Electronic Supplementary Information

Origins of regioselectivity in Ni-catalyzed hydrofunctionalization of alkenes via ligand-to-ligand hydrogen transfer mechanism

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Computational Details

The B3LYP density function and a mixed basis set of LANL2DZ for Ni and 6-31g(d) for other atoms were used for geometry optimizations for all intermediates and transition states. All minima have zero imaginary frequency and all transition states have only one imaginary frequency and were confirmed by intrinsic reaction coordinate (IRC) calculations. Single-point energies were calculated by using M06 and the def2-TZVP basis set. Solvation energy corrections were calculated using the SMD model[1] with the solvents used in experiments. All these calculations were carried out with Gaussian 09.[2]

Energy decomposition analysis (EDA) calculations at the M06/def2-TZVP level of theory were performed by using the second-generation EDA based on absolutely localized orbitals (ALMO-EDA2) implemented in Q-Chem 5.2.[3] The complementary occupied-virtual pairs (COVPs) were computed to figure out the direction of charge transfer and the most significant orbitals. To minimize the effect of early or late transition states in comparing each energy term among the LLHT transition states, we performed EDA calculations along the reaction coordinates obtained from IRC calculations. The reported energies in the bar charts are the average of $\Delta\Delta E$ values at the region of X–H (X = O, C) bond distances that correspond to the two regioisomeric LLHT transition states. The orbitals were visualized using IQmol (isovalue = 0.08 $Å^{-3}$).

Competing LLHT and Oxidative Addition Pathways

As shown in Fig. S1, for the Ni-catalyzed hydrofunctionalization of alkenes with MeOH, aldehyde, benzene and pyridine, the LLHT pathways (in black and blue) are superior to the pathway of oxidative addition followed by migratory insertion (in red). This suggests that the regioselectivity is determined by the LLHT pathway.

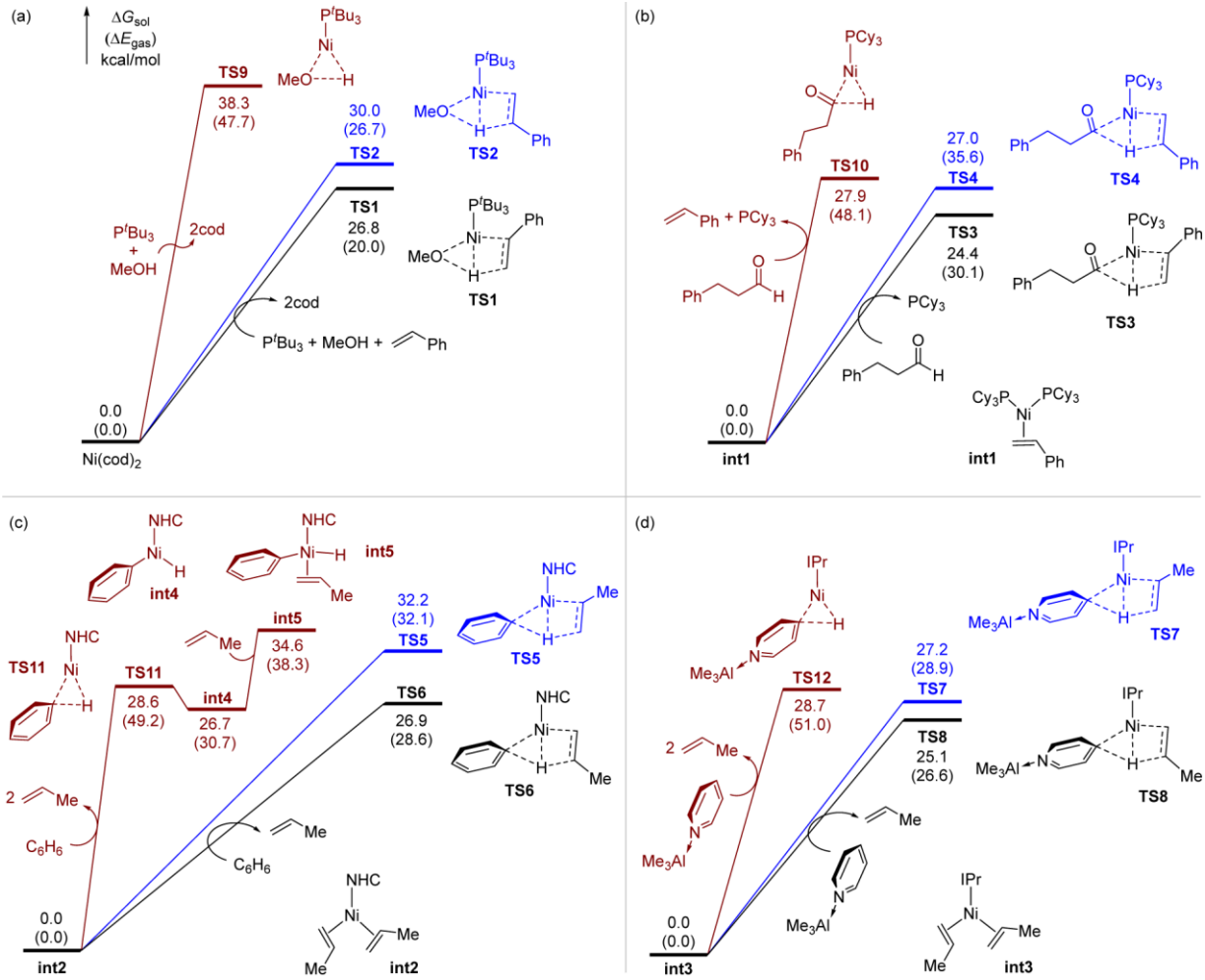

Fig. S1. Energy profiles for LLHT and oxidative addition pathways.

COVPs Results for TS1 and TS2

The most significant donor-acceptor interaction in **TS1** and **TS2** is from the combination of O–H σ and Ni occupied d orbitals (i.e., σ+d) to styrene π* orbital, which has been discussed in the main text (Fig. 1c). The other direction of charge transfer, i.e., from styrene π orbital to O–H σ* and Ni empty d orbitals, is stronger in **TS1** than in **TS2** (Fig. S2). This also contributes to the lower barrier of branched-selective **TS1**.

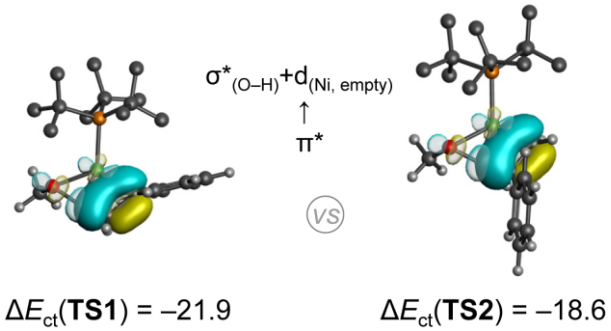

Fig. S2. Difference of charge transfer from $\pi_{(C=C)} \rightarrow \sigma^*_{(O–H)}+d_{(Ni,\ empty)}$ in **TS1** and **TS2**. Energies are given in kcal/mol.

EDA Results along IRC for TS3 and TS4 and NCI Plots

The EDA result along IRC shows that the charge transfer (ΔE_{ct}) and dispersion (ΔE_{disp}) energies are the positive contributors to the lower barrier of **TS3** than **TS4** (Fig. S3a). As shown in Fig. S3b, the COVPs results indicate the orbital interaction of $\sigma+d_{occupied}\rightarrow\pi^*$ is the most significant donor-acceptor interaction for stabilizing the branched-selective **TS3**. The orbital interaction of $\pi\rightarrow\sigma^*+d_{empty}$ also contributes to the lower barrier of **TS3**.

The dispersion interactions in **TS3** and **TS4** can be described by using NCI plots. As shown in Fig. S4, there are greater non-covalent interactions in **TS3** between PCy_3 and styrene (the larger green slice) than those in **TS4** (the smaller green slice), which is consistent with the computed larger dispersion energy in **TS3** than **TS4**. This is because the styrene phenyl group is proximal to the PCy_3 ligand in **TS3** while the phenyl group is distal to the ligand in **TS4**.

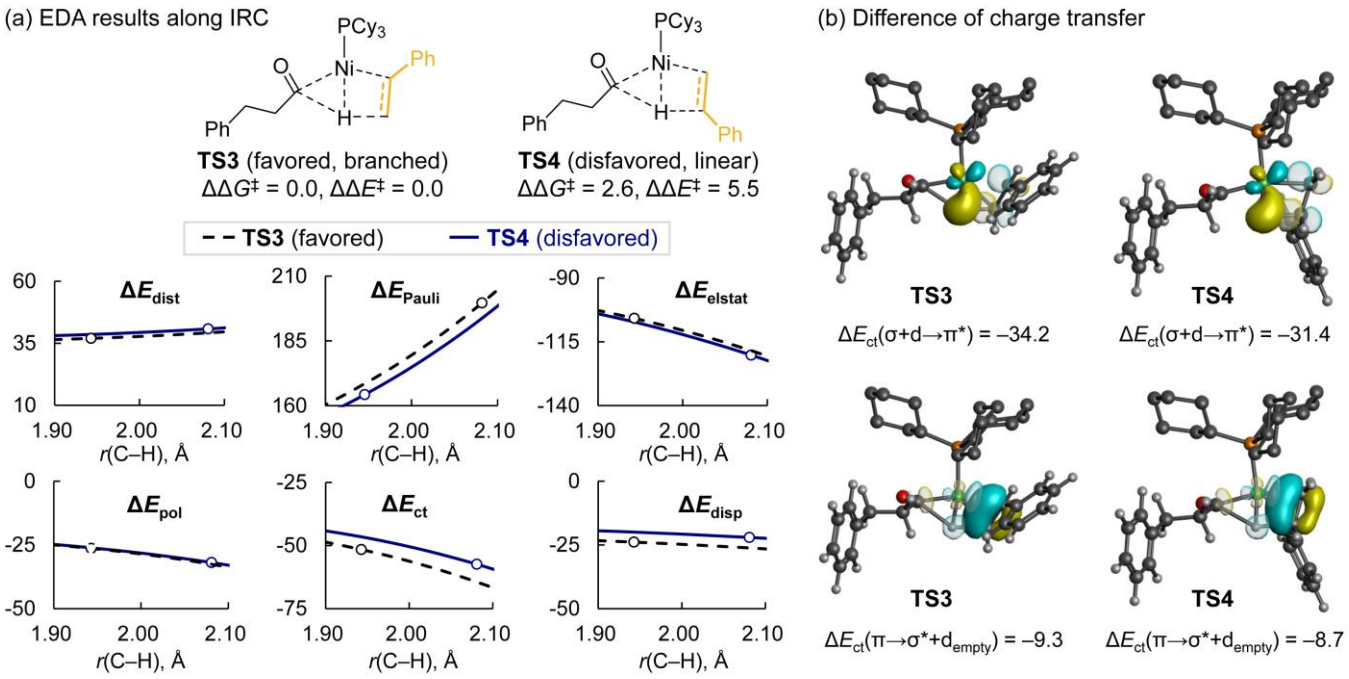

Fig. S3. EDA results for the two regioisomeric LLHT transition states with aldehyde and styrene. Energies are given in kcal/mol.

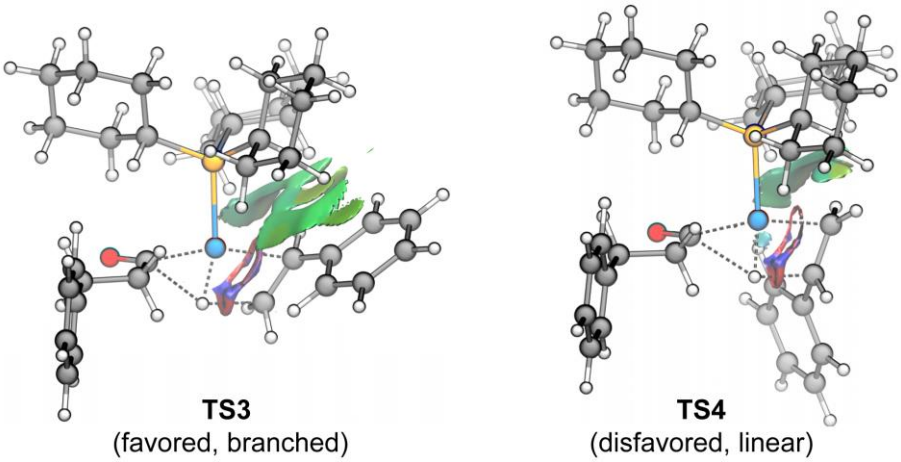

Fig. S4. The NCI plot between PCy_3Ni/aldehyde and styrene in **TS3** and **TS4**.

EDA Results along IRC for TS7 and TS8

As shown in Fig. S5, the EDA result along IRC shows that the lower barrier of **TS8** than **TS7** is mostly due to the weaker destabilizing effects, including distortion (ΔE_{dist}) and Pauli repulsion (ΔE_{Pauli}).

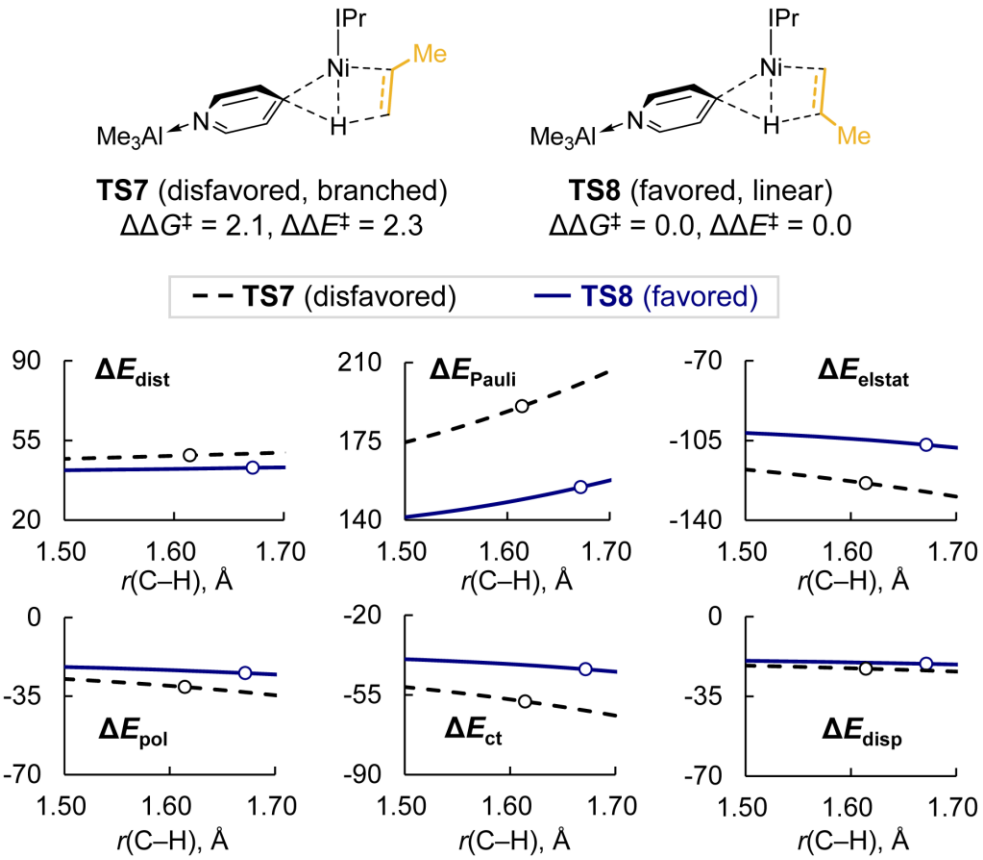

Fig. S5. EDA results for the two regioisomeric LLHT transition states with pyridine/$AlMe_3$ and propene. Energies are given in kcal/mol.

Energy Terms of EDA along IRC

Table S1. EDA energy terms of TS1 along IRC

Energy terms (in kcal/mol) / *r*(O-H) in **TS1** (in Å)	ΔE_{dist}	ΔE_{Pauli}	ΔE_{ct}	ΔE_{elstat}	ΔE_{pol}	ΔE_{disp}
1.24	69.6	264.2	-105.3	-175.7	-48.6	-19.2
1.29	72.8	277.8	-110.8	-179.8	-53.3	-20.1
1.35	75.7	293.3	-116.6	-184.4	-58.9	-21.1
1.40(TS)	78.1	310.4	-122.6	-189.2	-65.7	-22.2
1.45	80.2	329.8	-128.9	-194.7	-73.9	-23.4
1.50	82.0	349.8	-135.2	-200.0	-83.2	-24.6
1.55	83.7	365.0	-140.0	-203.4	-91.3	-25.7
1.59	85.1	378.2	-144.0	-205.7	-99.0	-26.6

Table S2. EDA energy terms of TS2 along IRC

Energy terms (in kcal/mol) / *r*(O-H) in **TS2** (in Å)	ΔE_{dist}	ΔE_{Pauli}	ΔE_{ct}	ΔE_{elstat}	ΔE_{pol}	ΔE_{disp}
1.22	68.2	258.8	-98.0	-176.7	-46.3	-16.4
1.27	71.4	269.4	-102.4	-179.9	-49.7	-17.2
1.32	74.2	282.0	-107.1	-183.7	-54.0	-18.1
1.38	76.6	296.5	-112.2	-188.1	-59.2	-19.1
1.43(TS)	78.6	312.9	-117.5	-193.0	-65.5	-20.2
1.48	80.2	331.6	-123.2	-198.6	-73.3	-21.3
1.54	81.6	351.5	-128.9	-204.3	-82.3	-22.5
1.58	82.9	369.7	-133.7	-209.0	-91.7	-23.5

Table S3. EDA energy terms of TS3 along IRC

Energy terms (in kcal/mol) / *r*(C-H) in **TS3** (in Å)	ΔE_{dist}	ΔE_{Pauli}	ΔE_{ct}	ΔE_{elstat}	ΔE_{pol}	ΔE_{disp}
1.85	36.1	152.8	-45.8	-99.6	-23.6	-22.7
1.90	36.5	159.8	-48.4	-102.5	-24.8	-23.3
1.94(TS)	37.0	168.0	-51.6	-105.8	-26.3	-23.9
1.99	37.6	177.2	-55.3	-109.6	-28.1	-24.6
2.04	38.4	187.7	-59.6	-113.8	-30.2	-25.3
2.08	39.3	199.6	-64.6	-118.6	-32.7	-26.2
2.13	40.3	213.1	-70.2	-123.8	-35.7	-27.1
2.17	41.5	228.1	-76.6	-129.6	-39.3	-28.1

Table S4. EDA energy terms of TS4 along IRC

Energy terms (in kcal/mol) / *r*(C-H) in **TS4** (in Å)	ΔE_{dist}	ΔE_{Pauli}	ΔE_{ct}	ΔE_{elstat}	ΔE_{pol}	ΔE_{disp}
1.86	37.8	150.3	-42.2	-101.2	-23.6	-18.9
1.90	38.1	156.8	-44.2	-104.1	-24.8	-19.4
1.95	38.6	164.3	-46.7	-107.5	-26.2	-20.0
1.99	39.2	172.8	-49.7	-111.3	-27.8	-20.6
2.04	40.0	182.5	-53.3	-115.5	-29.7	-21.3
2.08(TS)	40.8	193.5	-57.4	-120.2	-31.9	-22.1
2.13	41.8	205.8	-62.2	-125.4	-34.5	-22.9
2.17	43.0	219.7	-67.6	-131.2	-37.7	-23.8

Table S5. EDA energy terms of TS5 along IRC

Energy terms (in kcal/mol) / *r*(C-H) in **TS5** (in Å)	ΔE_{dist}	ΔE_{Pauli}	ΔE_{ct}	ΔE_{elstat}	ΔE_{pol}	ΔE_{disp}
1.22	55.9	203.1	-59.0	-140.9	-31.6	-24.3
1.31	58.3	213.2	-63.3	-144.3	-33.9	-25.0
1.37	59.7	220.1	-66.2	-146.7	-35.6	-25.6
1.42	61.1	228.5	-69.5	-149.6	-37.8	-26.2
1.47	62.3	238.4	-73.3	-153.1	-40.4	-26.9
1.53	63.5	249.8	-77.5	-157.2	-43.5	-27.7
1.58(TS)	64.7	262.9	-82.2	-161.8	-47.3	-28.6
1.63	65.9	277.6	-87.4	-167.0	-51.9	-29.6
1.69	67.1	294.1	-93.0	-172.7	-57.4	-30.6
1.84	71.7	351.7	-111.2	-191.0	-81.0	-34.1

Table S6. EDA energy terms of TS6 along IRC

Energy terms (in kcal/mol) / *r*(C-H) in **TS6** (in Å)	ΔE_{dist}	ΔE_{Pauli}	ΔE_{ct}	ΔE_{elstat}	ΔE_{pol}	ΔE_{disp}
1.28	51.6	196.3	-56.2	-137.1	-31.7	-21.9
1.39	53.9	207.1	-60.3	-141.2	-34.1	-22.7
1.44	55.0	214.3	-62.9	-144.0	-35.9	-23.3
1.49	56.0	223.0	-66.0	-147.3	-38.0	-23.9
1.55	57.0	233.1	-69.6	-151.3	-40.6	-24.6
1.60(TS)	58.1	244.7	-73.7	-155.7	-43.7	-25.4
1.65	59.1	257.9	-78.3	-160.7	-47.4	-26.3
1.71	60.1	272.9	-83.3	-166.3	-51.9	-27.3
1.76	61.2	289.6	-88.9	-172.4	-57.5	-28.3
1.81	62.4	308.2	-94.8	-178.9	-64.2	-29.4

Table S7. EDA energy terms of TS7 along IRC

Energy terms (in kcal/mol) / *r*(C-H) in **TS7** (in Å)	ΔE_{dist}	ΔE_{Pauli}	ΔE_{ct}	ΔE_{elstat}	ΔE_{pol}	ΔE_{disp}
1.40	45.5	164.6	-47.6	-114.1	-25.2	-20.6
1.45	46.3	169.6	-49.6	-115.9	-26.3	-21.1
1.51	47.0	175.5	-51.9	-118.1	-27.6	-21.6
1.56	47.7	182.5	-54.7	-120.7	-29.1	-22.2
1.61(TS)	48.5	190.6	-57.9	-123.7	-30.9	-22.9
1.67	49.2	199.8	-61.5	-127.2	-33.1	-23.6
1.72	50.0	210.4	-65.7	-131.2	-35.6	-24.4
1.77	50.8	222.4	-70.5	-135.7	-38.7	-25.3
1.82	51.8	235.9	-75.8	-140.7	-42.3	-26.3
1.87	52.8	251.0	-81.6	-146.2	-46.8	-27.4
1.92	54.0	267.6	-87.9	-152.1	-52.1	-28.5

Table S8. EDA energy terms of TS8 along IRC

Energy terms (in kcal/mol) / *r*(C-H) in **TS8** (in Å)	ΔE_{dist}	ΔE_{Pauli}	ΔE_{ct}	ΔE_{elstat}	ΔE_{pol}	ΔE_{disp}
1.40	41.2	137.1	-38.0	-100.3	-21.0	-18.9
1.46	41.6	139.1	-38.7	-100.9	-21.5	-19.1
1.51	42.0	141.9	-39.5	-101.9	-22.1	-19.4
1.56	42.3	145.3	-40.6	-103.2	-22.9	-19.8
1.62	42.6	149.5	-42.0	-104.8	-23.7	-20.2
1.67(TS)	43.0	154.6	-43.8	-106.9	-24.8	-20.7
1.72	43.3	160.5	-45.8	-109.3	-25.9	-21.3
1.78	43.7	167.5	-48.4	-112.1	-27.3	-21.9
1.83	44.2	175.6	-51.5	-115.5	-29.0	-22.5
1.88	44.7	184.9	-55.1	-119.3	-31.0	-23.3
1.93	45.4	195.5	-59.2	-123.7	-33.3	-24.1

Additional Discussions of Computational Results

Effects of electronic properties of aromatic substituents on LLHT

For the para-OMe and para-CO_2Me substituted styrene, we computed the Markovnikov and anti-Markovnikov LLHT transition states in the reactions with alcohol (**TS1a** vs **TS2a**; **TS1b** vs **TS2b**) and aldehyde (**TS3a** vs **TS4a**; **TS3b** vs **TS4b**). As shown in Fig. S6 and S7, the electronic properties of the para-substituents do not affect the regioselectivity, favoring the Markovnikov selectivity. The EDA results indicate that the charge transfer effect is also the dominant factor in controlling the regioselectivity. Compared with styrene, the para-OMe and para-CO_2Me can indeed increase and reduce the LUMO orbital coefficients of the two carbon atoms, respectively. However, the differences in orbital coefficients between the two carbon atoms are slightly changed (24% vs 12% for styrene; 25% vs 14% for para-OMe styrene; 17% vs 6% for para-CO_2Me styrene), which leads to comparable charge transfer effect ($\Delta\Delta E_{ct}$ = 6~8 kcal/mol) in the reactions of alcohol and aldehyde with styrenes. Thus, the electronic properties of styrene para-substituents exert a small influence on both the trends of regioselectivity and the charge transfer effect.

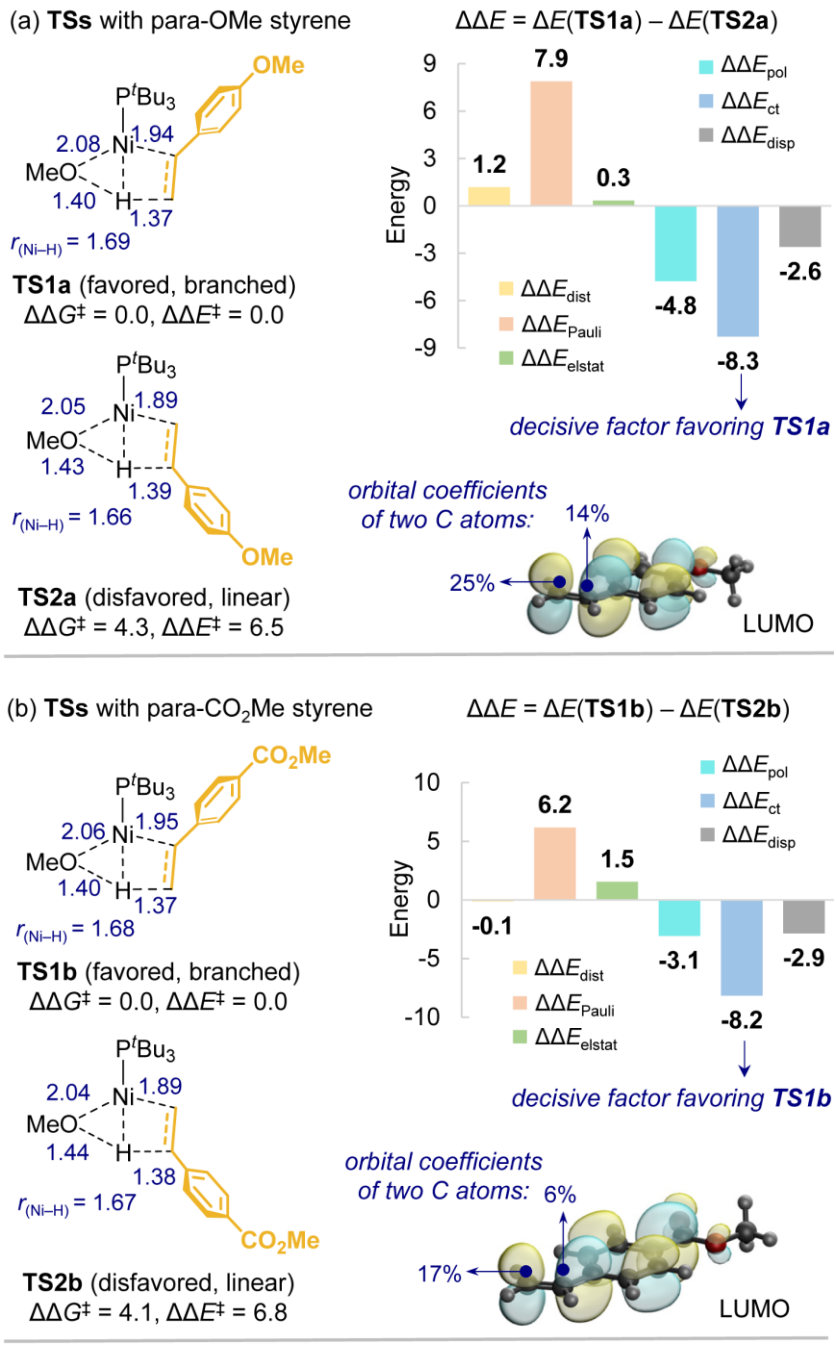

Fig. S6. EDA results for the two regioisomeric LLHT transition states with para-OMe and para-CO_2Me substituted styrene. Energies are given in kcal/mol.

