3LYP enthalpy: -2131.460151 a.u.
B3LYP free energy: -2131.519682 a.u.
M06 SCF energy in solution: -2132.14485248 a.u.
M06 enthalpy in solution: -2131.765267 a.u.
M06 free energy in solution: -2131.824798 a.u.
Three lowest frequencies (cm-1): 60.0553 89.5708 109.1310

Cartesian coordinates

ATOM	X	Y	Z
Ni	0.000002	0.000005	0.000000
C	2.242523	1.848550	0.556399
C	1.368943	1.518961	-0.635529
C	1.511488	0.426436	-1.477870
C	2.242397	-1.848557	-0.556805
C	1.369039	-1.518959	0.635280
C	1.511737	-0.426435	1.477598
C	2.621382	-0.615115	-1.404703
C	2.621623	0.615111	1.404252
C	-2.242408	-1.848684	0.556363
C	-1.369042	-1.518808	-0.635643
C	-1.511732	-0.426084	-1.477702
C	-2.242534	1.848677	-0.555956
C	-1.368946	1.518810	0.635891
C	-1.511484	0.426085	1.477974
C	-2.621618	0.615444	-1.404120
C	-2.621376	-0.615449	1.404571
H	1.693515	2.564961	1.190392
H	3.158187	2.384280	0.233739
H	0.774894	2.356927	-1.015561
H	0.992631	0.486177	-2.438544
H	3.158102	-2.384320	-0.234317
H	1.693253	-2.564940	-1.190714

H	0.775052	-2.356921	1.015420
H	0.993052	-0.486185	2.438364
H	3.542116	-0.153702	-1.016041
H	2.869397	-0.945134	-2.426600
H	2.869791	0.945139	2.426109
H	3.542300	0.153689	1.015463
H	-1.693275	-2.565231	1.190096
H	-3.158119	-2.384356	0.233743
H	-0.775056	-2.356682	-1.015976
H	-0.993040	-0.485602	-2.438479
H	-3.158204	2.384316	-0.233165
H	-1.693537	2.565253	-1.189774
H	-0.774897	2.356689	1.016117
H	-0.992619	0.485593	2.438658
H	-3.542303	0.153931	-1.015461
H	-2.869768	0.945724	-2.425900
H	-2.869374	-0.945719	2.426391
H	-3.542119	-0.153945	1.016040

int2

B3LYP SCF energy: -3564.80475987 a.u.
B3LYP enthalpy: -3564.103442 a.u.
B3LYP free energy: -3564.220439 a.u.
M06 SCF energy in solution: -3565.54061227 a.u.
M06 enthalpy in solution: -3564.839294 a.u.
M06 free energy in solution: -3564.956291 a.u.
Three lowest frequencies (cm-1): 7.9455 15.3856 36.8255

Cartesian coordinates

ATOM	X	Y	Z
Ni	-0.086229	-0.823340	0.428174
P	2.022380	0.057689	0.474371
C	2.495395	0.565174	2.278544
P	-1.884559	0.275803	-0.247647
C	-1.828793	1.981329	-1.145319
C	-0.907325	-2.456352	0.927050
N	0.276145	-2.574467	1.204404
C	-2.165398	-3.251404	0.991352
H	-2.556665	-3.423663	-0.023071
H	-1.989375	-4.222510	1.480713
H	-2.942429	-2.702016	1.544722
C	-1.230196	2.979258	-0.140922
H	-1.901881	3.150973	0.714651
H	-0.264911	2.622165	0.243914
H	-1.055728	3.950746	-0.634331
C	-0.873890	1.799877	-2.338141
H	-0.633712	2.783795	-2.775290
H	0.070038	1.330642	-2.032372
H	-1.326713	1.185941	-3.131514
C	-3.172191	2.511251	-1.670521
H	-2.984719	3.387800	-2.315393
H	-3.706773	1.766322	-2.280199
H	-3.835530	2.850830	-0.863404
C	3.868025	1.243434	2.408770

H	4.052678	1.483788	3.470697
H	4.679831	0.578460	2.080494
H	3.945072	2.181516	1.841102
C	1.385242	1.473031	2.842833
H	1.341439	2.459385	2.359018
H	0.395941	1.006164	2.731635
H	1.561914	1.645661	3.918450
C	2.509693	-0.741883	3.098551
H	3.333081	-1.405277	2.795951
H	2.653703	-0.493728	4.164268
H	1.572562	-1.306975	2.992680
C	-3.058446	0.542164	1.178234
C	-2.572464	0.199437	2.453623
C	-4.362224	1.070629	1.098128
C	-3.347704	0.377745	3.603118
H	-1.568423	-0.222576	2.535410
C	-5.141520	1.247648	2.245645
H	-4.789702	1.351017	0.136926
C	-4.637459	0.903844	3.503059
H	-2.939012	0.101660	4.578638
H	-6.151026	1.657131	2.153038
H	-5.248403	1.044370	4.398557
C	-2.791492	-0.794392	-1.471493
C	-4.172348	-1.050617	-1.482830
C	-1.992531	-1.438681	-2.436750
C	-4.738635	-1.900904	-2.439953
H	-4.822000	-0.604055	-0.730488
C	-2.557351	-2.275816	-3.401131
H	-0.909326	-1.295839	-2.417085
C	-3.936337	-2.509909	-3.407222
H	-5.815628	-2.088528	-2.423225
H	-1.914396	-2.759731	-4.141029
H	-4.380145	-3.172437	-4.154802
C	2.452428	1.478145	-0.654810
C	2.680095	1.174487	-2.013290
C	2.467657	2.833151	-0.283383
C	2.936384	2.176292	-2.950214
H	2.665154	0.133286	-2.344360
C	2.723979	3.840947	-1.221318
H	2.281200	3.126064	0.748681
C	2.963811	3.518846	-2.557828
H	3.116066	1.905332	-3.994031
H	2.737237	4.884880	-0.896775
H	3.168182	4.305272	-3.288783
C	3.413583	-1.105414	0.024377
C	4.692779	-0.640255	-0.339778
C	3.195564	-2.493200	0.072484
C	5.720529	-1.534540	-0.648367
H	4.891938	0.431224	-0.397211
C	4.228359	-3.386346	-0.236533
H	2.218094	-2.870401	0.378196
C	5.491029	-2.913336	-0.599260
H	6.704790	-1.150547	-0.930145
H	4.037606	-4.462033	-0.191727
H	6.294572	-3.613553	-0.843294

int3

B3LYP SCF energy: -3926.88187729 a.u.
B3LYP enthalpy: -3926.063408 a.u.
B3LYP free energy: -3926.199206 a.u.
M06 SCF energy in solution: -3927.70821352 a.u.
M06 enthalpy in solution: -3926.889744 a.u.
M06 free energy in solution: -3927.025542 a.u.
Three lowest frequencies (cm-1): 17.2001 20.6225 25.9463

