Electronic Supplementary Information (ESI)

Computational exploration of substrate and ligand effects in nickel-catalyzed C–Si bond carboxylation with CO_2

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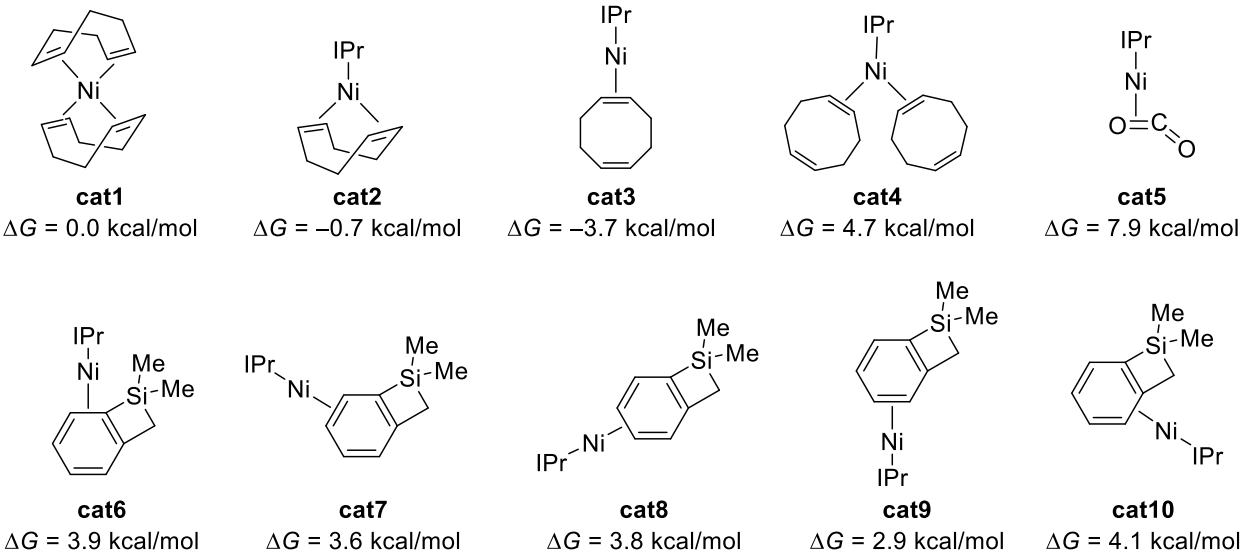
Possible active Ni(0) catalyst species

Because the 1:1 ratio of ligand and $Ni(COD)_2$ was employed in the experimental condition, we computed several possible Ni complexes ligated by one IPr ligand (Fig. S1). The complex **cat3** has the lowest energy and thus is chosen as the zero reference in the energy profile shown in the manuscript.



cat1 ΔG = 0.0 kcal/mol

cat2 ΔG = –0.7 kcal/mol

cat3 ΔG = –3.7 kcal/mol

cat4 ΔG = 4.7 kcal/mol

cat5 ΔG = 7.9 kcal/mol

cat6 ΔG = 3.9 kcal/mol

cat7 ΔG = 3.6 kcal/mol

cat8 ΔG = 3.8 kcal/mol

cat9 ΔG = 2.9 kcal/mol

cat10 ΔG = 4.1 kcal/mol

Fig. S1 Computed energies of Ni(0) complexes.

Stability difference between 14*e*- and 16*e*-Ni species

We compared several key 16*e*- and 14*e*- Ni(0) and Ni(II) intermediates along the reaction coordinate. As shown in Fig. S2, the computed energies show that 16*e* structures (**cat2** and **8**) are less stable than the 14*e* structures (**cat3** and **6**) for both Ni(0) and Ni(II) species, respectively. This is mostly because the Ni centers with more ligands lead to more steric repulsions with the bulky IPr ligand. The disfavored repulsive interactions are evidenced by the short H···H and H···O distances in the 3D structures of **cat2** and **8**, respectively. These distances are shorter than the sum of radii of Van der Waals of corresponding atoms, indicating repulsive interactions.

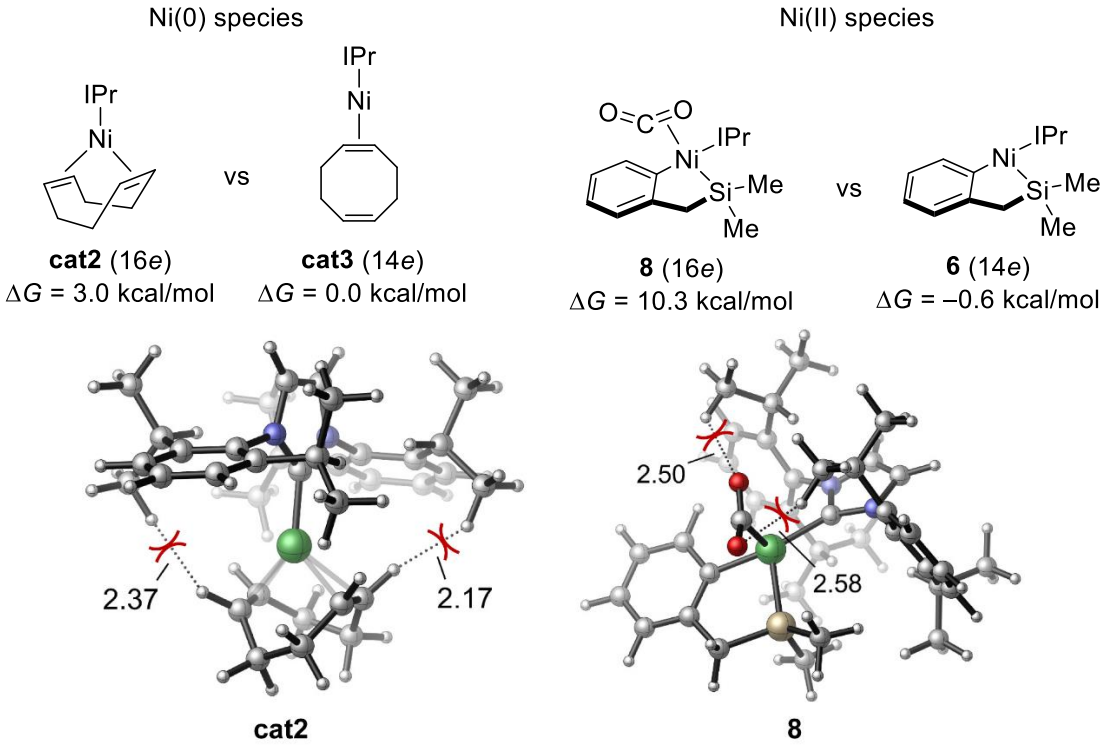


Fig. S2 Ni(0) and Ni(II) complexes with 14*e* and 16*e*.

Transition states of C–Si bond cleavages

The oxidative addition transition states of C(sp^2)–Si and C(sp^3)–Si bonds in substrates **1a-f** were shown in Fig. S3. In the transition states of C(sp^3)–Si bond cleavages with the 6-membered substrates **1e**, **1f** (**5-TSe** and **5-TSf**), the C–Si bond lengths are elongated to more than 2.1 Å while the Ni–C and Ni–Si bond distances are shortened to 2.0 and 2.3 Å, respectively. These transition states have the product-like structure, bearing the late transition state feature. In contrast, **4-TSe** is not that late transition state, which has a shorter C–Si distance (2.05 Å) and a longer Ni–Si distance (2.47 Å) compared to **5-TSe** and **5-TSf**.

To better explore the origin of difference in reactivity between C(sp^2)–Si and C(sp^3)–Si bond oxidative addition, we further performed the extended distortion/interaction analysis along the intrinsic reaction coordinate for **4-TSe** and **5-TSe**. As shown in Fig. S4b, the substrate distortion energies are almost identical, thus exerting no influence on the reactivity difference. The distortion energies of catalyst show that there is a small difference (<0.7 kcal/mol) of in these two transition states, indicating a marginal contribution for the reactivity difference (Fig. S4a). In contrast, as shown in Fig. 4c, there is a 4~9 kcal/mol difference for the interaction energy between catalyst and substrate. This demonstrates the stronger interaction in **4-TSe** is the major factor accounting for its lower barrier than **5-TSe**. Taken together, compared to **5-TSe**, **4-TSe** can achieve the enough favorable interactions with smaller deformations of the IPr-Ni and substrate, leading to the higher reactivity.

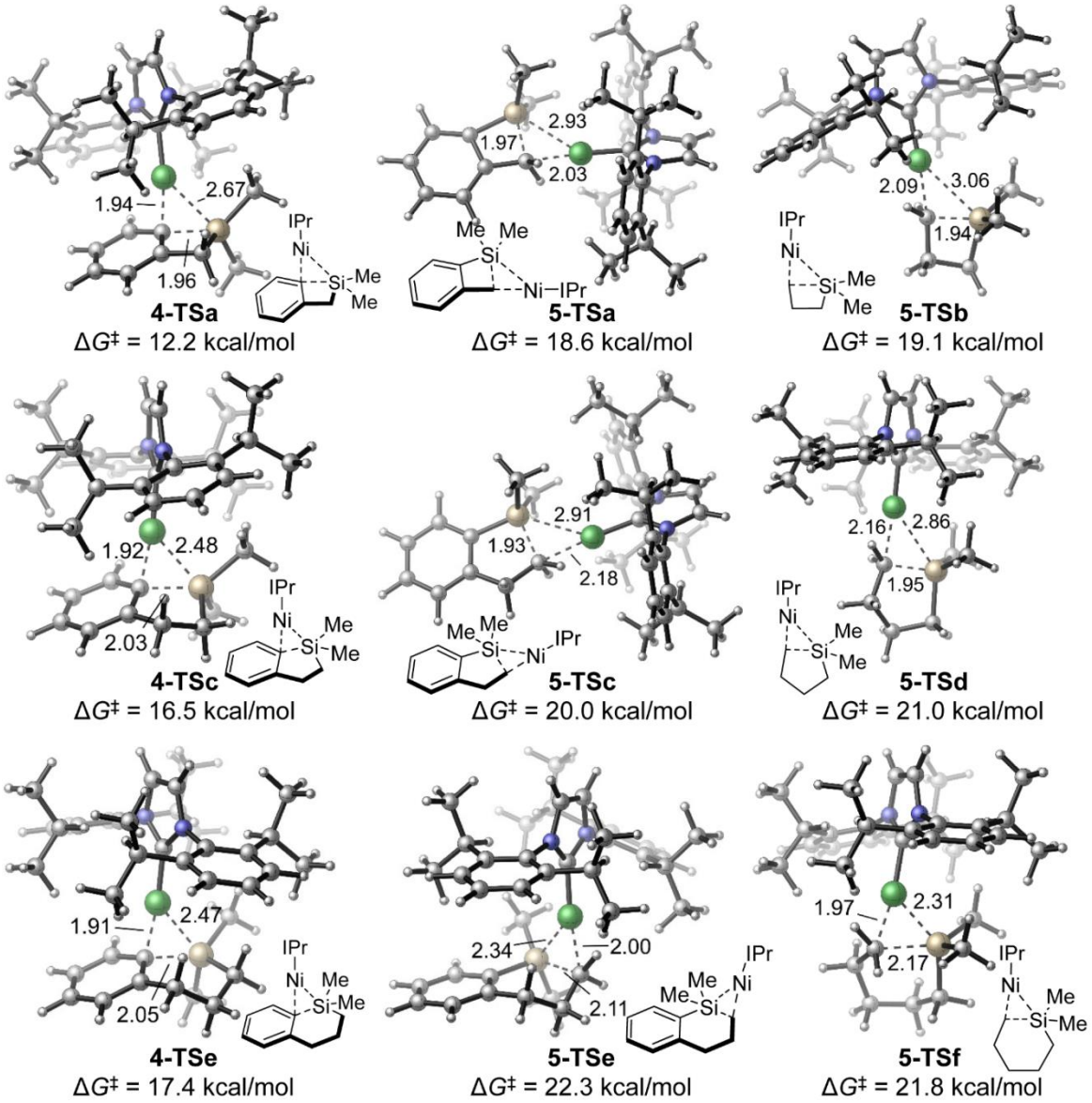


Fig. S3 Optimized oxidative addition transition states of C(sp^2)–Si and C(sp^3)–Si bond in the substrates **1a-f**.