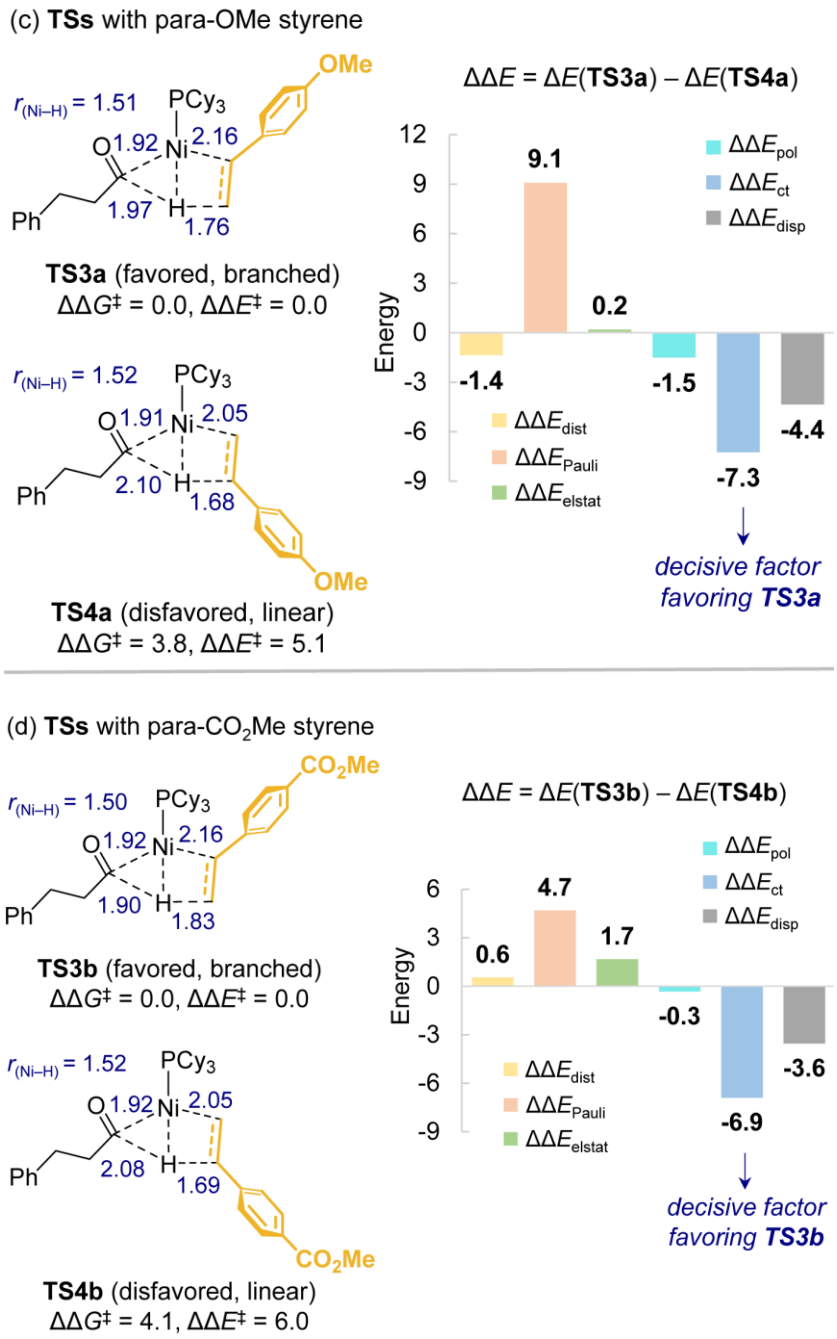

Fig. S7. EDA results for the two regioisomeric LLHT transition states with para-OMe and para-CO_2Me substituted styrene. Energies are given in kcal/mol.

Effects of ortho-substituents on LLHT

We computed the LLHT transition states with ortho-methyl substituted styrene and performed EDA calculations. As shown in Fig. S8, the results indicate that the Markovnikov selectivity in the reactions with alcohol and aldehyde is also favored over the anti-Markovnikov selectivity (**TS1c** vs **TS2c**; **TS3c** vs **TS4c**). While the charge transfer is still the dominant factor for controlling regioselectivity in P^tBu_3-Ni mediated LLHT (**TS1c** vs **TS2c**), the dispersion effect becomes more important in PCy_3-Ni mediated LLHT (**TS3c** vs **TS4c**) although the charge transfer is still a positive contributor. This is mostly

because the non-covalent interactions between ortho-Me substituted styrene and the PCy_3 ligand in **TS3c** are much greater, which is evidenced by the difference in NCI plots between **TS3c** and **TS4c**.

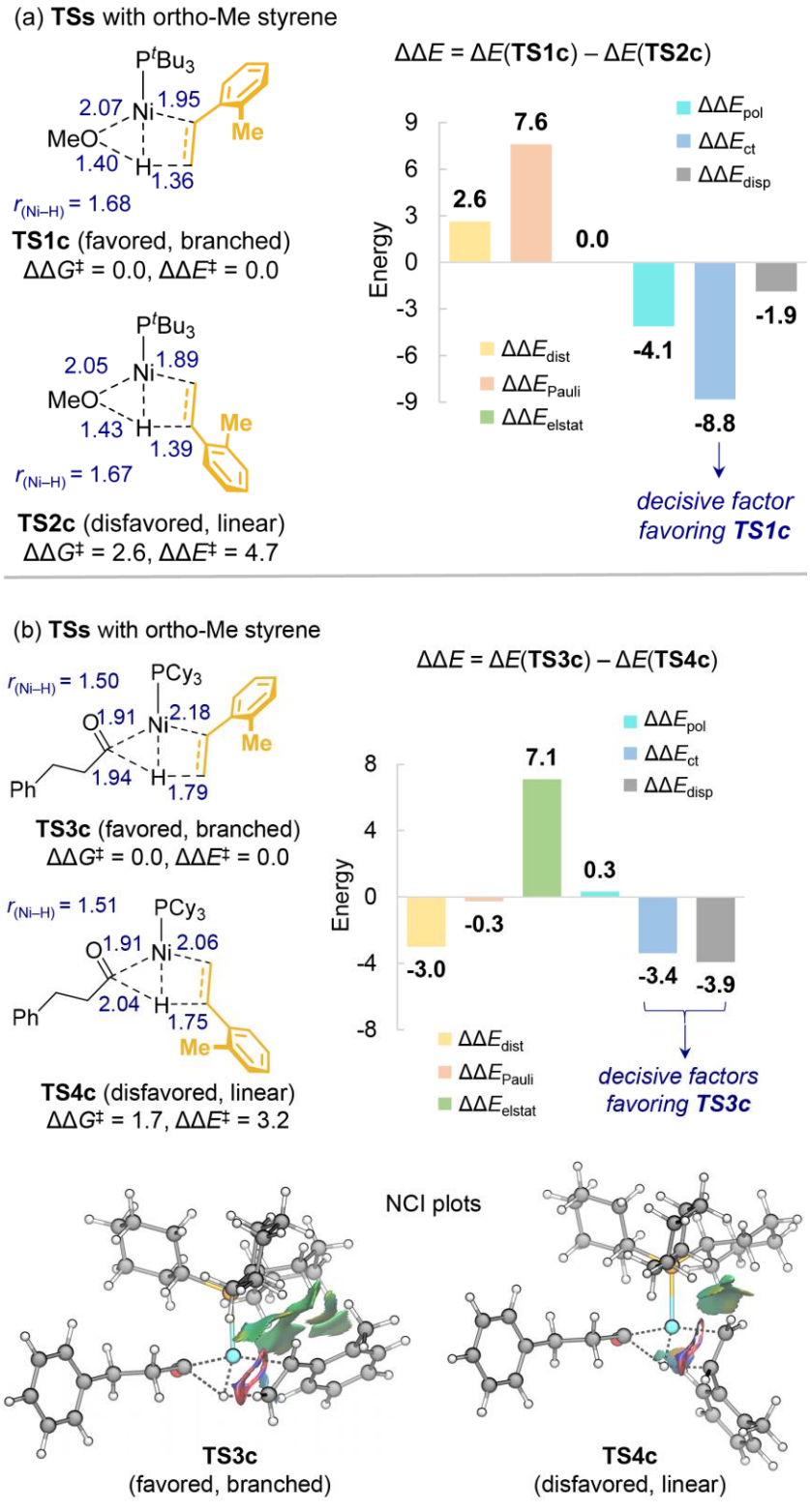

Fig. S8. EDA results for regioisomeric LLHT transition states with ortho-Me substituted styrene. Energies are given in kcal/mol.

Effects of alkenes with larger alkyl groups on LLHT

Taking the reaction of pyridine with 1-hexene for example, we computed the LLHT transition states (**TS7a** and **TS8a**, Fig. S9) and performed EDA calculations. The results show that Pauli repulsion is also the dominant factor for the favored anti-Markovnikov selectivity, which indicates that methyl and larger alkyl groups share the same conclusion for regioselectivity.

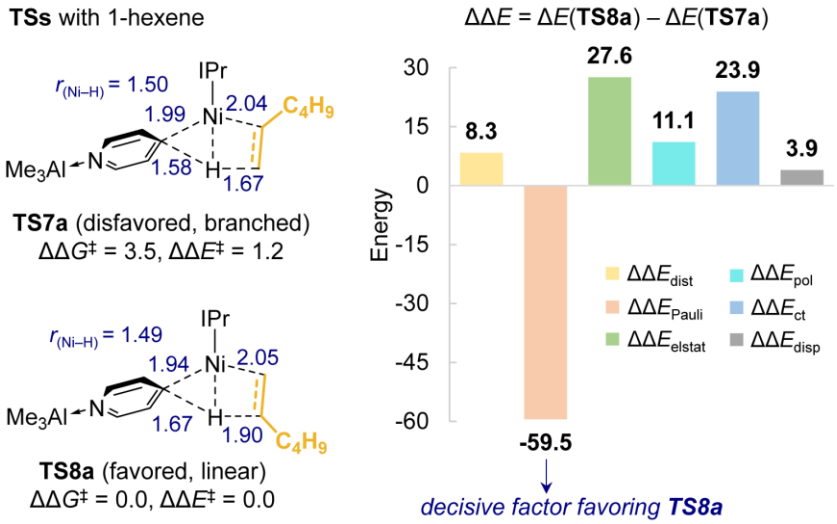

Fig. S9. EDA results for regioisomeric LLHT transition states with 1-hexene. Energies are given in kcal/mol.

Effects of ligands on LLHT

The choice of ligands in experiments mostly depends on the reaction efficiency when employing different types of ligands. In this regard, for the hydroarylation of styrene with MeOH reported by Zhou group (*Angew. Chem. Int. Ed.* 2018, 57, 461), although the selectivity is unchanged, the yield is dramatically decreased when replacing P^{t}Bu$_3$ with IPr (Fig. S10). For the hydroarylation of alkyl-substituted alkenes reported by Hiyama group (*J. Am. Chem. Soc.* 2010, 132, 13666), while IPr gives a good yield of linear product, the phosphine ligand (e.g., P^{i}Pr$_3$) is completely ineffective (Fig. S11). We further computed the barriers of LLHT and analyzed the key factor for regioselectivity. As shown in Fig. S10 and S11, both the regioselectivity of LLHT and the dominant factor, i.e., charge transfer for Markovnikov selectivity with styrene and Pauli repulsion for anti-Markovnikov selectivity with propene, are not affected by the change of ligands. However, for the reaction with styrene, the LLHT transition states with IPr ($\Delta G^‡$ = 32.9 kcal/mol for **TS1d**; $\Delta G^‡$ = 36.1 kcal/mol for **TS2d**) have higher barriers than those with P^{t}Bu$_3$ ($\Delta G^‡$ = 26.8 kcal/mol for **TS1**; $\Delta G^‡$ = 30.0 kcal/mol for **TS2**, Fig. S1). For the reaction with propene, the LLHT transition states with P^{t}Bu$_3$ ($\Delta G^‡$ = 35.2 kcal/mol for **TS7b**; $\Delta G^‡$ = 30.1 kcal/mol for **TS8b**) is less favorable than those with IPr ($\Delta G^‡$ = 27.2 kcal/mol for **TS7**; $\Delta G^‡$ = 25.1 kcal/mol for **TS8**, Fig. S1). These results indicate that the choice of ligands can affect the reactivity of LLHT. Moreover, it should be noted that ligands can exert influence on not only LLHT but also other reaction steps, such as transmetalation and reductive elimination. The uses of phosphine ligands for aryl-substituted alkenes and NHC ligands for alkyl-substituted alkenes are due to their capacity for promoting the overall reaction efficiency.

The electronic and steric effects of ligands on LLHT regioselectivity can be understood from two aspects: 1) The NHC-type ligands are typically bulkier than the phosphine ligands. Thus, the differences of geometry deformations between the two LLHT transition states with NHC-type ligands are expected to be greater than those with phosphine ligands. This is evidenced by the finding that the computed $\Delta\Delta E_{dist}$ values of **TS5** vs **TS6** ($\Delta\Delta E_{dist(TS6–TS5)}$ = –7.1 kcal/mol) and **TS7** vs **TS8** ($\Delta\Delta E_{dist(TS8–TS7)}$ = –6.3 kcal/mol) are larger than those of **TS1** vs **TS2** ($\Delta\Delta E_{dist(TS1–TS2)}$ = 0.6 kcal/mol) and **TS3** vs **TS4** ($\Delta\Delta E_{dist(TS3–TS4)}$ = –1.6 kcal/mol). 2) The NHC-type ligands are better electron donors than phosphine ligands, which can render the Ni fragments ligated by NHC-type ligands more electron-rich. This can enhance both Pauli repulsion and charge transfer effects with the olefin fragments, which is supported by the much greater $\Delta\Delta E_{Pauli}$ and $\Delta\Delta E_{ct}$ values of **TS5** vs **TS6** ($\Delta\Delta E_{Pauli(TS6–TS5)}$ = –23.9 kcal/mol; $\Delta\Delta E_{ct(TS6–TS5)}$ = 10.2 kcal/mol) and **TS7** vs **TS8** ($\Delta\Delta E_{Pauli(TS8–TS7)}$ = –47.1 kcal/mol; $\Delta\Delta E_{ct(TS8–TS7)}$ = 18.4 kcal/mol) than those of **TS1** vs **TS2** ($\Delta\Delta E_{Pauli(TS1–TS2)}$ = 5.4 kcal/mol; $\Delta\Delta E_{ct(TS1–TS2)}$ = –7.7 kcal/mol) and **TS3** vs **TS4** ($\Delta\Delta E_{Pauli(TS3–TS4)}$ = 4.9 kcal/mol; $\Delta\Delta E_{ct(TS3–TS4)}$ = –6.0 kcal/mol), respectively.

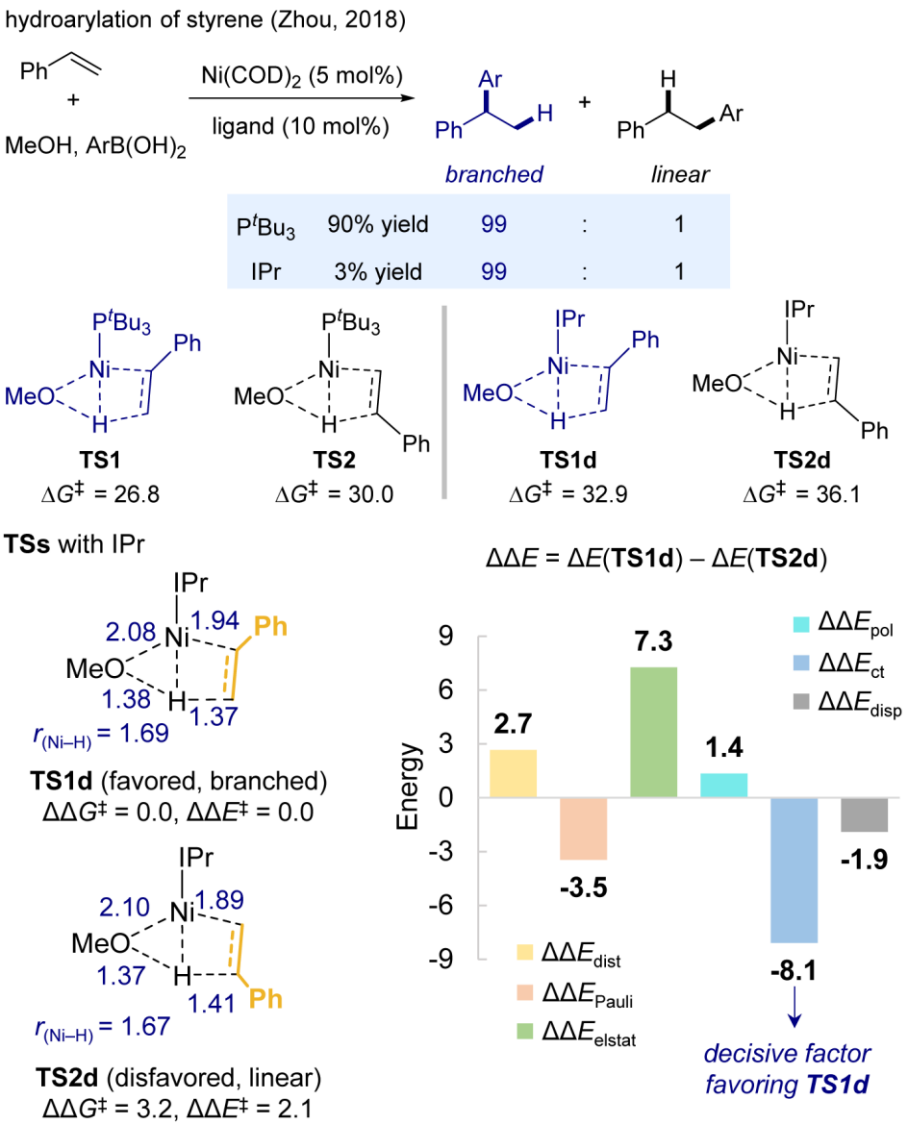

Fig. S10. EDA results for regioisomeric LLHT transition states with styrene and IPr. Energies are given in kcal/mol.

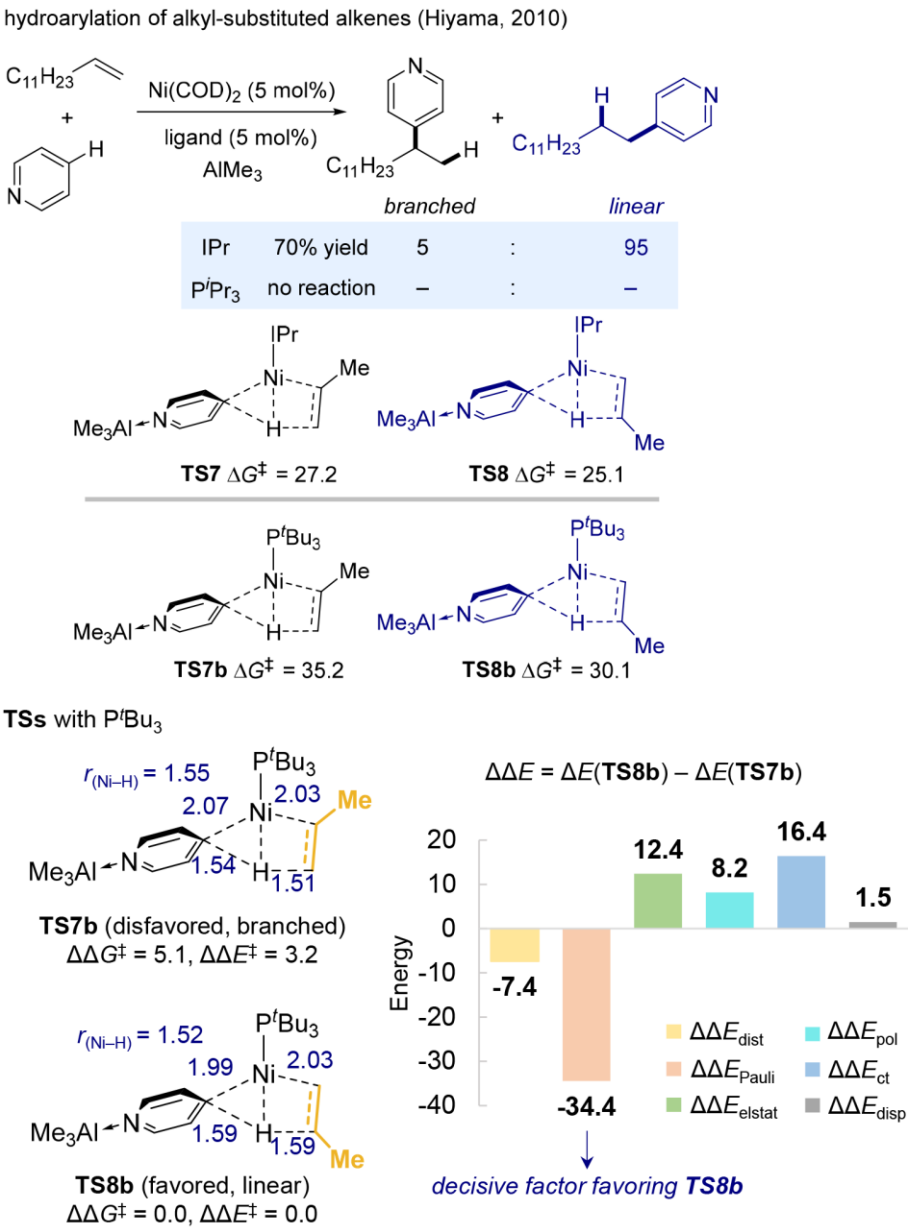

Fig. S11. EDA results for regioisomeric LLHT transition states with propene and P^{t}Bu$_3$. Energies are given in kcal/mol.

Effects of alkene types on LLHT

We computed the Markovnikov and anti-Markovnikov LLHT transition states by exchanging the alkene type (Fig. S12). As discussed in the manuscript, the transition states of **TS1**/**TS2** and **TS3**/**TS4** with styrene favor the Markovnikov selectivity, and the transition states of **TS5**/**TS6** and **TS7**/**TS8** with propene favor the anti-Markovnikov selectivity. After exchanging the alkene type in these transition states, the regioselectivity, i.e., the barrier difference between the two LLHT transition states, is not consistent with the alkene type. Except for the Markovnikov selectivity, styrene can also afford the anti-Markovnikov selectivity in the presence of NHC-type ligands (**TS5c** vs **TS6c**; **TS7c** vs **TS8c**). The regioselectivity with propene and P^{t}Bu$_3$ (**TS1e** vs **TS2e**) is significantly decreased and even reversed compared with other transition states with propene (**TS3e** vs **TS4e**; **TS5** vs **TS6**; **TS7** vs **TS8**). This indicates the regioselectivity is not merely determinized by the alkene type.

As shown in Fig. 13, the EDA results of **TS1e**/**TS2e**, together with those of **TS1**/**TS2** and **TS3**/**TS4** (Fig. 1 and 2 in the manuscript), reveal that charge transfer is the dominant factor for favoring the Markovnikov selectivity. The EDA results of **TS3e**/**TS4e**, together with those of **TS5**/**TS6** and **TS7**/**TS8** (Fig. 3 and 4 in the manuscript), suggest that the anti-Markovnikov selectivity is controlled by Pauli repulsion. However, although the combination of styrene with NHC-type ligands can afford the anti-Markovnikov selectivity, the EDA results of **TS7c**/**TS8c** show that Pauli repulsion is a negative contributor for the regioselectivity. Thus, the steric and electronic properties of ligands can also affect the interactions with alkenes and alter the intermolecular forces (i.e., the six EDA energy terms), which is critical for the trend of stability of LLHT transition states. The EDA results of **TS5c**/**TS6c** are not currently available due to the failure of EDA calculations with 206 atoms.

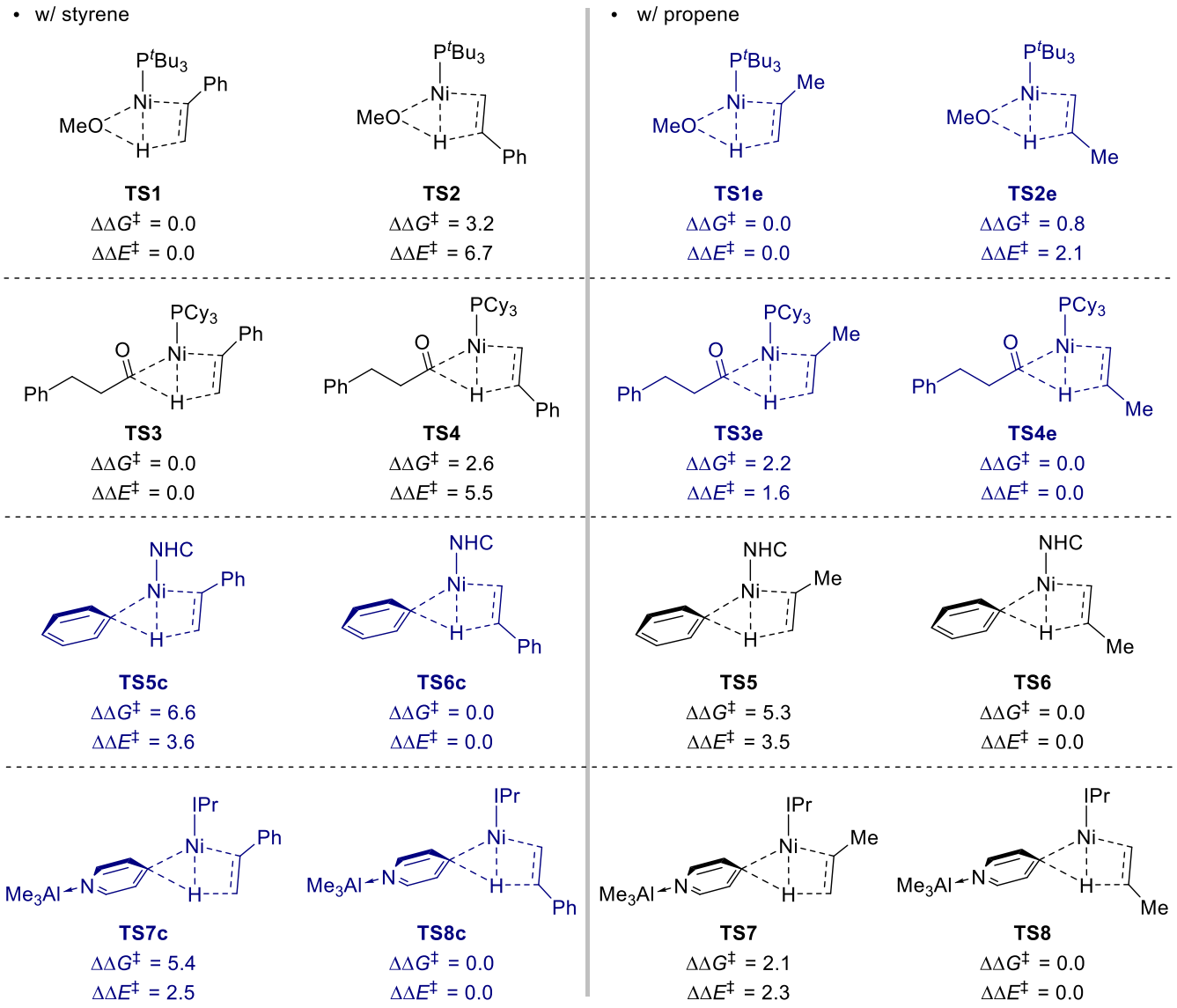

Fig. S12. Computed LLHT transition states with different alkenes. Energies are given in kcal/mol.