Cartesian coordinates

ATOM	X	Y	Z
Ni	-0.095053	0.468026	-0.245121
P	1.650660	-1.073564	-0.231233
C	1.470098	-2.551167	-1.462652
P	-2.131939	-0.322857	0.268258
C	-2.292368	-1.272167	1.942833
C	-0.466700	2.183417	-0.840686
N	0.714255	2.215553	-0.483969
C	-1.431379	3.140428	-1.453935
H	-1.571855	4.005432	-0.788068
H	-0.998767	3.513915	-2.396380
H	-2.407390	2.682876	-1.657076
C	-1.733752	-2.697670	1.800475
H	-2.295823	-3.316193	1.087010
H	-0.681677	-2.683768	1.490973
H	-1.776836	-3.198621	2.782423
C	-1.401311	-0.507692	2.943958
H	-1.374625	-1.057860	3.899660
H	-0.367927	-0.418815	2.579452
H	-1.784669	0.500409	3.157888
C	-3.727136	-1.313363	2.499584
H	-3.715495	-1.842920	3.467909
H	-4.129524	-0.306537	2.678086
H	-4.435705	-1.845189	1.848644
C	2.730420	-3.429031	-1.548912
H	2.551201	-4.246491	-2.268882
H	3.601496	-2.861077	-1.903965
H	3.000615	-3.891277	-0.588807
C	0.243871	-3.408491	-1.106044
H	0.356067	-3.954543	-0.159831
H	-0.667320	-2.799127	-1.045480
H	0.086422	-4.159680	-1.898605
C	1.212127	-1.919953	-2.846673
H	2.067245	-1.328450	-3.202296
H	1.035394	-2.724260	-3.580698
H	0.320438	-1.274865	-2.839090
C	-2.971378	-1.284297	-1.080763
C	-2.656607	-0.878333	-2.392480
C	-3.880256	-2.344195	-0.919188
C	-3.234653	-1.500457	-3.501022
H	-1.945963	-0.061197	-2.542828
C	-4.447269	-2.979969	-2.029400
H	-4.162203	-2.686975	0.075159
C	-4.129334	-2.559992	-3.322933

H	-2.977246	-1.161088	-4.507578
H	-5.146090	-3.806582	-1.877041
H	-4.575469	-3.056313	-4.188426
C	-3.341381	1.064390	0.549442
C	-4.654580	1.047575	0.050400
C	-2.929997	2.175292	1.309084
C	-5.532886	2.104431	0.313230
H	-5.002180	0.206082	-0.551266
C	-3.810983	3.224278	1.582646
H	-1.903249	2.238323	1.675504
C	-5.117009	3.192923	1.084011
H	-6.548935	2.073379	-0.089042
H	-3.466388	4.076115	2.174326
H	-5.804360	4.017607	1.288877
C	2.115883	-1.701747	1.450541
C	2.446266	-0.699566	2.386477
C	2.109051	-3.036885	1.885112
C	2.772984	-1.025958	3.703082
H	2.462704	0.349219	2.077815
C	2.426555	-3.362572	3.209872
H	1.860128	-3.844737	1.198557
C	2.761481	-2.361126	4.122349
H	3.036332	-0.229894	4.404084
H	2.415244	-4.409942	3.522896
H	3.013538	-2.617307	5.154538
C	3.262711	-0.357665	-0.807730
C	4.502490	-0.798111	-0.311285
C	3.252518	0.617860	-1.818508
C	5.697670	-0.284543	-0.820747
H	4.541404	-1.546954	0.481789
C	4.449065	1.120862	-2.337103
H	2.302884	1.006081	-2.188429
C	5.674638	0.672469	-1.839522
H	6.651445	-0.634165	-0.416880
H	4.418892	1.883383	-3.118641
H	6.609600	1.076396	-2.236103
Al	1.969786	3.730454	0.044503
C	0.709022	4.894537	1.093068
H	1.278650	5.701490	1.592622
H	-0.066054	5.401383	0.488450
H	0.186281	4.346069	1.900069
C	3.409211	2.974744	1.201563
H	3.015529	2.586314	2.160080
H	4.005964	2.171552	0.737019
H	4.122090	3.776444	1.473937
C	2.538415	4.533233	-1.699525
H	1.683577	4.834376	-2.334012
H	3.126138	5.453966	-1.521479
H	3.177142	3.871862	-2.311331

int4

B3LYP SCF energy: -2903.09749598 a.u.

B3LYP enthalpy: -2902.322864 a.u.

B3LYP free energy: -2902.437884 a.u.

M06 SCF energy in solution: -2903.66245029 a.u.
M06 enthalpy in solution: -2902.887818 a.u.
M06 free energy in solution: -2903.002838 a.u.
Three lowest frequencies (cm-1): 17.8085 23.6792 31.9278

Cartesian coordinates

ATOM	X	Y	Z
Ni	0.000177	0.000409	1.605261
N	-1.069800	0.134374	-1.181067
N	1.069594	-0.135096	-1.180994
C	-0.000108	-0.000057	-0.320545
C	-0.670701	0.091148	-2.515811
C	0.670456	-0.092845	-2.515756
C	2.456687	-0.264187	-0.808399
C	2.936843	-1.512264	-0.351084
C	4.300582	-1.614191	-0.038266
C	5.160089	-0.528211	-0.187425
C	4.668702	0.688186	-0.656742
C	3.312893	0.851738	-0.975414
C	2.045325	-2.747000	-0.254223
C	2.278881	-3.680033	-1.457967
C	2.212902	-3.501288	1.074180
C	2.824485	2.198502	-1.510279
C	3.301065	3.392911	-0.664913
C	3.239643	2.395175	-2.981900
C	-2.456862	0.263721	-0.808446
C	-2.936892	1.512025	-0.351568
C	-4.300558	1.614125	-0.038536
C	-5.160142	0.528121	-0.187177
C	-4.668890	-0.688472	-0.656104
C	-3.313115	-0.852229	-0.974866
C	-2.045245	2.746718	-0.255384
C	-2.213149	3.502177	1.072297
C	-2.278288	3.678755	-1.460004
C	-2.824776	-2.199198	-1.509287
C	-3.240309	-2.396561	-2.980703
C	-3.300954	-3.393293	-0.663237
C	1.124243	1.642332	1.812218
C	0.777174	1.161873	3.085902
C	-1.124266	-1.641186	1.813203
C	-0.776922	-1.160353	3.086648
H	-1.376036	0.194834	-3.334147
H	1.375770	-0.197060	-3.334041
H	4.698267	-2.566016	0.319691
H	6.219774	-0.630910	0.060284
H	5.352391	1.531661	-0.773467
H	1.002360	-2.407052	-0.294755
H	2.094854	-3.161874	-2.412423
H	1.605087	-4.551377	-1.410738
H	3.315196	-4.056369	-1.477223
H	3.213257	-3.952977	1.174285
H	1.479396	-4.320894	1.140611
H	2.052067	-2.833606	1.934174
H	1.725340	2.193415	-1.469818
H	4.393307	3.527577	-0.720269
H	3.025095	3.278963	0.392957

H	2.842292	4.323240	-1.037239
H	2.845198	3.347566	-3.372341
H	2.867875	1.587199	-3.629666
H	4.337283	2.420416	-3.081985
H	-4.698143	2.566086	0.319163
H	-6.219785	0.630970	0.060648
H	-5.352648	-1.531941	-0.772446
H	-1.002319	2.406586	-0.295261
H	-3.213450	3.954153	1.171689
H	-1.479523	4.321711	1.138253
H	-2.052709	2.835234	1.932942
H	-2.093913	3.159796	-2.413955
H	-1.604477	4.550111	-1.413249
H	-3.314588	4.055098	-1.479957
H	-1.725615	-2.193968	-1.469151
H	-4.337975	-2.421839	-3.080504
H	-2.845969	-3.349139	-3.370795
H	-2.868686	-1.588894	-3.628936
H	-3.024746	-3.278794	0.394513
H	-2.842112	-4.323723	-1.035227
H	-4.393183	-3.528177	-0.718265
H	0.618653	2.519730	1.394590
H	2.143967	1.486268	1.444417
H	-0.053410	1.663067	3.601437
H	-0.618856	-2.518855	1.395916
H	-2.143942	-1.485059	1.445332
H	0.053367	-1.661729	3.602490
C	-1.799395	-0.541259	4.014873
H	-2.324962	-1.321773	4.597316
H	-1.344997	0.149967	4.742984
H	-2.566812	0.018453	3.455512
C	1.799929	0.543774	4.014508
H	2.325610	1.324880	4.596036
H	1.345699	-0.146772	4.743372
H	2.567260	-0.016502	3.455580

int5

B3LYP SCF energy: -3033.35304828 a.u.
B3LYP enthalpy: -3032.569807 a.u.
B3LYP free energy: -3032.688758 a.u.
M06 SCF energy in solution: -3033.97185611 a.u.
M06 enthalpy in solution: -3033.188615 a.u.
M06 free energy in solution: -3033.307566 a.u.
Three lowest frequencies (cm-1): 16.2710 23.7871 29.7022