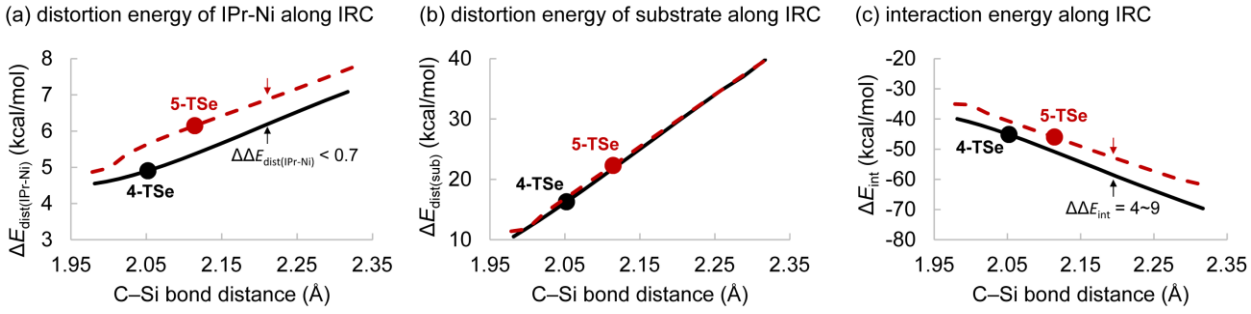
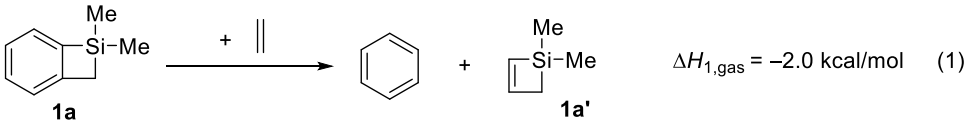
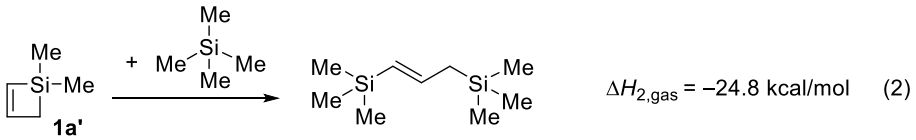


Fig. S4 Extended distortion/interaction analysis along the intrinsic reaction coordinates for transition states of C(sp^2)–Si and C(sp^3)–Si bond oxidative addition.

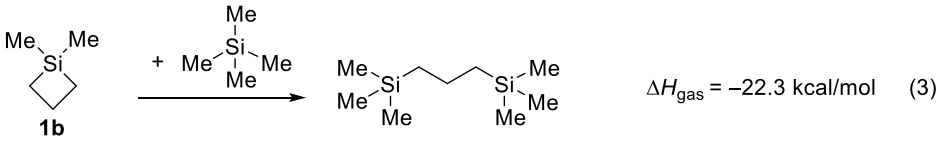
Calculations of ring strain energies of substrates 1a-f

The ring strain energy was calculated using the homodesmotic reactions shown in Fig. S5. For the benzocyclic substrates (**1a**, **1c**, **1e**), equations (1), (4), (7) were used to evaluated the additional strain that derived from the fusion of benzene and sila-cyclobutene **1a'**, sila-cyclopantene **1c'**, sila-cyclohexene **1e'**, respectively. The ring strain energies of sila-cyclobutene **1a'**, sila-cyclopantene **1c'**, sila-cyclohexene **1e'** were computed by using equations (2), (5), (8). The total ring strain energies of substrates **1a**, **1c**, **1e** were evaluated by combining equations (1) and (2), (4) and (5), (7) and (8), respectively.

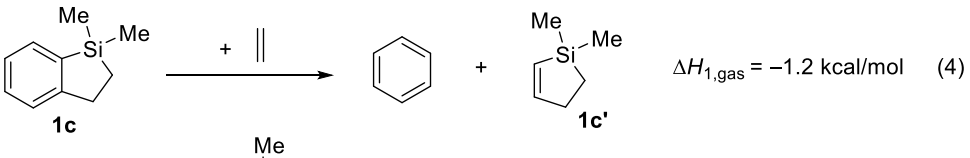


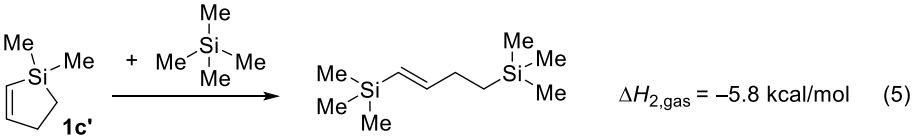


ring strain energy of **1a**: $\Delta H_{strain} = -(\Delta H_{1,gas} + \Delta H_{2,gas})$ = 26.8 kcal/mol

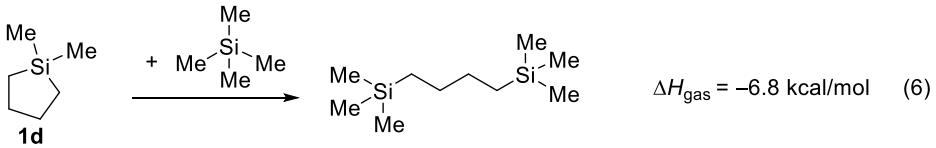


ring strain energy of **1b**: $\Delta H_{strain} = -\Delta H_{gas}$ = 22.3 kcal/mol

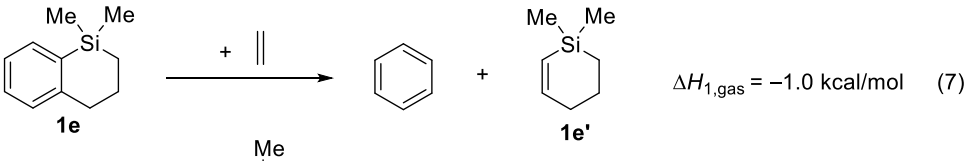


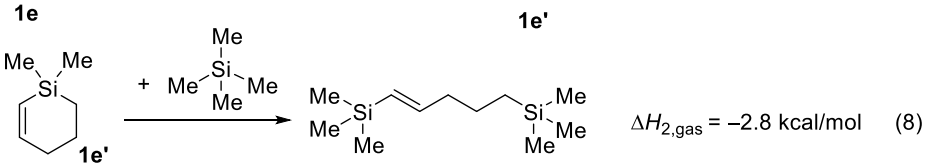


ring strain energy of **1c**: $\Delta H_{strain} = -\Delta H_{gas} = -(\Delta H_{1,gas} + \Delta H_{2,gas})$ = 7.0 kcal/mol

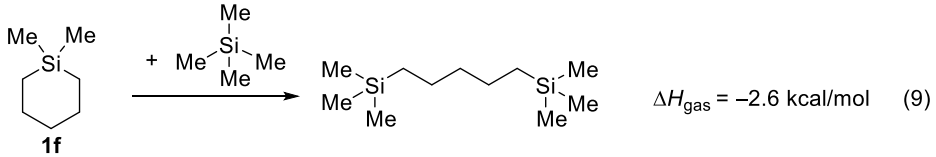


ring strain energy of **1d**: $\Delta H_{strain} = -\Delta H_{gas}$ = 6.8 kcal/mol





ring strain energy of **1e**: $\Delta H_{strain} = -\Delta H_{gas} = -(\Delta H_{1,gas} + \Delta H_{2,gas})$ = 3.8 kcal/mol



ring strain energy of **1f**: $\Delta H_{strain} = -\Delta H_{gas}$ = 2.6 kcal/mol

Fig. S5 Ring strain energies of substrates **1a-f** based on the homodesmotic reactions.

Relationships between the barrier of CO_2 insertion and other factors

We dissected the transition state of CO_2 insertion into three fragments (CO_2, IPr-Ni and substrate) to investigate the relationships between the barrier of CO_2 insertion and the distortion energies of these fragments. While the distortion energy of substrates ($\Delta E_{dist(sub)}$) excellently correlates with the barrier of CO_2 insertion ($\Delta G^{‡}$) (R^2 = 0.96, Fig. 5b in the manuscript), the distortion energies of both CO_2 ($\Delta E_{dist(CO2)}$, Fig. S6a) and catalyst ($\Delta E_{dist(IPr\text{-}Ni)}$, Fig. S6b) poorly correlate with the barrier of CO_2 insertion ($\Delta G^{‡}$).

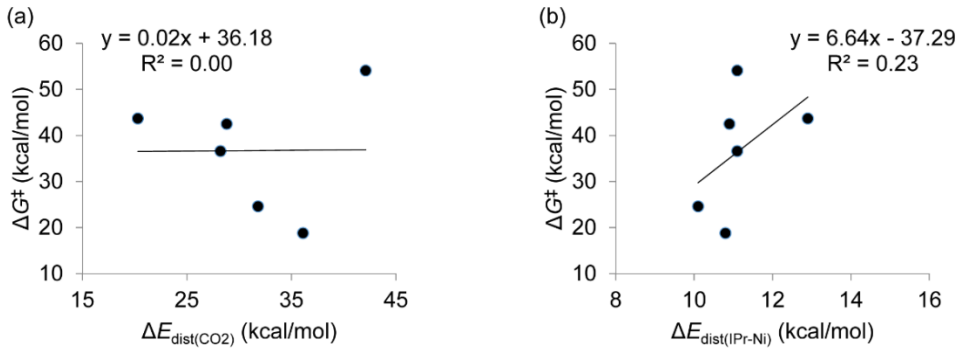
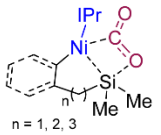


Fig. S6 Relationships between the barrier of CO_2 insertion ($\Delta G^{‡}$) and the distortion energies of CO_2 ($\Delta E_{dist(CO2)}$) and catalyst ($\Delta E_{dist(IPr\text{-}Ni)}$).