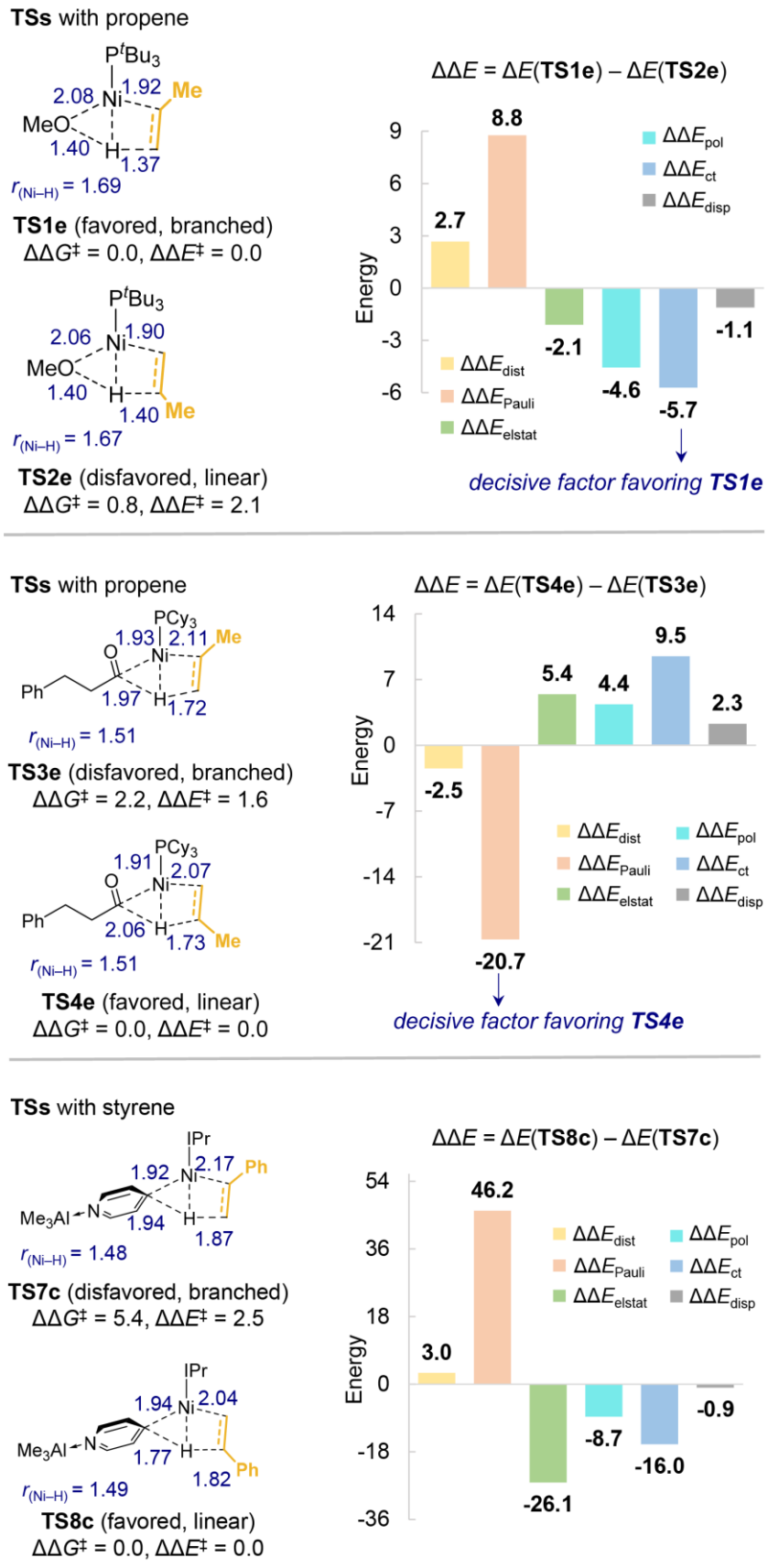

Fig. S13. EDA results for regioisomeric LLHT transition states with different alkenes. Energies are given in kcal/mol.

Cartesian Coordinates (Å) and Energies of the Optimized Structures

TS1
B3LYP SCF energy: -1409.54474059 a.u.
B3LYP enthalpy: -1408.955466 a.u.
B3LYP free energy: -1409.044623 a.u.
M06 SCF energy in solution: -2748.21765063 a.u.
M06 enthalpy in solution: -2747.628376 a.u.
M06 free energy in solution: -2747.717533 a.u.
Three lowest frequencies (cm-1): -1216.6892 24.0232 39.0716
Imaginary frequency: -1216.6892 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ni	0.223869	1.218438	-0.626901
P	-1.205299	-0.405921	0.025139
C	-1.324602	-1.956886	-1.145675
C	-1.994837	-1.546587	-2.476299
C	0.101229	-2.412426	-1.529577
C	-2.084045	-3.165437	-0.560534
H	-3.063364	-1.345371	-2.378077
H	-1.512513	-0.668486	-2.918585
H	-1.886619	-2.375636	-3.187919
H	0.704090	-2.738190	-0.683062
H	0.018847	-3.261175	-2.222192
H	0.640836	-1.612551	-2.037674
H	-2.157549	-3.943216	-1.332927
H	-1.561194	-3.610452	0.289718
H	-3.100440	-2.921699	-0.245554
C	-0.735517	-1.008431	1.812511
C	-1.872023	-1.671971	2.615865
C	0.450722	-1.995171	1.739158
C	-0.211352	0.221640	2.592995
H	-2.696164	-0.986062	2.825323
H	-2.281674	-2.553144	2.115966
H	-1.473212	-2.002281	3.584739
H	1.280210	-1.598564	1.147041
H	0.824303	-2.160548	2.758311
H	0.167306	-2.972706	1.341773
H	0.105683	-0.107047	3.592037
H	0.658146	0.663381	2.095870
H	-0.958317	1.004102	2.725493
C	-2.962094	0.437937	0.080141
C	-3.109781	1.315295	-1.189417
C	-4.164382	-0.522344	0.182898
C	-3.024056	1.427361	1.264962
H	-2.348691	2.100482	-1.207915
H	-3.064857	0.749932	-2.120485
H	-4.093418	1.804078	-1.153871
H	-4.112341	-1.179728	1.055230
H	-5.080223	0.076198	0.280570
H	-4.285894	-1.144689	-0.707185
H	-3.958649	1.998069	1.181595
H	-3.037012	0.935467	2.240096
H	-2.200644	2.143075	1.222511
O	-0.474971	3.129400	-0.235987

C	1.875838	0.723132	-1.525954
C	1.724450	2.200391	-1.593286
H	2.516729	2.768850	-1.097047
H	1.540155	2.573418	-2.604703
C	-0.032749	3.819589	0.906943
H	1.056605	3.720898	1.075142
H	-0.249678	4.895423	0.812766
H	-0.529060	3.462821	1.825687
H	0.663033	2.806649	-0.982030
C	2.907616	0.095482	-0.670664
C	3.484864	-1.135341	-1.040433
C	3.351508	0.683407	0.532740
C	4.448845	-1.755159	-0.245627
H	3.177924	-1.603055	-1.972914
C	4.317869	0.067221	1.325274
H	2.929029	1.633223	0.849996
C	4.871524	-1.158403	0.943937
H	4.877745	-2.702804	-0.562255
H	4.640422	0.546271	2.246514
H	5.625124	-1.637669	1.562830
H	1.722056	0.200290	-2.470528

TS2

B3LYP SCF energy:	-1409.53663466 a.u.		
B3LYP enthalpy:	-1408.948032 a.u.		
B3LYP free energy:	-1409.039231 a.u.		
M06 SCF energy in solution:	-2748.20989685 a.u.		
M06 enthalpy in solution:	-2747.621294 a.u.		
M06 free energy in solution:	-2747.712493 a.u.		
Three lowest frequencies (cm-1):	-1236.1913	19.0904	23.1746
Imaginary frequency:	-1236.1913 cm-1		

Cartesian coordinates

ATOM	X	Y	Z
Ni	-0.447612	0.552410	-0.458959
P	1.621672	-0.174959	-0.011123
C	2.678652	1.403829	0.400350
C	2.412450	2.451959	-0.708867
C	2.138588	2.024989	1.709299
C	4.200099	1.197424	0.537115
H	2.822205	2.171448	-1.679476
H	1.341792	2.639469	-0.830137
H	2.886837	3.398021	-0.415609
H	2.413860	1.445770	2.593957
H	2.586888	3.020397	1.828779
H	1.050558	2.141351	1.682904
H	4.658745	2.151655	0.830239
H	4.461018	0.463031	1.303718
H	4.670493	0.892783	-0.401718
C	1.471108	-1.273169	1.587088
C	2.764497	-1.433435	2.412584
C	0.370577	-0.662291	2.489974
C	0.964094	-2.681797	1.204368
H	3.583537	-1.872851	1.837792

H	3.112221	-0.487300	2.833793
H	2.562105	-2.105002	3.258182
H	-0.586647	-0.583006	1.965555
H	0.229235	-1.323956	3.355404
H	0.614251	0.329228	2.868138
H	0.710595	-3.218952	2.127568
H	0.058852	-2.637139	0.590720
H	1.712869	-3.280331	0.680927
C	2.548187	-1.194636	-1.383183
C	2.967809	-0.248228	-2.530640
C	3.799871	-1.954895	-0.895413
C	1.571632	-2.210430	-2.021360
H	2.129827	0.358762	-2.888394
H	3.790485	0.416073	-2.257895
H	3.315176	-0.859428	-3.373904
H	3.552236	-2.757913	-0.196684
H	4.288238	-2.422786	-1.761020
H	4.535780	-1.303994	-0.418191
H	2.105418	-2.749025	-2.816050
H	1.194986	-2.956498	-1.321934
H	0.715850	-1.705769	-2.471020
C	-1.347757	-0.390580	-1.832673
C	-2.359723	0.537810	-1.260125
H	-0.970799	-0.139517	-2.826764
H	-2.636155	1.347621	-1.944166
H	-1.529561	-1.458766	-1.709435
C	-3.559632	-0.041694	-0.558983
C	-4.832723	0.504432	-0.776514
C	-3.448802	-1.123943	0.328567
C	-5.960529	-0.019772	-0.142635
H	-4.941368	1.346522	-1.456854
C	-4.573737	-1.652417	0.960357
H	-2.469876	-1.552773	0.526972
C	-5.837070	-1.103364	0.727936
H	-6.936741	0.419543	-0.332276
H	-4.462297	-2.492131	1.642044
H	-6.713251	-1.513286	1.223099
O	-1.142033	2.027143	0.773696
H	-1.891975	1.346995	-0.234637
C	-1.156013	3.388294	0.423793
H	-1.871380	3.938282	1.055823
H	-0.168553	3.861392	0.561169
H	-1.450613	3.563311	-0.628709

TS3

B3LYP SCF energy:	-1950.30595981 a.u.		
B3LYP enthalpy:	-1949.478710 a.u.		
B3LYP free energy:	-1949.593995 a.u.		
M06 SCF energy in solution:	-3288.75321478 a.u.		
M06 enthalpy in solution:	-3287.925965 a.u.		
M06 free energy in solution:	-3288.041250 a.u.		
Three lowest frequencies (cm-1):	-454.7459	11.3874	15.2528
Imaginary frequency:	-454.7459 cm-1		

Cartesian coordinates

ATOM	X	Y	Z
Ni	-0.181047	0.333896	-1.683366
C	1.474432	-0.625271	-1.775367
O	1.575764	-1.721552	-2.302363
C	-1.741106	2.913557	-1.203770
C	-0.590635	3.705031	-1.007101
C	-0.620775	4.827361	-0.181021
C	-1.797385	5.191840	0.480188
C	-2.944660	4.414188	0.304741
C	-2.915115	3.292332	-0.523053
H	0.336531	3.434870	-1.504902
H	0.281094	5.420663	-0.052273
H	-1.819586	6.069583	1.120106
H	-3.869829	4.686779	0.806621
H	-3.821502	2.708480	-0.665699
C	2.708339	0.035496	-1.134581
H	2.919383	0.939542	-1.723933
H	2.441434	0.399616	-0.133311
C	3.953247	-0.871311	-1.077025
H	3.732466	-1.743575	-0.449821
H	4.143502	-1.261064	-2.082744
C	5.170950	-0.146476	-0.549612
C	6.013957	0.565281	-1.416057
C	5.473501	-0.139290	0.819616
C	7.119475	1.265502	-0.931447
H	5.802029	0.563760	-2.483497
C	6.578051	0.559077	1.310384
H	4.837990	-0.693827	1.507569
C	7.405665	1.265764	0.435576
H	7.761380	1.806192	-1.622571
H	6.795436	0.546594	2.375599
H	8.268443	1.807259	0.814501
C	-0.876249	1.623751	-3.198498
H	-1.148027	0.965432	-4.020097
H	-0.240381	2.456898	-3.485871
H	0.653310	0.760231	-2.861970
P	-1.054748	-0.732428	0.142163
C	-1.252313	0.473425	1.585055
C	-1.979436	0.033224	2.877354
C	0.104279	1.127629	1.938077
H	-1.863610	1.260647	1.121368
C	-2.198160	1.241648	3.805632
H	-1.385106	-0.707412	3.418526
H	-2.937183	-0.448507	2.658184
C	-0.074056	2.302084	2.917827
H	0.772386	0.376272	2.383835
H	0.592625	1.485920	1.024788
C	-0.861054	1.900354	4.173850
H	-2.727931	0.920499	4.711964
H	-2.844535	1.977602	3.305533
H	0.910854	2.698776	3.196691
H	-0.603239	3.113306	2.400450
H	-1.029719	2.778520	4.810194
H	-0.265323	1.192835	4.770092
C	0.030777	-2.186519	0.724902

C	-0.094979	-2.659546	2.188285
C	-0.083712	-3.400126	-0.228174
H	1.043967	-1.778847	0.604199
C	0.926131	-3.766651	2.518139
H	-1.112463	-3.030252	2.379529
H	0.076003	-1.828335	2.876240
C	0.959993	-4.479669	0.100461
H	-1.084380	-3.842587	-0.125868
H	0.043128	-3.082247	-1.265284
C	0.840266	-4.954765	1.553079
H	0.780238	-4.097860	3.554622
H	1.938057	-3.337743	2.468523
H	0.840655	-5.323265	-0.591171
H	1.964285	-4.070772	-0.079214
H	1.620723	-5.690288	1.786591
H	-0.124001	-5.467210	1.689781
C	-2.771523	-1.492073	-0.153256
C	-3.958347	-0.520717	0.047924
C	-2.873304	-2.089018	-1.579998
H	-2.879291	-2.309132	0.576279
C	-5.306489	-1.237426	-0.150498
H	-3.881625	0.297924	-0.677390
H	-3.941450	-0.057464	1.036529
C	-4.213922	-2.810426	-1.800943
H	-2.774568	-1.269744	-2.305692
H	-2.050294	-2.775267	-1.786686
C	-5.409571	-1.886192	-1.536964
H	-6.126651	-0.523472	0.000066
H	-5.420072	-2.010258	0.624262
H	-4.253987	-3.204265	-2.824506
H	-4.269982	-3.681286	-1.130677
H	-6.352224	-2.440187	-1.630910
H	-5.432580	-1.097160	-2.303404
C	-1.752035	1.749622	-2.108756
H	-2.677377	1.183439	-2.144235

TS4

B3LYP SCF energy:	-1950.30183700 a.u.		
B3LYP enthalpy:	-1949.475157 a.u.		
B3LYP free energy:	-1949.593396 a.u.		
M06 SCF energy in solution:	-3288.74559085 a.u.		
M06 enthalpy in solution:	-3287.918911 a.u.		
M06 free energy in solution:	-3288.037150 a.u.		
Three lowest frequencies (cm-1):	-568.1646	10.0913	12.0135
Imaginary frequency:	-568.1646 cm-1		

Cartesian coordinates

ATOM	X	Y	Z
Ni	-0.500154	1.023365	0.421295
C	1.049594	1.222170	-0.687099
O	0.906388	1.441836	-1.882704
C	2.466786	1.130983	-0.098427
H	2.588005	2.020692	0.537760
H	2.515649	0.277323	0.591619

C	3.591290	1.063161	-1.149354
H	3.466053	0.152369	-1.748176
H	3.464597	1.901348	-1.842700
C	4.970261	1.088871	-0.530173
C	5.611039	2.305623	-0.252150
C	5.634306	-0.098746	-0.190941
C	6.870132	2.335988	0.348690
H	5.117061	3.238534	-0.516574
C	6.894150	-0.074985	0.409864
H	5.159037	-1.053676	-0.407909
C	7.517380	1.144262	0.682900
H	7.349121	3.291034	0.550086
H	7.391592	-1.009085	0.659331
H	8.500036	1.165842	1.146758
C	-1.391915	2.611845	1.569216
H	0.048445	2.410320	0.697142
P	-0.903137	-1.170619	0.042421
C	-0.736617	-2.051038	1.709232
C	-1.061116	-3.556646	1.846026
C	0.629677	-1.746500	2.365106
H	-1.491166	-1.509367	2.298304
C	-1.086210	-3.964700	3.330725
H	-0.299799	-4.157578	1.341561
H	-2.014003	-3.809776	1.370280
C	0.650077	-2.185892	3.840379
H	1.427171	-2.270423	1.818082
H	0.848952	-0.674598	2.291722
C	0.256791	-3.660667	4.010978
H	-1.323314	-5.032888	3.417343
H	-1.891681	-3.422001	3.847585
H	1.644563	-2.004106	4.267326
H	-0.052386	-1.556647	4.406823
H	0.213286	-3.920369	5.076302
H	1.035676	-4.297718	3.566082
C	0.301706	-1.969834	-1.193650
C	0.520787	-3.495915	-1.128898
C	-0.018729	-1.547108	-2.647930
H	1.253708	-1.492264	-0.922689
C	1.596102	-3.960708	-2.130995
H	-0.423801	-4.020935	-1.332768
H	0.841695	-3.794514	-0.128387
C	1.080445	-1.996029	-3.624548
H	-0.963555	-2.015373	-2.956967
H	-0.141659	-0.463051	-2.710454
C	1.297796	-3.512795	-3.566233
H	1.693407	-5.052971	-2.078510
H	2.567330	-3.547185	-1.820861
H	0.812401	-1.684437	-4.641979
H	2.016578	-1.475345	-3.377526
H	2.114225	-3.813726	-4.235100
H	0.392454	-4.023804	-3.927000
C	-2.639453	-1.609489	-0.585043
C	-3.717354	-1.700090	0.521804
C	-3.114694	-0.586567	-1.647514
H	-2.561030	-2.598532	-1.061662
C	-5.087104	-2.095767	-0.060673

H	-3.808298	-0.726858	1.018741
H	-3.440711	-2.419767	1.296202
C	-4.480475	-0.971900	-2.241084
H	-3.190511	0.398035	-1.166956
H	-2.384999	-0.475823	-2.452009
C	-5.549737	-1.121625	-1.151958
H	-5.827245	-2.143776	0.748506
H	-5.019311	-3.110026	-0.481735
H	-4.786558	-0.217105	-2.976586
H	-4.382317	-1.920180	-2.790520
H	-6.498549	-1.459648	-1.587693
H	-5.745289	-0.138241	-0.699631
C	-2.116135	1.396916	1.624637
H	-3.054950	1.325883	1.083663
H	-2.042820	0.787090	2.522188
H	-0.792213	2.865980	2.442017
C	-1.896529	3.801953	0.819758
C	-1.895658	5.057170	1.444190
C	-2.407130	3.702177	-0.483624
C	-2.410946	6.180022	0.794306
H	-1.496259	5.153329	2.451540
C	-2.920519	4.822692	-1.134195
H	-2.374741	2.744610	-0.996263
C	-2.928008	6.066332	-0.496840
H	-2.404674	7.143540	1.297322
H	-3.304323	4.727146	-2.146578
H	-3.324533	6.940099	-1.006889

TS5

B3LYP SCF energy:	-4071.43461044 a.u.		
B3LYP enthalpy:	-4069.647606 a.u.		
B3LYP free energy:	-4069.905824 a.u.		
M06 SCF energy in solution:	-5408.95911442 a.u.		
M06 enthalpy in solution:	-5407.172110 a.u.		
M06 free energy in solution:	-5407.430328 a.u.		
Three lowest frequencies (cm-1):	-1110.7791	11.2443	12.0153
Imaginary frequency:	-1110.7791 cm-1		

Cartesian coordinates

ATOM	X	Y	Z
Ni	0.135580	0.031887	-2.444769
N	0.417275	0.894114	0.387831
N	-0.708586	-0.948263	0.229537
C	-0.047634	-0.011426	-0.547076
C	0.040484	0.533708	1.681923
H	0.301338	1.131579	2.537408
C	-0.632530	-0.629587	1.586445
H	-1.067379	-1.258998	2.342790
C	-1.684745	-0.171650	-3.242183
H	-2.059709	-1.163118	-2.983936
C	-0.724183	-0.120781	-4.315604
H	-0.483961	-1.042421	-4.849221
H	0.717813	0.131494	-3.868046
C	2.084086	0.270638	-3.085130

C	2.914299	-0.809204	-3.454929
C	2.681028	1.549064	-3.111864
C	4.252247	-0.629631	-3.820791
H	2.506866	-1.816874	-3.481275
C	4.019634	1.738884	-3.465428
H	2.095467	2.425104	-2.846188
C	4.812822	0.649308	-3.830023
H	5.848558	0.796567	-4.127173
C	-1.449380	-2.111222	-0.208836
C	-2.849630	-2.153939	-0.021259
C	-0.764304	-3.243155	-0.717084
C	-3.550958	-3.315121	-0.381296
C	-1.500083	-4.372953	-1.068577
C	-2.887057	-4.419208	-0.909842
H	-4.625683	-3.325219	-0.255640
H	-1.001156	-5.246571	-1.471024
C	1.262322	2.044799	0.151670
C	2.611367	2.015393	0.595020
C	0.729765	3.210447	-0.431225
C	3.410564	3.134399	0.377085
C	1.563376	4.322128	-0.619569
C	2.901667	4.284128	-0.232392
H	4.452645	3.127545	0.674627
H	1.145315	5.207295	-1.080013
C	-0.751850	3.329115	-0.814695
H	-1.061664	2.345260	-1.180461
C	3.200317	0.828347	1.372711
H	2.707096	-0.077303	1.004178
C	0.764543	-3.307274	-0.818955
H	1.118467	-2.302210	-1.074799
C	-3.651105	-1.009577	0.620145
H	-3.114018	-0.077620	0.405226
H	4.442801	2.741634	-3.461211
H	4.853029	-1.489516	-4.111859
O	3.782354	5.312856	-0.390043
O	-3.492295	-5.580576	-1.288373
C	3.328463	6.493930	-1.033006
H	4.191884	7.160520	-1.076527
H	2.974612	6.288340	-2.051474
H	2.523684	6.980306	-0.465678
C	-4.903226	-5.673160	-1.168262
H	-5.410864	-4.908733	-1.770699
H	-5.170213	-6.664028	-1.540305
H	-5.227314	-5.579207	-0.123074
C	1.422588	-3.686481	0.514210
C	2.775884	-3.367567	0.713470
C	0.750524	-4.395980	1.512442
C	3.458656	-3.764793	1.867000
H	3.311260	-2.822420	-0.061112
C	1.400544	-4.790802	2.691895
H	-0.295822	-4.653720	1.376908
C	2.751410	-4.474366	2.850544
H	3.271161	-4.790079	3.753820
C	1.209923	-4.221577	-1.974816
C	1.880759	-5.430128	-1.774922
C	0.903843	-3.835432	-3.288699

C	2.255142	-6.243151	-2.856550
H	2.120173	-5.752242	-0.766143
C	1.266292	-4.619432	-4.386458
H	0.365571	-2.903985	-3.449761
C	1.942220	-5.825027	-4.151491
H	2.227284	-6.448427	-4.997124
C	-5.060713	-0.848308	0.005970
C	-6.201555	-0.674770	0.796291
C	-5.214739	-0.831916	-1.390157
C	-7.469436	-0.482861	0.223581
H	-6.115143	-0.690485	1.877562
C	-6.460695	-0.635298	-1.990044
H	-4.346606	-0.987786	-2.022032
C	-7.582358	-0.461950	-1.166992
H	-8.560085	-0.312680	-1.622223
C	-3.704856	-1.130198	2.152284
C	-3.820135	-2.360405	2.803515
C	-3.668113	0.038671	2.929590
C	-3.893852	-2.441671	4.203573
H	-3.840928	-3.277741	2.221881
C	-3.745266	-0.008127	4.323399
H	-3.564597	1.001615	2.435261
C	-3.856735	-1.260530	4.946258
H	-3.909342	-1.312400	6.032641
C	-0.961457	4.305243	-1.985032
C	-1.531969	5.570708	-1.823230
C	-0.525115	3.927418	-3.264305
C	-1.673097	6.450944	-2.907564
H	-1.873985	5.884707	-0.841385
C	-0.649938	4.780773	-4.363453
H	-0.067501	2.950275	-3.398628
C	-1.224650	6.044337	-4.166336
H	-1.322703	6.722738	-5.012382
C	-1.651426	3.659460	0.383265
C	-1.177582	4.308708	1.528185
C	-3.018198	3.355953	0.302926
C	-2.038189	4.654131	2.579336
H	-0.122072	4.554080	1.606257
C	-3.907400	3.702597	1.326256
H	-3.400717	2.865524	-0.589794
C	-3.398481	4.350320	2.460585
H	-4.079783	4.631417	3.261913
C	4.707294	0.626748	1.132198
C	5.667047	1.104531	2.030820
C	5.139546	-0.080195	-0.000559
C	7.036412	0.889810	1.822224
H	5.349397	1.634608	2.923739
C	6.499249	-0.328948	-0.223479
H	4.406691	-0.439631	-0.719692
C	7.433277	0.162091	0.699182
H	8.492092	-0.035312	0.538380
C	2.896014	0.911931	2.878546
C	2.759920	2.126058	3.555961
C	2.780110	-0.280901	3.609792
C	2.511985	2.166894	4.938742
H	2.839139	3.060934	3.007528

C	2.534191	-0.273242	4.983547
H	2.870365	-1.231585	3.090160
C	2.400191	0.963042	5.635086
H	2.200234	0.982450	6.705312
C	2.367962	3.495939	5.646233
H	2.162819	3.361393	6.713173
H	3.280424	4.098744	5.555353
H	1.550012	4.091216	5.220476
C	2.421420	-1.565583	5.760459
H	1.556562	-1.554024	6.434774
H	2.319032	-2.424567	5.090144
H	3.310463	-1.733811	6.383129
C	8.054709	1.438042	2.796498
H	8.241510	2.505968	2.619656
H	7.712570	1.339081	3.833078
H	9.015285	0.919844	2.705983
C	6.969220	-1.106319	-1.431760
H	7.823491	-1.746650	-1.183006
H	6.173243	-1.734837	-1.840003
H	7.289045	-0.431531	-2.236068
C	-0.194230	4.342005	-5.736863
H	0.620931	3.613285	-5.674054
H	-1.013658	3.869116	-6.295274
H	0.154683	5.191662	-6.334237
C	-2.317989	7.804921	-2.712112
H	-2.003796	8.267999	-1.769654
H	-2.065684	8.491086	-3.527495
H	-3.412816	7.723146	-2.679745
C	-1.498080	5.327589	3.820983
H	-1.038876	4.597933	4.501995
H	-0.727022	6.065974	3.573124
H	-2.290133	5.839448	4.377800
C	-5.386230	3.413669	1.192809
H	-5.910355	3.570207	2.141428
H	-5.851008	4.071665	0.446847
H	-5.571337	2.382610	0.870903
C	-6.594426	-0.583695	-3.495542
H	-6.536401	0.449377	-3.863836
H	-5.796412	-1.148270	-3.988905
H	-7.555683	-0.991624	-3.827866
C	-8.687911	-0.332064	1.106735
H	-9.001221	-1.298584	1.523916
H	-8.489476	0.332954	1.955159
H	-9.538020	0.075419	0.549728
C	-3.994140	-3.789235	4.882787
H	-4.815738	-4.386915	4.469534
H	-3.074723	-4.374035	4.747834
H	-4.164361	-3.683924	5.959060
C	-3.706849	1.258179	5.148724
H	-2.929393	1.207960	5.921082
H	-3.506204	2.133898	4.524129
H	-4.660717	1.426116	5.665968
C	0.958396	-4.162979	-5.794749
H	-0.043450	-3.723630	-5.864683
H	1.670925	-3.396515	-6.127862
H	1.012597	-4.993459	-6.506520