Cartesian coordinates

ATOM	X	Y	Z
Ni	0.072244	-0.971928	-1.011754
N	1.150083	1.022595	0.924431
N	-0.982739	1.275362	0.769558
N	-0.620184	-4.577435	-1.419570
C	0.043424	0.479567	0.296807
C	0.812910	2.090509	1.751253
C	-0.526607	2.258194	1.646177

C	-0.206425	-3.928608	-0.340808
C	-0.729507	-2.688559	0.100945
C	-1.746927	-2.088031	-0.681744
C	-2.182740	-2.790067	-1.833121
C	-1.601504	-4.007738	-2.150102
C	0.788133	-1.596620	-2.815447
C	1.123808	-0.257211	-2.525999
C	1.842334	-2.686269	-2.837716
C	2.521545	0.616199	0.733397
C	3.349170	1.385763	-0.120073
C	3.018065	-0.491860	1.456610
C	4.688834	0.993796	-0.255496
C	4.364158	-0.842157	1.277003
C	5.192084	-0.111420	0.427522
C	2.849184	2.635628	-0.844971
C	2.157299	-1.252212	2.461878
C	2.392971	-2.769942	2.436215
C	2.359744	-0.691537	3.883526
C	3.318625	2.727696	-2.307139
C	3.260920	3.913535	-0.085713
C	-2.381805	1.154282	0.448430
C	-2.859001	1.680705	-0.774524
C	-3.247036	0.561672	1.398688
C	-4.235261	1.590275	-1.029801
C	-5.106598	1.012434	-0.107755
C	-4.615095	0.506424	1.093592
C	-1.941113	2.375859	-1.776126
C	-2.190423	1.928095	-3.224820
C	-2.048982	3.906832	-1.640241
C	-2.747205	-0.000734	2.728709
C	-3.217066	-1.445702	2.973619
C	-3.150290	0.907220	3.906288
H	1.553772	2.628289	2.334307
H	-1.195203	2.978081	2.108299
H	0.575220	-4.420321	0.252720
H	-0.497407	-2.345313	1.109744
H	-2.991090	-2.389351	-2.450122
H	-1.939499	-4.569866	-3.028619
H	-0.046702	-1.768775	-3.508056
H	0.590450	0.574153	-3.003394
H	2.151982	-0.020922	-2.229635
H	2.617179	-2.515345	-2.071121
H	2.359353	-2.714965	-3.817004
H	4.774002	-1.697783	1.816647
H	5.350326	1.562821	-0.911634
H	1.106893	-1.081913	2.186672
H	1.750137	2.589190	-0.859347
H	3.403999	-0.820402	4.212842
H	1.711091	-1.215171	4.605109
H	2.123020	0.382448	3.935278
H	1.646893	-3.281326	3.065471
H	3.385199	-3.042090	2.830772
H	2.313088	-3.171698	1.415087
H	4.358508	4.010617	-0.049249
H	2.893761	3.919496	0.950965
H	2.860694	4.808959	-0.588747

H	2.834748	3.585576	-2.801328
H	3.065924	1.822547	-2.876612
H	4.406431	2.887267	-2.382023
H	6.238030	-0.402300	0.300640
H	-4.633549	1.986478	-1.966016
H	-6.175890	0.956495	-0.327421
H	-0.909442	2.089595	-1.531274
H	-2.125534	0.833648	-3.321592
H	-1.433872	2.370131	-3.892549
H	-3.177508	2.247562	-3.597297
H	-1.354197	4.407649	-2.334235
H	-1.805413	4.240930	-0.619385
H	-3.068336	4.257646	-1.872534
H	-1.648181	-0.021021	2.689218
H	-2.941596	-2.110247	2.141268
H	-4.309330	-1.506516	3.105913
H	-2.756647	-1.843571	3.892490
H	-2.776492	1.934697	3.778303
H	-2.744852	0.516419	4.853798
H	-4.246584	0.962678	4.008470
H	-5.306814	0.054274	1.807700
H	1.415978	-3.686327	-2.669374
H	-2.353235	-1.268219	-0.299347

int6

B3LYP SCF energy: -3395.44304291 a.u.
B3LYP enthalpy: -3394.541842 a.u.
B3LYP free energy: -3394.680303 a.u.
M06 SCF energy in solution: -3396.15290465 a.u.
M06 enthalpy in solution: -3395.251704 a.u.
M06 free energy in solution: -3395.390165 a.u.
Three lowest frequencies (cm-1): 14.5513 19.6754 21.1393

Cartesian coordinates

ATOM	X	Y	Z
Ni	0.106221	-0.060844	-1.397156
Al	-5.396863	-0.250840	0.102414
N	1.515497	-0.890413	1.141866
N	1.516018	1.255569	0.927162
N	-3.598213	0.012170	-0.873875
C	1.074856	0.108886	0.302144
C	2.184298	-0.376065	2.248838
C	2.197923	0.969823	2.107555
C	-2.625074	0.745116	-0.354954
C	-1.484823	1.196328	-1.076522
C	-1.378298	0.814724	-2.464917
C	-2.474877	0.052660	-3.002537
C	-3.512402	-0.341406	-2.206143
C	-6.555515	1.097220	-0.811430
C	-5.910370	-2.147984	-0.262249
C	-4.976869	0.203236	2.011061
C	0.430795	-1.235225	-3.089372
C	1.607370	-0.992838	-2.384419
C	-0.311414	-2.545660	-3.006106