We also analyzed the substrate effect on the reactivity of disfavored CO_2 insertion into the Ni–Si bond using the distortion/interaction model (Fig. S7a). The results show that the barrier of CO_2 insertion linearly correlates with the substrate distortion energy (R^2 = 0.84, Fig. S7b), and further excellently correlates with the ring strain energy (R^2 = 0.98, Fig. S7c). This result is same with the CO_2 insertion into the Ni–C bond shown in Fig. 5 in the manuscript.

(a)



10-TSa~10-TSf
CO_2 insertion transition state

substrate (ΔH_{strain})	barrier $\Delta G^{‡}$	$\Delta E_{dist(sub)}$	$\Delta E_{dist(IPr\text{-}Ni)}$	$\Delta E_{dist(CO_2)}$
1a (26.8)	21.8	48.6	11.2	42.2
1b (22.3)	29.6	52.4	11.6	44.0
1c (7.0)	43.6	84.6	16.3	43.0
1d (6.8)	43.2	72.9	13.5	47.8
1e (3.8)	48.9	75.6	13.2	47.3
1f (2.6)	51.4	79.2	13.2	48.8

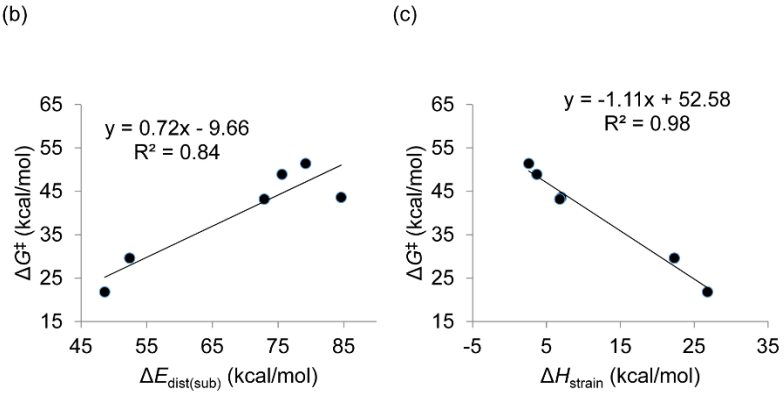


Fig. S7 Relationships of the activation free energies ($\Delta G^{‡}$) of CO_2 insertion into the Ni–Si bond with the distortion energy of substrates **1a-f** ($\Delta E_{dist(sub)}$) and the substrate ring strain energy (ΔH_{strain}).

Based on the three-fragment dissection of transition state structures, we studied the effect of NHC ligands on the reactivity of CO_2 insertion. The distortion energies of CO_2 ($\Delta E_{dist(CO2)}$), catalyst ($\Delta E_{dist(LNi)}$) and substrate ($\Delta E_{dist(sub)}$) show relatively poor correlations with the barrier of CO_2 insertion (Fig. S8). These results indicate the three-fragment dissection of transition state structures is not effective to describe the origin of CO_2 insertion reactivity. Instead, as shown in Fig. 6 in the manuscript, the distortion of nickelacycles with NHC ligands is a better descriptor for the reactivity, which is further ascribed to the steric hindrance ($\%V_{bur}$) of NHC ligands. The electronic property of NHC ligands shows a relatively poor correlation with the barrier of CO_2 insertion (Fig. S9). These results indicate that the steric property of NHC ligands is the major factor that determines the reactivity of CO_2 insertion.

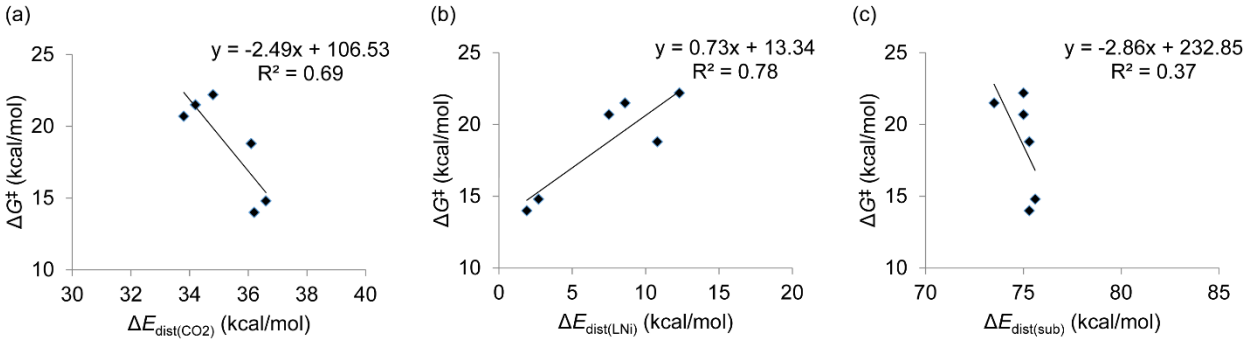


Fig. S8 Relationships between the barrier of CO_2 insertion ($\Delta G^{‡}$) and the distortion energies of separated fragments ($\Delta E_{dist(CO2)}$, $\Delta E_{dist(LNi)}$, , $\Delta E_{dist(sub)}$).

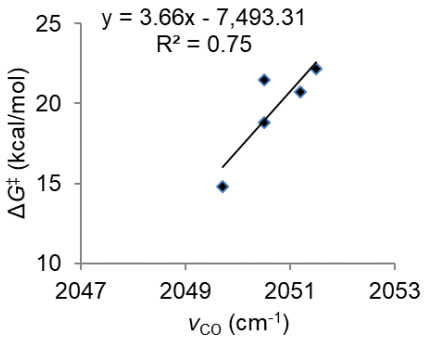
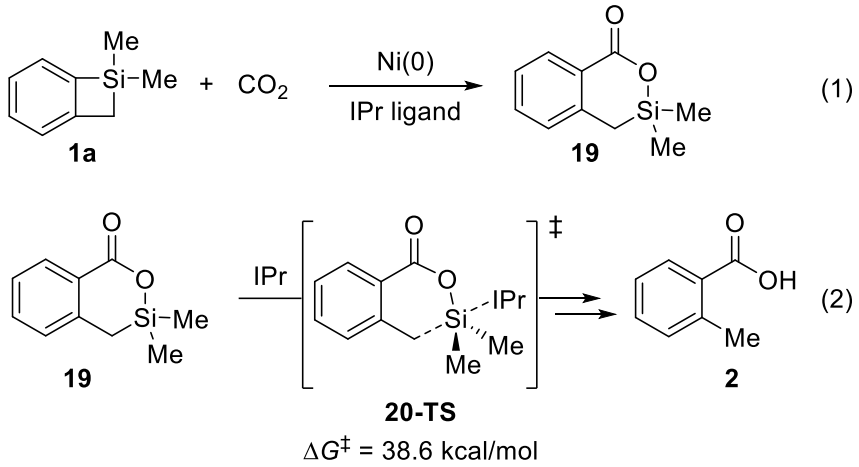


Fig. S9 Relationship between the barrier of CO_2 insertion ($\Delta G^{‡}$) and the TEP parameter (ν_{co}) of NHC ligands.

C(sp^3)–Si bond cleavage in silalactone 19

The reaction reported by Murakami group generally has two major steps (equations 1 and 2, Fig. S10). Our computational study mainly focuses on the first step shown in equation 1. This is because the Ni catalyst is critical for the reaction. The control experiment from Murakami group shows that no carboxylated product was obtained in in the presence of only IPr ligand without $Ni(COD)_2$. Their experimental results also show that the IPr ligand plays an important role in breaking the C(sp^3)–Si bond in intermediate **19**. We further computed the transition state of C(sp^3)–Si cleavage via the S_N2 mechanism with IPr, which gives an extremely high barrier (**20-TS**, $\Delta G^{‡}$ = 38.6 kcal/mol). This indicates the high temperature is mainly used to promote the C(sp^3)–Si cleavage of **19**.



$\Delta G^{‡}$ = 38.6 kcal/mol

Fig. S10 Two major steps in the Ni-catalyzed carboxylation with benzosilacyclobutene **1a**.

Cartesian coordinates (Å) and energies of key optimized structures

1a
B3LYP SCF energy: -639.68878809 a.u.
B3LYP enthalpy: -639.495306 a.u.
B3LYP free energy: -639.542676 a.u.
M06 SCF energy in solution: -639.48726605 a.u.
M06 enthalpy in solution: -639.293784 a.u.
M06 free energy in solution: -639.341154 a.u.
Three lowest frequencies (cm-1): 66.6229 117.5004 148.2486

Cartesian coordinates

ATOM	X	Y	Z
Si	1.481919	0.002497	-0.000014
C	0.555355	1.695552	-0.000206
H	0.672506	2.331636	0.885809
H	0.672479	2.331447	-0.886360
C	2.488950	-0.400058	-1.548470
H	1.931467	-0.154171	-2.458817
H	3.429202	0.165107	-1.564207
H	2.743730	-1.466170	-1.589955
C	2.489085	-0.399396	1.548526
H	1.931220	-0.154216	2.458829
H	2.745044	-1.465226	1.589907
H	3.428712	0.166811	1.564457
C	-0.726602	0.860164	-0.000096
C	-0.331404	-0.496701	0.000064
C	-1.292324	-1.510890	0.000193
C	-2.643634	-1.156166	0.000158
C	-3.029779	0.192062	-0.000001
C	-2.077790	1.215385	-0.000130
H	-4.088034	0.442490	-0.000024
H	-2.388028	2.258152	-0.000254
H	-3.408753	-1.929188	0.000256
H	-1.007564	-2.561340	0.000319

1b
B3LYP SCF energy: -487.26050813 a.u.
B3LYP enthalpy: -487.093568 a.u.
B3LYP free energy: -487.135664 a.u.
M06 SCF energy in solution: -487.14054783 a.u.
M06 enthalpy in solution: -486.973608 a.u.
M06 free energy in solution: -487.015704 a.u.
Three lowest frequencies (cm-1): 107.2257 142.1435 158.1008

Cartesian coordinates

ATOM	X	Y	Z
C	-1.033439	-0.255844	-1.208725
C	-1.985753	0.035502	0.000107
C	-1.033304	-0.255643	1.208881
H	-1.128032	-1.295981	-1.544357
H	-1.167004	0.392303	-2.080255
H	-2.912462	-0.552191	0.000208
H	-2.275661	1.092979	0.000035

H	-1.127862	-1.295723	1.544700
H	-1.166768	0.392653	2.080315
Si	0.426589	-0.018543	-0.000023
C	1.834573	-1.283396	0.000000
H	1.452233	-2.310475	0.000103
H	2.472319	-1.164328	-0.884832
H	2.472418	-1.164187	0.884742
C	1.140523	1.735128	-0.000200
H	1.764507	1.910980	0.884780
H	1.764430	1.910837	-0.885263
H	0.344039	2.488245	-0.000226

1c

B3LYP SCF energy: -679.03003683 a.u.
B3LYP enthalpy: -678.806140 a.u.
B3LYP free energy: -678.855840 a.u.
M06 SCF energy in solution: -678.80654005 a.u.
M06 enthalpy in solution: -678.582643 a.u.
M06 free energy in solution: -678.632343 a.u.
Three lowest frequencies (cm-1): 72.5983 87.5945 142.0958

Cartesian coordinates

ATOM	X	Y	Z
C	-0.997790	0.867875	-0.010592
C	-0.370043	-0.396285	0.016443
C	-1.164117	-1.551907	0.044244
C	-2.556227	-1.459845	0.039480
C	-3.168642	-0.203055	0.007423
C	-2.393959	0.956982	-0.017310
H	-0.697616	-2.535411	0.061834
H	-3.164292	-2.360913	0.055273
H	-4.253406	-0.128717	-0.002912
H	-2.877866	1.931632	-0.044995
C	-0.085359	2.088671	0.005252
H	-0.490996	2.885632	-0.631572
Si	1.498925	-0.168240	-0.010081
C	2.308519	-0.509621	1.668976
H	2.224106	-1.568185	1.943447
H	3.376080	-0.256853	1.653025
H	1.837076	0.076696	2.466088
C	2.379969	-1.177236	-1.347028
H	3.444362	-0.917250	-1.403380
H	2.317369	-2.253210	-1.142992
H	1.938228	-0.999881	-2.334098
H	-0.067388	2.502729	1.024176
C	1.355864	1.689540	-0.417091
H	1.473508	1.819514	-1.501133
H	2.106603	2.328873	0.059586

1d

B3LYP SCF energy: -526.59979209 a.u.
B3LYP enthalpy: -526.402398 a.u.
B3LYP free energy: -526.447020 a.u.