C	2.984307	-7.545173	-2.611530
H	3.962388	-7.373718	-2.143996
H	2.419037	-8.200945	-1.937600
H	3.153450	-8.091069	-3.545378
C	4.932810	-3.475504	2.039264
H	5.187171	-3.306319	3.091440
H	5.541486	-4.321334	1.691192
H	5.240251	-2.592920	1.470790
C	0.641451	-5.536804	3.766437
H	-0.074925	-4.879750	4.277716
H	0.067510	-6.371261	3.346016
H	1.316901	-5.942382	4.526818
H	-0.746303	0.749368	-4.976501
C	-2.699087	0.946040	-3.091195
H	-3.581797	0.782604	-3.730064
H	-3.067270	1.032821	-2.062993
H	-2.276401	1.915045	-3.374347

TS6

B3LYP SCF energy:	-4071.44150779 a.u.		
B3LYP enthalpy:	-4069.654565 a.u.		
B3LYP free energy:	-4069.914959 a.u.		
M06 SCF energy in solution:	-5408.96531249 a.u.		
M06 enthalpy in solution:	-5407.178370 a.u.		
M06 free energy in solution:	-5407.438764 a.u.		
Three lowest frequencies (cm-1):	-1053.7021	12.4928	13.5605
Imaginary frequency:	-1053.7021 cm-1		

Cartesian coordinates

ATOM	X	Y	Z
Ni	-0.078872	0.034048	-2.415268
N	-0.390185	-0.919097	0.388982
N	0.546538	1.028543	0.307745
C	0.006471	0.051791	-0.507198
C	-0.091831	-0.555396	1.703769
H	-0.320447	-1.196367	2.537260
C	0.466651	0.670829	1.654699
H	0.823096	1.318309	2.437012
C	1.798696	0.180689	-3.053117
C	0.971961	0.149811	-4.224308
H	-0.557690	-0.040325	-3.863890
C	-1.955727	-0.295300	-3.129118
C	-2.904648	0.704384	-3.429583
C	-2.390664	-1.630182	-3.281418
C	-4.204736	0.395251	-3.843406
H	-2.630709	1.753065	-3.353635
C	-3.690757	-1.949535	-3.679454
H	-1.701181	-2.446857	-3.080876
C	-4.606245	-0.935683	-3.970763
H	-5.612332	-1.180756	-4.303488
C	1.241306	2.219203	-0.124414
C	2.642593	2.290636	0.025924
C	0.516821	3.323984	-0.635489
C	3.318548	3.438374	-0.413632

C	1.222259	4.452985	-1.044914
C	2.616589	4.512575	-0.956754
H	4.397105	3.466272	-0.326307
H	0.698851	5.311356	-1.447940
C	-1.072613	-2.152100	0.069483
C	-2.438331	-2.300438	0.424317
C	-0.367902	-3.214710	-0.528102
C	-3.089635	-3.484184	0.088438
C	-1.054337	-4.398655	-0.833161
C	-2.412761	-4.529149	-0.546811
H	-4.142410	-3.612821	0.311761
H	-0.508669	-5.205592	-1.303931
C	1.142324	-3.143527	-0.796659
H	1.361203	-2.113458	-1.095364
C	-3.187188	-1.238536	1.242328
H	-2.767058	-0.265112	0.969260
C	-1.017700	3.334300	-0.681709
H	-1.331543	2.345836	-1.037019
C	3.456664	1.187340	0.720358
H	2.929283	0.242547	0.554091
H	-3.988350	-2.992566	-3.768698
H	-4.902229	1.198622	-4.073296
O	-3.158494	-5.635726	-0.827267
O	3.189999	5.663368	-1.410020
C	-2.529094	-6.719252	-1.493542
H	-3.306270	-7.471920	-1.639266
H	-2.128179	-6.415195	-2.469053
H	-1.717453	-7.148557	-0.891096
C	4.604182	5.771741	-1.368882
H	5.086665	4.987044	-1.965805
H	4.841246	6.748445	-1.794910
H	4.984217	5.723960	-0.339554
C	-1.648614	3.529765	0.702046
C	-2.969872	3.103478	0.904932
C	-0.991757	4.191357	1.742920
C	-3.640932	3.348028	2.106893
H	-3.493135	2.597171	0.096336
C	-1.627634	4.430607	2.970648
H	0.029559	4.534227	1.600259
C	-2.950182	4.010238	3.133539
H	-3.460979	4.209384	4.074311
C	-1.560038	4.351973	-1.700378
C	-2.167503	5.553247	-1.317487
C	-1.426556	4.078721	-3.067443
C	-2.644451	6.464220	-2.269239
H	-2.283072	5.784818	-0.263150
C	-1.900172	4.963149	-4.043261
H	-0.942926	3.155364	-3.375718
C	-2.510633	6.151231	-3.625918
H	-2.891812	6.844535	-4.373830
C	4.855211	1.008009	0.105221
C	6.014938	1.500164	0.711383
C	4.974899	0.335885	-1.120071
C	7.274997	1.335853	0.115288
H	5.944912	2.012903	1.666400
C	6.214738	0.156236	-1.739899

H	4.079490	-0.038160	-1.607037
C	7.357501	0.667405	-1.108482
H	8.329645	0.540340	-1.582228
C	3.526445	1.383474	2.243806
C	3.503109	2.642665	2.848337
C	3.646139	0.248546	3.061889
C	3.599007	2.784719	4.243096
H	3.399983	3.533193	2.234500
C	3.744768	0.356994	4.449873
H	3.647362	-0.736891	2.603076
C	3.719442	1.636510	5.026577
H	3.788628	1.734681	6.108826
C	1.558963	-4.028259	-1.983606
C	2.212426	-5.254308	-1.816820
C	1.237187	-3.613092	-3.282537
C	2.546482	-6.057073	-2.916447
H	2.469477	-5.593536	-0.817570
C	1.554117	-4.392211	-4.400236
H	0.714102	-2.669932	-3.418158
C	2.206750	-5.614796	-4.198817
H	2.453826	-6.234014	-5.059702
C	1.987549	-3.430367	0.450873
C	1.502765	-4.139099	1.552796
C	3.329728	-3.017804	0.457301
C	2.328798	-4.439996	2.647365
H	0.467088	-4.467045	1.566592
C	4.183541	-3.317386	1.522049
H	3.722283	-2.472243	-0.398314
C	3.663662	-4.029651	2.614146
H	4.317920	-4.272816	3.449980
C	-4.691117	-1.158908	0.932190
C	-5.638890	-1.868514	1.683358
C	-5.140386	-0.333595	-0.105170
C	-7.007763	-1.765049	1.417557
H	-5.310088	-2.495669	2.506630
C	-6.508667	-0.195169	-0.383591
H	-4.416589	0.204060	-0.714156
C	-7.426153	-0.916469	0.386273
H	-8.490525	-0.810418	0.180982
C	-2.954503	-1.408625	2.754783
C	-2.733398	-2.653343	3.349891
C	-2.997100	-0.271149	3.576039
C	-2.562299	-2.778617	4.738836
H	-2.686793	-3.544761	2.730154
C	-2.828495	-0.362632	4.958791
H	-3.148030	0.704712	3.121604
C	-2.610478	-1.627560	5.526137
H	-2.471691	-1.711711	6.602832
C	-2.323225	-4.138259	5.356825
H	-2.248200	-4.074376	6.447175
H	-3.135900	-4.835512	5.117704
H	-1.395336	-4.591467	4.984635
C	-2.891562	0.870348	5.831799
H	-2.129841	0.843375	6.619818
H	-2.741839	1.781551	5.244066
H	-3.866761	0.954739	6.330442

C	-8.019255	-2.528225	2.243294
H	-8.653336	-1.849518	2.828583
H	-8.687732	-3.123116	1.608667
H	-7.528768	-3.210368	2.945058
C	-6.988664	0.702154	-1.501366
H	-8.015662	1.040797	-1.325818
H	-6.350874	1.585337	-1.610766
H	-6.970803	0.175800	-2.463437
C	1.213737	-3.915468	-5.794564
H	0.248452	-3.397461	-5.817181
H	1.968467	-3.211387	-6.170351
H	1.166900	-4.749840	-6.502595
C	3.279977	-7.364593	-2.717295
H	3.006361	-7.838109	-1.767973
H	3.065172	-8.073081	-3.524755
H	4.367762	-7.212255	-2.699756
C	1.772697	-5.182039	3.841822
H	1.181671	-4.515556	4.484638
H	1.111740	-6.000238	3.533038
H	2.571481	-5.607407	4.458427
C	5.641948	-2.918938	1.482412
H	6.018936	-2.676049	2.482064
H	6.262387	-3.737445	1.092553
H	5.803186	-2.049061	0.838261
C	6.322475	-0.587972	-3.051911
H	6.580412	-1.643542	-2.891812
H	5.377036	-0.563024	-3.603466
H	7.101687	-0.159417	-3.692275
C	8.518443	1.852781	0.803642
H	8.340611	2.823387	1.280597
H	8.851912	1.164693	1.592128
H	9.348584	1.968641	0.098873
C	3.555375	4.159124	4.872941
H	4.297571	4.830573	4.424008
H	2.573989	4.632061	4.736072
H	3.753187	4.112587	5.948651
C	3.882031	-0.872988	5.318564
H	3.190244	-0.842255	6.168996
H	3.679763	-1.785756	4.749771
H	4.895543	-0.956249	5.733477
C	-1.751230	4.637428	-5.512469
H	-0.700731	4.683459	-5.827640
H	-2.109058	3.625333	-5.735421
H	-2.314364	5.339471	-6.136040
C	-3.274247	7.768780	-1.835010
H	-3.765690	7.671607	-0.860937
H	-2.521593	8.563587	-1.740971
H	-4.020572	8.114690	-2.558629
C	-5.090327	2.952215	2.280385
H	-5.326219	2.737713	3.328410
H	-5.758248	3.762420	1.957313
H	-5.341149	2.066701	1.687896
C	-0.885599	5.122491	4.092255
H	-0.161302	4.446865	4.567352
H	-0.323882	5.989664	3.725368
H	-1.570490	5.470011	4.872716

H	0.977045	-0.783180	-4.793425
H	2.370850	-0.711785	-2.803306
H	2.270771	1.121021	-2.774094
C	0.839525	1.384174	-5.106137
H	-0.093875	1.387683	-5.681630
H	0.873289	2.300411	-4.507523
H	1.671951	1.426184	-5.821116

TS7

B3LYP SCF energy:	-2057.75000396 a.u.		
B3LYP enthalpy:	-2056.846124 a.u.		
B3LYP free energy:	-2056.985513 a.u.		
M06 SCF energy in solution:	-3396.12085186 a.u.		
M06 enthalpy in solution:	-3395.216972 a.u.		
M06 free energy in solution:	-3395.356361 a.u.		
Three lowest frequencies (cm-1):	-899.4300	15.2461	15.8632
Imaginary frequency:	-899.4300 cm-1		

Cartesian coordinates

ATOM	X	Y	Z
Ni	-0.543287	-0.190286	-1.467992
Al	6.204244	-1.290829	-0.551497
N	-0.934929	1.346493	1.069608
N	-2.364646	-0.258939	0.889525
N	4.187660	-0.948708	-0.884232
C	-1.296733	0.315183	0.231759
C	-1.757618	1.412436	2.191877
C	-2.645546	0.400040	2.085741
C	3.690411	0.273747	-1.165592
C	2.338903	0.507054	-1.377316
C	1.391800	-0.538144	-1.292395
C	1.947026	-1.808794	-1.015879
C	3.310320	-1.971730	-0.816193
C	6.222591	-1.880345	1.363027
C	6.614053	-2.722620	-1.888748
C	7.030634	0.498286	-0.907161
C	-1.096236	-0.628102	-3.438502
C	-2.173671	-0.082095	-2.707811
C	0.237056	2.189242	0.955620
C	0.199749	3.325216	0.119306
C	1.355409	1.879541	1.759038
C	1.343772	4.131352	0.071008
C	2.468392	2.726358	1.675426
C	2.469917	3.834522	0.835417
C	-1.058380	3.726617	-0.644693
C	1.379669	0.709317	2.740897
C	2.611258	-0.197353	2.566029
C	1.292548	1.222226	4.194415
C	-0.766266	4.358704	-2.016422
C	-1.924035	4.677705	0.210004
C	-3.121781	-1.422529	0.480602
C	-4.446507	-1.244942	0.024372
C	-2.545955	-2.704532	0.636856
C	-5.183651	-2.392235	-0.299687

C	-4.630877	-3.661846	-0.180801
C	-3.326890	-3.811844	0.283972
C	-5.113363	0.124810	-0.096247
C	-5.834445	0.318828	-1.444682
C	-6.108557	0.360055	1.060669
C	-1.157894	-2.906353	1.243288
C	-0.443985	-4.171881	0.738089
C	-1.241816	-2.933885	2.785547
H	-1.617375	2.159459	2.956399
H	-3.439944	0.079664	2.739802
H	4.420240	1.075115	-1.218110
H	2.025535	1.522854	-1.599774
H	0.393015	-0.624550	-2.557775
H	1.313724	-2.689346	-0.966222
H	3.739806	-2.945922	-0.600081
H	5.870992	-1.100477	2.054732
H	7.242095	-2.140495	1.685273
H	5.606828	-2.772337	1.553155
H	6.025857	-3.641843	-1.747116
H	7.669719	-3.026691	-1.826499
H	6.447486	-2.397964	-2.926204
H	6.872843	0.864793	-1.932435
H	8.121347	0.436374	-0.774787
H	6.691593	1.292720	-0.225119
H	3.346361	2.510418	2.276420
H	1.350789	5.010859	-0.564470
H	0.497917	0.089298	2.556085
H	-1.641703	2.820481	-0.825225
H	2.165246	1.835260	4.448099
H	1.260115	0.379789	4.895138
H	0.398923	1.834706	4.359587
H	2.555923	-1.037884	3.267772
H	3.548117	0.332562	2.769367
H	2.667187	-0.603827	1.553837
H	-1.379146	5.601187	0.439881
H	-2.214566	4.214657	1.159289
H	-2.840556	4.950180	-0.327124
H	-1.702872	4.500585	-2.566937
H	-0.109625	3.723746	-2.621205
H	-0.294415	5.343803	-1.925773
H	3.346211	4.475000	0.782293
H	-6.204869	-2.286200	-0.652575
H	-5.218010	-4.537988	-0.442750
H	-4.333491	0.889842	-0.028268
H	-5.177238	0.103825	-2.291510
H	-6.180563	1.354783	-1.536298
H	-6.716569	-0.325787	-1.530102
H	-6.560553	1.355625	0.980052
H	-5.626429	0.287879	2.040933
H	-6.917274	-0.379750	1.034788
H	-0.537237	-2.053294	0.955057
H	-0.441762	-4.228748	-0.356071
H	-0.905142	-5.089103	1.122715
H	0.596134	-4.168223	1.081375
H	-1.671969	-2.010876	3.187463
H	-0.242292	-3.056425	3.219217

H	-1.862959	-3.771794	3.124844
H	-2.913726	-4.809479	0.384794
H	-0.627851	-0.034968	-4.224513
H	-1.042685	-1.703300	-3.604452
H	-2.900802	-0.783708	-2.304586
C	-2.695902	1.304418	-3.021586
H	-3.160960	1.780144	-2.151677
H	-1.893746	1.962836	-3.371993
H	-3.457833	1.270832	-3.815244

TS8

B3LYP SCF energy:	-2057.75575217 a.u.		
B3LYP enthalpy:	-2056.851577 a.u.		
B3LYP free energy:	-2056.990731 a.u.		
M06 SCF energy in solution:	-3396.12480495 a.u.		
M06 enthalpy in solution:	-3395.220630 a.u.		
M06 free energy in solution:	-3395.359784 a.u.		
Three lowest frequencies (cm-1):	-608.8499	11.6719	17.5556
Imaginary frequency:	-608.8499 cm-1		

Cartesian coordinates

ATOM	X	Y	Z
Ni	0.546138	-0.236847	-1.416697
Al	-6.129972	-1.409679	-0.325641
N	2.341932	-0.101189	0.995093
N	0.896964	1.496549	0.986967
N	-4.111020	-1.105939	-0.661613
C	1.280952	0.390153	0.266375
C	2.595339	0.678029	2.123685
C	1.696768	1.686681	2.111170
C	-3.185462	-2.074663	-0.505265
C	-1.832799	-1.870048	-0.742896
C	-1.339346	-0.609877	-1.151563
C	-2.337028	0.379150	-1.321935
C	-3.671379	0.104180	-1.069738
C	-6.551967	0.015493	1.020174
C	-6.915164	-1.120825	-2.143212
C	-6.196613	-3.287218	0.367752
C	1.327799	-0.599098	-3.386405
C	2.278499	-0.068753	-2.512630
C	3.157243	-1.253161	0.679319
C	4.477081	-1.040402	0.223137
C	2.636403	-2.547052	0.906074
C	5.268479	-2.169841	-0.027126
C	3.470135	-3.636509	0.625439
C	4.771114	-3.454091	0.162506
C	5.080878	0.351085	0.029538
C	1.248632	-2.767547	1.506562
C	0.609793	-4.108075	1.106048
C	1.301455	-2.652453	3.046284
C	5.771431	0.523176	-1.337789
C	6.078307	0.679743	1.161361
C	-0.235171	2.352534	0.713448
C	-0.137920	3.323006	-0.304789

C	-1.380124	2.223908	1.529462
C	-1.248468	4.149756	-0.519544
C	-2.398926	4.029365	0.255422
C	-2.456915	3.082085	1.273283
C	1.135163	3.547330	-1.115900
C	0.874775	3.548099	-2.633456
C	1.834290	4.850590	-0.676224
C	-1.472106	1.231444	2.687764
C	-2.709483	0.320182	2.598631
C	-1.442861	1.972436	4.041477
H	3.382937	0.434758	2.818032
H	1.538710	2.510360	2.788585
H	-3.566451	-3.038699	-0.182866
H	-1.160537	-2.712663	-0.615642
H	-0.355708	-0.713924	-2.499242
H	-2.075797	1.380585	-1.650306
H	-4.436199	0.865898	-1.190580
H	-6.015303	-0.124722	1.970165
H	-7.623724	0.016422	1.269414
H	-6.321669	1.033795	0.671443
H	-6.721663	-0.116199	-2.548363
H	-8.009229	-1.236860	-2.125684
H	-6.540494	-1.838325	-2.887764
H	-5.853977	-4.043153	-0.354664
H	-7.234909	-3.556968	0.613075
H	-5.620350	-3.440323	1.292705
H	0.846253	0.080563	-4.088806
H	2.535832	0.985963	-2.555106
H	3.017656	-0.726760	-2.065934
H	3.101386	-4.644375	0.780951
H	6.287246	-2.038460	-0.379019
H	0.592482	-1.975450	1.133880
H	4.269634	1.083998	0.077308
H	1.958999	-3.420981	3.470611
H	0.300802	-2.790266	3.472382
H	1.672494	-1.674588	3.369680
H	-0.433350	-4.131367	1.439268
H	1.114074	-4.962528	1.572472
H	0.623645	-4.259192	0.020831
H	6.925537	-0.016032	1.150638
H	5.613313	0.616823	2.150767
H	6.475273	1.694294	1.038883
H	6.109230	1.559566	-1.453972
H	5.096263	0.291305	-2.166349
H	6.655141	-0.118035	-1.431979
H	5.399438	-4.316590	-0.043128
H	-1.205376	4.908081	-1.295902
H	-3.248441	4.681727	0.071986
H	1.820130	2.721367	-0.907905
H	0.393375	2.616941	-2.950376
H	1.820753	3.646705	-3.179239
H	0.232998	4.382179	-2.939217
H	2.771093	4.989530	-1.229153
H	2.070709	4.834898	0.393747
H	1.200543	5.725216	-0.864399
H	-0.595116	0.578863	2.650651

H	-2.712897	-0.253718	1.669422
H	-3.646629	0.884632	2.648518
H	-2.708582	-0.387148	3.436494
H	-0.546988	2.595162	4.148461
H	-1.456893	1.254029	4.869401
H	-2.315062	2.627099	4.152477
H	-3.355663	3.002028	1.877246
C	1.343748	-2.053542	-3.813151
H	0.347338	-2.417228	-4.084361
H	1.992246	-2.172264	-4.692186
H	1.738824	-2.695991	-3.019369

TS9

B3LYP SCF energy:	-1099.87265589 a.u.		
B3LYP enthalpy:	-1099.428006 a.u.		
B3LYP free energy:	-1099.503576 a.u.		
M06 SCF energy in solution:	-2438.66131865 a.u.		
M06 enthalpy in solution:	-2438.216669 a.u.		
M06 free energy in solution:	-2438.292239 a.u.		
Three lowest frequencies (cm-1):	-1077.3718	36.5835	44.4541
Imaginary frequency:	-1077.3718 cm-1		

Cartesian coordinates

ATOM	X	Y	Z
Ni	-1.752674	0.305902	0.155032
P	0.400090	0.000378	-0.002601
C	1.083623	-0.464973	1.759972
C	0.349914	0.431074	2.789324
C	0.669156	-1.912718	2.104633
C	2.605676	-0.329707	1.960731
H	0.591794	1.489560	2.695686
H	-0.738194	0.326277	2.703915
H	0.637796	0.116060	3.801684
H	1.220275	-2.663808	1.534455
H	0.882584	-2.092778	3.166501
H	-0.403150	-2.073885	1.951440
H	2.863081	-0.650453	2.979689
H	3.177159	-0.954484	1.268762
H	2.952924	0.701201	1.853150
C	0.820469	-1.438455	-1.239850
C	2.242084	-2.025412	-1.128982
C	-0.216525	-2.567466	-1.022012
C	0.603096	-0.950639	-2.689645
H	3.021267	-1.272941	-1.275790
H	2.420261	-2.515109	-0.168004
H	2.374794	-2.789850	-1.906769
H	-1.237206	-2.180915	-1.107047
H	-0.071815	-3.333523	-1.796034
H	-0.121800	-3.060676	-0.054549
H	0.661815	-1.818353	-3.359937
H	-0.384550	-0.496973	-2.819100
H	1.363595	-0.239487	-3.019981
C	1.281009	1.625617	-0.611029
C	1.237856	2.679448	0.517555

C	2.740414	1.467130	-1.081355
C	0.435885	2.220885	-1.764308
H	0.222505	2.812906	0.905227
H	1.905400	2.446044	1.350348
H	1.562525	3.643846	0.105541
H	2.827392	0.834995	-1.968897
H	3.137532	2.455073	-1.352334
H	3.393016	1.055932	-0.306600
H	0.853632	3.200239	-2.034802
H	0.437489	1.606062	-2.664220
H	-0.604393	2.362924	-1.456350
O	-3.548166	0.665923	0.064607
C	-4.558394	-0.326609	-0.036921
H	-4.186038	-1.349769	0.107575
H	-5.302215	-0.122378	0.743449
H	-5.064093	-0.274517	-1.013434
H	-2.700112	0.491427	-1.031005

TS10

B3LYP SCF energy:	-1640.65597371 a.u.		
B3LYP enthalpy:	-1639.970567 a.u.		
B3LYP free energy:	-1640.071060 a.u.		
M06 SCF energy in solution:	-2979.21660687 a.u.		
M06 enthalpy in solution:	-2978.531200 a.u.		
M06 free energy in solution:	-2978.631693 a.u.		
Three lowest frequencies (cm-1):	-125.6037	5.6475	13.9153
Imaginary frequency:	-125.6037 cm-1		

Cartesian coordinates

ATOM	X	Y	Z
Ni	-0.010580	0.123866	-1.591512
C	-1.764517	0.744439	-1.862719
O	-1.535870	1.882118	-2.313646
H	-1.441228	-0.205653	-2.527229
P	1.496600	-0.031411	-0.042544
C	1.420931	1.472539	1.094323
C	2.474865	1.539521	2.216983
C	1.407886	2.782762	0.275264
H	0.430009	1.384969	1.563047
C	2.248561	2.762404	3.124623
H	3.476967	1.613194	1.772505
H	2.463319	0.622496	2.819072
C	1.196613	4.007040	1.183579
H	2.363519	2.896825	-0.257944
H	0.623276	2.738306	-0.489025
C	2.232839	4.067139	2.315409
H	3.026509	2.800227	3.898146
H	1.289092	2.648635	3.650493
H	1.233698	4.923554	0.581456
H	0.186912	3.960397	1.617531
H	2.028707	4.920609	2.974385
H	3.231122	4.236457	1.884620
C	3.277172	-0.037101	-0.696829
C	4.338122	-0.768704	0.152986

C	3.329377	-0.528145	-2.161397
H	3.540728	1.031416	-0.707348
C	5.745964	-0.599811	-0.447803
H	4.101396	-1.840178	0.195912
H	4.332295	-0.405651	1.186456
C	4.736829	-0.371452	-2.760166
H	3.028879	-1.584826	-2.205409
H	2.596419	0.024305	-2.762507
C	5.800355	-1.076832	-1.906104
H	6.475767	-1.148300	0.161760
H	6.033960	0.460950	-0.400649
H	4.749906	-0.760968	-3.786023
H	4.979861	0.699349	-2.829405
H	6.800452	-0.907155	-2.324718
H	5.628206	-2.163091	-1.937092
C	1.351776	-1.512849	1.113560
C	0.103118	-1.406167	2.015993
C	1.302900	-2.825925	0.300843
H	2.240485	-1.535529	1.759765
C	-0.058554	-2.642390	2.918209
H	-0.787874	-1.295892	1.380733
H	0.153886	-0.509017	2.643496
C	1.152502	-4.058404	1.208445
H	0.452049	-2.774268	-0.392927
H	2.200252	-2.930989	-0.320567
C	-0.086492	-3.944553	2.106891
H	-0.973920	-2.543382	3.515554
H	0.777812	-2.678244	3.632140
H	1.096408	-4.964975	0.592284
H	2.050125	-4.162386	1.836308
H	-0.153705	-4.810103	2.778170
H	-0.990164	-3.961987	1.480100
C	-2.933415	0.440858	-0.942992
H	-2.786864	-0.536221	-0.467322
H	-2.956321	1.207431	-0.159089
C	-4.277389	0.454498	-1.716737
H	-4.383456	1.436031	-2.192621
H	-4.230145	-0.288492	-2.523900
C	-5.465846	0.167866	-0.825581
C	-6.131876	1.207586	-0.161313
C	-5.909786	-1.145562	-0.617429
C	-7.207709	0.943931	0.687782
H	-5.806020	2.233938	-0.317319
C	-6.984864	-1.414719	0.231104
H	-5.410654	-1.964758	-1.131518
C	-7.637686	-0.369596	0.887927
H	-7.713802	1.765316	1.188775
H	-7.316190	-2.440163	0.374483
H	-8.477521	-0.576443	1.545971

TS11

B3LYP SCF energy:	-3953.53172616 a.u.
B3LYP enthalpy:	-3951.832637 a.u.
B3LYP free energy:	-3952.085149 a.u.