C	1.428387	-2.316863	0.917466
C	2.600532	-3.012926	0.530022
C	0.204582	-2.983516	1.157385
C	2.507569	-4.402403	0.360302
C	0.171019	-4.371931	0.960321
C	1.306646	-5.076044	0.564942
C	3.955862	-2.330101	0.334044
C	-1.027932	-2.250073	1.679893
C	-2.351107	-2.883342	1.232879
C	-0.977486	-2.132862	3.216972
C	4.668369	-2.750968	-0.964322
C	4.882168	-2.584924	1.540397
C	1.384280	2.615777	0.455218
C	2.281902	3.086574	-0.532176
C	0.422585	3.463108	1.057932
C	2.168505	4.425599	-0.934018
C	1.219331	5.272762	-0.367059
C	0.362172	4.795107	0.621545
C	3.399539	2.218606	-1.104758
C	3.562720	2.371391	-2.625289
C	4.729595	2.503172	-0.379350
C	-0.517265	2.991041	2.167247
C	-1.954707	3.516172	2.003896
C	0.018633	3.381062	3.559876
H	2.586328	-1.014579	3.028476
H	2.629672	1.747810	2.728574
H	-2.769432	1.052448	0.684260
H	-0.981986	2.084289	-0.691552
H	-2.495927	-0.202491	-4.064731
H	-4.353064	-0.918292	-2.596091
H	-6.185441	2.132846	-0.695097
H	-7.579541	1.083140	-0.392694
H	-6.663953	0.915892	-1.896824
H	-6.038323	-2.367838	-1.338715
H	-6.890578	-2.361359	0.205072
H	-5.206325	-2.899641	0.136505
H	-4.145258	-0.367892	2.464100
H	-5.864240	-0.008505	2.637006
H	-4.753213	1.276153	2.162254
H	0.248239	-0.654137	-4.000314
H	2.318847	-0.242948	-2.745148
H	2.032449	-1.775527	-1.754148
H	-0.048848	-3.103118	-2.093607
H	-0.063029	-3.187044	-3.872053
H	-0.760187	-4.913939	1.127401
H	3.392954	-4.966347	0.060054
H	-1.004993	-1.230822	1.266057
H	3.780875	-1.245791	0.269116
H	-0.992901	-3.130454	3.686323
H	-1.850222	-1.571694	3.587733
H	-0.070574	-1.613351	3.562638
H	-3.192429	-2.241600	1.527275
H	-2.520794	-3.867368	1.698958
H	-2.394914	-3.009368	0.140681
H	5.109329	-3.658893	1.639616
H	4.432367	-2.255087	2.488470

H	5.837386	-2.049274	1.416331
H	5.582228	-2.150990	-1.102234
H	4.032168	-2.606824	-1.849469
H	4.978251	-3.807780	-0.939425
H	1.255286	-6.158324	0.421223
H	2.844123	4.815471	-1.697658
H	1.150068	6.313362	-0.693981
H	3.136937	1.169514	-0.914228
H	2.608842	2.215932	-3.152275
H	4.285663	1.631987	-3.005136
H	3.944179	3.366598	-2.904753
H	5.529143	1.848018	-0.762446
H	4.644436	2.332729	0.705113
H	5.048160	3.547764	-0.529911
H	-0.557841	1.891640	2.119785
H	-2.342308	3.358578	0.987218
H	-2.023753	4.593689	2.223322
H	-2.628238	3.000673	2.705970
H	1.019115	2.968992	3.754491
H	-0.655582	3.010652	4.348782
H	0.083998	4.476952	3.659532
H	-0.373276	5.470025	1.062764
H	-1.404905	-2.406965	-3.013990
H	-0.816032	1.446963	-3.161570

int7

B3LYP SCF energy: -3829.02689844 a.u.
B3LYP enthalpy: -3827.775578 a.u.
B3LYP free energy: -3827.937289 a.u.
M06 SCF energy in solution: -3829.91342009 a.u.
M06 enthalpy in solution: -3828.662100 a.u.
M06 free energy in solution: -3828.823811 a.u.
Three lowest frequencies (cm-1): 16.7698 17.6985 31.5264

Cartesian coordinates

ATOM	X	Y	Z
C	-2.239368	2.452622	1.083549
C	-2.413966	2.422633	2.487551
C	-3.716711	2.303287	2.996049
H	-3.870649	2.275943	4.077566
C	-4.818489	2.229299	2.148158
C	-4.635905	2.283005	0.766278
C	-3.356702	2.412898	0.210199
H	-5.825503	2.138664	2.564301
H	-5.506955	2.237290	0.109893
C	-0.619877	4.180372	0.438202
C	0.621635	4.179553	-0.443162
H	-1.458705	4.744338	-0.000148
H	1.460762	4.743556	-0.005424
C	2.239977	2.450201	-1.087064
C	3.357667	2.411743	-0.214105
C	4.636617	2.280746	-0.770494
H	5.507960	2.236097	-0.114429
C	4.818591	2.224595	-2.152365

C	3.716469	2.297273	-2.999912
C	2.413951	2.417771	-2.491079
H	5.825412	2.133089	-2.568785
H	3.869976	2.268059	-4.081442
N	-0.949820	2.747304	0.532320
N	0.950793	2.746212	-0.535664
H	0.430903	4.600666	-1.445107
H	-0.428895	4.602506	1.439668
Ni	-0.000132	-0.000077	-0.000033
C	0.000250	1.901908	-0.001251
C	-2.999702	1.073647	-1.876741
H	-3.919865	0.483455	-1.748688
H	-2.767812	1.113118	-2.953592
H	-2.180750	0.545143	-1.360127
C	-4.280612	3.261123	-2.026989
H	-4.017544	3.386897	-3.089737
H	-5.245127	2.728656	-1.998928
H	-4.436311	4.262832	-1.594498
C	-3.171019	2.486720	-1.300817
H	-2.227701	3.023898	-1.484629
C	-1.243372	2.557926	3.456306
H	-0.320142	2.511552	2.859605
C	-1.273236	3.910626	4.194245
H	-2.162593	3.991098	4.840946
H	-0.383683	4.024139	4.835784
H	-1.298582	4.762096	3.496446
C	1.188110	1.392883	-4.466779
H	1.157376	0.422999	-3.951818
H	0.288544	1.472882	-5.098027
H	2.061182	1.394465	-5.139880
C	1.243008	2.551828	-3.459583
H	0.319994	2.506380	-2.862477
C	1.272766	3.903502	-4.199413
H	2.161889	3.982945	-4.846564
H	0.382985	4.016228	-4.840776
H	1.298480	4.755948	-3.502821
C	3.172531	2.488196	1.296855
H	2.229611	3.026281	1.480078
C	-2.239788	-2.452309	-1.083781
C	-2.413838	-2.422275	-2.487846
C	-3.716363	-2.302511	-2.996816
H	-3.869905	-2.275101	-4.078388
C	-4.818433	-2.228225	-2.149334
C	-4.636393	-2.282028	-0.767386
C	-3.357429	-2.412259	-0.210842
H	-5.825262	-2.137275	-2.565859
H	-5.507678	-2.236081	-0.111332
C	-0.621514	-4.180546	-0.436915
C	0.621065	-4.179879	0.443009
H	-1.460253	-4.743449	0.003006
H	1.459800	-4.743468	0.003945
C	2.239309	-2.450692	1.087330
C	3.357079	-2.412348	0.214473
C	4.635992	-2.281499	0.770985
H	5.507399	-2.236917	0.114999
C	4.817841	-2.225366	2.152872