M06 SCF energy in solution: -526.45807442 a.u.
M06 enthalpy in solution: -526.260680 a.u.
M06 free energy in solution: -526.305302 a.u.
Three lowest frequencies (cm-1): 60.1806 146.6710 151.7705

Cartesian coordinates

ATOM	X	Y	Z
C	1.951610	-0.599723	-0.485342
C	1.951398	0.599538	0.485598
C	0.618729	0.598490	1.276722
C	0.618886	-0.599242	-1.276389
H	2.825904	-0.574548	-1.148992
H	2.030067	-1.528413	0.098338
H	2.029441	1.528248	-0.098117
H	2.825748	0.574770	1.149196
H	0.678831	-0.118374	2.107378
H	0.403577	1.576812	1.721510
H	0.403893	-1.577801	-1.720739
H	0.678721	0.117266	-2.107368
Si	-0.674561	-0.000129	-0.000015
C	-1.770456	1.393183	-0.671180
H	-2.387541	1.043618	-1.508233
H	-2.449237	1.776228	0.100585
H	-1.169992	2.236318	-1.033362
C	-1.772208	-1.392242	0.670692
H	-2.389696	-1.041558	1.506983
H	-2.450677	-1.775010	-0.101477
H	-1.172934	-2.235782	1.033894

1e
B3LYP SCF energy: -718.34611195 a.u.
B3LYP enthalpy: -718.091964 a.u.
B3LYP free energy: -718.144063 a.u.
M06 SCF energy in solution: -718.10376783 a.u.
M06 enthalpy in solution: -717.849620 a.u.
M06 free energy in solution: -717.901719 a.u.
Three lowest frequencies (cm-1): 48.0718 84.0918 146.1893

Cartesian coordinates

ATOM	X	Y	Z
C	-2.546857	0.851350	-0.080613
C	-1.144465	0.845827	-0.117029
C	-0.456255	-0.387226	-0.028150
C	-1.214081	-1.567335	0.091972
C	-2.607242	-1.551793	0.118297
C	-3.276504	-0.330353	0.031595
H	-3.074305	1.801593	-0.140718
H	-0.703354	-2.526518	0.167956
H	-3.165193	-2.480256	0.209796
H	-4.362917	-0.296492	0.057795
C	0.936671	2.290289	0.440052
H	1.280605	3.331419	0.371405
H	0.798027	2.083194	1.510674
C	1.998196	1.341280	-0.151549
H	2.960118	1.475750	0.360934

H	2.172174	1.608583	-1.204076
C	-0.421629	2.177365	-0.272924
H	-0.265412	2.379338	-1.345049
H	-1.084041	2.976432	0.082830
Si	1.432063	-0.468263	-0.043545
C	2.056884	-1.270882	1.556424
H	1.658892	-2.284770	1.683807
H	3.151739	-1.343302	1.558898
H	1.758163	-0.688347	2.435850
C	2.053356	-1.471306	-1.526145
H	3.150087	-1.496720	-1.551489
H	1.701166	-2.509075	-1.488766
H	1.706918	-1.038435	-2.471810

1f

B3LYP SCF energy: -565.91830550 a.u.
B3LYP enthalpy: -565.690515 a.u.
B3LYP free energy: -565.736932 a.u.
M06 SCF energy in solution: -565.75647815 a.u.
M06 enthalpy in solution: -565.528688 a.u.
M06 free energy in solution: -565.575105 a.u.
Three lowest frequencies (cm-1): 83.5803 135.4631 151.2649

Cartesian coordinates

ATOM	X	Y	Z
Si	0.916436	0.000022	-0.019753
C	-0.201068	-1.491695	-0.392764
H	0.233718	-2.424719	-0.008681
H	-0.263749	-1.614715	-1.484679
C	-1.626152	-1.296403	0.174185
H	-1.588924	-1.295950	1.273792
H	-2.257034	-2.152663	-0.103129
C	-2.311747	0.000351	-0.296924
H	-3.351254	-0.000144	0.057534
H	-2.363595	0.001560	-1.396643
C	-1.626330	1.296208	0.176901
H	-2.257117	2.153009	-0.098955
H	-1.589409	1.293654	1.276505
C	-0.201128	1.492435	-0.389473
H	-0.263835	1.617209	-1.481212
H	0.233684	2.424861	-0.003993
C	1.442290	-0.002651	1.803376
H	2.045633	-0.887382	2.041462
H	2.045229	0.881523	2.044498
H	0.577508	-0.004008	2.477459
C	2.459506	0.001848	-1.119368
H	3.082270	0.885589	-0.933138
H	3.082063	-0.882797	-0.936827
H	2.192484	0.004111	-2.183049

3

B3LYP SCF energy: -1969.03620881 a.u.
B3LYP enthalpy: -1968.235208 a.u.

B3LYP free energy: -1968.360284 a.u.
M06 SCF energy in solution: -1969.95733210 a.u.
M06 enthalpy in solution: -1969.156331 a.u.
M06 free energy in solution: -1969.281407 a.u.
Three lowest frequencies (cm-1): 14.0826 21.1842 25.0810

Cartesian coordinates

ATOM	X	Y	Z
C	-1.774400	-1.907268	0.659262
C	-2.563699	-2.447738	-0.378185
C	-3.954163	-2.447231	-0.206079
H	-4.588546	-2.857925	-0.986353
C	-4.535616	-1.930647	0.948288
C	-3.733470	-1.412680	1.962382
C	-2.337978	-1.392398	1.846116
H	-5.616642	-1.937413	1.061505
H	-4.198786	-1.024832	2.863396
C	0.436823	-3.059773	0.726206
C	1.716376	-2.711999	0.453939
H	0.007578	-3.996390	1.045577
H	2.630636	-3.283813	0.483631
C	2.878440	-0.625248	-0.266741
C	3.207592	-0.473949	-1.629343
C	4.358949	0.259670	-1.942089
H	4.632238	0.402530	-2.983895
C	5.163246	0.800480	-0.942562
C	4.830897	0.612646	0.396523
C	3.683073	-0.100019	0.765325
H	6.055013	1.362730	-1.207473
H	5.471036	1.028382	1.169479
C	-1.953413	-3.060673	-1.636749
H	-0.890301	-2.803784	-1.654504
C	-1.475220	-0.898538	3.004428
H	-0.478756	-0.684659	2.609172
C	2.372367	-1.084763	-2.750586
H	1.576227	-1.678608	-2.292753
N	-0.341407	-1.922615	0.514566
N	1.696325	-1.368231	0.085960
C	3.359188	-0.306288	2.242442
H	2.370658	-0.769418	2.308713
C	0.420060	-0.839723	0.116349
Ni	-0.104989	0.936921	-0.229192
Si	-2.543357	2.881631	-1.412647
C	-2.992558	3.199113	0.435445
H	-3.514283	4.125966	0.701071
H	-3.495516	2.367293	0.943729
C	-2.571660	-2.505249	-2.932732
H	-2.055409	-2.927207	-3.803311
H	-3.632859	-2.763943	-3.025587
H	-2.484755	-1.415892	-2.978549
C	-2.061247	-4.599627	-1.602647
H	-3.109572	-4.921275	-1.587751
H	-1.587616	-5.037985	-2.489237
H	-1.572935	-5.019625	-0.716167
C	-1.334782	-2.003508	4.072749
H	-0.684093	-1.667019	4.888899
H	-2.309972	-2.261890	4.503485

H	-0.902691	-2.917973	3.650659
C	-1.990402	0.407525	3.632374
H	-2.971518	0.283457	4.106125
H	-1.294668	0.741403	4.411162
H	-2.061204	1.202828	2.884282
C	4.369095	-1.271004	2.897179
H	5.385262	-0.859181	2.873598
H	4.104438	-1.449682	3.946262
H	4.391960	-2.239380	2.384120
C	3.286249	1.022216	3.017846
H	2.999735	0.832666	4.059414
H	4.253282	1.539212	3.032961
H	2.545072	1.693621	2.574246
C	3.208986	-2.038732	-3.625548
H	2.571417	-2.519471	-4.377017
H	4.005908	-1.508702	-4.160379
H	3.677961	-2.825787	-3.023874
C	1.687586	0.001126	-3.601823
H	2.421206	0.665527	-4.074725
H	1.090203	-0.459666	-4.398342
H	1.021631	0.605684	-2.977153
C	-3.294984	1.376676	-2.272842
H	-3.252868	0.492904	-1.628537
H	-4.344312	1.559152	-2.539180
H	-2.752708	1.146993	-3.198872
C	-2.765657	4.401354	-2.523921
H	-2.376703	5.303760	-2.039086
H	-2.230165	4.275885	-3.473460
H	-3.823513	4.571457	-2.761404
C	-1.482086	3.233683	0.674158
C	-0.872831	2.778117	-0.554261
C	0.552714	2.794735	-0.672354
C	1.303970	3.317341	0.425708
C	0.681384	3.778079	1.575848
C	-0.729632	3.748015	1.714619
H	1.285798	4.188851	2.381853
H	-1.201598	4.149560	2.608901
H	1.051353	2.688994	-1.635088
H	2.386438	3.379627	0.338872

4-TSa

B3LYP SCF energy: -1969.02690653 a.u.
B3LYP enthalpy: -1968.226775 a.u.
B3LYP free energy: -1968.349898 a.u.
M06 SCF energy in solution: -1969.95106074 a.u.
M06 enthalpy in solution: -1969.150929 a.u.
M06 free energy in solution: -1969.274052 a.u.
Three lowest frequencies (cm-1): -126.0491 19.7971 23.4326
Imaginary frequency: -126.0491 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-2.382695	-1.103587	0.859133
C	-3.320404	-1.717315	0.000144
C	-4.654441	-1.294672	0.080061