M06 SCF energy in solution: -5291.08771555 a.u.
M06 enthalpy in solution: -5289.388626 a.u.
M06 free energy in solution: -5289.641138 a.u.
Three lowest frequencies (cm-1): -612.7443 13.2706 14.4894
Imaginary frequency: -612.7443 cm-1

Cartesian coordinates

ATOM	X	Y	Z
N	-0.131003	-1.006330	0.649437
N	0.115136	1.133826	0.721421
C	0.043529	0.090017	-0.163929
C	-0.164994	-0.652788	1.995098
H	-0.292846	-1.383673	2.776391
C	-0.020486	0.693460	2.040695
H	-0.014660	1.380435	2.871638
C	-0.358775	-2.323945	0.108390
C	-1.678839	-2.779835	-0.047140
C	0.742233	-3.115357	-0.294337
C	-1.901815	-3.995235	-0.708403
C	0.487642	-4.328280	-0.926653
C	-0.825017	-4.759402	-1.161653
H	-2.923449	-4.317576	-0.867786
H	1.303707	-4.956279	-1.264311
C	0.324482	2.522440	0.387757
C	1.618560	3.064122	0.480514
C	-0.781966	3.333302	0.038703
C	1.793576	4.440275	0.276151
C	-0.565782	4.690854	-0.177882
C	0.708415	5.254029	-0.044266
H	2.788678	4.854646	0.374575
H	-1.386633	5.338109	-0.464944
C	-2.195657	2.758286	-0.108890
H	-2.073084	1.706740	-0.387644
C	-2.855216	-2.020278	0.573241
H	-2.555081	-0.971047	0.644458
C	2.851300	2.196971	0.760142
H	2.487388	1.229073	1.117662
C	2.174857	-2.682783	0.039501
H	2.234582	-1.607619	-0.162596
O	0.784177	6.599012	-0.254042
O	-0.944513	-5.946804	-1.817666
C	-2.246445	-6.415035	-2.133845
H	-2.102811	-7.348910	-2.680322
H	-2.836285	-6.612468	-1.228578
H	-2.787814	-5.701047	-2.767536
C	2.053107	7.225367	-0.153432
H	2.760281	6.825570	-0.892219
H	1.880477	8.283988	-0.356284
H	2.481389	7.113098	0.851374
C	-4.105365	-2.029381	-0.316277
C	-4.111351	-1.212440	-1.456844
C	-5.237210	-2.799308	-0.033609
C	-5.219716	-1.156248	-2.307322
H	-3.232932	-0.608503	-1.681471
C	-6.362839	-2.768117	-0.870713
H	-5.256668	-3.419072	0.858433

C	-6.339271	-1.940381	-1.996328
H	-7.213646	-1.896415	-2.643504
C	-3.117408	-2.482338	2.015966
C	-3.500538	-1.528047	2.972501
C	-2.997305	-3.815611	2.417685
C	-3.767315	-1.886020	4.296300
H	-3.581325	-0.484667	2.677919
C	-3.261942	-4.207899	3.739689
H	-2.679930	-4.568077	1.701258
C	-3.643835	-3.234170	4.663805
H	-3.844305	-3.526323	5.693446
C	2.484073	-2.861592	1.532768
C	1.857038	-3.833993	2.319022
C	3.446572	-2.036215	2.128672
C	2.169698	-3.984424	3.677798
H	1.105916	-4.480793	1.873800
C	3.786559	-2.164663	3.478830
H	3.943864	-1.283895	1.520226
C	3.133254	-3.142597	4.240781
H	3.381678	-3.248128	5.295382
C	3.225109	-3.338877	-0.864243
C	3.960495	-4.461748	-0.466782
C	3.444745	-2.803521	-2.138528
C	4.899499	-5.052686	-1.320767
H	3.809498	-4.878010	0.525320
C	4.379794	-3.369798	-3.014096
H	2.872104	-1.934908	-2.457742
C	5.099077	-4.492595	-2.587953
H	5.830893	-4.940145	-3.258558
C	3.691140	1.896649	-0.493826
C	4.757792	0.990230	-0.369892
C	3.450859	2.472235	-1.742330
C	5.567313	0.655000	-1.456103
H	4.973114	0.555370	0.603833
C	4.258069	2.170651	-2.852569
H	2.625801	3.164858	-1.869611
C	5.307910	1.264669	-2.693453
H	5.944223	1.030320	-3.545467
C	3.689061	2.783063	1.906293
C	3.330227	2.494631	3.230355
C	4.784693	3.622233	1.679359
C	4.029028	3.037291	4.313629
H	2.487835	1.831796	3.418974
C	5.509656	4.178178	2.742769
H	5.096383	3.829123	0.658708
C	5.117315	3.879851	4.051003
H	5.674684	4.304688	4.884281
C	-2.948902	3.414412	-1.277395
C	-3.889707	4.428742	-1.087718
C	-2.656894	2.997202	-2.585696
C	-4.538686	5.030598	-2.177717
H	-4.135091	4.754358	-0.080198
C	-3.281075	3.582448	-3.690385
H	-1.917383	2.213859	-2.737870
C	-4.222937	4.598847	-3.466881
H	-4.719249	5.060738	-4.319204

C	-3.015006	2.776303	1.187171
C	-4.178045	1.993266	1.244437
C	-2.688190	3.569139	2.291078
C	-5.014392	2.005945	2.364744
H	-4.448479	1.380103	0.386685
C	-3.496698	3.590907	3.437673
H	-1.795296	4.187360	2.262399
C	-4.655897	2.809582	3.456832
H	-5.299926	2.831566	4.334439
C	-3.124695	-5.658947	4.144703
H	-3.786223	-6.304451	3.553269
H	-2.101350	-6.024056	3.990038
H	-3.374565	-5.805030	5.200463
C	-4.182772	-0.849110	5.315638
H	-4.084513	0.165085	4.916846
H	-5.228929	-0.987495	5.619474
H	-3.575126	-0.917100	6.226437
C	-5.204353	-0.277091	-3.537102
H	-6.219606	-0.061264	-3.886690
H	-4.701683	0.676447	-3.342118
H	-4.669656	-0.763058	-4.364373
C	-7.571290	-3.622843	-0.560090
H	-7.422386	-4.660788	-0.887836
H	-7.776053	-3.652490	0.516148
H	-8.467744	-3.248050	-1.065113
C	4.843178	-1.275459	4.095189
H	4.683750	-0.221545	3.838522
H	4.849122	-1.360297	5.186995
H	5.846480	-1.545133	3.739653
C	1.463620	-5.030944	4.510703
H	1.856713	-5.062462	5.532007
H	0.386181	-4.829993	4.573927
H	1.578340	-6.032136	4.076947
C	4.613671	-2.765293	-4.380039
H	5.220463	-3.423894	-5.010376
H	3.666449	-2.572747	-4.895967
H	5.136541	-1.802794	-4.303156
C	5.664824	-6.284321	-0.890863
H	5.782487	-6.323100	0.197485
H	5.145669	-7.203672	-1.194616
H	6.663349	-6.314083	-1.340879
C	6.715757	5.050286	2.475095
H	6.574393	5.668706	1.581775
H	6.925528	5.715952	3.319111
H	7.615198	4.442941	2.306389
C	3.605996	2.744024	5.735487
H	4.470773	2.662164	6.403371
H	2.965704	3.543193	6.132913
H	3.039129	1.809325	5.800385
C	3.978678	2.819432	-4.189631
H	4.780022	2.616315	-4.907725
H	3.040944	2.447801	-4.621456
H	3.879878	3.907513	-4.093561
C	6.683191	-0.354328	-1.310440
H	7.057945	-0.391879	-0.281825
H	6.336214	-1.363371	-1.568700

H	7.526107	-0.118188	-1.969802
C	-2.939684	3.148934	-5.098815
H	-2.410142	3.944724	-5.638990
H	-2.296482	2.263669	-5.103344
H	-3.842751	2.917131	-5.677198
C	-5.574596	6.108299	-1.948060
H	-5.235148	6.839976	-1.205439
H	-5.802785	6.647869	-2.873153
H	-6.515860	5.684284	-1.573180
C	-3.107768	4.432174	4.632779
H	-2.381981	3.909766	5.270971
H	-2.643692	5.375678	4.324587
H	-3.976432	4.669609	5.256002
C	-6.292372	1.197106	2.377852
H	-6.661548	1.046539	3.397813
H	-7.085630	1.704907	1.813222
H	-6.148886	0.213003	1.918583
Ni	0.140917	0.034991	-2.083928
C	0.223253	-0.109763	-3.946618
C	-0.931809	-0.459010	-4.680426
C	1.460529	-0.172949	-4.624801
C	-0.848383	-0.916673	-5.998745
H	-1.910273	-0.383825	-4.210009
C	1.546199	-0.627126	-5.944089
H	2.367846	0.131842	-4.108283
C	0.391955	-1.004932	-6.635965
H	-1.753665	-1.198459	-6.533435
H	2.514466	-0.675555	-6.439032
H	0.456680	-1.348870	-7.665498
H	0.103463	1.230902	-2.928825

TS12

B3LYP SCF energy: -1939.83799865 a.u.
B3LYP enthalpy: -1939.022248 a.u.
B3LYP free energy: -1939.155736 a.u.
M06 SCF energy in solution: -3278.24149975 a.u.
M06 enthalpy in solution: -3277.425749 a.u.
M06 free energy in solution: -3277.559237 a.u.
Three lowest frequencies (cm-1): -599.5447 13.7607 15.6905
Imaginary frequency: -599.5447 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ni	-0.170967	-0.015705	-0.336396
C	-1.986961	-0.044501	-0.685984
C	-2.757321	1.141499	-0.676999
C	-4.138238	1.080388	-0.565570
H	-2.279471	2.114580	-0.745492
C	-4.106521	-1.229537	-0.548348
H	-4.745433	1.980288	-0.533962
H	-4.689468	-2.143684	-0.500995
H	-0.698866	-0.030308	-1.712648
C	-2.722748	-1.250828	-0.660112
H	-2.217088	-2.210695	-0.715279

N	-4.817041	-0.084177	-0.494173
N	2.512195	1.107771	0.341069
N	2.556034	-1.041838	0.334250
C	2.066221	2.478529	0.241685
C	2.167082	-2.429272	0.228098
C	1.712250	0.016821	0.128786
C	3.811909	0.737073	0.663811
C	3.839598	-0.620383	0.659404
C	2.215972	3.149902	-0.988120
C	1.513587	3.094944	1.382217
C	1.643717	-3.074017	1.366716
C	2.341971	-3.087515	-1.005451
C	1.787457	4.481645	-1.052283
C	1.098067	4.426709	1.259264
C	1.284326	-4.421441	1.237951
C	1.970331	-4.435951	-1.075312
C	1.233711	5.115294	0.056799
C	1.446290	-5.097778	0.031758
C	2.797966	2.480721	-2.229211
C	1.335324	2.363855	2.709621
C	1.437610	-2.357126	2.697792
C	2.891940	-2.387577	-2.244234
H	4.582663	1.464748	0.864308
H	4.639457	-1.317253	0.855247
H	1.884596	5.027224	-1.986537
H	0.661128	4.929987	2.116783
H	0.870590	-4.946938	2.093685
H	2.088706	-4.972491	-2.012365
H	3.090158	1.460925	-1.961491
H	1.807055	1.380175	2.622544
H	1.870989	-1.355555	2.615728
H	3.141368	-1.357853	-1.971252
Al	-6.884021	-0.056214	-0.289379
C	-7.100538	0.798898	1.507877
H	-6.663802	1.807272	1.565867
H	-8.163808	0.911713	1.767524
H	-6.645719	0.210316	2.318105
C	-7.371066	-1.995035	-0.397229
H	-8.463011	-2.108571	-0.321530
H	-7.085095	-2.471579	-1.346797
H	-6.950113	-2.609396	0.412872
C	-7.441269	1.067305	-1.849439
H	-7.147875	0.630806	-2.815288
H	-8.535645	1.177431	-1.880718
H	-7.035064	2.089781	-1.828174
H	1.161683	-6.143651	-0.045953
H	0.905284	6.148569	-0.016455
C	2.031001	3.097893	3.872078
H	1.581408	4.079367	4.060880
H	1.942968	2.513189	4.795081
H	3.096453	3.252329	3.667622
C	-0.157727	2.128491	3.014534
H	-0.274161	1.560192	3.944891
H	-0.695575	3.076564	3.131254
H	-0.642833	1.567243	2.207732
C	1.741890	2.367594	-3.346325

H	1.402088	3.355095	-3.680073
H	2.162872	1.848226	-4.215450
H	0.869525	1.804213	-2.999317
C	4.064795	3.205082	-2.724852
H	3.845177	4.230060	-3.045244
H	4.829398	3.258013	-1.941189
H	4.494300	2.675264	-3.583073
C	4.187099	-3.054545	-2.747261
H	4.010967	-4.086692	-3.071385
H	4.589868	-2.502752	-3.604549
H	4.956115	-3.077479	-1.966478
C	1.829137	-2.313003	-3.358160
H	2.225341	-1.770350	-4.224721
H	1.531676	-3.312118	-3.697638
H	0.933961	-1.790244	-3.005749
C	2.160701	-3.069210	3.857098
H	3.231817	-3.179297	3.653518
H	2.047831	-2.493738	4.783196
H	1.750961	-4.069113	4.039707
C	-0.063632	-2.181205	3.002579
H	-0.568993	-1.635478	2.197570
H	-0.563989	-3.150179	3.114186
H	-0.202943	-1.622244	3.935442

TS1a

B3LYP SCF energy:	-1524.06513100 a.u.
B3LYP enthalpy:	-1523.440749 a.u.
B3LYP free energy:	-1523.536788 a.u.
M06 SCF energy in solution:	-2862.72508931 a.u.
M06 enthalpy in solution:	-2862.100707 a.u.
M06 free energy in solution:	-2862.196746 a.u.
Three lowest frequencies (cm-1):	-1222.0173 17.9715 27.3512
Imaginary frequency:	-1222.0173 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ni	-0.565748	1.366268	-0.565337
P	-1.549996	-0.577676	0.031039
C	-1.432381	-2.032817	-1.257191
C	-2.301480	-1.697048	-2.489413
C	0.015575	-2.122531	-1.787971
C	-1.846027	-3.419821	-0.722369
H	-3.372815	-1.752582	-2.288473
H	-2.071168	-0.703254	-2.887482
H	-2.081677	-2.428207	-3.278469
H	0.752975	-2.353786	-1.020596
H	0.059317	-2.921426	-2.540956
H	0.312509	-1.189132	-2.267215
H	-1.808946	-4.141662	-1.549794
H	-1.165401	-3.786698	0.050308
H	-2.861068	-3.439232	-0.320121
C	-0.801840	-1.179291	1.719045
C	-1.686934	-2.137102	2.542578
C	0.561305	-1.863221	1.474420

C	-0.493574	0.082360	2.561478
H	-2.620907	-1.672455	2.867297
H	-1.934274	-3.054146	2.001449
H	-1.140808	-2.430887	3.449452
H	1.228387	-1.245086	0.866867
H	1.049273	-2.016339	2.446006
H	0.464974	-2.846137	1.007627
H	-0.020684	-0.229779	3.502653
H	0.206352	0.741253	2.037870
H	-1.379380	0.664304	2.813923
C	-3.435596	-0.151102	0.284845
C	-3.880975	0.753951	-0.892297
C	-4.388986	-1.358212	0.396010
C	-3.603566	0.720237	1.549535
H	-3.294768	1.676949	-0.914087
H	-3.820773	0.268405	-1.866523
H	-4.932539	1.029759	-0.731970
H	-4.120903	-2.037896	1.209673
H	-5.401103	-0.985071	0.603967
H	-4.450232	-1.938949	-0.527857
H	-4.643515	1.071661	1.582987
H	-3.422040	0.174570	2.478254
H	-2.962435	1.603013	1.505348
O	-1.617756	3.047062	0.056948
C	1.053422	1.316705	-1.638917
C	0.594125	2.727663	-1.538869
H	1.296634	3.406682	-1.046333
H	0.241800	3.138865	-2.489095
C	-1.233272	3.739267	1.218844
H	-0.137734	3.876613	1.295651
H	-1.686556	4.743263	1.236034
H	-1.552918	3.219014	2.138281
H	-0.511345	3.036381	-0.795493
C	2.279844	0.854638	-0.952670
C	3.063740	-0.173888	-1.500218
C	2.723548	1.407502	0.270084
C	4.219883	-0.647552	-0.873934
H	2.770552	-0.613434	-2.450657
C	3.871080	0.952662	0.903118
H	2.153480	2.208879	0.732706
C	4.630873	-0.084130	0.338569
H	4.790191	-1.441213	-1.343755
H	4.203346	1.385190	1.842138
H	0.911255	0.855696	-2.617330
O	5.740142	-0.462473	1.042500
C	6.548663	-1.495902	0.508568
H	7.365925	-1.636666	1.218724
H	5.990531	-2.437011	0.408426
H	6.963724	-1.220754	-0.470630

TS2a

B3LYP SCF energy: -1524.05704383 a.u.

B3LYP enthalpy: -1523.432774 a.u.

B3LYP free energy: -1523.529391 a.u.

M06 SCF energy in solution: -2862.71757955 a.u.
M06 enthalpy in solution: -2862.093310 a.u.
M06 free energy in solution: -2862.189927 a.u.
Three lowest frequencies (cm-1): -1217.9133 14.8461 22.3091
Imaginary frequency: -1217.9133 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ni	0.168491	0.697971	-0.487950
P	2.141434	-0.235318	0.017425
C	3.237782	1.182296	0.773594
C	3.160551	2.397979	-0.184053
C	2.593625	1.646160	2.100850
C	4.719590	0.844564	1.030905
H	3.667652	2.234890	-1.135085
H	2.123449	2.675247	-0.392235
H	3.645697	3.255386	0.301367
H	2.733664	0.925499	2.910310
H	3.086639	2.575974	2.414404
H	1.524520	1.849237	1.981977
H	5.197971	1.709222	1.510986
H	4.850058	-0.010680	1.699061
H	5.274069	0.645261	0.109954
C	1.769216	-1.554074	1.398221
C	2.961163	-1.920195	2.306584
C	0.613686	-1.013622	2.276491
C	1.233993	-2.852901	0.754380
H	3.815557	-2.311660	1.748580
H	3.304232	-1.074128	2.906436
H	2.642973	-2.703040	3.008473
H	-0.282632	-0.809471	1.682802
H	0.358530	-1.778713	3.022356
H	0.861464	-0.098554	2.811508
H	0.857631	-3.503525	1.554473
H	0.402017	-2.657829	0.070430
H	2.002223	-3.415598	0.219401
C	3.147026	-1.095217	-1.408568
C	3.740864	-0.018092	-2.343614
C	4.293684	-2.014576	-0.936373
C	2.181644	-1.921135	-2.290351
H	2.980867	0.695717	-2.677480
H	4.566174	0.534150	-1.889418
H	4.139450	-0.517148	-3.236599
H	3.929235	-2.892372	-0.397345
H	4.835408	-2.382732	-1.818274
H	5.018296	-1.501053	-0.300461
H	2.763326	-2.383331	-3.099447
H	1.676037	-2.723904	-1.754328
H	1.420369	-1.284605	-2.743245
C	-0.691155	-0.025853	-2.013758
C	-1.679753	0.903233	-1.407890
H	-0.227761	0.304587	-2.946043
H	-1.854735	1.799970	-2.012740
H	-0.943141	-1.087009	-2.024257
C	-2.960419	0.350123	-0.841613
C	-4.166222	1.035169	-1.016798

C	-3.000332	-0.850174	-0.109475
C	-5.374556	0.553579	-0.502417
H	-4.172568	1.969265	-1.574751
C	-4.190252	-1.346329	0.405573
H	-2.080692	-1.403360	0.061817
C	-5.390934	-0.646932	0.213447
H	-6.284357	1.119442	-0.669193
H	-4.215588	-2.273549	0.970187
O	-0.518190	2.081854	0.853167
H	-1.229842	1.568149	-0.275110
C	-0.403717	3.468420	0.656535
H	-1.149379	4.005615	1.264512
H	0.590219	3.846382	0.951439
H	-0.561612	3.772644	-0.396015
O	-6.507707	-1.216659	0.761949
C	-7.741229	-0.536900	0.614941
H	-8.486302	-1.149721	1.126502
H	-7.712919	0.459271	1.077366
H	-8.023790	-0.432026	-0.441699

TS1b

B3LYP SCF energy:	-1637.42282105 a.u.		
B3LYP enthalpy:	-1636.785645 a.u.		
B3LYP free energy:	-1636.885949 a.u.		
M06 SCF energy in solution:	-2976.07465087 a.u.		
M06 enthalpy in solution:	-2975.437475 a.u.		
M06 free energy in solution:	-2975.537779 a.u.		
Three lowest frequencies (cm-1):	-1227.2534	18.1346	24.2842
Imaginary frequency:	-1227.2534 cm-1		

Cartesian coordinates

ATOM	X	Y	Z
Ni	-1.121726	1.390739	-0.546977
P	-1.911609	-0.644082	0.056238
C	-1.829624	-2.030766	-1.306233
C	-2.849051	-1.726809	-2.427447
C	-0.444755	-1.981907	-1.989086
C	-2.076990	-3.464773	-0.792021
H	-3.885852	-1.883747	-2.123515
H	-2.745445	-0.703766	-2.803966
H	-2.652231	-2.407597	-3.266014
H	0.390557	-2.147103	-1.310213
H	-0.408247	-2.766809	-2.756678
H	-0.291669	-1.021131	-2.482348
H	-2.069895	-4.151762	-1.649165
H	-1.295008	-3.802043	-0.107437
H	-3.040620	-3.580039	-0.291532
C	-0.943777	-1.253601	1.627556
C	-1.672900	-2.298738	2.497205
C	0.426637	-1.836733	1.216337
C	-0.631017	-0.004363	2.486519
H	-2.598072	-1.914309	2.932584
H	-1.910213	-3.213646	1.947928
H	-1.017677	-2.581463	3.332389

H	0.993397	-1.151878	0.579510
H	1.017483	-2.000090	2.127072
H	0.343842	-2.801880	0.711393
H	-0.036777	-0.315865	3.355891
H	-0.039266	0.723532	1.921873
H	-1.522172	0.500089	2.859320
C	-3.782987	-0.370059	0.522699
C	-4.413765	0.539692	-0.562484
C	-4.629641	-1.649542	0.674537
C	-3.878583	0.438656	1.835231
H	-3.900556	1.504384	-0.606722
H	-4.423682	0.092274	-1.556454
H	-5.459007	0.730863	-0.282548
H	-4.231371	-2.337687	1.424912
H	-5.638826	-1.362344	0.999267
H	-4.743566	-2.196955	-0.264483
H	-4.932499	0.702502	1.994654
H	-3.553542	-0.121033	2.715093
H	-3.316679	1.371838	1.762296
O	-2.237609	2.945425	0.216056
C	0.409944	1.499467	-1.750833
C	-0.141498	2.866182	-1.555573
H	0.544572	3.580216	-1.090623
H	-0.596529	3.282095	-2.458847
C	-1.812615	3.629885	1.370780
H	-0.731569	3.863867	1.358769
H	-2.350701	4.585903	1.465029
H	-2.002975	3.051550	2.290502
H	-1.203984	3.063051	-0.720666
C	1.703813	1.102712	-1.164854
C	2.494850	0.115482	-1.790238
C	2.204369	1.672384	0.028051
C	3.710179	-0.294361	-1.253703
H	2.148735	-0.325881	-2.721229
C	3.418577	1.269120	0.565899
H	1.626322	2.437359	0.538912
C	4.186588	0.277416	-0.064512
H	4.300613	-1.052144	-1.757121
H	3.795543	1.711176	1.482722
H	0.225734	1.061292	-2.731861
C	5.473808	-0.116366	0.559544
O	5.917235	0.351939	1.591999
O	6.123859	-1.073971	-0.148794
C	7.377734	-1.494464	0.403628
H	7.238073	-1.915737	1.403193
H	7.760388	-2.252387	-0.281230
H	8.072195	-0.652382	0.471025

TS2b

B3LYP SCF energy:	-1637.41467830 a.u.
B3LYP enthalpy:	-1636.778013 a.u.
B3LYP free energy:	-1636.879455 a.u.
M06 SCF energy in solution:	-2976.06646751 a.u.
M06 enthalpy in solution:	-2975.429802 a.u.

M06 free energy in solution: -2975.531244 a.u.
Three lowest frequencies (cm-1): -1204.1891 19.5303 20.2549
Imaginary frequency: -1204.1891 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ni	-0.700463	0.822256	0.413004
P	-2.589835	-0.296567	-0.016341
C	-3.760962	0.952388	-0.938855
C	-3.774740	2.271431	-0.127261
C	-3.131908	1.300453	-2.308208
C	-5.214001	0.489768	-1.162717
H	-4.268329	2.179602	0.840448
H	-2.761549	2.647370	0.039304
H	-4.322415	3.029615	-0.702698
H	-3.217854	0.485121	-3.030647
H	-3.678675	2.155081	-2.728609
H	-2.079012	1.583439	-2.212560
H	-5.739523	1.255113	-1.749856
H	-5.277792	-0.447808	-1.720566
H	-5.767126	0.369310	-0.227477
C	-2.098784	-1.728937	-1.239708
C	-3.245128	-2.281096	-2.111195
C	-0.970973	-1.206337	-2.162386
C	-1.482508	-2.900415	-0.443437
H	-4.079777	-2.669575	-1.522252
H	-3.636860	-1.535261	-2.806931
H	-2.858527	-3.112049	-2.716635
H	-0.111822	-0.848502	-1.587300
H	-0.631495	-2.035715	-2.797329
H	-1.282162	-0.394097	-2.817263
H	-1.035981	-3.606270	-1.155581
H	-0.686014	-2.562574	0.227226
H	-2.218536	-3.457455	0.140680
C	-3.558660	-1.059380	1.487174
C	-4.229407	0.072474	2.297736
C	-4.640312	-2.091064	1.103126
C	-2.560411	-1.729301	2.460841
H	-3.521339	0.866961	2.554764
H	-5.084995	0.516934	1.784600
H	-4.604116	-0.351313	3.238534
H	-4.215020	-2.996432	0.662941
H	-5.174016	-2.397978	2.012843
H	-5.383107	-1.691232	0.409063
H	-3.126114	-2.121921	3.316333
H	-2.014304	-2.564572	2.023955
H	-1.832941	-1.009948	2.839028
C	0.136700	0.356344	2.043960
C	1.094663	1.270967	1.358473
H	-0.375013	0.770283	2.915521
H	1.192909	2.242118	1.855444
H	0.458665	-0.673871	2.199934
C	2.426082	0.726952	0.923690
C	3.584820	1.506626	1.067012
C	2.557538	-0.551617	0.353660
C	4.831373	1.029957	0.670923

H	3.506514	2.500667	1.501356
C	3.798320	-1.035440	-0.041022
H	1.674625	-1.169555	0.217107
C	4.950226	-0.250405	0.113595
H	5.715401	1.645752	0.794330
H	3.898878	-2.023373	-0.478906
O	-0.049690	2.061757	-1.070781
H	0.658612	1.751546	0.141030
C	-0.262161	3.451043	-1.069668
H	0.474537	3.952042	-1.717756
H	-1.263573	3.715005	-1.450029
H	-0.172630	3.904104	-0.063683
C	6.249506	-0.819562	-0.327124
O	6.393454	-1.926545	-0.812095
O	7.284998	0.034052	-0.130819
C	8.567277	-0.460361	-0.537562
H	8.571615	-0.689709	-1.606843
H	9.274137	0.339981	-0.314747
H	8.825847	-1.366538	0.017503

TS3a

B3LYP SCF energy:	-2064.82615063 a.u.		
B3LYP enthalpy:	-2063.963598 a.u.		
B3LYP free energy:	-2064.085528 a.u.		
M06 SCF energy in solution:	-3403.25979221 a.u.		
M06 enthalpy in solution:	-3402.397240 a.u.		
M06 free energy in solution:	-3402.519170 a.u.		
Three lowest frequencies (cm-1):	-500.3584	9.4153	13.7930
Imaginary frequency:	-500.3584 cm-1		

Cartesian coordinates

ATOM	X	Y	Z
Ni	-0.004141	-0.191051	-1.777244
C	1.882794	-0.530942	-1.783824
O	2.352079	-1.575245	-2.209379
C	-2.408525	1.701682	-1.590608
C	-1.623619	2.869270	-1.464027
C	-2.086109	3.986504	-0.782464
C	-3.358716	3.982797	-0.189590
C	-4.153324	2.835492	-0.290292
C	-3.674326	1.720070	-0.983196
H	-0.631795	2.897841	-1.906420
H	-1.477163	4.881206	-0.694391
H	-5.143430	2.799879	0.150300
H	-4.317643	0.847744	-1.069872
C	2.817107	0.550651	-1.212573
H	2.715032	1.432978	-1.860675
H	2.434570	0.867316	-0.233085
C	4.294229	0.123317	-1.108910
H	4.363297	-0.765417	-0.470330
H	4.637860	-0.189233	-2.100921
C	5.175315	1.224789	-0.564106
C	5.766821	2.165458	-1.420201
C	5.398463	1.355195	0.814450