C	3.715629	-2.297879	3.000318
C	2.413149	-2.418242	2.491362
H	5.824632	-2.133951	2.569387
H	3.869033	-2.268617	4.081862
N	-0.950536	-2.747330	-0.532012
N	0.950104	-2.746537	0.535891
H	0.431718	-4.601607	1.444938
H	-0.432162	-4.603818	-1.438185
C	-0.000197	-1.902117	0.001285
C	-1.187782	-1.400567	-4.465057
H	-1.156875	-0.429938	-3.951509
H	-0.288203	-1.481666	-5.096148
H	-2.060836	-1.402953	-5.138188
C	-1.242949	-2.558022	-3.456167
H	-0.319915	-2.511911	-2.859144
C	-1.273014	-3.910781	-4.194003
H	-2.162171	-3.991000	-4.841010
H	-0.383267	-4.024660	-4.835208
H	-1.298906	-4.762188	-3.496147
C	-3.000506	-1.072948	1.876077
H	-2.181301	-0.544738	1.359565
H	-3.920446	-0.482455	1.747842
H	-2.768805	-1.112435	2.952966
C	-1.188943	1.400349	4.465108
H	-1.157996	0.429765	3.951474
H	-0.289650	1.481179	5.096642
H	-2.062326	1.402854	5.137810
C	-4.282382	-3.259833	2.026185
H	-4.019664	-3.385597	3.089020
H	-5.246650	-2.726937	1.997798
H	-4.438406	-4.261527	1.593772
C	-3.172246	-2.486004	1.300242
H	-2.229221	-3.023566	1.484422
C	1.271721	-3.903520	4.199933
H	0.381821	-4.016091	4.841157
H	1.297583	-4.756158	3.503580
H	2.160722	-3.982775	4.847274
C	1.242071	-2.552045	3.459736
H	0.319148	-2.506760	2.862478
C	4.282312	-3.263713	-2.020990
H	4.019711	-3.391331	-3.083634
H	5.246582	-2.730774	-1.993436
H	4.438277	-4.264647	-1.586804
C	3.000446	-1.076532	-1.874759
H	2.769066	-1.117832	-2.951648
H	2.181077	-0.547484	-1.359354
H	3.920308	-0.485761	-1.747248
C	3.172098	-2.488622	-1.296518
H	2.229088	-3.026478	-1.479929
C	3.000524	1.076195	1.875213
H	2.181160	0.547206	1.359741
H	3.920311	0.485267	1.747912
H	2.768988	1.117640	2.952063
C	1.187006	-1.392823	4.466605
H	1.156222	-0.423085	3.951368
H	0.287401	-1.472720	5.097811

H	2.060038	-1.394145	5.139762
C	4.282814	3.263112	2.021403
H	4.020073	3.390921	3.083989
H	5.246959	2.729935	1.994071
H	4.439091	4.263957	1.587123

int8

B3LYP SCF energy: -3128.40976745 a.u.
B3LYP enthalpy: -3127.630329 a.u.
B3LYP free energy: -3127.751885 a.u.
M06 SCF energy in solution: -3129.11936982 a.u.
M06 enthalpy in solution: -3128.339931 a.u.
M06 free energy in solution: -3128.461487 a.u.
Three lowest frequencies (cm-1): 18.9838 20.7818 30.6874

Cartesian coordinates

ATOM	X	Y	Z
C	-0.753821	-3.641816	-1.424392
O	-2.077185	-3.889604	-1.279174
O	0.094242	-4.447903	-1.107968
C	-2.418631	-5.160462	-0.734034
H	-2.030308	-5.974560	-1.365004
H	-2.002519	-5.280320	0.277967
H	-3.514859	-5.195398	-0.699888
C	-0.482925	-2.310330	-2.021830
C	-1.523555	-1.406167	-2.372545
C	0.870846	-1.968480	-2.293054
C	-1.211448	-0.185102	-2.995056
H	-2.559254	-1.674178	-2.165704
C	1.179322	-0.753135	-2.926628
C	0.140075	0.151221	-3.254888
Ni	-0.022519	-0.299733	-1.152608
C	0.178657	0.609743	0.472228
N	1.338122	0.793817	1.181063
N	-0.787045	1.279842	1.177838
C	1.201416	1.674875	2.350647
C	2.630094	0.313159	0.792749
C	-0.317988	1.869510	2.440893
C	-2.165251	1.375335	0.804161
H	1.627791	1.207309	3.252945
H	1.737874	2.626768	2.189108
C	3.088939	-0.921379	1.313474
C	3.452334	1.106271	-0.044148
H	-0.757548	1.342841	3.306124
H	-0.609945	2.929371	2.518946
C	-2.596423	2.494380	0.050816
C	-3.084556	0.394584	1.249302
C	4.353062	-1.380575	0.916938
C	2.236447	-1.755692	2.265521
C	4.712593	0.606734	-0.403899
C	3.028736	2.492335	-0.524891
C	-3.950944	2.577159	-0.302803
C	-1.635176	3.600136	-0.377791
C	-4.429809	0.526914	0.875765

C	-2.659345	-0.760705	2.151051
C	5.156317	-0.630513	0.059360
H	4.718101	-2.340660	1.288309
C	3.030656	-2.284857	3.470754
C	1.524553	-2.892527	1.514748
H	1.449766	-1.094210	2.659167
H	5.361065	1.198531	-1.054960
C	3.071708	2.629181	-2.055340
C	3.872026	3.593859	0.145881
H	1.981668	2.639168	-0.223680
C	-4.860693	1.600214	0.097729
H	-4.301867	3.424091	-0.897735
C	-2.111029	4.991173	0.076043
C	-1.367760	3.563768	-1.891921
H	-0.672428	3.403992	0.116009
H	-5.155027	-0.222454	1.202056
C	-3.107785	-2.130136	1.618253
C	-3.159178	-0.547088	3.593515
H	-1.559969	-0.771291	2.171052
H	6.138921	-1.006407	-0.238155
H	3.557073	-1.475358	4.001809
H	3.781890	-3.034693	3.174081
H	2.351777	-2.776412	4.186472
H	0.904405	-2.485806	0.704914
H	0.874951	-3.467253	2.195728
H	2.244415	-3.595036	1.064827
H	2.433640	1.871630	-2.530554
H	4.094217	2.515739	-2.450603
H	2.708544	3.623378	-2.363455
H	3.829026	3.529212	1.244696
H	3.514668	4.593928	-0.150774
H	4.932617	3.519398	-0.145600
H	-5.912927	1.681888	-0.187724
H	-2.294405	5.023114	1.162007
H	-3.045022	5.289991	-0.427004
H	-1.352552	5.754354	-0.163781
H	-0.940243	2.591969	-2.175787
H	-0.654694	4.353598	-2.181447
H	-2.293927	3.719907	-2.469777
H	-2.745712	-2.301426	0.595017
H	-4.205795	-2.230007	1.614546
H	-2.711023	-2.935119	2.258768
H	-2.822958	0.417105	4.006570
H	-2.790935	-1.347779	4.256143
H	-4.260901	-0.556486	3.639106
H	0.378543	1.102862	-3.735334
H	-2.010236	0.509031	-3.262701
H	1.652860	-2.676234	-2.016231
H	2.218983	-0.500637	-3.142247

int9

B3LYP SCF energy: -3490.48351575 a.u.

B3LYP enthalpy: -3489.587264 a.u.

B3LYP free energy: -3489.732993 a.u.

M06 SCF energy in solution: -3491.27587884 a.u.
M06 enthalpy in solution: -3490.379627 a.u.
M06 free energy in solution: -3490.525356 a.u.
Three lowest frequencies (cm-1): 14.9849 18.8592 20.5700