H	-5.397421	-1.750892	-0.567699
C	-5.041832	-0.299508	0.970873
C	-4.099511	0.287065	1.812813
C	-2.755013	-0.102164	1.784421
H	-6.080692	0.017360	1.014387
H	-4.417503	1.055024	2.510395
C	-0.603711	-2.778138	1.341849
C	0.722504	-2.885630	1.097183
H	-1.291374	-3.450951	1.829068
H	1.425152	-3.671744	1.325562
C	2.462341	-1.437135	0.056223
C	2.863060	-1.669156	-1.275578
C	4.197389	-1.404777	-1.610154
H	4.533232	-1.568603	-2.630522
C	5.102830	-0.945148	-0.657584
C	4.686541	-0.737515	0.654787
C	3.360958	-0.973290	1.040560
H	6.135288	-0.752204	-0.937579
H	5.401523	-0.383362	1.392341
C	-2.943520	-2.835248	-0.971535
H	-1.851738	-2.885878	-1.021105
C	-1.756981	0.487146	2.779074
H	-0.764441	0.428365	2.323895
C	1.908427	-2.197988	-2.340944
H	0.930720	-2.343686	-1.874025
N	-1.013860	-1.550659	0.820499
N	1.103740	-1.718800	0.437962
C	2.940599	-0.743424	2.489960
H	1.854224	-0.854278	2.546857
C	0.039698	-0.850523	0.251719
Ni	0.139164	0.892600	-0.396740
Si	-1.037694	2.501551	-2.180288
C	-1.764310	3.787265	-0.943064
H	-2.081522	4.757937	-1.343275
H	-2.562259	3.411716	-0.290589
C	-3.449880	-2.580490	-2.403958
H	-3.087312	-3.370142	-3.072943
H	-4.544800	-2.585797	-2.458494
H	-3.097882	-1.619007	-2.787761
C	-3.454409	-4.200105	-0.463675
H	-4.549572	-4.213108	-0.408598
H	-3.142382	-5.003950	-1.141181
H	-3.070710	-4.432501	0.535613
C	-1.742124	-0.348455	4.076982
H	-1.000757	0.049272	4.780721
H	-2.722243	-0.324442	4.569482
H	-1.490939	-1.396321	3.879248
C	-2.004004	1.971321	3.095908
H	-2.938729	2.132465	3.646416
H	-1.190211	2.352040	3.723507
H	-2.029476	2.574562	2.182828
C	3.567245	-1.800768	3.421560
H	4.662117	-1.738016	3.413855
H	3.230100	-1.650716	4.454172
H	3.291310	-2.817621	3.119843
C	3.271422	0.679939	2.975312
H	2.902525	0.822292	3.998324

H	4.351967	0.866317	2.987997
H	2.801711	1.432497	2.334898
C	2.370191	-3.563859	-2.885639
H	1.643330	-3.949963	-3.610315
H	3.338531	-3.491062	-3.394776
H	2.471722	-4.301003	-2.080868
C	1.716649	-1.176875	-3.477686
H	2.657090	-0.975857	-4.004903
H	0.995603	-1.554474	-4.213076
H	1.337310	-0.231465	-3.075099
C	-2.165748	1.056252	-2.665588
H	-2.633880	0.596784	-1.791731
H	-2.957667	1.428266	-3.333510
H	-1.607879	0.280562	-3.200901
C	-0.465433	3.299152	-3.805367
H	0.082842	4.230114	-3.624645
H	0.201118	2.621801	-4.354440
H	-1.319106	3.521937	-4.458551
C	-0.392687	3.812322	-0.280701
C	0.380856	2.758395	-0.849734
C	1.749974	2.626243	-0.524047
C	2.307106	3.524471	0.407582
C	1.535410	4.549104	0.957836
C	0.184506	4.716756	0.605413
H	1.995744	5.248370	1.652454
H	-0.389679	5.545602	1.014045
H	2.394396	1.915203	-1.034001
H	3.358549	3.442292	0.673364

4-TSc

B3LYP SCF energy: -2008.35911953 a.u.
B3LYP enthalpy: -2007.528395 a.u.
B3LYP free energy: -2007.653572 a.u.
M06 SCF energy in solution: -2009.26395968 a.u.
M06 enthalpy in solution: -2008.433235 a.u.
M06 free energy in solution: -2008.558412 a.u.
Three lowest frequencies (cm-1): -122.1362 11.5383 18.5345
Imaginary frequency: -122.1362 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	2.632054	-1.142990	0.263700
C	3.394389	-0.505764	1.263766
C	4.706855	-0.132885	0.944668
H	5.317515	0.360307	1.695888
C	5.240103	-0.384407	-0.315368
C	4.468786	-1.022374	-1.284799
C	3.152363	-1.417956	-1.019531
H	6.260500	-0.087114	-0.543245
H	4.899411	-1.218847	-2.261602
C	1.025421	-2.755482	1.271920
C	-0.314569	-2.802467	1.454367
H	1.806989	-3.437658	1.567610
H	-0.936594	-3.535589	1.942104
C	-2.254600	-1.355062	0.852275

C	-2.757480	-0.380243	1.744049
C	-4.132919	-0.121103	1.712837
H	-4.550563	0.625122	2.380681
C	-4.979815	-0.811512	0.848919
C	-4.465398	-1.786083	0.000743
C	-3.095301	-2.080979	-0.020265
H	-6.044877	-0.594361	0.844430
H	-5.137253	-2.327077	-0.658732
C	2.852380	-0.237201	2.665053
H	1.796532	-0.521047	2.680631
C	2.340705	-2.168441	-2.071443
H	1.282745	-2.030739	-1.829651
C	-1.864030	0.310131	2.773013
H	-0.853298	0.354020	2.357685
N	1.294692	-1.573764	0.585029
N	-0.843443	-1.653052	0.868311
C	-3.136717	-3.121959	-2.363874
H	-2.660551	-3.889520	-2.985286
H	-4.216709	-3.307056	-2.392836
H	-2.945451	-2.148945	-2.824051
C	-2.275155	1.759302	3.080030
H	-3.241573	1.819080	3.595040
H	-1.530068	2.218479	3.739743
H	-2.328386	2.362099	2.168265
C	-1.812759	-0.521104	4.073339
H	-1.146961	-0.047331	4.804957
H	-2.809143	-0.601066	4.525424
H	-1.444265	-1.536346	3.890367
C	2.921748	1.255640	3.036238
H	2.366289	1.863435	2.315654
H	2.484883	1.417603	4.029164
H	3.955620	1.620025	3.068459
C	3.579118	-1.102881	3.714172
H	3.493509	-2.170794	3.482400
H	4.646941	-0.858219	3.763315
H	3.151658	-0.937110	4.710237
C	2.550103	-1.631836	-3.498122
H	2.373017	-0.552645	-3.550072
H	3.561927	-1.829499	-3.871044
H	1.852047	-2.123018	-4.185844
C	2.645706	-3.680428	-2.014857
H	2.427067	-4.097869	-1.026058
H	2.040737	-4.222728	-2.751621
H	3.702253	-3.874989	-2.236074
C	-2.888317	-4.581923	-0.325563
H	-3.970846	-4.737036	-0.243857
H	-2.480985	-5.377514	-0.960915
H	-2.462179	-4.699897	0.676089
C	-2.578132	-3.194994	-0.930190
H	-1.490519	-3.094491	-1.000860
C	0.145300	-0.848800	0.324466
Ni	0.031436	0.895553	-0.348615
C	-1.119011	3.623237	-0.418293
C	-0.052815	2.762199	-0.803982
C	1.244699	3.016392	-0.298591
C	1.462566	4.058411	0.618098
C	0.401905	4.877610	0.998445

C	-0.881004	4.670723	0.469434
H	2.095694	2.441151	-0.655150
H	2.462135	4.245399	1.003725
H	0.572677	5.703081	1.685671
H	-1.693166	5.340544	0.746178
C	-2.463882	3.372356	-1.076351
H	-2.994533	2.575982	-0.535254
H	-3.099622	4.265414	-1.013955
C	-2.212287	2.924241	-2.536287
H	-2.057170	3.811971	-3.165265
H	-3.075772	2.387788	-2.947642
Si	-0.607664	1.864754	-2.535101
C	-1.123444	0.120435	-3.132013
H	-1.883732	-0.303081	-2.470858
H	-1.550799	0.207443	-4.143552
H	-0.283216	-0.578124	-3.171619
C	0.652931	2.487049	-3.818055
H	0.885657	3.548031	-3.673389
H	1.595556	1.929185	-3.749651
H	0.268240	2.356125	-4.838048

4-TSe

B3LYP SCF energy: -2047.67223148 a.u.
B3LYP enthalpy: -2046.811330 a.u.
B3LYP free energy: -2046.938875 a.u.
M06 SCF energy in solution: -2048.55972892 a.u.
M06 enthalpy in solution: -2047.698827 a.u.
M06 free energy in solution: -2047.826372 a.u.
Three lowest frequencies (cm-1): -110.9846 14.5181 20.4527
Imaginary frequency: -110.9846 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	2.928963	-0.654763	0.156506
C	3.456854	0.111183	1.216081
C	4.664035	0.786848	0.994239
H	5.092656	1.386032	1.792692
C	5.322907	0.700430	-0.227773
C	4.784990	-0.068914	-1.257175
C	3.580340	-0.762889	-1.091295
H	6.259479	1.230873	-0.379624
H	5.310913	-0.129745	-2.204601
C	1.714326	-2.681190	0.930023
C	0.418405	-3.033267	1.100258
H	2.628042	-3.210461	1.150165
H	-0.026937	-3.931698	1.497636
C	-1.787879	-1.931869	0.758263
C	-2.368460	-1.438229	1.944667
C	-3.766718	-1.446107	2.038743
H	-4.241606	-1.068480	2.940051
C	-4.554849	-1.936015	1.001965
C	-3.956805	-2.436616	-0.152438
C	-2.564545	-2.448556	-0.301488
H	-5.637820	-1.934503	1.094657
H	-4.583269	-2.825010	-0.949264