C	6.550702	3.204735	-0.916948
H	5.614229	2.076659	-2.494031
C	6.181519	2.392260	1.323822
H	4.957083	0.629594	1.495255
C	6.760605	3.322907	0.458698
H	7.002659	3.919586	-1.600171
H	6.344064	2.470195	2.396052
H	7.373635	4.129519	0.852138
C	-1.049769	0.612603	-3.423919
H	-1.034477	-0.179339	-4.168935
H	-0.751942	1.586899	-3.803226
H	0.645589	0.410417	-2.995911
P	-0.507247	-1.280899	0.166135
C	-1.071709	-0.017728	1.456179
C	-1.620273	-0.471312	2.830378
C	0.013507	1.065703	1.656310
H	-1.901255	0.469402	0.923605
C	-2.205165	0.732470	3.592243
H	-0.821088	-0.901910	3.440178
H	-2.378560	-1.253639	2.726875
C	-0.519251	2.257294	2.471499
H	0.881419	0.628652	2.171981
H	0.367887	1.420067	0.682165
C	-1.140090	1.817958	3.805375
H	-2.608974	0.398758	4.557105
H	-3.048348	1.151696	3.023888
H	0.293119	2.974232	2.647433
H	-1.275781	2.782445	1.873067
H	-1.573118	2.682805	4.324134
H	-0.352380	1.421250	4.463462
C	0.979677	-2.236382	0.873413
C	0.984372	-2.576102	2.378550
C	1.278623	-3.510512	0.048324
H	1.810079	-1.539624	0.695138
C	2.297795	-3.263713	2.803561
H	0.132976	-3.229185	2.619763
H	0.869263	-1.669736	2.976998
C	2.607413	-4.159694	0.467178
H	0.473495	-4.240074	0.211470
H	1.311823	-3.273160	-1.017376
C	2.614529	-4.504354	1.961047
H	2.243367	-3.523030	3.868996
H	3.121620	-2.541519	2.701865
H	2.779154	-5.060029	-0.136302
H	3.431503	-3.469715	0.236969
H	3.583017	-4.926909	2.257841
H	1.860085	-5.280973	2.157897
C	-1.890190	-2.577079	0.040087
C	-3.322933	-2.012694	0.178177
C	-1.799934	-3.351723	-1.299735
H	-1.725539	-3.286711	0.865414
C	-4.377297	-3.132721	0.115590
H	-3.509690	-1.302718	-0.635952
H	-3.450306	-1.453371	1.107454
C	-2.845588	-4.476980	-1.378836
H	-1.962690	-2.642787	-2.123274

H	-0.803014	-3.767993	-1.454201
C	-4.270912	-3.945294	-1.181520
H	-5.380365	-2.697453	0.213615
H	-4.242823	-3.802598	0.977965
H	-2.759209	-4.990310	-2.345000
H	-2.626750	-5.229365	-0.606341
H	-4.992950	-4.771716	-1.176173
H	-4.537239	-3.301917	-2.033329
C	-1.956543	0.523015	-2.354512
H	-2.616004	-0.339050	-2.332488
O	-3.722072	5.134097	0.451645
C	-5.002366	5.186576	1.055623
H	-5.108700	4.432051	1.847296
H	-5.087461	6.182325	1.495116
H	-5.804522	5.046944	0.318210

TS4a

B3LYP SCF energy: -2064.82279354 a.u.
B3LYP enthalpy: -2063.960396 a.u.
B3LYP free energy: -2064.083307 a.u.
M06 SCF energy in solution: -3403.25267834 a.u.
M06 enthalpy in solution: -3402.390281 a.u.
M06 free energy in solution: -3402.513192 a.u.
Three lowest frequencies (cm-1): -585.3294 8.3138 13.5026
Imaginary frequency: -585.3294 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ni	-0.710883	0.140495	0.481554
C	0.162006	1.446231	-0.612309
O	-0.159620	1.524598	-1.791332
C	1.225739	2.405477	-0.054152
H	0.695942	3.079069	0.636160
H	1.923590	1.840172	0.578684
C	1.980979	3.215123	-1.126044
H	2.503284	2.520049	-1.795272
H	1.245040	3.736669	-1.747000
C	2.965700	4.195852	-0.531288
C	2.569365	5.497235	-0.188895
C	4.295152	3.824951	-0.281946
C	3.468073	6.396637	0.386383
H	1.544825	5.808647	-0.382752
C	5.198812	4.719823	0.293281
H	4.626726	2.823532	-0.550625
C	4.788016	6.011017	0.630714
H	3.138808	7.401783	0.638190
H	6.225840	4.410562	0.471840
H	5.490640	6.711421	1.074558
C	-2.447455	0.534905	1.704568
H	-1.324471	1.471395	0.876058
P	0.621153	-1.627866	0.024224
C	1.434156	-2.094490	1.667888
C	2.340903	-3.341905	1.783687
C	2.141055	-0.875236	2.302780

H	0.544301	-2.291923	2.283547
C	2.661931	-3.632080	3.261482
H	3.285513	-3.174823	1.258854
H	1.883096	-4.220573	1.318066
C	2.514718	-1.149413	3.770288
H	3.052054	-0.638160	1.733294
H	1.492674	0.006746	2.241479
C	3.349193	-2.429474	3.925894
H	3.300348	-4.522062	3.333794
H	1.732333	-3.869489	3.800043
H	3.056803	-0.288532	4.181856
H	1.590219	-1.246420	4.358747
H	3.535437	-2.634279	4.987797
H	4.334324	-2.278466	3.459834
C	1.984449	-1.253407	-1.244935
C	3.253008	-2.132486	-1.253642
C	1.404614	-1.154352	-2.676761
H	2.291852	-0.239548	-0.951726
C	4.287980	-1.624643	-2.277341
H	2.989112	-3.174585	-1.486254
H	3.724556	-2.135867	-0.268283
C	2.444154	-0.617671	-3.673525
H	1.100215	-2.156582	-3.008104
H	0.520244	-0.512020	-2.685467
C	3.704500	-1.490892	-3.688928
H	5.156883	-2.295720	-2.279913
H	4.655572	-0.641577	-1.947070
H	1.997739	-0.568343	-4.674680
H	2.708255	0.413918	-3.400325
H	4.456389	-1.075497	-4.372078
H	3.449025	-2.489662	-4.073963
C	-0.217968	-3.213742	-0.590261
C	-0.847188	-4.079298	0.528599
C	-1.317977	-2.895542	-1.634199
H	0.565227	-3.812114	-1.080989
C	-1.459048	-5.372704	-0.040680
H	-1.634399	-3.504989	1.032291
H	-0.115202	-4.342627	1.296157
C	-1.941269	-4.177232	-2.213801
H	-2.098415	-2.299297	-1.143221
H	-0.932411	-2.277988	-2.447496
C	-2.514667	-5.080693	-1.114744
H	-1.896659	-5.960458	0.776621
H	-0.657515	-5.989453	-0.474280
H	-2.723525	-3.909671	-2.935539
H	-1.174031	-4.729268	-2.777170
H	-2.892112	-6.017200	-1.544773
H	-3.376155	-4.580764	-0.647833
C	-2.069982	-0.830269	1.661862
H	-2.682446	-1.521109	1.089821
H	-1.567773	-1.257211	2.527139
H	-2.188957	1.083835	2.609276
C	-3.666168	1.057971	1.021341
C	-4.474527	1.995123	1.670740
C	-4.060892	0.626500	-0.258094
C	-5.650167	2.482081	1.091359

H	-4.191010	2.353649	2.658035
C	-5.222889	1.100086	-0.848475
H	-3.432768	-0.070960	-0.805421
C	-6.031066	2.031349	-0.176358
H	-6.249298	3.205043	1.633189
H	-5.522546	0.775332	-1.840071
O	-7.151836	2.435438	-0.843870
C	-7.989122	3.396500	-0.224584
H	-7.454674	4.337564	-0.036934
H	-8.805871	3.579930	-0.925396
H	-8.402256	3.023764	0.722628

TS3b

B3LYP SCF energy: -2178.18373457 a.u.
B3LYP enthalpy: -2177.308526 a.u.
B3LYP free energy: -2177.435657 a.u.
M06 SCF energy in solution: -3516.60920109 a.u.
M06 enthalpy in solution: -3515.733993 a.u.
M06 free energy in solution: -3515.861124 a.u.
Three lowest frequencies (cm-1): -469.6618 8.9274 9.4398
Imaginary frequency: -469.6618 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ni	0.406601	-0.375826	-1.799034
C	2.273531	0.055681	-1.760801
O	3.113543	-0.742075	-2.141759
C	-2.573177	0.351100	-1.794413
C	-2.366284	1.747942	-1.743353
C	-3.288720	2.589197	-1.136165
C	-4.453651	2.071351	-0.547942
C	-4.669691	0.685258	-0.580274
C	-3.744501	-0.153826	-1.190891
H	-1.469302	2.174341	-2.182660
H	-3.125957	3.661813	-1.104655
H	-5.568604	0.273148	-0.134920
H	-3.938461	-1.222907	-1.225347
C	2.697091	1.422278	-1.199660
H	2.330585	2.178334	-1.909034
H	2.149157	1.612778	-0.267159
C	4.216538	1.571745	-0.989795
H	4.554182	0.815981	-0.270319
H	4.720656	1.338172	-1.933699
C	4.602025	2.952998	-0.509734
C	4.841033	3.990594	-1.422883
C	4.703772	3.240623	0.858789
C	5.167201	5.274556	-0.984289
H	4.776993	3.785401	-2.489711
C	5.029975	4.522949	1.303636
H	4.532076	2.446910	1.583577
C	5.262411	5.546044	0.382431
H	5.353119	6.062041	-1.710371
H	5.107905	4.721420	2.369717
H	5.520080	6.544407	0.725856

C	-0.783888	-0.143505	-3.505243
H	-0.398868	-0.884947	-4.201261
H	-0.878548	0.854633	-3.923610
H	0.875658	0.415609	-2.988314
P	0.328012	-1.503171	0.196847
C	-0.817345	-0.583453	1.388016
C	-1.194566	-1.187793	2.761783
C	-0.341691	0.877825	1.566955
H	-1.741977	-0.536319	0.795336
C	-2.299216	-0.346441	3.427976
H	-0.328512	-1.199683	3.429055
H	-1.520698	-2.228522	2.669050
C	-1.404080	1.730494	2.282924
H	0.592741	0.895544	2.147165
H	-0.116540	1.318837	0.588857
C	-1.846170	1.108888	3.615527
H	-2.567239	-0.790499	4.395484
H	-3.206457	-0.372152	2.806771
H	-1.014345	2.743488	2.445353
H	-2.275843	1.832904	1.623349
H	-2.652058	1.705632	4.061077
H	-1.007909	1.134246	4.328048
C	2.035414	-1.683275	1.025591
C	2.073248	-1.899937	2.552594
C	2.906408	-2.751726	0.321737
H	2.497750	-0.707352	0.824087
C	3.516418	-1.942269	3.092002
H	1.557794	-2.836149	2.811671
H	1.544069	-1.093469	3.064448
C	4.347640	-2.755873	0.857552
H	2.471579	-3.745095	0.499614
H	2.921248	-2.578950	-0.756566
C	4.382779	-2.982209	2.373197
H	3.493718	-2.136548	4.172203
H	3.970367	-0.948001	2.965212
H	4.925286	-3.531225	0.338587
H	4.826210	-1.796867	0.612832
H	5.413585	-2.942967	2.747705
H	4.005107	-3.990913	2.598667
C	-0.331310	-3.277476	0.067795
C	-1.871144	-3.403284	0.119384
C	0.167076	-3.953764	-1.234417
H	0.081248	-3.827493	0.927135
C	-2.316407	-4.875973	0.058340
H	-2.302749	-2.864417	-0.732362
H	-2.286112	-2.941119	1.017647
C	-0.264041	-5.428081	-1.310809
H	-0.249244	-3.404673	-2.090349
H	1.251921	-3.884006	-1.332097
C	-1.786036	-5.583414	-1.195658
H	-3.412301	-4.928842	0.093123
H	-1.951135	-5.398493	0.954949
H	0.095298	-5.867080	-2.250192
H	0.222955	-5.989083	-0.499146
H	-2.064613	-6.644749	-1.182169
H	-2.262548	-5.146366	-2.085769

C	-1.640227	-0.560310	-2.472695
H	-1.886837	-1.616560	-2.422296
C	-5.406044	3.021815	0.078254
O	-5.253706	4.228578	0.122603
O	-6.488762	2.399525	0.608594
C	-7.449802	3.268208	1.222535
H	-8.240626	2.614942	1.593519
H	-6.995425	3.827156	2.045350
H	-7.849396	3.978549	0.493349

TS4b

B3LYP SCF energy: -2178.17865959 a.u.
B3LYP enthalpy: -2177.304108 a.u.
B3LYP free energy: -2177.432652 a.u.
M06 SCF energy in solution: -3516.60058252 a.u.
M06 enthalpy in solution: -3515.726031 a.u.
M06 free energy in solution: -3515.854575 a.u.
Three lowest frequencies (cm-1): -561.4415 9.7390 11.5277
Imaginary frequency: -561.4415 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ni	0.318096	-0.006685	-0.584144
C	-0.273802	1.433482	0.534330
O	0.133455	1.479744	1.687052
C	-1.223384	2.523960	0.018178
H	-0.664074	3.082593	-0.747104
H	-2.050834	2.046927	-0.524456
C	-1.752077	3.478107	1.106374
H	-2.312374	2.896384	1.848712
H	-0.895100	3.903437	1.639338
C	-2.624653	4.575408	0.540321
C	-2.064671	5.781387	0.093184
C	-4.011450	4.406623	0.417498
C	-2.861351	6.783188	-0.462909
H	-0.991780	5.936528	0.188448
C	-4.813682	5.404964	-0.137773
H	-4.467727	3.482938	0.768950
C	-4.240628	6.598402	-0.581613
H	-2.405308	7.711448	-0.798184
H	-5.887320	5.253060	-0.217971
H	-4.863226	7.379087	-1.010676
C	2.022096	0.094572	-1.877797
H	1.116784	1.216627	-0.994544
P	-1.248847	-1.540274	-0.017009
C	-2.245776	-1.865939	-1.592578
C	-3.343592	-2.955009	-1.635916
C	-2.800924	-0.544812	-2.172653
H	-1.446085	-2.194484	-2.272285
C	-3.816313	-3.176402	-3.084785
H	-4.208595	-2.646653	-1.041766
H	-2.996238	-3.898855	-1.203685
C	-3.330493	-0.740825	-3.604443
H	-3.613042	-0.174531	-1.529678

H	-2.020498	0.225288	-2.168529
C	-4.361873	-1.875336	-3.692294
H	-4.585529	-3.958938	-3.107675
H	-2.976621	-3.543901	-3.693216
H	-3.764803	0.198445	-3.969736
H	-2.482665	-0.970297	-4.266858
H	-4.660925	-2.035955	-4.735784
H	-5.271682	-1.581408	-3.148175
C	-2.440547	-0.964306	1.346810
C	-3.808877	-1.665949	1.471608
C	-1.742531	-0.933026	2.728374
H	-2.633392	0.079120	1.058937
C	-4.684778	-1.017651	2.562674
H	-3.665130	-2.732032	1.700351
H	-4.353827	-1.614465	0.526756
C	-2.619433	-0.249015	3.789282
H	-1.553214	-1.964482	3.055561
H	-0.780851	-0.418822	2.659489
C	-3.979296	-0.944473	3.922105
H	-5.629242	-1.570974	2.645994
H	-4.949221	0.000873	2.241191
H	-2.092366	-0.246956	4.751586
H	-2.764406	0.805175	3.512690
H	-4.613070	-0.422182	4.650091
H	-3.829289	-1.962885	4.311019
C	-0.611854	-3.232536	0.556030
C	-0.216282	-4.189803	-0.593699
C	0.605290	-3.069246	1.501104
H	-1.431081	-3.703165	1.120475
C	0.256116	-5.551558	-0.051835
H	0.593655	-3.738709	-1.179220
H	-1.047434	-4.350529	-1.284478
C	1.088475	-4.422245	2.050354
H	1.417631	-2.593147	0.936753
H	0.379916	-2.397663	2.331942
C	1.432264	-5.402675	0.922241
H	0.533802	-6.202094	-0.891156
H	-0.582439	-6.045271	0.461473
H	1.959698	-4.263931	2.698439
H	0.302508	-4.857167	2.685821
H	1.712512	-6.380253	1.334553
H	2.310585	-5.030407	0.374537
C	1.434370	-1.194067	-1.821795
H	1.950251	-1.978932	-1.276110
H	0.833490	-1.525921	-2.665503
H	1.830280	0.682981	-2.773810
C	3.343150	0.381955	-1.243990
C	4.330267	1.048825	-1.985363
C	3.648178	-0.024892	0.065694
C	5.593939	1.283880	-1.449541
H	4.108162	1.377972	-2.997793
C	4.907223	0.206761	0.605156
H	2.880687	-0.502007	0.668620
C	5.894025	0.859254	-0.148581
H	6.349376	1.795644	-2.035206
H	5.145802	-0.101611	1.617743

C	7.224286	1.077186	0.480605
O	7.526574	0.715579	1.601939
O	8.085174	1.729747	-0.337742
C	9.387101	1.969025	0.213546
H	9.942028	2.495710	-0.563801
H	9.316624	2.580736	1.117172
H	9.878896	1.025088	0.464532

TS1c

B3LYP SCF energy: -1448.85754784 a.u.
B3LYP enthalpy: -1448.239108 a.u.
B3LYP free energy: -1448.332431 a.u.
M06 SCF energy in solution: -2787.51276873 a.u.
M06 enthalpy in solution: -2786.894329 a.u.
M06 free energy in solution: -2786.987652 a.u.
Three lowest frequencies (cm-1): -1200.0942 21.4062 32.0590
Imaginary frequency: -1200.0942 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ni	0.067576	1.205626	-0.581821
P	-1.321475	-0.464410	0.054428
C	-0.948823	-2.227863	-0.672754
C	-1.181212	-2.195773	-2.200257
C	0.551777	-2.545755	-0.485485
C	-1.769288	-3.385895	-0.067633
H	-2.234997	-2.116151	-2.474328
H	-0.633617	-1.374695	-2.674782
H	-0.807151	-3.134439	-2.629315
H	0.836356	-2.715825	0.552147
H	0.784094	-3.465261	-1.039792
H	1.176787	-1.743427	-0.875675
H	-1.516893	-4.312570	-0.601123
H	-1.532113	-3.551550	0.986562
H	-2.847892	-3.241999	-0.155720
C	-1.374909	-0.598946	1.992771
C	-2.640980	-1.252120	2.584551
C	-0.142936	-1.383047	2.496183
C	-1.225418	0.829563	2.567063
H	-3.547576	-0.678708	2.377857
H	-2.795622	-2.273017	2.226588
H	-2.534239	-1.302289	3.676929
H	0.791018	-1.000398	2.073020
H	-0.083059	-1.266662	3.586425
H	-0.210016	-2.454361	2.293797
H	-1.173887	0.763682	3.662337
H	-0.302347	1.300348	2.214758
H	-2.055180	1.488708	2.314365
C	-3.069093	0.109245	-0.591409
C	-2.880188	0.684149	-2.018780
C	-4.165777	-0.973650	-0.615932
C	-3.569919	1.298183	0.259355
H	-2.209914	1.548392	-2.003174
H	-2.503787	-0.042843	-2.739070

H	-3.858037	1.028541	-2.382739
H	-4.337764	-1.424997	0.365201
H	-5.109506	-0.507389	-0.929857
H	-3.955102	-1.775325	-1.328562
H	-4.473083	1.700446	-0.219295
H	-3.850282	1.012945	1.275951
H	-2.827222	2.099490	0.285114
O	-0.866578	3.055635	-0.532414
C	1.840828	0.781404	-1.268249
C	1.589682	2.239783	-1.445729
H	2.266259	2.889820	-0.883480
H	1.515757	2.545337	-2.494052
C	-0.697054	3.927407	0.558092
H	0.336182	3.927699	0.954150
H	-0.931476	4.962787	0.263318
H	-1.361237	3.666027	1.398758
H	0.404452	2.786420	-1.055358
C	2.874529	0.310418	-0.311540
C	3.816497	-0.690011	-0.666332
C	2.953162	0.867826	0.980692
C	4.760784	-1.103755	0.282572
C	3.904493	0.450614	1.907972
H	2.241070	1.641851	1.257735
C	4.813017	-0.550646	1.561414
H	5.480711	-1.870063	0.002713
H	3.932763	0.902116	2.896486
H	1.796160	0.206342	-2.191483
H	5.559243	-0.891671	2.274052
C	3.860922	-1.292069	-2.055119
H	2.951633	-1.854656	-2.300353
H	3.976340	-0.520944	-2.826899
H	4.705221	-1.982534	-2.148000

TS2c

B3LYP SCF energy: -1448.85174036 a.u.
B3LYP enthalpy: -1448.233184 a.u.
B3LYP free energy: -1448.327101 a.u.
M06 SCF energy in solution: -2787.50813336 a.u.
M06 enthalpy in solution: -2786.889577 a.u.
M06 free energy in solution: -2786.983494 a.u.
Three lowest frequencies (cm-1): -1227.8825 14.7800 27.2998
Imaginary frequency: -1227.8825 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ni	0.310073	0.523713	0.318915
P	-1.811907	-0.139485	0.048145
C	-2.788898	1.407069	-0.610831
C	-2.435331	2.607387	0.302524
C	-2.250104	1.768437	-2.014606
C	-4.322852	1.271935	-0.685011
H	-2.836085	2.517399	1.312377
H	-1.352966	2.745362	0.374987
H	-2.861181	3.518895	-0.137732

H	-2.582220	1.068836	-2.785864
H	-2.644830	2.755646	-2.289567
H	-1.156889	1.822761	-2.026228
H	-4.734048	2.186819	-1.133080
H	-4.645293	0.433025	-1.307295
H	-4.785998	1.164097	0.299747
C	-1.767815	-1.503189	-1.340504
C	-3.089941	-1.726231	-2.102633
C	-0.662795	-1.112645	-2.352073
C	-1.324931	-2.851590	-0.730669
H	-3.914337	-2.017859	-1.446892
H	-3.399407	-0.844942	-2.669404
H	-2.946268	-2.538972	-2.827669
H	0.306133	-0.978589	-1.861876
H	-0.562162	-1.923170	-3.086772
H	-0.876915	-0.195874	-2.898702
H	-1.121375	-3.551596	-1.551410
H	-0.404109	-2.753137	-0.147223
H	-2.091028	-3.310096	-0.101234
C	-2.756018	-0.850789	1.592263
C	-3.091618	0.299119	2.567912
C	-4.059431	-1.608414	1.260907
C	-1.820037	-1.798633	2.378336
H	-2.209778	0.904408	2.802243
H	-3.881155	0.957663	2.199441
H	-3.450016	-0.139070	3.508430
H	-3.875431	-2.528994	0.700870
H	-4.548359	-1.898227	2.200932
H	-4.772322	-1.003634	0.695954
H	-2.366493	-2.172283	3.254822
H	-1.493076	-2.666143	1.805954
H	-0.932612	-1.273147	2.733694
C	1.211655	-0.271938	1.780986
C	2.250016	0.512105	1.057996
H	0.883993	0.136243	2.739969
H	2.572293	1.391337	1.619458
H	1.331884	-1.355438	1.807687
C	3.392758	-0.221601	0.400972
C	4.709600	0.290484	0.441805
C	3.160298	-1.426979	-0.278947
C	5.737048	-0.432784	-0.178740
C	4.193185	-2.134619	-0.890276
H	2.146018	-1.813736	-0.331507
C	5.494438	-1.636053	-0.839627
H	6.750162	-0.038144	-0.139713
H	3.979429	-3.066117	-1.408343
O	1.035241	1.780009	-1.124603
H	1.785240	1.200851	-0.054321
C	1.129497	3.172501	-0.964515
H	1.869867	3.590847	-1.665345
H	0.169519	3.677632	-1.166139
H	1.440533	3.472513	0.054860
H	6.311841	-2.173287	-1.313284
C	5.042360	1.591784	1.139698
H	4.499484	2.441997	0.707340
H	4.794474	1.561545	2.208737

H	6.111603	1.810697	1.057327

TS3c

B3LYP SCF energy:	-1989.61790811 a.u.		
B3LYP enthalpy:	-1988.761060 a.u.		
B3LYP free energy:	-1988.880538 a.u.		
M06 SCF energy in solution:	-3328.04830057 a.u.		
M06 enthalpy in solution:	-3327.191452 a.u.		
M06 free energy in solution:	-3327.310930 a.u.		
Three lowest frequencies (cm-1):	-432.8117	6.5356	11.2662
Imaginary frequency:	-432.8117 cm-1		

Cartesian coordinates

ATOM	X	Y	Z
Ni	0.129508	-1.382798	0.338876
C	-1.463879	-1.602163	-0.691700
O	-1.384822	-1.843780	-1.886074
C	-2.839226	-1.484581	-0.014029
H	-2.919528	-2.353855	0.655294
H	-2.840799	-0.611712	0.653059
C	-4.031753	-1.448006	-0.988416
H	-3.941689	-0.566410	-1.633970
H	-3.961475	-2.317373	-1.650854
C	-5.364229	-1.433175	-0.273530
C	-6.001624	-2.630506	0.083918
C	-5.985183	-0.225183	0.075364
C	-7.217120	-2.622742	0.769609
H	-5.540911	-3.578778	-0.185938
C	-7.201067	-0.210838	0.760937
H	-5.512252	0.715402	-0.201273
C	-7.822098	-1.411288	1.111523
H	-7.695155	-3.563426	1.031479
H	-7.666333	0.738151	1.016036
H	-8.770775	-1.402988	1.641719
C	0.844223	-2.795564	1.740447
H	0.963504	-3.824186	1.410170
H	0.183124	-2.672077	2.595049
H	-0.496652	-2.732638	0.560468
P	0.497710	0.840878	-0.102719
C	0.923021	1.667714	1.548289
C	1.327871	3.158480	1.635827
C	-0.161522	1.353013	2.604621
H	1.813630	1.089092	1.832565
C	1.848060	3.486535	3.047947
H	0.469570	3.803639	1.432872
H	2.085305	3.413485	0.888053
C	0.313420	1.716833	4.022449
H	-1.077631	1.914758	2.371219
H	-0.429634	0.289950	2.561130
C	0.789225	3.174061	4.115921
H	2.138421	4.543829	3.098513
H	2.758107	2.902177	3.250618
H	-0.492863	1.531381	4.743593
H	1.141757	1.048920	4.302168

H	1.184432	3.380163	5.118691
H	-0.070531	3.845815	3.974782
C	-1.019652	1.736394	-0.843486
C	-1.168688	3.244942	-0.551617
C	-1.154910	1.479547	-2.365159
H	-1.859932	1.228136	-0.350862
C	-2.463061	3.828643	-1.149820
H	-0.303844	3.792144	-0.953314
H	-1.186564	3.422110	0.526314
C	-2.458871	2.060840	-2.937831
H	-0.312553	1.953738	-2.886672
H	-1.112912	0.409401	-2.579189
C	-2.584302	3.561214	-2.653416
H	-2.503639	4.905924	-0.942475
H	-3.325799	3.380865	-0.633932
H	-2.496794	1.867001	-4.017195
H	-3.318059	1.533347	-2.498436
H	-3.536870	3.950150	-3.035203
H	-1.787618	4.101341	-3.186519
C	1.924522	1.244067	-1.281248
C	3.314482	1.301881	-0.608117
C	1.980337	0.203056	-2.427690
H	1.712660	2.235660	-1.709268
C	4.412958	1.660340	-1.626863
H	3.542356	0.323153	-0.171077
H	3.337658	2.029833	0.207258
C	3.066341	0.555186	-3.458048
H	2.201182	-0.778383	-1.989247
H	1.015043	0.102571	-2.927186
C	4.447923	0.674577	-2.801817
H	5.385729	1.682904	-1.118746
H	4.234930	2.677977	-2.006580
H	3.082424	-0.207937	-4.246511
H	2.809371	1.506217	-3.949290
H	5.198035	0.988741	-3.539293
H	4.758674	-0.312761	-2.432962
C	1.882814	-1.874164	1.538556
H	1.979599	-1.071131	2.260623
C	3.084498	-2.225863	0.751175
C	4.377033	-1.807337	1.159314
C	2.971694	-3.029071	-0.400445
C	5.488046	-2.196945	0.401386
C	4.090170	-3.410011	-1.138976
H	1.983721	-3.343209	-0.727664
C	5.359881	-2.989991	-0.740204
H	6.477527	-1.879227	0.723578
H	3.967109	-4.027159	-2.025160
H	6.241695	-3.279939	-1.305118
C	4.583722	-0.983014	2.411050
H	5.649960	-0.816580	2.593747
H	4.107184	0.004320	2.343609
H	4.166472	-1.478408	3.296625