Cartesian coordinates

ATOM	X	Y	Z
C	-2.733413	1.727447	-0.829549
O	-2.567439	3.012254	-0.530397
O	-3.749242	1.116682	-0.474431
C	-3.615626	3.674351	0.190724
H	-4.541453	3.682517	-0.401538
H	-3.806648	3.169463	1.148104
H	-3.259181	4.697026	0.359276
C	-1.645856	1.127102	-1.598597
C	-0.533391	1.902040	-2.047188
C	-1.726257	-0.256221	-1.937905
C	0.448151	1.315373	-2.858394
H	-0.471187	2.956867	-1.780852
C	-0.738082	-0.840760	-2.740986
C	0.369892	-0.065975	-3.170275
Ni	0.297887	0.101391	-1.055336
C	1.356596	-0.393716	0.424245
N	2.370414	0.328802	0.987848
N	1.320595	-1.577332	1.101680
C	3.067362	-0.356326	2.088775
C	2.797845	1.627069	0.560915
C	2.319637	-1.696410	2.175717
C	0.406201	-2.649966	0.843640
H	4.138796	-0.481895	1.858624
H	2.999140	0.228880	3.020637
C	3.822454	1.733916	-0.410966
C	2.238298	2.778708	1.165506
H	2.978521	-2.564097	2.004391
H	1.828779	-1.845837	3.151668
C	-0.826407	-2.693952	1.538116
C	0.781186	-3.679575	-0.053022
C	4.237924	3.015312	-0.801149
C	4.501627	0.507703	-1.015746
C	2.689904	4.036992	0.741829
C	1.203645	2.683953	2.283316
C	-1.701339	-3.756530	1.270108
C	-1.205495	-1.650303	2.584995
C	-0.128630	-4.721112	-0.285211
C	2.143159	-3.703245	-0.742878
C	3.674108	4.158619	-0.237760
H	5.022237	3.120544	-1.555023
C	5.991440	0.443241	-0.631471
C	4.318181	0.432465	-2.540446
H	4.009478	-0.381168	-0.595775
H	2.267835	4.939082	1.191258
C	-0.063894	3.501822	1.990419
C	1.814980	3.087908	3.639150
H	0.895223	1.630824	2.353405
C	-1.363314	-4.757319	0.360735
H	-2.664447	-3.802382	1.783585

C	-1.201650	-2.259471	4.000428
C	-2.549992	-0.971626	2.282928
H	-0.436428	-0.864711	2.556888
H	0.135115	-5.520513	-0.982203
C	2.021812	-3.656623	-2.274720
C	2.982083	-4.912176	-0.288487
H	2.680854	-2.792961	-0.440174
H	4.011543	5.148920	-0.554898
H	6.131023	0.470548	0.461035
H	6.555633	1.289348	-1.056707
H	6.450408	-0.484800	-1.010148
H	3.250102	0.402471	-2.797070
H	4.791955	-0.477872	-2.942954
H	4.772463	1.296422	-3.052564
H	-0.523306	3.199201	1.038812
H	0.147388	4.582648	1.939818
H	-0.806949	3.352629	2.791121
H	2.708063	2.489904	3.880867
H	1.083839	2.950304	4.452769
H	2.119957	4.147429	3.640337
H	-2.062162	-5.573874	0.161792
H	-0.232361	-2.723130	4.244895
H	-1.973962	-3.039330	4.102358
H	-1.410025	-1.485397	4.757310
H	-2.552279	-0.513504	1.284447
H	-2.756086	-0.179943	3.021494
H	-3.391124	-1.681643	2.325068
H	1.483047	-2.752230	-2.590182
H	1.483481	-4.533457	-2.669972
H	3.019730	-3.641405	-2.743199
H	3.094965	-4.939091	0.807148
H	3.989920	-4.876008	-0.734027
H	2.518617	-5.864237	-0.594673
Al	-5.603010	0.424813	-0.476627
H	1.145787	-0.526857	-3.785685
H	1.288579	1.913655	-3.214675
H	-2.574922	-0.842728	-1.584865
H	-0.809286	-1.896414	-3.007410
C	-6.416902	1.602372	-1.868325
H	-6.488158	2.664607	-1.567801
H	-5.869551	1.572051	-2.828734
H	-7.450652	1.279164	-2.093555
C	-5.367748	-1.485006	-0.993551
H	-4.685659	-2.035511	-0.319704
H	-6.333459	-2.023854	-0.962565
H	-4.980873	-1.609542	-2.021924
C	-6.170740	0.758789	1.404196
H	-6.185235	1.830950	1.675213
H	-7.198499	0.386272	1.574341
H	-5.530385	0.246147	2.144994

int10

B3LYP SCF energy: -3054.41246496 a.u.

B3LYP enthalpy: -3053.615898 a.u.

B3LYP free energy: -3053.736878 a.u.
M06 SCF energy in solution: -3055.05648017 a.u.
M06 enthalpy in solution: -3054.259913 a.u.
M06 free energy in solution: -3054.380893 a.u.
Three lowest frequencies (cm-1): 15.5171 18.6892 28.3103

Cartesian coordinates

ATOM	X	Y	Z
C	0.212767	-0.454328	0.470557
C	-0.234047	-1.687810	2.474546
C	1.271620	-1.392326	2.404928
H	-0.717167	-1.200561	3.339227
H	-0.452076	-2.766410	2.544774
H	1.637817	-0.840379	3.287145
H	1.877293	-2.312060	2.323017
N	1.381295	-0.578306	1.186794
N	-0.729358	-1.127008	1.209883
C	2.656285	-0.080886	0.771647
C	3.505771	-0.895752	-0.016381
C	3.078282	1.194938	1.218805
C	4.754244	-0.383002	-0.398016
C	4.332789	1.665480	0.805440
C	5.162686	0.889483	-0.002542
H	5.422177	-0.992730	-1.011951
H	4.670216	2.654368	1.124842
H	6.137956	1.273264	-0.314017
C	-2.098786	-1.297516	0.833162
C	-3.068535	-0.365122	1.275806
C	-2.472331	-2.438824	0.081837
C	-4.405814	-0.569807	0.906440
C	-3.822167	-2.597244	-0.263383
C	-4.781910	-1.668879	0.136164
H	-5.167976	0.142721	1.230989
H	-4.129671	-3.466610	-0.850285
H	-5.829402	-1.808530	-0.144397
C	2.194614	2.059579	2.113153
H	1.405017	1.407652	2.515086
C	3.120078	-2.315713	-0.423321
H	2.079236	-2.474794	-0.107391
C	-1.462750	-3.510646	-0.321125
H	-0.470808	-3.160238	-0.002125
C	-2.704023	0.810759	2.177887
H	-1.606400	0.874646	2.199367
Ni	-0.014398	0.365153	-1.181592
O	-2.306672	3.715106	-1.310606
C	-2.755498	5.008248	-1.006689
H	-3.797557	4.931022	-0.664219
H	-2.153871	5.480077	-0.203587
H	-2.721598	5.674563	-1.892766
C	-1.574492	1.303288	-2.485316
H	-2.622218	1.537289	-2.297806
C	-0.590531	2.276584	-2.194815
C	-0.974912	3.669328	-1.757599
H	-0.282735	4.027062	-0.968355
H	-0.847637	4.359826	-2.621106
C	-1.197301	0.049081	-3.010978

C	0.163761	-0.232976	-3.269206
H	-1.963650	-0.696585	-3.230995
H	0.451197	-1.198159	-3.692111
C	0.777895	1.977161	-2.423626
C	1.153531	0.732363	-2.973442
H	1.544061	2.722499	-2.194959
H	2.207167	0.518833	-3.163049
C	2.954123	2.653164	3.310545
H	3.710057	3.391772	2.997296
H	2.255055	3.173448	3.985578
H	3.471130	1.873029	3.892020
C	1.484585	3.152280	1.296240
H	0.884339	2.689798	0.498881
H	0.814535	3.748679	1.937986
H	2.212290	3.840605	0.833744
C	-3.194577	0.567415	3.619170
H	-2.814095	-0.381455	4.029758
H	-2.866272	1.382273	4.285782
H	-4.295657	0.524547	3.662656
C	-3.219713	2.157765	1.648457
H	-4.321768	2.193814	1.626808
H	-2.883671	2.975461	2.308167
H	-2.848052	2.365056	0.634904
C	3.998618	-3.358327	0.294276
H	3.962095	-3.239796	1.388862
H	3.666731	-4.381400	0.051342
H	5.054626	-3.270413	-0.010124
C	3.155929	-2.525052	-1.945661
H	4.170427	-2.393360	-2.355950
H	2.827206	-3.545721	-2.201709
H	2.485139	-1.815244	-2.448520
C	-1.745104	-4.842508	0.399520
H	-2.716279	-5.266729	0.095813
H	-0.968106	-5.587542	0.160537
H	-1.769670	-4.715801	1.493709
C	-1.392192	-3.710667	-1.843453
H	-1.127087	-2.768058	-2.341749
H	-0.625775	-4.460927	-2.099268
H	-2.350986	-4.063917	-2.257319

int11

B3LYP SCF energy: -3416.47920338 a.u.
B3LYP enthalpy: -3415.564722 a.u.
B3LYP free energy: -3415.706002 a.u.
M06 SCF energy in solution: -3417.21545151 a.u.
M06 enthalpy in solution: -3416.300970 a.u.
M06 free energy in solution: -3416.442250 a.u.
Three lowest frequencies (cm-1): 12.1217 19.9915 22.7374