C	2.783969	0.200812	2.582459
H	1.820407	-0.311739	2.518970
C	3.026577	-1.632371	-2.217148
H	1.944956	-1.711214	-2.069112
C	-1.535303	-0.948045	3.125788
H	-0.484783	-0.955278	2.823656
N	1.714829	-1.399579	0.383455
N	-0.350429	-1.960660	0.653837
C	-2.684723	-2.716794	-2.845608
H	-2.108921	-3.060560	-3.712573
H	-3.660613	-3.214380	-2.888943
H	-2.846789	-1.640041	-2.952229
C	-1.875118	0.499920	3.523010
H	-2.919606	0.603359	3.840251
H	-1.242930	0.817498	4.361100
H	-1.699375	1.184439	2.687717
C	-1.677038	-1.902892	4.328670
H	-1.036684	-1.573399	5.155583
H	-2.709409	-1.932858	4.697052
H	-1.388823	-2.926587	4.063324
C	2.487748	1.655818	2.989648
H	1.859420	2.150568	2.242923
H	1.958831	1.676288	3.950320
H	3.406956	2.242356	3.107969
C	3.622043	-0.518983	3.658470
H	3.793550	-1.569691	3.397349
H	4.602023	-0.043648	3.786348
H	3.107890	-0.489737	4.626640
C	3.253389	-1.030322	-3.615242
H	2.914911	0.009293	-3.666948
H	4.309531	-1.057459	-3.908608
H	2.695759	-1.605901	-4.362573
C	3.617973	-3.057358	-2.157806
H	3.393766	-3.551351	-1.206990
H	3.205608	-3.677107	-2.963269
H	4.708164	-3.031446	-2.275897
C	-1.776752	-4.580909	-1.403874
H	-2.758063	-5.058349	-1.293311
H	-1.292243	-5.005965	-2.291198
H	-1.173047	-4.848863	-0.530679
C	-1.924832	-3.051028	-1.549577
H	-0.920284	-2.625584	-1.640591
C	0.431706	-0.907993	0.208552
Ni	-0.101428	0.816725	-0.287588
C	-1.729495	3.121257	0.287855
C	-0.635208	2.642130	-0.497260
C	0.620639	3.288910	-0.358688
C	0.817535	4.332663	0.551195
C	-0.259560	4.786911	1.310195
C	-1.516701	4.189886	1.167537
H	1.449779	2.983692	-0.992222
H	1.796508	4.795518	0.651474
H	-0.130728	5.612927	2.005669
H	-2.350503	4.558521	1.762226
C	-3.122643	2.519805	0.190954
H	-3.108018	1.482552	0.551123
H	-3.787492	3.072034	0.866915

Si	-1.133834	1.804306	-2.303086
C	-0.392857	0.424303	-3.404879
H	-0.557782	-0.577222	-3.002442
H	-0.851303	0.485222	-4.404093
H	0.686124	0.562173	-3.527412
C	-0.818889	3.362175	-3.367239
H	0.252755	3.593641	-3.418888
H	-1.171850	3.203897	-4.395265
H	-1.323742	4.247587	-2.964527
C	-3.720653	2.532074	-1.229666
H	-3.662316	3.552475	-1.633860
H	-4.790565	2.289384	-1.159485
C	-3.015729	1.544589	-2.176887
H	-3.452981	1.613135	-3.184361
H	-3.202539	0.520266	-1.824438

5-TSa

B3LYP SCF energy: -1969.01916884 a.u.
B3LYP enthalpy: -1968.219565 a.u.
B3LYP free energy: -1968.346016 a.u.
M06 SCF energy in solution: -1969.93702802 a.u.
M06 enthalpy in solution: -1969.137424 a.u.
M06 free energy in solution: -1969.263875 a.u.
Three lowest frequencies (cm-1): -67.9185 8.6194 15.6317
Imaginary frequency: -67.9185 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	1.940306	-2.351317	-0.185988
C	1.804661	-2.899815	-1.477774
C	1.571972	-4.276726	-1.581423
H	1.453642	-4.724979	-2.564167
C	1.487387	-5.080607	-0.447721
C	1.639061	-4.518113	0.816826
C	1.870552	-3.146209	0.976807
H	1.306406	-6.147547	-0.550165
H	1.574613	-5.153763	1.695820
C	3.467365	-0.389026	0.010558
C	3.308728	0.947691	0.151997
H	4.356871	-0.996669	-0.051189
H	4.032463	1.741806	0.247694
C	1.383623	2.512799	0.327074
C	1.250958	3.334197	-0.813754
C	0.773488	4.637583	-0.627838
H	0.666213	5.295044	-1.485547
C	0.434305	5.106996	0.639066
C	0.570078	4.276985	1.747744
C	1.050168	2.967069	1.619379
H	0.064266	6.121727	0.761041
H	0.304358	4.652244	2.732157
N	2.189856	-0.940546	-0.051106
N	1.935311	1.192825	0.171070
C	1.196765	0.023743	0.053996
Ni	-0.589581	-0.278835	0.124522
C	-4.043110	-1.050088	0.409159

C	-4.748241	-0.071926	-0.325580
C	-6.142580	-0.123249	-0.392921
C	-6.813793	-1.151680	0.276605
C	-6.102075	-2.117682	1.002616
C	-4.706853	-2.081205	1.079125
H	-6.646527	-2.907967	1.514125
H	-4.161412	-2.834165	1.643500
Si	-3.146562	0.794840	-0.833945
C	-2.949963	2.550469	-0.167994
H	-3.104735	2.572376	0.916358
H	-1.952318	2.952830	-0.372294
H	-3.692187	3.218334	-0.625777
C	-2.783806	0.700444	-2.685950
H	-3.466988	1.351483	-3.247416
H	-1.756470	1.007157	-2.906793
H	-2.916472	-0.322464	-3.055620
C	-2.568492	-0.720773	0.287617
H	-2.101194	-0.505040	1.286489
H	-1.996798	-1.559650	-0.191611
C	0.732072	-2.709773	3.196680
H	0.460305	-3.762720	3.338555
H	0.855129	-2.259625	4.189481
H	-0.097628	-2.205370	2.690181
C	3.230356	-3.185067	3.117474
H	3.358534	-2.714188	4.099478
H	3.093211	-4.260496	3.281344
H	4.160200	-3.050939	2.552749
C	2.029194	-2.564217	2.377959
H	2.225594	-1.493133	2.277118
C	2.972629	-2.541516	-3.706202
H	2.757303	-3.547736	-4.084592
H	3.044489	-1.872856	-4.572387
H	3.953926	-2.571829	-3.218783
C	0.506739	-1.970086	-3.434500
H	0.558098	-1.319018	-4.315944
H	0.169850	-2.959519	-3.767292
H	-0.243026	-1.564402	-2.746987
C	1.879983	-2.046713	-2.739656
H	2.145964	-1.028730	-2.440809
C	3.033698	3.380247	-2.607857
H	3.315568	3.010348	-3.601071
H	3.041753	4.476557	-2.641101
H	3.804585	3.061238	-1.898615
C	1.640475	2.850986	-2.208146
H	1.693372	1.758464	-2.175599
C	0.600960	3.222442	-3.281133
H	0.554533	4.304032	-3.454206
H	0.865262	2.752836	-4.235871
H	-0.401202	2.883139	-3.001104
C	1.210987	2.097358	2.862106
H	1.554867	1.111152	2.539947
C	2.275858	2.674753	3.815261
H	1.985329	3.661870	4.194430
H	2.413026	2.013609	4.679297
H	3.244351	2.782546	3.313534
C	-0.132500	1.887614	3.584603
H	0.001071	1.227321	4.450063

H	-0.552780	2.832759	3.948613
H	-0.858182	1.423552	2.908631
H	-7.899029	-1.207243	0.236503
H	-6.709967	0.617734	-0.952584

5-TSb

B3LYP SCF energy: -1816.59270149 a.u.
B3LYP enthalpy: -1815.819416 a.u.
B3LYP free energy: -1815.940451 a.u.
M06 SCF energy in solution: -1817.58996719 a.u.
M06 enthalpy in solution: -1816.816682 a.u.
M06 free energy in solution: -1816.937717 a.u.
Three lowest frequencies (cm-1): -73.2512 19.3013 20.7951
Imaginary frequency: -73.2512 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	2.843621	-0.495704	0.296907
C	3.347789	0.274650	1.364740
C	4.570379	0.931013	1.176146
H	4.978311	1.538447	1.979469
C	5.270927	0.820125	-0.021991
C	4.759399	0.041868	-1.056943
C	3.540443	-0.633891	-0.921201
H	6.218463	1.337827	-0.147837
H	5.313357	-0.041434	-1.987936
C	1.513744	-2.507840	0.923355
C	0.200570	-2.834578	0.936886
H	2.390377	-3.076815	1.191775
H	-0.302466	-3.746549	1.218961
C	-1.932571	-1.687613	0.374247
C	-2.702382	-1.395221	1.520576
C	-4.096737	-1.400839	1.388822
H	-4.716210	-1.169870	2.250501
C	-4.704151	-1.700810	0.171516
C	-3.923419	-2.004048	-0.939934
C	-2.524604	-2.007782	-0.864296
H	-5.788175	-1.701610	0.091380
H	-4.406284	-2.244777	-1.883175
N	1.596845	-1.193925	0.467683
N	-0.499377	-1.713025	0.490886
C	0.347836	-0.657487	0.181091
Ni	0.024382	0.988020	-0.507147
C	-0.281628	4.260377	-2.076196
C	-1.810629	4.569963	-2.084039
Si	-2.011896	3.270861	-0.691992
C	-3.479188	2.092593	-0.834535
H	-3.502104	1.606773	-1.816108
H	-3.441586	1.304304	-0.076073
H	-4.420999	2.644966	-0.710818
C	-1.945834	4.070539	1.021767
H	-2.858169	4.651475	1.209986
H	-1.855026	3.320072	1.814258
H	-1.092492	4.753393	1.108004
C	-0.261153	2.844015	-1.414979

H	-0.280551	2.058061	-2.203323
H	0.653828	2.702198	-0.776827
C	2.608565	-0.566254	-3.269702
H	3.471340	-0.011670	-3.658268
H	2.200624	-1.171209	-4.089105
H	1.845546	0.155659	-2.959153
C	3.996804	-2.561732	-2.513152
H	3.558726	-3.180046	-3.305706
H	4.929087	-2.137157	-2.903812
H	4.256247	-3.218386	-1.674625
C	3.003625	-1.465212	-2.082310
H	2.092713	-1.967104	-1.744422
C	3.460949	-0.017802	3.886212
H	4.346560	0.616502	4.009593
H	2.879064	0.045260	4.813526
H	3.805318	-1.052019	3.770778
C	2.087098	1.867341	2.867001
H	1.522274	1.958008	3.803106
H	2.913503	2.587820	2.901481
H	1.426617	2.137847	2.036100
C	2.602263	0.426392	2.686629
H	1.724435	-0.225065	2.653457
C	-2.703398	-1.779752	4.046215
H	-2.143192	-1.571243	4.965193
H	-3.737729	-1.459641	4.217496
H	-2.709896	-2.864751	3.891290
C	-2.057729	-1.042998	2.858745
H	-1.010001	-1.355308	2.817420
C	-2.064048	0.482811	3.076572
H	-3.089088	0.872532	3.110339
H	-1.573058	0.739393	4.023617
H	-1.528615	0.982556	2.262148
C	-1.701554	-2.366464	-2.096974
H	-0.644875	-2.287776	-1.828742
C	-1.961952	-3.818782	-2.542824
H	-3.004804	-3.967920	-2.847431
H	-1.326022	-4.075161	-3.398638
H	-1.746572	-4.528200	-1.735564
C	-1.944916	-1.374139	-3.249087
H	-1.315980	-1.629492	-4.110645
H	-2.989270	-1.385921	-3.583749
H	-1.693563	-0.356690	-2.931542
H	0.245448	4.974827	-1.433201
H	0.203886	4.292077	-3.059379
H	-2.074299	5.620945	-1.927780
H	-2.271843	4.240464	-3.023573