TS4c

B3LYP SCF energy: -1989.61770092 a.u.
B3LYP enthalpy: -1988.761459 a.u.
B3LYP free energy: -1988.881864 a.u.
M06 SCF energy in solution: -3328.04412334 a.u.
M06 enthalpy in solution: -3327.187881 a.u.
M06 free energy in solution: -3327.308286 a.u.
Three lowest frequencies (cm-1): -488.5851 10.1953 12.8761
Imaginary frequency: -488.5851 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ni	-0.657307	0.836063	0.290347
C	0.848581	1.354236	-0.767472
O	0.677907	1.543616	-1.965334
C	2.242348	1.544780	-0.153216
H	2.163013	2.406428	0.526015
H	2.465232	0.688660	0.498183
C	3.371881	1.768147	-1.177264
H	3.431431	0.895900	-1.839575
H	3.098609	2.615217	-1.815483
C	4.709824	2.009930	-0.515667
C	5.110445	3.304235	-0.152146
C	5.571542	0.944497	-0.216833
C	6.327652	3.527070	0.493107
H	4.460799	4.146135	-0.383172
C	6.790397	1.160970	0.428149
H	5.284723	-0.066619	-0.500353
C	7.173039	2.454960	0.787212
H	6.618748	4.539662	0.761404
H	7.443883	0.319449	0.644982
H	8.122980	2.627011	1.286433
C	-1.993831	2.196920	1.263578
H	-0.421434	2.315274	0.499359
P	-0.508923	-1.412866	0.037980
C	-0.255481	-2.097871	1.785486
C	-0.212864	-3.619014	2.062070
C	0.947943	-1.409138	2.469108
H	-1.158010	-1.711524	2.281234
C	-0.244449	-3.886083	3.578246
H	0.707965	-4.052523	1.661971
H	-1.037687	-4.144401	1.570000
C	0.972188	-1.696254	3.980987
H	1.883533	-1.766938	2.014330
H	0.907336	-0.327070	2.295978
C	0.934229	-3.200993	4.285636
H	-0.222807	-4.967676	3.763802
H	-1.191781	-3.515258	3.997063
H	1.862341	-1.238302	4.430687
H	0.102111	-1.210890	4.447618
H	0.879459	-3.367451	5.368902
H	1.872933	-3.663168	3.945567
C	0.933180	-1.994661	-1.057871
C	1.432190	-3.446255	-0.899326
C	0.661468	-1.698012	-2.553097
H	1.750067	-1.331196	-0.739376
C	2.658761	-3.728805	-1.789401

H	0.625926	-4.150356	-1.151701
H	1.713394	-3.644344	0.136804
C	1.905750	-1.957495	-3.418457
H	-0.143382	-2.356791	-2.906939
H	0.330871	-0.665035	-2.686066
C	2.404871	-3.399196	-3.264780
H	2.957907	-4.778672	-1.673391
H	3.503038	-3.123544	-1.426739
H	1.670661	-1.741123	-4.468155
H	2.701860	-1.256580	-3.128280
H	3.318292	-3.558096	-3.852016
H	1.648911	-4.089688	-3.667959
C	-2.037817	-2.290229	-0.659776
C	-3.137117	-2.598698	0.383739
C	-2.665797	-1.460377	-1.808396
H	-1.688590	-3.248665	-1.073231
C	-4.319826	-3.347446	-0.256985
H	-3.500860	-1.659017	0.816455
H	-2.747583	-3.193181	1.213848
C	-3.850146	-2.195223	-2.458312
H	-3.008015	-0.501205	-1.398451
H	-1.924482	-1.214341	-2.571772
C	-4.926201	-2.563735	-1.428533
H	-5.083343	-3.546635	0.506116
H	-3.972899	-4.328429	-0.614603
H	-4.278438	-1.569410	-3.251455
H	-3.484279	-3.110698	-2.947123
H	-5.728196	-3.144475	-1.901753
H	-5.390175	-1.642895	-1.045631
C	-2.418412	0.855553	1.358543
H	-3.247517	0.525744	0.739836
H	-2.274459	0.315232	2.292165
H	-1.536125	2.625698	2.153891
C	-2.710410	3.179624	0.383514
C	-3.605261	4.101244	0.974169
C	-2.539458	3.180450	-1.007153
C	-4.305339	4.984453	0.144292
C	-3.250125	4.066642	-1.818542
C	-4.137745	4.972754	-1.241241
H	-4.995702	5.693331	0.596507
H	-3.097729	4.052569	-2.894427
H	-4.693352	5.671511	-1.861329
H	-1.816974	2.500139	-1.451145
C	-3.823804	4.138761	2.470103
H	-4.132076	3.160724	2.859411
H	-2.910027	4.421468	3.010426
H	-4.598133	4.865910	2.733567

TS7a

B3LYP SCF energy:	-2175.68936555 a.u.
B3LYP enthalpy:	-2174.695310 a.u.
B3LYP free energy:	-2174.843467 a.u.
M06 SCF energy in solution:	-3514.00827069 a.u.
M06 enthalpy in solution:	-3513.014215 a.u.

M06 free energy in solution: -3513.162372 a.u.
Three lowest frequencies (cm-1): -995.9637 12.8700 17.1962
Imaginary frequency: -995.9637 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ni	0.442223	-0.139037	-1.105032
Al	-6.455237	0.064306	-1.528123
N	0.486770	-0.260261	1.882962
N	1.809709	1.264060	1.121753
N	-4.382208	0.047007	-1.483025
C	0.922119	0.295985	0.701244
C	1.092503	0.335212	2.987310
C	1.911368	1.298565	2.511796
C	-3.730004	-1.071790	-1.101359
C	-2.347488	-1.155875	-1.041668
C	-1.532363	-0.047728	-1.367487
C	-2.243196	1.099231	-1.784278
C	-3.632086	1.114866	-1.822048
C	-6.876531	1.948868	-2.055860
C	-6.863421	-1.342790	-2.890489
C	-6.911632	-0.420153	0.362829
C	1.167513	-0.568649	-3.013313
C	2.200817	-0.587307	-2.040377
C	-0.569395	-1.236213	2.045221
C	-0.287251	-2.604969	1.845316
C	-1.833929	-0.780337	2.473982
C	-1.331350	-3.516394	2.044737
C	-2.838673	-1.738690	2.664357
C	-2.596395	-3.089862	2.444077
C	1.116823	-3.096119	1.503786
C	-2.134413	0.685652	2.781911
C	-3.370267	1.213925	2.031660
C	-2.297064	0.896687	4.302452
C	1.130403	-4.357622	0.624449
C	1.930653	-3.340114	2.793708
C	2.560965	2.178401	0.290147
C	3.954895	1.990983	0.167521
C	1.894288	3.276235	-0.301120
C	4.674104	2.926329	-0.589136
C	4.038360	4.000000	-1.201278
C	2.663858	4.170126	-1.055278
C	4.706362	0.845687	0.844949
C	5.678114	0.126280	-0.110112
C	5.476875	1.344042	2.086600
C	0.405551	3.538339	-0.077134
C	-0.264653	4.302545	-1.231587
C	0.182185	4.294997	1.250868
H	0.867462	0.024809	3.994940
H	2.547429	2.005434	3.018812
H	-4.359647	-1.915999	-0.836260
H	-1.905373	-2.094643	-0.721273
H	-0.357917	-0.368602	-2.367693
H	-1.714278	1.995743	-2.093757
H	-4.185113	1.996227	-2.131415
H	-6.495067	2.703061	-1.351089

H	-7.967162	2.091886	-2.086419
H	-6.510224	2.226217	-3.055589
H	-6.459635	-1.103873	-3.885102
H	-7.949419	-1.463854	-3.019336
H	-6.476099	-2.337349	-2.623119
H	-6.491269	-1.385541	0.683170
H	-8.000496	-0.504494	0.496497
H	-6.569987	0.332657	1.088630
H	-3.825594	-1.418822	2.984399
H	-1.152146	-4.576075	1.896183
H	-1.281951	1.287462	2.454336
H	1.616931	-2.304251	0.939686
H	-3.155554	0.334617	4.688141
H	-2.464231	1.957101	4.524576
H	-1.410967	0.569320	4.858296
H	-3.519270	2.275125	2.264817
H	-4.286213	0.685208	2.315937
H	-3.248654	1.117019	0.950500
H	1.460716	-4.116727	3.409058
H	2.010175	-2.432350	3.401267
H	2.947126	-3.671255	2.548934
H	2.154711	-4.572036	0.300566
H	0.510658	-4.233408	-0.270330
H	0.772131	-5.241711	1.164389
H	-3.391692	-3.815366	2.592819
H	5.747490	2.807921	-0.700944
H	4.613956	4.710967	-1.787953
H	3.970818	0.106707	1.178046
H	5.180878	-0.186993	-1.031858
H	6.088061	-0.766004	0.377106
H	6.526588	0.763254	-0.384998
H	5.991629	0.509874	2.577857
H	4.816356	1.812073	2.823659
H	6.232788	2.085675	1.802453
H	-0.096275	2.569084	-0.002039
H	-0.066052	3.831325	-2.200766
H	0.069802	5.345067	-1.287906
H	-1.349004	4.322604	-1.077765
H	0.577423	3.740539	2.108018
H	-0.888560	4.458568	1.420949
H	0.674234	5.275010	1.226531
H	2.183580	5.019317	-1.528677
H	0.856304	-1.508974	-3.471686
H	1.064047	0.293233	-3.672407
H	2.833002	0.297759	-1.979248
C	2.869231	-1.897792	-1.667070
H	3.343250	-1.813645	-0.679550
H	2.111088	-2.686895	-1.576032
C	3.928357	-2.356420	-2.691337
H	4.673985	-1.559769	-2.831421
H	3.443910	-2.488899	-3.669213
C	4.641179	-3.654978	-2.291673
H	5.132825	-3.512696	-1.318271
H	3.893187	-4.447177	-2.141917
C	5.675496	-4.120090	-3.322521
H	6.454719	-3.362306	-3.471574

H	5.206989	-4.307165	-4.296558
H	6.168068	-5.046932	-3.006497

TS8a

B3LYP SCF energy: -2175.69514137 a.u.
B3LYP enthalpy: -2174.701328 a.u.
B3LYP free energy: -2174.851743 a.u.
M06 SCF energy in solution: -3514.01132735 a.u.
M06 enthalpy in solution: -3513.017514 a.u.
M06 free energy in solution: -3513.167929 a.u.
Three lowest frequencies (cm-1): -639.9689 12.6504 16.3231
Imaginary frequency: -639.9689 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ni	-0.540849	0.553517	-0.767080
Al	6.034015	2.156598	0.391328
N	-1.886496	-1.340815	1.139546
N	-0.280465	-2.302450	0.073227
N	4.038697	1.711683	0.073115
C	-0.903284	-1.084617	0.208465
C	-1.862127	-2.670479	1.559675
C	-0.863036	-3.275954	0.881146
C	3.047563	2.186636	0.855232
C	1.707476	1.901080	0.630484
C	1.301699	1.068690	-0.437829
C	2.363603	0.598220	-1.246280
C	3.679986	0.926977	-0.966067
C	6.848175	0.338927	0.618783
C	6.532390	3.104632	-1.299503
C	5.987781	3.288754	2.042923
C	-1.664537	1.840561	-2.064383
C	-2.384476	0.714670	-1.657154
C	-2.868577	-0.409130	1.649182
C	-4.210677	-0.545696	1.229893
C	-2.471257	0.552705	2.605108
C	-5.156254	0.329519	1.781584
C	-3.458815	1.406695	3.111429
C	-4.786973	1.299941	2.706145
C	-4.672641	-1.617467	0.241450
C	-1.039285	0.625795	3.133458
C	-0.632434	2.028513	3.615558
C	-0.827830	-0.399257	4.269576
C	-5.559840	-1.055239	-0.887164
C	-5.419904	-2.754048	0.971846
C	0.888015	-2.585837	-0.728502
C	0.743512	-2.770932	-2.118761
C	2.128753	-2.731306	-0.070674
C	1.897368	-3.068738	-2.855684
C	3.137583	-3.195033	-2.235626
C	3.246489	-3.036392	-0.857356
C	-0.609454	-2.728511	-2.823517
C	-0.611208	-1.776968	-4.034043
C	-1.050071	-4.148048	-3.236749

C	2.286120	-2.617324	1.445009
C	3.379535	-1.617084	1.861617
C	2.557541	-4.003622	2.067074
H	-2.551176	-3.047158	2.297931
H	-0.502849	-4.291996	0.897783
H	3.364377	2.819162	1.678536
H	0.973543	2.346605	1.294590
H	0.099182	1.758542	-1.360204
H	2.166648	-0.035794	-2.105371
H	4.495629	0.561043	-1.583023
H	6.475044	-0.187713	1.509590
H	7.939796	0.410047	0.737890
H	6.680477	-0.329032	-0.239846
H	6.408625	2.487242	-2.201864
H	7.588519	3.412997	-1.284279
H	5.945653	4.020666	-1.461363
H	5.431994	4.230625	1.921946
H	7.011547	3.579191	2.323254
H	5.569552	2.778266	2.923525
H	-1.214117	1.825441	-3.057458
H	-2.502967	-0.135967	-2.322782
H	-3.124919	0.813553	-0.869195
H	-3.188032	2.161179	3.841843
H	-6.196019	0.248855	1.479630
H	-0.366599	0.360377	2.312518
H	-3.784633	-2.050072	-0.229715
H	-1.489193	-0.181320	5.117046
H	0.207062	-0.360381	4.629326
H	-1.029758	-1.422856	3.938219
H	0.441498	2.046083	3.829995
H	-1.148584	2.313519	4.539882
H	-0.841764	2.795618	2.861662
H	-6.329411	-2.376817	1.454042
H	-4.803439	-3.218778	1.748239
H	-5.714985	-3.535730	0.262128
H	-5.783171	-1.847367	-1.611359
H	-5.069839	-0.236355	-1.421456
H	-6.518668	-0.685208	-0.506978
H	-5.535452	1.971546	3.118120
H	1.820173	-3.217492	-3.928777
H	4.019383	-3.427530	-2.826648
H	-1.349728	-2.348966	-2.114440
H	-0.316084	-0.764713	-3.738195
H	-1.614365	-1.726092	-4.473993
H	0.073903	-2.113611	-4.820529
H	-2.042294	-4.121981	-3.703043
H	-1.099850	-4.818169	-2.370996
H	-0.351321	-4.587442	-3.958303
H	1.343561	-2.248266	1.859631
H	3.170192	-0.616830	1.476113
H	4.372102	-1.913294	1.505997
H	3.428838	-1.557846	2.955469
H	1.768730	-4.724331	1.822236
H	2.618948	-3.926107	3.158825
H	3.506589	-4.417915	1.707455
H	4.216841	-3.146540	-0.382894

C	-1.959495	3.228798	-1.523080
H	-1.049025	3.842090	-1.526456
H	-2.284079	3.151690	-0.476987
C	-3.048501	3.944395	-2.344844
H	-3.964699	3.337629	-2.336049
H	-2.729324	4.003514	-3.396008
C	-3.360707	5.355843	-1.830136
H	-2.439445	5.955390	-1.834898
H	-3.679254	5.294731	-0.779615
C	-4.439728	6.070164	-2.650912
H	-4.132976	6.179903	-3.698401
H	-5.382669	5.509487	-2.639717
H	-4.643183	7.072510	-2.257043

TS1d

B3LYP SCF energy: -1754.71230522 a.u.
B3LYP enthalpy: -1753.910472 a.u.
B3LYP free energy: -1754.032605 a.u.
M06 SCF energy in solution: -3093.12582189 a.u.
M06 enthalpy in solution: -3092.323989 a.u.
M06 free energy in solution: -3092.446122 a.u.
Three lowest frequencies (cm-1): -1208.7720 12.3821 17.2115
Imaginary frequency: -1208.7720 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ni	-0.309214	0.068077	-1.449625
O	-1.482336	1.442384	-2.480026
C	0.744711	-1.376900	-2.188999
C	0.044115	-0.667440	-3.300501
H	0.713043	-0.212118	-4.036921
H	-0.727558	-1.272215	-3.787334
C	-0.918807	2.670288	-2.860711
H	0.132925	2.580563	-3.192368
H	-1.483447	3.116124	-3.697099
H	-0.931642	3.398789	-2.032386
H	-0.747936	0.417709	-3.044045
C	2.224427	-1.350764	-2.114447
C	2.939959	-2.530373	-1.835744
C	2.973082	-0.183201	-2.364556
C	4.335586	-2.547741	-1.808687
H	2.387795	-3.451545	-1.659706
C	4.365459	-0.197683	-2.338819
H	2.449274	0.746174	-2.573511
C	5.057618	-1.380357	-2.060467
H	4.858209	-3.478125	-1.599023
H	4.915037	0.720252	-2.532879
H	6.144249	-1.390331	-2.042805
H	0.331848	-2.355136	-1.936887
N	0.306234	0.612952	1.470159
N	-1.696187	-0.076204	1.065773
C	-0.495482	0.173196	0.445433
C	-0.387593	0.650483	2.679278
C	-1.641910	0.211772	2.425954

C	1.718858	0.914347	1.396728
C	2.134712	2.171428	0.908026
C	2.628240	-0.042811	1.894152
C	3.508808	2.438220	0.903500
C	3.990504	0.282160	1.869021
C	4.428865	1.505023	1.374443
C	1.135440	3.239500	0.468970
C	2.184345	-1.375424	2.495426
C	2.946435	-2.577414	1.909484
C	2.319858	-1.355381	4.032798
C	1.670017	4.158204	-0.642442
C	0.679240	4.082486	1.679849
C	-2.885776	-0.597552	0.429213
C	-3.921914	0.296315	0.094208
C	-2.992600	-1.992044	0.232879
C	-5.091358	-0.246519	-0.454300
C	-5.221543	-1.614748	-0.665637
C	-4.181018	-2.476136	-0.325745
C	-3.826370	1.800304	0.330834
C	-4.170807	2.605453	-0.935569
C	-4.710949	2.226884	1.520536
C	-1.895946	-2.962711	0.665195
C	-1.685212	-4.119118	-0.328085
C	-2.185248	-3.512350	2.078294
H	0.080535	0.979742	3.592800
H	-2.496222	0.081495	3.070841
H	4.715831	-0.435592	2.240009
H	3.866321	3.392286	0.531367
H	1.126284	-1.520454	2.257470
H	0.255120	2.729603	0.066326
H	3.366691	-1.225145	4.332142
H	1.963132	-2.299679	4.461149
H	1.743146	-0.541055	4.484740
H	2.527619	-3.511206	2.303923
H	4.008949	-2.558012	2.178776
H	2.878204	-2.597696	0.818975
H	1.529704	4.610327	2.128520
H	0.220029	3.461999	2.456489
H	-0.058800	4.831407	1.368543
H	0.864282	4.804828	-1.005806
H	2.049085	3.582656	-1.493405
H	2.474147	4.813128	-0.286691
H	5.490803	1.735816	1.359686
H	-5.908116	0.416333	-0.723271
H	-6.136810	-2.013486	-1.095401
H	-2.788416	2.035844	0.583840
H	-3.531843	2.284877	-1.763115
H	-4.005319	3.674366	-0.752114
H	-5.222172	2.484048	-1.223599
H	-4.609750	3.302941	1.705627
H	-4.440046	1.698685	2.442452
H	-5.768984	2.019976	1.319165
H	-0.954796	-2.407349	0.708676
H	-1.534351	-3.748150	-1.347142
H	-2.533997	-4.812808	-0.342516
H	-0.800201	-4.698810	-0.041138

H	-2.254381	-2.706405	2.816976
H	-1.388009	-4.194934	2.396879
H	-3.131743	-4.066121	2.096162
H	-4.297838	-3.542422	-0.491265

TS2d

B3LYP SCF energy: -1754.71071050 a.u.
B3LYP enthalpy: -1753.908621 a.u.
B3LYP free energy: -1754.031475 a.u.
M06 SCF energy in solution: -3093.12029853 a.u.
M06 enthalpy in solution: -3092.318209 a.u.
M06 free energy in solution: -3092.441063 a.u.
Three lowest frequencies (cm-1): -1274.1088 14.1594 20.8549
Imaginary frequency: -1274.1088 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ni	-0.162422	0.806355	-0.656358
O	0.302153	2.792359	-0.147831
C	-1.396691	0.215883	-1.962278
C	-1.504908	1.695680	-1.936972
H	-1.133415	2.164394	-2.858193
C	1.306452	3.480777	-0.856195
H	1.253065	3.308106	-1.947720
H	1.212517	4.567814	-0.696641
H	2.315937	3.183694	-0.533840
H	-0.607501	2.358963	-1.083293
H	-2.246883	-0.356063	-1.589101
N	1.994700	-0.871866	0.444495
N	0.060313	-1.745886	0.805368
C	0.659354	-0.662275	0.211792
C	2.214975	-2.045140	1.160573
C	0.997596	-2.590204	1.394455
C	3.063146	0.021462	0.064625
C	3.547504	0.932658	1.025361
C	3.612739	-0.081702	-1.228683
C	4.620416	1.752664	0.653473
C	4.679818	0.767423	-1.547740
C	5.182471	1.673223	-0.617818
C	2.951333	1.054903	2.424959
C	3.098586	-1.073470	-2.267346
C	2.521637	-0.347335	-3.497875
C	4.189673	-2.083522	-2.673199
C	2.338995	2.450263	2.659494
C	3.988990	0.705161	3.510168
C	-1.360501	-1.997182	0.865504
C	-2.130809	-1.321766	1.834097
C	-1.915149	-2.946922	-0.017348
C	-3.497868	-1.620990	1.894614
C	-4.072000	-2.553443	1.035656
C	-3.286080	-3.210281	0.092669
C	-1.527917	-0.333267	2.827911
C	-2.285819	1.006438	2.859864
C	-1.448756	-0.959637	4.235624

C	-1.079264	-3.698363	-1.050734
C	-1.677439	-3.613224	-2.467886
C	-0.881063	-5.170580	-0.634310
H	3.207082	-2.368388	1.433647
H	0.706986	-3.486952	1.918165
H	5.124821	0.714245	-2.537335
H	5.016108	2.467297	1.369585
H	2.279051	-1.641014	-1.817750
H	2.136468	0.330345	2.512266
H	5.039788	-1.587712	-3.156294
H	3.786345	-2.816361	-3.382185
H	4.573042	-2.628485	-1.802939
H	2.113736	-1.073103	-4.211670
H	3.289219	0.237669	-4.018087
H	1.716706	0.333608	-3.202326
H	4.830761	1.407584	3.503971
H	4.396540	-0.303113	3.369960
H	3.528091	0.749717	4.503914
H	1.882406	2.493147	3.656300
H	1.569577	2.672199	1.912144
H	3.104371	3.234905	2.614973
H	6.013301	2.320895	-0.885202
H	-4.119877	-1.116963	2.628106
H	-5.135013	-2.769722	1.101716
H	-0.506527	-0.110392	2.509008
H	-2.343219	1.454886	1.863493
H	-1.766573	1.711261	3.519486
H	-3.307324	0.890359	3.241048
H	-0.980946	-0.260515	4.938956
H	-0.858404	-1.883357	4.232022
H	-2.447045	-1.203223	4.618788
H	-0.091430	-3.229682	-1.092233
H	-1.819640	-2.573417	-2.776716
H	-2.645826	-4.122330	-2.534045
H	-1.005121	-4.095778	-3.187202
H	-0.405384	-5.251959	0.349495
H	-0.248326	-5.694417	-1.360686
H	-1.840937	-5.698017	-0.582745
H	-3.744601	-3.937501	-0.571122
H	-0.916490	-0.241448	-2.830007
C	-2.822111	2.296791	-1.484350
C	-2.877985	3.293391	-0.496307
C	-4.026623	1.883867	-2.077305
C	-4.098913	3.854481	-0.113791
H	-1.952922	3.614488	-0.024923
C	-5.246525	2.444095	-1.696686
H	-4.001945	1.118415	-2.849153
C	-5.287876	3.433434	-0.711281
H	-4.118301	4.622367	0.656020
H	-6.165684	2.109417	-2.172044
H	-6.237400	3.871838	-0.414380

TS7b
B3LYP SCF energy: -1712.56977078 a.u.