Cartesian coordinates

ATOM	X	Y	Z
C	1.160592	0.099519	0.448766
C	2.646287	-0.417469	2.252403
C	2.259296	1.063511	2.341362

H	2.420212	-0.969170	3.178021
H	3.720770	-0.559884	2.041770
H	1.668117	1.283824	3.246915
H	3.133413	1.733927	2.349556
N	1.450162	1.259209	1.128349
N	1.824225	-0.896672	1.129490
C	1.124201	2.589648	0.701426
C	2.028077	3.281586	-0.145460
C	-0.036305	3.232859	1.197483
C	1.722621	4.597953	-0.519733
C	-0.293406	4.552647	0.797386
C	0.570383	5.230712	-0.059479
H	2.405459	5.141542	-1.177352
H	-1.185394	5.062581	1.167344
H	0.349854	6.258192	-0.360657
C	1.994658	-2.243261	0.665131
C	1.151626	-3.269857	1.158087
C	3.065932	-2.546694	-0.213646
C	1.377255	-4.585995	0.728819
C	3.246385	-3.877978	-0.615894
C	2.409976	-4.891632	-0.155197
H	0.736591	-5.390088	1.097040
H	4.063077	-4.126243	-1.298448
H	2.568060	-5.923956	-0.478282
C	-0.979167	2.555316	2.186436
H	-0.748893	1.479172	2.166860
C	3.337529	2.664051	-0.627132
H	3.350758	1.618786	-0.290343
C	4.048978	-1.488682	-0.708355
H	3.712833	-0.518184	-0.319332
C	0.044603	-2.987545	2.168787
H	-0.148272	-1.904769	2.138128
Ni	0.116775	-0.078933	-1.082565
O	-3.827844	-0.553709	-0.298128
C	-3.216676	-0.675436	0.995599
H	-3.694665	0.061750	1.647676
H	-3.380681	-1.689377	1.391401
H	-2.139816	-0.468096	0.907558
C	-0.893115	-1.602725	-2.337222
H	-0.998503	-2.682570	-2.206478
C	-1.895883	-0.729344	-1.848162
C	-3.179570	-1.327629	-1.324820
H	-3.915035	-1.383297	-2.141088
H	-3.012652	-2.351784	-0.950924
C	0.227183	-1.085273	-3.020279
C	0.362312	0.310384	-3.201471
H	0.984277	-1.766888	-3.412005
H	1.225489	0.707298	-3.739347
C	-1.745487	0.670969	-2.015103
C	-0.617408	1.190105	-2.686068
H	-2.520057	1.343051	-1.641900
H	-0.509483	2.268840	-2.813708
Al	-5.863013	-0.285374	-0.416064
C	-6.055487	0.316942	-2.302972
H	-5.941866	-0.478360	-3.061687
H	-7.072417	0.728565	-2.446918

H	-5.357697	1.129823	-2.575428
C	-6.490340	-2.124326	0.020554
H	-6.188399	-2.460270	1.029810
H	-7.595476	-2.168359	0.003319
H	-6.144026	-2.893107	-0.694570
C	-6.162079	1.109418	0.971147
H	-6.043526	0.758107	2.012045
H	-5.519248	1.999596	0.846629
H	-7.203890	1.473747	0.892281
C	-0.740867	3.071255	3.619869
H	-1.374764	2.529432	4.341211
H	0.307955	2.952691	3.932831
H	-0.986842	4.143211	3.697916
C	-2.457594	2.719039	1.802597
H	-2.781510	3.770797	1.846637
H	-2.652776	2.349318	0.785386
H	-3.101866	2.161907	2.500596
C	-1.270314	-3.704330	1.825392
H	-1.181496	-4.798542	1.917590
H	-2.070858	-3.391092	2.514670
H	-1.591424	-3.479015	0.797439
C	0.490077	-3.352064	3.598968
H	0.687200	-4.433368	3.686705
H	1.412693	-2.826546	3.888769
H	-0.292243	-3.092510	4.331338
C	5.469529	-1.744481	-0.170638
H	5.886303	-2.686465	-0.563192
H	6.150467	-0.930916	-0.470425
H	5.484643	-1.812503	0.928821
C	4.053461	-1.367520	-2.240888
H	4.751150	-0.577785	-2.564010
H	4.367983	-2.305504	-2.726758
H	3.050978	-1.106980	-2.606873
C	4.554951	3.371760	-0.002301
H	4.622297	4.422155	-0.329806
H	4.505417	3.374052	1.098292
H	5.491232	2.870819	-0.299098
C	3.442324	2.640286	-2.160688
H	3.462652	3.656286	-2.587395
H	4.367838	2.132141	-2.477264
H	2.590333	2.101573	-2.598710

int12

B3LYP SCF energy: -1677.32657999 a.u.
B3LYP enthalpy: -1676.553848 a.u.
B3LYP free energy: -1676.675141 a.u.
M06 SCF energy in solution: -3015.77102446 a.u.
M06 enthalpy in solution: -3014.998292 a.u.
M06 free energy in solution: -3015.119585 a.u.
Three lowest frequencies (cm-1): 9.6795 16.4048 19.3841