5-TSc

B3LYP SCF energy:	-2008.35408832 a.u.
B3LYP enthalpy:	-2007.523717 a.u.
B3LYP free energy:	-2007.652392 a.u.
M06 SCF energy in solution:	-2009.25458756 a.u.
M06 enthalpy in solution:	-2008.424216 a.u.
M06 free energy in solution:	-2008.552891 a.u.
Three lowest frequencies (cm-1):	-77.2571 9.1688 15.9008

Imaginary frequency: -77.2571 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	2.600346	-1.952822	0.152139
C	2.712853	-2.694697	-1.041734
C	2.787695	-4.089169	-0.938585
H	2.869840	-4.686346	-1.842631
C	2.758439	-4.723128	0.300782
C	2.657420	-3.967833	1.466056
C	2.580295	-2.570390	1.419458
H	2.817600	-5.806986	0.358771
H	2.635189	-4.471030	2.428851
C	3.685058	0.289498	0.096581
C	3.258672	1.569399	-0.010433
H	4.677764	-0.124304	0.182583
H	3.804171	2.499470	-0.042683
C	1.063740	2.714248	-0.217481
C	0.674555	3.144734	-1.502628
C	-0.058500	4.334376	-1.598397
H	-0.376129	4.685525	-2.576267
C	-0.380903	5.076691	-0.466185
C	0.021073	4.636151	0.792171
C	0.746259	3.447874	0.946305
H	-0.946126	5.999921	-0.563880
H	-0.233542	5.223616	1.669531
C	2.740581	-2.036691	-2.417706
H	2.721801	-0.952909	-2.273101
C	2.446373	-1.774956	2.713556
H	2.489644	-0.711675	2.460742
C	1.031822	2.375205	-2.769793
H	1.590477	1.483197	-2.475008
N	2.548675	-0.515441	0.077626
N	1.866562	1.526658	-0.091368
C	0.039215	3.011302	3.357600
H	0.379922	2.590653	4.311025
H	-0.322242	4.026254	3.560147
H	-0.808607	2.414969	3.006352
C	-0.229654	1.888428	-3.507099
H	-0.853485	2.725082	-3.844229
H	0.048285	1.301748	-4.391093
H	-0.830707	1.252347	-2.848755
C	1.938847	3.207672	-3.696937
H	2.225806	2.620226	-4.577326
H	1.432376	4.112921	-4.052389
H	2.855807	3.518830	-3.183356
C	1.486353	-2.403281	-3.234322
H	0.582153	-2.096135	-2.697561
H	1.501430	-1.894968	-4.206418
H	1.428264	-3.482457	-3.421389
C	4.030983	-2.376139	-3.188058
H	4.923241	-2.085850	-2.621431
H	4.106509	-3.448967	-3.400969
H	4.051156	-1.846636	-4.148062
C	1.075506	-2.028037	3.370069
H	0.269627	-1.768827	2.675324
H	0.957703	-3.079872	3.657994

H	0.964565	-1.417501	4.274726
C	3.600956	-2.060516	3.692387
H	4.574737	-1.851882	3.234368
H	3.504296	-1.432620	4.586092
H	3.605703	-3.105595	4.023563
C	2.370570	3.857949	2.841066
H	2.080948	4.911750	2.933379
H	2.702825	3.512557	3.827485
H	3.226912	3.805978	2.159741
C	1.191361	3.001045	2.336104
H	1.540626	1.967343	2.257370
C	1.383923	0.227592	-0.045376
Ni	-0.290136	-0.462933	-0.212116
C	-4.706267	-1.898903	-0.420326
C	-4.782136	-0.655715	0.236797
C	-6.044694	-0.119678	0.529154
C	-7.209270	-0.802178	0.172203
C	-7.120071	-2.034334	-0.483477
C	-5.871516	-2.583935	-0.779714
H	-6.127315	0.842387	1.032578
H	-8.183879	-0.375755	0.397123
H	-8.025802	-2.563986	-0.768931
H	-5.807207	-3.541874	-1.292752
C	-3.307699	-2.442625	-0.665465
H	-3.070150	-3.185195	0.110764
H	-3.250405	-2.978906	-1.621256
Si	-3.047694	0.026432	0.573561
C	-2.629428	-0.174289	2.410395
H	-2.686525	-1.227560	2.710224
H	-1.617394	0.181104	2.628870
H	-3.338737	0.386162	3.033747
C	-2.938297	1.832446	0.027541
H	-3.102440	1.920298	-1.052668
H	-3.714510	2.427429	0.528196
H	-1.966371	2.278930	0.255374
C	-2.263466	-1.286162	-0.611941
H	-1.294496	-1.829599	-0.369742
H	-2.174387	-0.842502	-1.615688

5-TSd

B3LYP SCF energy: -1855.92736861 a.u.
B3LYP enthalpy: -1855.123412 a.u.
B3LYP free energy: -1855.245513 a.u.
M06 SCF energy in solution: -1856.90600872 a.u.
M06 enthalpy in solution: -1856.102052 a.u.
M06 free energy in solution: -1856.224153 a.u.
Three lowest frequencies (cm-1): -47.2382 18.6291 19.8642
Imaginary frequency: -47.2382 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-1.398077	5.353691	-1.121341
C	-0.112861	4.519068	-1.264550
C	-0.450417	3.028880	-0.977869
C	-2.045601	5.008744	0.236988

H	-1.184173	6.425799	-1.225517
H	-2.084336	5.089142	-1.938814
H	0.628498	4.872120	-0.533328
H	0.340932	4.639267	-2.256895
H	-0.959898	2.605631	-1.858347
H	0.570395	2.534597	-0.887462
H	-3.108549	5.276774	0.266537
H	-1.554993	5.578754	1.038689
Si	-1.717918	3.130595	0.495677
C	-1.051441	2.867360	2.250590
H	-1.761939	3.260208	2.991371
H	-0.873529	1.809220	2.463098
H	-0.102097	3.398808	2.389141
C	-3.305242	2.141731	0.200955
H	-3.141192	1.065086	0.305130
H	-4.084603	2.442606	0.913831
H	-3.694814	2.322712	-0.808628
C	-1.940462	-1.806451	-0.085630
C	-2.519488	-1.787411	-1.371950
C	-3.916868	-1.823883	-1.458618
H	-4.389895	-1.811468	-2.436592
C	-4.710179	-1.885410	-0.316268
C	-4.116217	-1.904451	0.942732
C	-2.723679	-1.861496	1.087453
H	-5.792823	-1.918101	-0.407107
H	-4.743527	-1.951879	1.828263
C	0.196504	-3.034096	0.219531
C	1.507366	-2.707442	0.295174
H	-0.301591	-3.989417	0.273479
H	2.385125	-3.320113	0.430583
C	2.834299	-0.605712	0.157200
C	3.507964	-0.406358	-1.065561
C	4.738653	0.260668	-1.031564
H	5.276699	0.432828	-1.959884
C	5.284761	0.705519	0.169387
C	4.605344	0.488003	1.364898
C	3.369448	-0.170386	1.386830
H	6.242739	1.219213	0.174025
H	5.041241	0.835376	2.297558
N	-0.507238	-1.843316	0.037579
N	1.586235	-1.323572	0.155069
C	0.337203	-0.743370	-0.016598
C	2.401357	0.921827	3.462512
H	1.827985	1.614198	2.838338
H	1.831034	0.735158	4.380519
H	3.337516	1.415026	3.749784
C	3.431781	-1.397238	3.600452
H	4.426806	-1.014753	3.858042
H	2.891260	-1.579401	4.537166
H	3.566413	-2.360059	3.094212
C	2.657197	-0.400195	2.715726
H	1.680123	-0.841216	2.499653
C	3.875141	-1.911572	-3.073066
H	3.425177	-2.282271	-4.001898
H	4.846629	-1.471860	-3.328294
H	4.060565	-2.771576	-2.419181
C	2.944671	-0.884096	-2.399795

H	1.991975	-1.383520	-2.203651
C	2.645165	0.301189	-3.337272
H	1.932768	0.985640	-2.864570
H	3.554422	0.863076	-3.583066
H	2.208680	-0.057259	-4.277747
C	-2.060162	-0.587734	-3.564391
H	-1.950283	0.363190	-3.032692
H	-1.401926	-0.566202	-4.441295
H	-3.092095	-0.663081	-3.927209
C	-1.681723	-1.764065	-2.646403
H	-0.638184	-1.614675	-2.358408
C	-1.777624	-3.109107	-3.393819
H	-2.804596	-3.313711	-3.720148
H	-1.139019	-3.099374	-4.285362
H	-1.458119	-3.942253	-2.757351
C	-2.704147	-0.836440	3.420465
H	-2.170054	-0.836786	4.378088
H	-2.626226	0.165723	2.987858
H	-3.761429	-1.030387	3.636126
C	-2.103059	-1.898858	2.481366
H	-1.038198	-1.670850	2.377916
C	-2.223035	-3.304358	3.105232
H	-1.746311	-3.328742	4.092522
H	-3.273792	-3.591966	3.232002
H	-1.742739	-4.064883	2.479689
Ni	0.002585	1.009508	-0.361606

5-TSe

B3LYP SCF energy: -2047.66340022 a.u.
B3LYP enthalpy: -2046.802628 a.u.
B3LYP free energy: -2046.929609 a.u.
M06 SCF energy in solution: -2048.55238759 a.u.
M06 enthalpy in solution: -2047.691615 a.u.
M06 free energy in solution: -2047.818596 a.u.
Three lowest frequencies (cm-1): -54.6300 15.5507 20.2142
Imaginary frequency: -54.6300 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	5.060596	-1.402552	-0.573698
C	3.736814	-1.429552	-1.033939
C	2.808439	-2.318467	-0.441734
C	3.267151	-3.150483	0.597637
C	4.586852	-3.117230	1.051307
C	5.489647	-2.232852	0.461655
H	5.768800	-0.721155	-1.042033
H	2.575453	-3.845072	1.069777
H	4.905759	-3.776005	1.855589
H	6.523129	-2.194149	0.797784
C	2.348652	-1.109177	-3.169105
H	2.374267	-0.526817	-4.101426
H	2.686632	-2.118828	-3.435937
C	3.341860	-0.498506	-2.167475
H	2.902555	0.422075	-1.753560
H	4.251036	-0.191371	-2.699890