B3LYP enthalpy: -1711.878529 a.u.
B3LYP free energy: -1711.986488 a.u.
M06 SCF energy in solution: -3051.19454040 a.u.
M06 enthalpy in solution: -3050.503299 a.u.
M06 free energy in solution: -3050.611258 a.u.
Three lowest frequencies (cm-1): -1113.8631 13.1084 23.9659
Imaginary frequency: -1113.8631 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ni	-0.871135	1.395618	-0.285000
Al	5.877013	-0.392008	0.080502
N	3.885359	0.215058	-0.005271
C	3.172047	0.522482	1.096043
C	1.847831	0.940525	1.039337
C	1.161831	1.035103	-0.189902
C	1.954470	0.757603	-1.324881
C	3.274436	0.346213	-1.199423
C	6.155923	-0.694330	2.039035
C	5.840212	-2.041311	-1.053609
C	6.815314	1.187549	-0.709383
C	-0.632718	3.437354	-0.693545
C	-2.005364	3.068345	-0.518010
H	3.699011	0.420120	2.039370
H	1.349970	1.178947	1.974711
H	0.353525	2.333195	-0.407121
H	1.545771	0.858097	-2.327429
H	3.881882	0.107917	-2.067542
H	6.078898	0.216477	2.651511
H	7.170205	-1.084279	2.211828
H	5.470963	-1.436639	2.475363
H	5.160633	-2.812843	-0.662853
H	6.837726	-2.503608	-1.095653
H	5.548164	-1.860981	-2.099113
H	6.501198	1.410187	-1.740012
H	7.902301	1.022878	-0.750510
H	6.664822	2.108035	-0.126695
H	-0.176315	4.088965	0.055715
H	-0.267524	3.622146	-1.705239
H	-2.585089	2.977011	-1.436069
C	-2.770685	3.606469	0.676398
H	-3.684691	3.039013	0.872395
H	-2.160778	3.585170	1.587689
H	-3.072587	4.652376	0.513896
P	-2.131272	-0.511443	-0.014192
C	-2.413483	-0.774100	1.897151
C	-3.885044	-0.538959	-0.882292
C	-1.147504	-2.055750	-0.704145
C	-1.125554	-0.316692	2.619513
H	-1.264417	-0.436703	3.702468
H	-0.240490	-0.885209	2.333681
H	-0.927333	0.742393	2.421917
C	-2.755225	-2.212011	2.339958
H	-2.927114	-2.211452	3.424821
H	-3.663064	-2.595197	1.868549
H	-1.946073	-2.918919	2.146565

C	-3.533273	0.157798	2.408812
H	-4.528773	-0.153972	2.086194
H	-3.528894	0.130889	3.506334
H	-3.373625	1.195998	2.106211
C	-4.613162	0.806170	-0.666523
H	-4.059949	1.634560	-1.107092
H	-5.588901	0.751235	-1.167606
H	-4.801749	1.037345	0.380983
C	-4.835541	-1.661592	-0.409663
H	-5.163336	-1.517614	0.623108
H	-5.738039	-1.640304	-1.035456
H	-4.406526	-2.660498	-0.493286
C	-3.695616	-0.662340	-2.411513
H	-4.657036	-0.454392	-2.898779
H	-2.969979	0.063684	-2.794091
H	-3.388553	-1.661648	-2.725538
C	-1.938881	-3.372961	-0.847256
H	-2.726070	-3.312764	-1.602067
H	-1.243988	-4.157498	-1.175482
H	-2.386063	-3.709986	0.090901
C	-0.585624	-1.678121	-2.096261
H	0.125227	-2.453658	-2.410171
H	-1.354275	-1.613686	-2.866590
H	-0.048404	-0.729228	-2.066092
C	0.075513	-2.338810	0.197862
H	-0.200429	-2.739484	1.175536
H	0.695777	-3.098610	-0.294561
H	0.696740	-1.454245	0.342340

TS8b

B3LYP SCF energy: -1712.57527638 a.u.
B3LYP enthalpy: -1711.884431 a.u.
B3LYP free energy: -1711.994744 a.u.
M06 SCF energy in solution: -3051.19983811 a.u.
M06 enthalpy in solution: -3050.508993 a.u.
M06 free energy in solution: -3050.619306 a.u.
Three lowest frequencies (cm-1): -1028.7552 8.6076 12.7126
Imaginary frequency: -1028.7552 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ni	-0.871390	1.376436	-0.291663
Al	5.742007	-0.577155	0.034237
N	3.789169	0.140172	-0.046341
C	3.119252	0.546942	1.050469
C	1.804040	0.991607	1.003777
C	1.085697	1.013440	-0.210441
C	1.829823	0.628735	-1.347898
C	3.142866	0.195730	-1.229182
C	6.654167	0.567306	-1.330036
C	6.255678	-0.242038	1.939246
C	5.486024	-2.495037	-0.477779
C	-0.833645	3.491366	-0.556169
C	-2.143501	2.933699	-0.558121

H	3.675567	0.503965	1.981429
H	1.335746	1.308033	1.932393
H	0.279229	2.362868	-0.440635
H	1.380914	0.648526	-2.337945
H	3.717803	-0.121611	-2.094270
H	6.243434	0.464154	-2.345697
H	7.719512	0.303579	-1.407826
H	6.619843	1.638064	-1.081638
H	6.209265	0.817317	2.232692
H	7.299306	-0.551544	2.100208
H	5.661204	-0.807440	2.672551
H	4.861749	-3.049389	0.238260
H	6.449825	-3.023989	-0.520343
H	5.023833	-2.624765	-1.467887
H	-0.430681	3.790522	-1.526889
H	-2.673892	2.864683	-1.504540
H	-2.776038	3.105520	0.310171
C	-0.344717	4.339697	0.608900
H	0.748308	4.357195	0.683176
H	-0.686510	5.374598	0.481515
H	-0.744168	3.971533	1.559977
P	-2.131909	-0.518969	0.020413
C	-1.210685	-2.223607	-0.265285
C	-2.794202	-0.510906	1.853811
C	-3.665921	-0.497418	-1.194748
C	-4.432579	-1.826708	-1.363475
H	-4.827642	-2.210228	-0.419137
H	-5.290936	-1.649086	-2.025463
H	-3.831509	-2.610492	-1.828760
C	-4.692414	0.564392	-0.739703
H	-4.237270	1.542049	-0.584839
H	-5.447998	0.672291	-1.529069
H	-5.223843	0.278269	0.170355
C	-3.154481	-0.045473	-2.584913
H	-2.496460	-0.775203	-3.057600
H	-4.017214	0.094754	-3.249793
H	-2.617627	0.904457	-2.523662
C	-4.011213	-1.417191	2.134190
H	-4.243123	-1.370753	3.206924
H	-4.908699	-1.095825	1.601246
H	-3.825737	-2.464432	1.887916
C	-1.658466	-0.922805	2.817283
H	-0.737705	-0.360087	2.633412
H	-1.979340	-0.705149	3.844357
H	-1.430025	-1.989540	2.773146
C	-3.157965	0.942693	2.234437
H	-3.968503	1.359982	1.635881
H	-3.480191	0.959810	3.284154
H	-2.290033	1.601330	2.135174
C	-1.955644	-3.471414	0.257656
H	-1.409069	-4.365211	-0.071671
H	-1.983090	-3.504078	1.350193
H	-2.977791	-3.560602	-0.111202
C	0.187140	-2.209157	0.397640
H	0.649621	-3.190614	0.228295
H	0.837302	-1.459666	-0.048328

H	0.166695	-2.045314	1.473571
C	-0.940529	-2.395755	-1.777375
H	-0.249122	-3.237248	-1.912572
H	-1.838183	-2.624291	-2.354807
H	-0.461824	-1.509372	-2.206430

TS1e

B3LYP SCF energy: -1217.80501994 a.u.
B3LYP enthalpy: -1217.272436 a.u.
B3LYP free energy: -1217.354577 a.u.
M06 SCF energy in solution: -2556.55125486 a.u.
M06 enthalpy in solution: -2556.018671 a.u.
M06 free energy in solution: -2556.100812 a.u.
Three lowest frequencies (cm-1): -1225.0929 33.9464 65.0116
Imaginary frequency: -1225.0929 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ni	1.509581	-0.122286	-0.299120
P	-0.714889	-0.002254	-0.008018
C	-1.786825	-1.420760	-0.799065
C	-1.731685	-1.308568	-2.339431
C	-1.152787	-2.789713	-0.462476
C	-3.265591	-1.446124	-0.358894
H	-2.285743	-0.452077	-2.727866
H	-0.701790	-1.254505	-2.707101
H	-2.188287	-2.210176	-2.768513
H	-1.142343	-3.014684	0.603732
H	-1.741580	-3.575052	-0.955629
H	-0.129204	-2.851928	-0.834432
H	-3.791329	-2.223950	-0.929308
H	-3.379109	-1.696784	0.699086
H	-3.782757	-0.502124	-0.541417
C	-1.118619	0.095256	1.892318
C	-2.467304	0.746711	2.261710
C	-1.079072	-1.317814	2.514689
C	0.029598	0.883513	2.567615
H	-2.526792	1.794206	1.957561
H	-3.322249	0.218685	1.831526
H	-2.585384	0.722025	3.353892
H	-0.156234	-1.850121	2.264776
H	-1.114467	-1.215129	3.607202
H	-1.931218	-1.936020	2.223738
H	-0.139408	0.892102	3.653080
H	0.998421	0.408249	2.380524
H	0.098070	1.919027	2.236024
C	-1.224065	1.680836	-0.852593
C	-0.469331	1.769291	-2.203546
C	-2.733139	1.891976	-1.088402
C	-0.688029	2.861446	-0.012578
H	0.612478	1.755923	-2.041971
H	-0.735139	0.979698	-2.906767
H	-0.723716	2.727520	-2.677370
H	-3.319146	1.839795	-0.166210
H	-2.882911	2.894571	-1.511462

H	-3.155820	1.180737	-1.802416
H	-0.851419	3.785517	-0.583203
H	-1.205081	2.980886	0.942273
H	0.387442	2.765046	0.153331
O	2.451224	1.725986	-0.449573
C	2.285930	-1.859434	-0.517432
C	3.355465	-0.857497	-0.753533
H	4.171504	-0.881534	-0.023123
H	3.731095	-0.817040	-1.780602
C	3.074762	2.307607	0.667548
H	3.659897	1.580015	1.261864
H	3.770311	3.101900	0.351930
H	2.344953	2.766699	1.356716
H	3.045632	0.476372	-0.655011
H	1.934823	-2.373318	-1.416554
C	2.400012	-2.774084	0.688440
H	1.447964	-3.265655	0.917442
H	3.140565	-3.571511	0.518043
H	2.717345	-2.223293	1.582209

TS2e

B3LYP SCF energy: -1217.80208942 a.u.
B3LYP enthalpy: -1217.269688 a.u.
B3LYP free energy: -1217.352838 a.u.
M06 SCF energy in solution: -2556.54874922 a.u.
M06 enthalpy in solution: -2556.016348 a.u.
M06 free energy in solution: -2556.099498 a.u.
Three lowest frequencies (cm-1): -1295.0733 27.1599 48.8007
Imaginary frequency: -1295.0733 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ni	-1.415571	-0.263328	0.111049
P	0.811442	-0.033891	-0.037252
C	1.158786	1.763928	-0.693005
C	0.272864	1.991262	-1.943885
C	0.657563	2.772724	0.366770
C	2.619489	2.100609	-1.052747
H	0.591189	1.413689	-2.811965
H	-0.774960	1.755227	-1.739596
H	0.328267	3.052495	-2.221519
H	1.301360	2.813358	1.248661
H	0.668529	3.775445	-0.081047
H	-0.367743	2.550946	0.680073
H	2.674302	3.158622	-1.343883
H	3.307049	1.958764	-0.214909
H	2.989740	1.518637	-1.901477
C	1.469061	-0.181564	1.788512
C	2.835357	0.478698	2.064848
C	0.404545	0.440078	2.725748
C	1.557079	-1.670147	2.191575
H	3.634116	0.081114	1.433179
H	2.808474	1.563493	1.938062
H	3.117676	0.284650	3.108742

H	-0.560064	-0.066577	2.618819
H	0.739826	0.315726	3.764666
H	0.235443	1.502368	2.556125
H	1.735809	-1.724765	3.273412
H	0.623034	-2.201308	1.984759
H	2.378681	-2.199780	1.704132
C	1.787746	-1.291534	-1.152847
C	1.524197	-0.966877	-2.639890
C	3.313350	-1.321562	-0.923414
C	1.224094	-2.715048	-0.934258
H	0.454119	-0.875281	-2.853042
H	2.027984	-0.056980	-2.972402
H	1.913259	-1.792272	-3.250311
H	3.579398	-1.698148	0.067507
H	3.768036	-2.001869	-1.656473
H	3.781685	-0.343412	-1.052976
H	1.758018	-3.404585	-1.602135
H	1.350848	-3.084672	0.082684
H	0.161857	-2.759861	-1.179564
C	-2.035228	-2.063530	0.067162
C	-3.218387	-1.226246	0.351070
H	-1.999638	-2.546435	-0.912428
H	-1.655802	-2.704319	0.865390
O	-2.455574	1.437282	0.638914
H	-2.975746	0.144871	0.527282
C	-3.096298	2.289550	-0.277947
H	-3.977185	2.766665	0.182687
H	-2.424348	3.099679	-0.607631
H	-3.444202	1.770554	-1.188922
C	-4.335182	-1.193219	-0.698098
H	-4.917155	-2.123598	-0.677523
H	-5.031820	-0.363462	-0.530668
H	-3.921961	-1.081609	-1.707305
H	-3.603352	-1.356787	1.370126

TS3e

B3LYP SCF energy: -1758.56453527 a.u.
B3LYP enthalpy: -1757.793423 a.u.
B3LYP free energy: -1757.902016 a.u.
M06 SCF energy in solution: -3097.08608773 a.u.
M06 enthalpy in solution: -3096.314975 a.u.
M06 free energy in solution: -3096.423568 a.u.
Three lowest frequencies (cm-1): -543.3306 12.0676 15.1159
Imaginary frequency: -543.3306 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ni	0.316139	-1.005917	-1.610709
C	-1.239510	0.111045	-1.816981
O	-1.195220	1.136509	-2.482788
C	-2.555310	-0.284710	-1.123632
H	-2.776919	-1.323327	-1.405538
H	-2.377338	-0.313429	-0.039107
C	-3.747152	0.638109	-1.444836

H	-3.481419	1.665878	-1.173462
H	-3.904463	0.642401	-2.529583
C	-5.011001	0.215892	-0.730568
C	-5.872980	-0.738223	-1.291633
C	-5.339477	0.741940	0.527390
C	-7.020959	-1.157322	-0.617780
H	-5.641964	-1.151747	-2.271441
C	-6.486379	0.327027	1.206338
H	-4.689844	1.491579	0.975472
C	-7.332193	-0.626452	0.636010
H	-7.676119	-1.894928	-1.074795
H	-6.722757	0.753240	2.178307
H	-8.227853	-0.948708	1.160593
C	0.776369	-2.540680	-2.993277
H	0.988053	-2.063307	-3.947672
H	0.070508	-3.367658	-3.055074
H	-0.579092	-1.516378	-2.710197
P	1.289995	0.085098	0.127032
C	1.159105	-0.992814	1.676967
C	1.843596	-0.576342	3.000184
C	-0.310305	-1.389340	1.946378
H	1.664861	-1.906518	1.335848
C	1.782485	-1.728994	4.019557
H	1.337074	0.288471	3.437357
H	2.882490	-0.271412	2.838848
C	-0.405501	-2.507632	2.999335
H	-0.871658	-0.510125	2.294928
H	-0.784752	-1.717694	1.014712
C	0.330262	-2.145704	4.297269
H	2.276149	-1.425059	4.951617
H	2.345513	-2.591848	3.633607
H	-1.459604	-2.730784	3.207555
H	0.030948	-3.426125	2.580004
H	0.301973	-2.990080	4.997625
H	-0.192560	-1.312913	4.790756
C	0.448666	1.751739	0.494492
C	0.655549	2.398968	1.879421
C	0.743235	2.790139	-0.614351
H	-0.616133	1.493100	0.412450
C	-0.185449	3.682728	2.035932
H	1.718928	2.635201	2.030977
H	0.366126	1.709358	2.675265
C	-0.135613	4.041747	-0.461273
H	1.794908	3.099592	-0.543680
H	0.582177	2.349373	-1.601058
C	0.062144	4.695309	0.911561
H	0.020015	4.134556	3.015240
H	-1.250203	3.405582	2.039351
H	0.099119	4.753146	-1.263107
H	-1.188703	3.757661	-0.595864
H	-0.602566	5.560750	1.029313
H	1.091051	5.078652	0.985589
C	3.134419	0.491645	-0.056760
C	4.082987	-0.679202	0.294125
C	3.459933	0.967683	-1.495128
H	3.345201	1.317719	0.639797

C	5.560014	-0.262569	0.169650
H	3.889644	-1.517250	-0.386480
H	3.904460	-1.053167	1.305273
C	4.932088	1.391283	-1.634984
H	3.248118	0.143952	-2.189193
H	2.813028	1.791868	-1.799865
C	5.889865	0.262232	-1.233753
H	6.203285	-1.115914	0.420593
H	5.776296	0.519970	0.912145
H	5.125912	1.708409	-2.667596
H	5.117253	2.270172	-0.999343
H	6.930952	0.606542	-1.278199
H	5.801011	-0.561462	-1.957444
C	1.740730	-2.528337	-1.972414
H	2.683325	-2.033806	-2.195654
C	1.798492	-3.646360	-0.951909
H	2.295725	-4.537398	-1.364826
H	2.356995	-3.362852	-0.053761
H	0.794144	-3.952970	-0.635590

TS4e

B3LYP SCF energy:	-1758.56880486 a.u.
B3LYP enthalpy:	-1757.797951 a.u.
B3LYP free energy:	-1757.906715 a.u.
M06 SCF energy in solution:	-3097.08915101 a.u.
M06 enthalpy in solution:	-3096.318297 a.u.
M06 free energy in solution:	-3096.427061 a.u.
Three lowest frequencies (cm-1):	-500.3481 12.9182 15.6069
Imaginary frequency:	-500.3481 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ni	0.309382	-1.505506	-1.080038
C	-1.210098	-0.509883	-1.677515
O	-1.139850	0.194694	-2.675390
C	-2.538043	-0.598388	-0.904717
H	-2.891521	-1.633959	-1.017276
H	-2.335534	-0.480787	0.169185
C	-3.617777	0.395523	-1.374713
H	-3.249464	1.418475	-1.229684
H	-3.751813	0.272912	-2.454826
C	-4.932495	0.210334	-0.651480
C	-5.884847	-0.709534	-1.115356
C	-5.224465	0.928370	0.517274
C	-7.085591	-0.909965	-0.433341
H	-5.682169	-1.269878	-2.025961
C	-6.424000	0.732623	1.203948
H	-4.503997	1.654787	0.888802
C	-7.360046	-0.189241	0.731176
H	-7.810390	-1.624888	-0.815014
H	-6.630055	1.304827	2.105280
H	-8.296421	-0.340753	1.261728
C	0.681387	-3.589561	-1.465536
H	-0.585884	-2.467731	-1.826996

P	1.338417	0.133901	0.097089
C	1.470071	-0.469193	1.886630
C	2.227258	0.348794	2.958768
C	0.082459	-0.884974	2.426373
H	2.038907	-1.399333	1.742670
C	2.390256	-0.481130	4.245727
H	1.672394	1.256828	3.209927
H	3.205915	0.679400	2.596396
C	0.210069	-1.678324	3.739130
H	-0.530596	0.011804	2.598982
H	-0.446034	-1.487090	1.677344
C	1.025489	-0.920259	4.797357
H	2.933233	0.105394	4.998011
H	3.005925	-1.368577	4.036509
H	-0.788345	-1.917918	4.126685
H	0.700741	-2.639400	3.525232
H	1.156654	-1.542285	5.691833
H	0.464955	-0.028989	5.116092
C	0.414338	1.796774	0.082185
C	0.651184	2.778803	1.248219
C	0.589368	2.530567	-1.269600
H	-0.634718	1.473510	0.137044
C	-0.245748	4.027219	1.133441
H	1.706531	3.087334	1.273542
H	0.437695	2.294471	2.203776
C	-0.331682	3.757371	-1.371806
H	1.629581	2.873302	-1.360284
H	0.383609	1.850690	-2.099822
C	-0.093774	4.736995	-0.216597
H	-0.020881	4.713930	1.959911
H	-1.294500	3.719865	1.260765
H	-0.170727	4.253950	-2.337012
H	-1.378963	3.422731	-1.366078
H	-0.786675	5.585854	-0.279469
H	0.921153	5.154669	-0.297207
C	3.109628	0.539210	-0.446347
C	4.195518	-0.396400	0.136943
C	3.221112	0.518386	-1.991735
H	3.321881	1.560444	-0.094653
C	5.602527	0.027532	-0.324000
H	4.005798	-1.424790	-0.193687
H	4.170188	-0.411655	1.229496
C	4.621005	0.942452	-2.466873
H	3.008502	-0.500753	-2.341448
H	2.466765	1.158432	-2.452995
C	5.718167	0.062944	-1.853536
H	6.348122	-0.657265	0.100430
H	5.828119	1.024895	0.082042
H	4.664786	0.900250	-3.562606
H	4.796018	1.992502	-2.188518
H	6.711349	0.421163	-2.153054
H	5.622338	-0.960089	-2.246311
C	1.758480	-2.959566	-0.819043
H	2.635880	-2.685324	-1.397263
H	1.927656	-3.147218	0.239559
C	-0.204424	-4.586885	-0.742300

H	0.277662	-5.573769	-0.748956
H	-0.358016	-4.296416	0.302093
H	-1.186268	-4.686414	-1.215790
H	0.778484	-3.762592	-2.536615

TS7c

B3LYP SCF energy: -2249.48391187 a.u.
B3LYP enthalpy: -2248.523252 a.u.
B3LYP free energy: -2248.667400 a.u.
M06 SCF energy in solution: -3587.78121199 a.u.
M06 enthalpy in solution: -3586.820552 a.u.
M06 free energy in solution: -3586.964700 a.u.
Three lowest frequencies (cm-1): -311.6494 14.5997 20.1117
Imaginary frequency: -311.6494 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ni	-0.448761	0.105290	-1.242244
Al	6.386474	-0.204979	-1.286278
N	-0.568703	0.092634	1.822329
N	-1.957808	-1.297179	0.932505
N	4.319476	-0.174654	-1.331012
C	-0.996564	-0.362272	0.598476
C	-1.251659	-0.521342	2.869018
C	-2.112175	-1.401119	2.314039
C	3.657549	0.926788	-0.917395
C	2.274094	1.007245	-0.875344
C	1.464825	-0.084830	-1.261905
C	2.184715	-1.213731	-1.707648
C	3.574073	-1.226718	-1.725355
C	6.836369	-1.975120	-2.108245
C	6.866553	1.405013	-2.374461
C	6.754971	-0.041811	0.678418
C	-1.719569	0.134731	-2.945226
C	-2.395953	0.793337	-1.921203
C	0.565174	0.953088	2.101935
C	0.417609	2.353268	2.010283
C	1.757901	0.343735	2.547931
C	1.528317	3.139879	2.340228
C	2.833742	1.182574	2.867628
C	2.725841	2.563906	2.758183
C	-0.909100	3.004772	1.630140
C	1.909633	-1.164416	2.743742
C	3.149338	-1.741478	2.036590
C	1.941538	-1.515406	4.246993
C	-0.744939	4.378374	0.960986
C	-1.828648	3.128609	2.864926
C	-2.690792	-2.171205	0.037577
C	-4.082318	-1.977621	-0.122652
C	-2.011711	-3.257714	-0.565576
C	-4.776409	-2.878136	-0.942832
C	-4.124258	-3.927512	-1.577670
C	-2.758101	-4.113311	-1.385094
C	-4.867815	-0.869302	0.580519

C	-5.861778	-0.154182	-0.357839
C	-5.636516	-1.419368	1.802279
C	-0.542632	-3.567509	-0.277647
C	0.160110	-4.332543	-1.412244
C	-0.408855	-4.360342	1.041878
H	-1.042681	-0.282394	3.899077
H	-2.803481	-2.096973	2.759363
H	4.280206	1.762624	-0.612101
H	1.831952	1.934314	-0.524774
H	0.112539	0.258375	-2.606041
H	1.666035	-2.096191	-2.068089
H	4.131272	-2.093740	-2.066796
H	6.470895	-2.841647	-1.536792
H	7.928977	-2.093231	-2.164998
H	6.468035	-2.089808	-3.138662
H	6.508278	1.338104	-3.412078
H	7.958347	1.529483	-2.432280
H	6.475252	2.348871	-1.965854
H	6.286065	0.845565	1.130609
H	7.832954	0.045748	0.880390
H	6.403423	-0.913710	1.249937
H	3.769835	0.745047	3.200116
H	1.456083	4.219810	2.274546
H	1.036470	-1.658281	2.307749
H	-1.408975	2.353424	0.906556
H	2.815419	-1.069609	4.735985
H	2.000037	-2.601652	4.383245
H	1.049857	-1.155745	4.772845
H	3.184123	-2.828110	2.182321
H	4.083293	-1.329486	2.432896
H	3.123102	-1.542585	0.963094
H	-1.370894	3.771800	3.626361
H	-2.031973	2.155599	3.324463
H	-2.789464	3.573320	2.579509
H	-1.711642	4.718516	0.580374
H	-0.050692	4.335781	0.115514
H	-0.383148	5.137174	1.665149
H	3.574341	3.195982	3.006035
H	-5.844585	-2.751314	-1.086442
H	-4.681119	-4.609618	-2.214403
H	-4.153896	-0.120908	0.941827
H	-5.386715	0.185237	-1.282944
H	-6.288738	0.719353	0.148272
H	-6.699208	-0.805159	-0.632295
H	-6.175459	-0.610512	2.309433
H	-4.974115	-1.890688	2.534541
H	-6.371852	-2.170350	1.490573
H	-0.014172	-2.617981	-0.155935
H	0.020387	-3.844253	-2.383069
H	-0.197074	-5.365499	-1.497678
H	1.234916	-4.382115	-1.208771
H	-0.827975	-3.814231	1.892737
H	0.647093	-4.560322	1.258383
H	-0.927621	-5.324099	0.969647
H	-2.266331	-4.949247	-1.869516
H	-1.421739	0.661339	-3.846335

H	-1.846685	-0.938827	-3.065355
H	-3.070262	0.219885	-1.298998
C	-2.567298	2.260149	-1.895739
C	-3.627926	2.830827	-1.167200
C	-1.743688	3.128191	-2.640401
C	-3.885436	4.200634	-1.215154
H	-4.274052	2.186178	-0.578218
C	-1.997739	4.497816	-2.684453
H	-0.898695	2.727253	-3.192274
C	-3.075750	5.042190	-1.981397
H	-4.725000	4.609780	-0.658600
H	-1.351174	5.143064	-3.273551
H	-3.277726	6.108830	-2.025577

TS8c

B3LYP SCF energy: -2249.49037044 a.u.
B3LYP enthalpy: -2248.530235 a.u.
B3LYP free energy: -2248.677489 a.u.
M06 SCF energy in solution: -3587.78612937 a.u.
M06 enthalpy in solution: -3586.825994 a.u.
M06 free energy in solution: -3586.973248 a.u.
Three lowest frequencies (cm-1): -559.2022 16.4063 16.8832
Imaginary frequency: -559.2022 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ni	-0.503236	0.381284	-0.940570
Al	6.093119	1.686907	0.451320
N	-2.099215	-1.128772	1.113779
N	-0.499671	-2.326008	0.308315
N	4.095476	1.321683	0.052874
C	-1.048922	-1.068620	0.224705
C	-2.185705	-2.380126	1.722998
C	-1.190927	-3.134328	1.207087
C	3.096759	1.974030	0.682615
C	1.754878	1.740213	0.410328
C	1.355156	0.778192	-0.543531
C	2.425238	0.124666	-1.196790
C	3.744059	0.410647	-0.879460
C	6.815215	-0.164076	0.722352
C	6.710151	2.608408	-1.214384
C	6.023108	2.820504	2.101506
C	-1.448010	1.597367	-2.456364
C	-2.262873	0.568835	-1.953116
C	-3.054958	-0.086015	1.414212
C	-4.370995	-0.215078	0.916377
C	-2.667972	0.979704	2.257514
C	-5.299872	0.772233	1.271431
C	-3.639578	1.937950	2.573980
C	-4.940895	1.839657	2.087082
C	-4.826341	-1.392016	0.052751
C	-1.268995	1.066514	2.865531
C	-0.801831	2.509721	3.121966
C	-1.194343	0.245495	4.171601

C	-5.590767	-0.952901	-1.212053
C	-5.695327	-2.369073	0.873838
C	0.688395	-2.798534	-0.366157
C	0.611800	-3.163442	-1.725738
C	1.870960	-2.945232	0.391339
C	1.777446	-3.649125	-2.332729
C	2.962815	-3.783830	-1.615099
C	3.002741	-3.442639	-0.266433
C	-0.686972	-3.115256	-2.525460
C	-0.535053	-2.335294	-3.844461
C	-1.217425	-4.540454	-2.785515
C	1.950093	-2.626898	1.883920
C	3.100386	-1.664487	2.231144
C	2.063843	-3.924818	2.711569
H	-2.940980	-2.603675	2.458706
H	-0.899288	-4.155220	1.393586
H	3.408539	2.704514	1.422774
H	1.017608	2.329937	0.945777
H	0.207578	1.433577	-1.721757
H	2.235831	-0.623436	-1.960640
H	4.567008	-0.098315	-1.372791
H	6.339800	-0.688771	1.564466
H	7.891549	-0.131874	0.949069
H	6.712465	-0.816092	-0.158246
H	6.589622	1.996309	-2.120738
H	7.779303	2.862145	-1.156420
H	6.178015	3.553072	-1.398786
H	5.560512	3.807242	1.949558
H	7.044557	3.021269	2.458388
H	5.498210	2.344931	2.943652
H	-0.970574	1.430660	-3.420924
H	-2.398989	-0.331875	-2.545077
H	-3.064825	0.805214	-1.263504
H	-3.377011	2.770184	3.217882
H	-6.318533	0.701136	0.902523
H	-0.565918	0.625540	2.152786
H	-3.936446	-1.935133	-0.280123
H	-1.888215	0.643534	4.922027
H	-0.182164	0.288305	4.590579
H	-1.444903	-0.807444	4.005444
H	0.255127	2.507515	3.409086
H	-1.354696	2.984326	3.941200
H	-0.911939	3.136487	2.230079
H	-6.614761	-1.880123	1.216770
H	-5.169851	-2.741462	1.759422
H	-5.981776	-3.233072	0.262846
H	-5.816143	-1.829607	-1.830349
H	-5.009233	-0.251836	-1.817605
H	-6.546280	-0.475331	-0.967258
H	-5.676911	2.594870	2.349452
H	1.751103	-3.940036	-3.378879
H	3.854982	-4.163827	-2.105489
H	-1.436117	-2.590726	-1.926802
H	-0.173294	-1.318339	-3.659140
H	-1.501818	-2.267097	-4.357555
H	0.165612	-2.823745	-4.531225

H	-2.173365	-4.502790	-3.321592
H	-1.375811	-5.084953	-1.847703
H	-0.514564	-5.122131	-3.393398
H	1.020993	-2.129416	2.177294
H	2.999233	-0.716208	1.698924
H	4.081515	-2.084835	1.985550
H	3.094700	-1.454306	3.307248
H	1.232667	-4.611455	2.513542
H	2.064918	-3.694130	3.783229
H	2.993650	-4.459055	2.483963
H	3.930390	-3.557833	0.285780
C	-1.605673	3.039065	-2.109707
C	-2.259539	3.470472	-0.943442
C	-1.096796	4.010367	-2.985256
C	-2.402524	4.829912	-0.670101
H	-2.653122	2.741950	-0.241473
C	-1.239447	5.371026	-2.712276
H	-0.583819	3.694241	-3.891132
C	-1.893625	5.787263	-1.551858
H	-2.913333	5.142480	0.237140
H	-0.838090	6.104515	-3.406477
H	-2.004834	6.846166	-1.335133

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