Cartesian coordinates

ATOM	X	Y	Z
N	0.330264	-1.262867	-1.196784

N	-1.744100	-0.649918	-0.916788
C	-0.484855	-0.498496	-0.411718
C	-0.365852	-1.980931	-2.281115
C	-1.829412	-1.539738	-2.089417
C	1.754052	-1.356629	-1.060418
C	2.574747	-0.436692	-1.749705
C	3.963605	-0.561095	-1.616697
C	4.525762	-1.572403	-0.841155
C	3.701498	-2.482859	-0.185025
C	2.307265	-2.398186	-0.283476
C	1.996088	0.681125	-2.611042
C	1.437205	-3.415400	0.447530
C	-2.921453	-0.026951	-0.385915
C	-3.673942	-0.701202	0.601167
C	-4.831039	-0.081819	1.088503
C	-5.241643	1.158296	0.606053
C	-4.497156	1.800772	-0.379456
C	-3.330804	1.224279	-0.897399
C	-3.247686	-2.054215	1.161520
C	-2.540913	1.958879	-1.975422
H	0.038205	-1.690662	-3.258611
H	-2.224971	-0.999566	-2.958515
H	4.613610	0.141508	-2.131452
H	4.147469	-3.272968	0.413411
H	0.912117	0.538141	-2.656526
H	0.392295	-3.176313	0.228658
H	-5.417754	-0.576204	1.858106
H	-4.825289	2.767651	-0.751884
H	-2.390641	-2.401124	0.576047
H	-1.689612	1.328694	-2.250469
C	-3.383365	2.186259	-3.245862
H	-4.237225	2.846120	-3.051581
H	-2.775263	2.655391	-4.028746
H	-3.778549	1.242901	-3.640923
C	-1.961876	3.285463	-1.447003
H	-1.369036	3.779926	-2.226427
H	-2.756643	3.977725	-1.142997
H	-1.312386	3.107133	-0.583883
C	1.703486	-4.851944	-0.043260
H	2.727921	-5.171725	0.181811
H	1.021985	-5.556885	0.448042
H	1.560647	-4.939793	-1.126713
C	1.606530	-3.309199	1.974945
H	0.945681	-4.021508	2.484020
H	2.635748	-3.529128	2.283626
H	1.353289	-2.300689	2.316008
C	-4.357972	-3.114456	1.032373
H	-3.992783	-4.090716	1.373134
H	-5.234818	-2.862434	1.640160
H	-4.694177	-3.220206	-0.005766
C	-2.766270	-1.921746	2.619443
H	-2.432741	-2.893479	3.004609
H	-1.927119	-1.219808	2.676204
H	-3.567906	-1.557358	3.273421
C	2.238396	2.061847	-1.971880
H	3.309441	2.276334	-1.874699

H	1.793365	2.852044	-2.589425
H	1.789522	2.108934	-0.975267
C	2.529786	0.632181	-4.055856
H	2.345447	-0.343356	-4.521286
H	2.039708	1.399269	-4.667309
H	3.609021	0.820525	-4.097307
H	-6.143529	1.622841	0.996585
H	5.606357	-1.655680	-0.754882
H	-2.501082	-2.383253	-1.887925
H	-0.235235	-3.065037	-2.175888
Ni	-0.024532	0.499143	1.100205
C	2.526300	2.552497	1.900444
C	1.401165	3.411533	1.812961
C	0.156984	2.972619	2.225010
C	-0.027998	1.662543	2.754405
C	1.099535	0.794196	2.799172
C	2.381153	1.259725	2.382962
H	1.050368	-0.138557	3.356634
H	3.229187	0.588496	2.457690
O	3.705727	3.102482	1.473854
C	4.869330	2.297109	1.536507
H	5.095098	1.994988	2.568762
H	4.771089	1.397928	0.913664
H	5.685498	2.915589	1.156670
H	1.548221	4.414083	1.422943
H	-0.690660	3.652100	2.181656
H	-0.949857	1.419598	3.277998

int13

B3LYP SCF energy: -2039.53129190 a.u.
B3LYP enthalpy: -2038.640215 a.u.
B3LYP free energy: -2038.783848 a.u.
M06 SCF energy in solution: -3377.91962411 a.u.
M06 enthalpy in solution: -3377.028547 a.u.
M06 free energy in solution: -3377.172180 a.u.
Three lowest frequencies (cm-1): 10.6718 16.3365 18.6415

Cartesian coordinates

ATOM	X	Y	Z
O	4.345608	0.994075	0.122088
Ni	-0.141782	0.145187	-0.807653
C	3.161099	1.007174	-0.649526
C	2.570484	2.257382	-0.927817
C	2.643826	-0.176092	-1.132671
C	1.438401	2.299958	-1.721296
H	3.026132	3.162565	-0.538872
C	1.487004	-0.149748	-1.966551
H	3.152686	-1.112524	-0.927262
C	0.876099	1.108980	-2.264311
H	0.992000	3.258974	-1.970614
C	4.129413	0.895117	1.547553
H	5.105762	1.008147	2.017618
H	3.458389	1.697754	1.865678
H	3.693333	-0.077403	1.791550

C	6.018391	1.345435	-2.503849
Al	6.203862	0.550919	-0.690922
C	6.231076	-1.439727	-0.545795
C	7.368503	1.537663	0.597258
H	6.964822	1.253346	-3.057971
H	5.250062	0.859513	-3.120108
H	5.522554	-1.936417	-1.223892
H	7.226365	-1.830567	-0.805692
H	8.388086	1.600120	0.187370
H	7.472629	1.065613	1.584875
H	6.017805	-1.807993	0.468703
H	7.047899	2.576048	0.765223
H	5.779592	2.417916	-2.479086
N	-1.931049	-1.543735	0.752541
N	-2.623481	0.523491	0.687805
C	-1.617571	-0.302599	0.285255
C	-3.238892	-1.616853	1.433151
C	-3.642101	-0.135773	1.528901
C	-1.182413	-2.737712	0.479613
C	-1.419886	-3.451993	-0.715355
C	-0.674737	-4.615156	-0.946119
C	0.263982	-5.065441	-0.021998
C	0.467037	-4.361017	1.161836
C	-0.254052	-3.193872	1.440973
C	-2.453844	-3.006492	-1.745540
C	-0.000842	-2.435351	2.739623
C	-2.663581	1.942588	0.477606
C	-2.015806	2.800512	1.393106
C	-2.091004	4.181036	1.170736
C	-2.793523	4.698969	0.086243
C	-3.441797	3.838505	-0.795843
C	-3.398036	2.450576	-0.616593
C	-1.239218	2.274452	2.596126
C	-4.107642	1.536540	-1.610556
H	-3.947656	-2.207741	0.838306
H	-4.649745	0.057822	1.145839
H	-0.832418	-5.176708	-1.863055
H	1.198572	-4.723311	1.878757
H	-2.928881	-2.094221	-1.372738
H	-0.774461	-1.666338	2.831221
H	-1.591754	4.859754	1.857023
H	-3.989562	4.251264	-1.638525
H	-1.321185	1.183480	2.598660
H	-4.072314	0.518423	-1.210219
C	-5.590659	1.908911	-1.796397
H	-5.709417	2.896973	-2.255652
H	-6.084050	1.182210	-2.452695
H	-6.125117	1.921269	-0.839429
C	-3.364859	1.510765	-2.960937
H	-3.863152	0.830318	-3.662466
H	-3.337843	2.506838	-3.419081
H	-2.334039	1.169044	-2.821028
C	-0.099927	-3.340782	3.981512
H	0.689388	-4.100983	3.996977
H	0.004531	-2.743207	4.894905
H	-1.063752	-3.861105	4.023404

C	1.353148	-1.701335	2.689376
H	1.513805	-1.126138	3.610001
H	2.183318	-2.410744	2.584503
H	1.380924	-1.012719	1.838257
C	-1.826026	2.789960	3.924902
H	-1.290103	2.350991	4.775031
H	-1.740616	3.879799	4.007918
H	-2.887431	2.533488	4.022406
C	0.260933	2.607439	2.484572
H	0.809064	2.181737	3.334456
H	0.676216	2.195656	1.559110
H	0.432003	3.690642	2.485007
C	-1.800244	-2.645981	-3.093111
H	-1.272834	-3.502657	-3.529057
H	-2.562390	-2.321483	-3.812174
H	-1.083229	-1.828884	-2.962493
C	-3.557381	-4.067030	-1.932020
H	-4.044094	-4.313025	-0.980988
H	-4.325567	-3.701406	-2.623857
H	-3.154642	-4.998298	-2.347225
H	-2.839109	5.773711	-0.069631
H	0.834621	-5.968571	-0.221991
H	-3.594625	0.247408	2.556609
H	-3.142453	-2.096978	2.412877
H	1.252099	-1.038700	-2.547849
H	0.154177	1.195176	-3.073830