Si	0.988865	-2.452440	-0.987206
C	0.802617	-4.031072	-2.057156
H	1.124660	-4.912324	-1.488101
H	-0.252246	-4.182324	-2.325124
H	1.382683	-4.005155	-2.986153
C	-0.046696	-2.955409	0.551463
H	-1.112991	-2.930036	0.304171
H	0.201082	-3.981819	0.862034
H	0.118675	-2.281009	1.396052
C	-3.198029	-0.259580	0.219130
C	-3.644426	-1.204224	1.171076
C	-4.635931	-2.110056	0.773489
H	-4.997026	-2.848398	1.482888
C	-5.166707	-2.081928	-0.512732
C	-4.723218	-1.130546	-1.426195
C	-3.738427	-0.195554	-1.082918
H	-5.933018	-2.796982	-0.800442
H	-5.156206	-1.104476	-2.421805
C	-2.501825	1.806746	1.416874
C	-1.345231	2.485725	1.599765
H	-3.500684	1.999750	1.773756
H	-1.129013	3.386811	2.151821
C	1.011994	2.232631	0.844499
C	1.909007	1.780249	1.834741
C	3.222587	2.262291	1.788768
H	3.938371	1.931950	2.535020
C	3.627867	3.157490	0.802162
C	2.721245	3.593476	-0.159965
C	1.394383	3.144507	-0.160739
H	4.653014	3.518298	0.785384
H	3.046171	4.296872	-0.921492
N	-2.202383	0.706778	0.615198
N	-0.360857	1.793415	0.900244
C	-0.865550	0.680161	0.257516
C	0.920859	3.439468	-2.643130
H	1.114905	2.376418	-2.818933
H	0.167929	3.774410	-3.366743
H	1.844431	3.993293	-2.848493
C	0.099288	5.160682	-0.966358
H	0.998086	5.780710	-1.067772
H	-0.638661	5.518701	-1.694271
H	-0.307266	5.326081	0.037864
C	0.416403	3.670883	-1.206794
H	-0.518836	3.113781	-1.103565
C	1.180105	1.632141	4.245771
H	0.841016	0.958165	5.041697
H	2.081057	2.146898	4.601282
H	0.402533	2.388260	4.089807
C	1.472295	0.839278	2.954056
H	0.539976	0.360329	2.639472
C	2.486931	-0.284883	3.226743
H	2.723858	-0.843456	2.316826
H	3.424886	0.099681	3.644324
H	2.072291	-0.986909	3.960139
C	-2.783926	-2.652554	3.102351
H	-2.070554	-3.146464	2.437574
H	-2.336745	-2.597511	4.101932

H	-3.674497	-3.287021	3.181855
C	-3.129477	-1.234638	2.609740
H	-2.208516	-0.644519	2.650279
C	-4.150316	-0.584231	3.568690
H	-5.090890	-1.148100	3.576717
H	-3.758537	-0.568596	4.592758
H	-4.385132	0.446179	3.282249
C	-2.970425	0.299317	-3.463496
H	-2.625982	1.099838	-4.129240
H	-2.162845	-0.433081	-3.365713
H	-3.821627	-0.189010	-3.951998
C	-3.344623	0.882404	-2.089242
H	-2.453946	1.389181	-1.710456
C	-4.465508	1.934098	-2.220488
H	-4.165111	2.730706	-2.911837
H	-5.388913	1.485234	-2.606184
H	-4.697239	2.394319	-1.253147
Ni	0.018608	-0.329264	-1.049119
C	0.892679	-1.153011	-2.652368
H	0.509665	-0.091158	-2.730338
H	0.263358	-1.724251	-3.345666

5-TSf

B3LYP SCF energy: -1895.24098070 a.u.
B3LYP enthalpy: -1894.406838 a.u.
B3LYP free energy: -1894.528644 a.u.
M06 SCF energy in solution: -1896.20515677 a.u.
M06 enthalpy in solution: -1895.371014 a.u.
M06 free energy in solution: -1895.492820 a.u.
Three lowest frequencies (cm-1): -68.6335 12.2475 24.6671
Imaginary frequency: -68.6335 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-2.165046	4.743367	-0.150852
H	-2.565971	5.755628	0.006606
H	-2.642151	4.110153	0.613447
C	-0.636628	4.741509	0.037742
H	-0.378065	5.270639	0.967147
H	-0.178749	5.325760	-0.775265
Si	0.187426	3.004430	0.133906
C	-2.196429	-1.565350	0.377696
C	-2.858450	-1.754961	-0.853721
C	-4.253349	-1.630473	-0.869522
H	-4.789847	-1.771057	-1.803371
C	-4.964800	-1.339224	0.290625
C	-4.290414	-1.170610	1.496685
C	-2.896009	-1.278535	1.569749
H	-6.047462	-1.249442	0.256411
H	-4.856270	-0.951605	2.397109
C	-0.156294	-2.924938	0.808248
C	1.179570	-2.726763	0.720642
H	-0.728233	-3.793334	1.094449
H	2.010115	-3.387382	0.912859
C	2.674199	-0.864200	0.038260

C	3.194357	-0.922371	-1.271136
C	4.489317	-0.431550	-1.480692
H	4.914044	-0.461863	-2.480201
C	5.243140	0.085375	-0.431651
C	4.712590	0.121003	0.855115
C	3.420193	-0.349158	1.120467
H	6.247319	0.458365	-0.615500
H	5.311870	0.521960	1.666888
N	-0.764506	-1.729077	0.433331
N	1.365099	-1.413475	0.292737
C	3.448024	-1.504797	3.368883
H	4.539789	-1.435413	3.446669
H	3.036273	-1.499134	4.385282
H	3.206705	-2.471073	2.913143
C	2.879052	-0.328411	2.547856
H	1.793137	-0.455080	2.493373
C	3.090626	-2.818916	-2.940376
H	2.501134	-3.266868	-3.749333
H	4.097877	-2.626445	-3.328665
H	3.179356	-3.558195	-2.136023
C	2.421080	-1.522865	-2.440960
H	1.421083	-1.785132	-2.086077
C	2.238795	-0.511260	-3.587545
H	1.721839	0.384916	-3.229276
H	3.198912	-0.205315	-4.019544
H	1.639853	-0.954767	-4.392317
C	-2.487330	-1.231706	-3.321054
H	-2.304556	-0.179826	-3.079593
H	-1.878115	-1.492919	-4.194552
H	-3.538976	-1.337979	-3.611696
C	-2.120048	-2.138957	-2.132773
H	-1.049387	-2.009092	-1.954967
C	-2.362160	-3.623152	-2.475940
H	-3.423914	-3.816946	-2.670571
H	-1.798765	-3.907091	-3.373001
H	-2.048120	-4.279957	-1.656768
C	-2.189737	-1.128693	2.914381
H	-1.124624	-0.973749	2.716435
C	-2.330362	-2.415471	3.755134
H	-1.798133	-2.311807	4.708362
H	-3.383814	-2.623722	3.978051
H	-1.921614	-3.288045	3.234333
C	0.162753	-0.761230	0.087919
Ni	-0.198931	0.889517	-0.706922
C	-0.141651	2.568859	1.977224
H	-1.220676	2.521286	2.165037
H	0.287850	1.609554	2.274500
H	0.269328	3.357981	2.624987
C	2.046685	3.328466	-0.139595
H	2.388926	4.163806	0.487472
H	2.658998	2.451281	0.092687
H	2.243767	3.599128	-1.184621
C	-2.684566	0.087526	3.718211
H	-2.067231	0.217888	4.614489
H	-2.623198	1.006641	3.128625
H	-3.721279	-0.035275	4.052700
C	3.146722	1.005069	3.269719

H	2.783564	1.856085	2.686498
H	2.634140	1.013203	4.238610
H	4.214332	1.157131	3.466659
C	-2.233138	2.797599	-1.852367
H	-2.589795	2.569538	-2.868444
H	-2.796794	2.135220	-1.181437
C	-0.726626	2.470168	-1.760906
H	-0.504576	1.548249	-2.378496
H	-0.138132	3.242582	-2.276534
C	-2.593040	4.259203	-1.542626
H	-3.678828	4.384719	-1.657017
H	-2.127143	4.908835	-2.299936

6

B3LYP SCF energy: -1969.05407357 a.u.
B3LYP enthalpy: -1968.251980 a.u.
B3LYP free energy: -1968.374901 a.u.
M06 SCF energy in solution: -1969.97362185 a.u.
M06 enthalpy in solution: -1969.171528 a.u.
M06 free energy in solution: -1969.294449 a.u.
Three lowest frequencies (cm-1): 15.0808 19.8096 24.8389

Cartesian coordinates

ATOM	X	Y	Z
C	2.079108	-1.806769	0.456887
C	2.960833	-1.221512	1.390079
C	4.334917	-1.347906	1.150881
H	5.040034	-0.907491	1.848497
C	4.812583	-2.029194	0.036092
C	3.921108	-2.598858	-0.868250
C	2.536696	-2.501827	-0.682527
H	5.883122	-2.115213	-0.129911
H	4.307115	-3.124922	-1.735352
C	-0.007077	-2.746920	1.431378
C	-1.301499	-2.358275	1.524496
H	0.501237	-3.622127	1.803335
H	-2.150257	-2.823271	1.999678
C	-2.647415	-0.401297	0.805420
C	-2.876124	0.623239	1.746879
C	-4.113845	1.278027	1.706693
H	-4.316490	2.074041	2.416970
C	-5.089359	0.921641	0.781760
C	-4.844724	-0.103743	-0.127147
C	-3.622441	-0.787372	-0.140279
H	-6.043615	1.441487	0.770062
H	-5.615107	-0.376630	-0.841436
N	0.655821	-1.754835	0.717166
N	-1.403097	-1.137940	0.863521
C	-0.189560	-0.729589	0.359559
Ni	0.390103	0.986626	-0.342576
C	1.434441	3.327302	-1.897969
C	1.139134	2.687562	-0.670472
C	1.535327	3.330333	0.519322
C	2.209429	4.557238	0.501270
Si	-0.348367	1.405574	-2.397723

C	2.038911	-3.008125	-3.136379
H	1.244313	-3.344459	-3.811553
H	2.270352	-1.966009	-3.376406
H	2.927213	-3.612284	-3.355120
C	1.583049	-3.163542	-1.673995
H	0.611802	-2.666680	-1.583493
C	1.386300	-4.657994	-1.340118
H	0.689041	-5.120478	-2.048948
H	2.338732	-5.198159	-1.402438
H	0.984656	-4.802649	-0.331803
C	2.548655	-1.459217	3.870274
H	3.584570	-1.762487	4.063964
H	2.170301	-0.957845	4.769119
H	1.956905	-2.368100	3.715917
C	2.471892	-0.514838	2.651912
H	1.419531	-0.251759	2.503869
C	3.228712	0.795542	2.936777
H	3.214403	1.464730	2.071136
H	2.760543	1.316980	3.780046
H	4.274055	0.613884	3.211464
C	-1.865673	1.003558	2.824550
H	-0.929588	0.479009	2.613881
C	-1.550038	2.510650	2.820835
H	-0.775077	2.733637	3.564084
H	-1.187071	2.835912	1.840985
H	-2.429815	3.112684	3.076048
C	-3.895209	-1.588130	-2.551445
H	-3.587777	-2.374756	-3.250066
H	-4.988164	-1.522259	-2.600229
H	-3.481928	-0.639322	-2.904627
C	-3.405029	-1.929038	-1.131153
H	-2.328274	-2.118101	-1.193931
C	-4.083570	-3.225800	-0.640036
H	-5.167550	-3.087380	-0.548918
H	-3.906513	-4.043169	-1.349192
H	-3.705218	-3.541817	0.337654
C	-2.351005	0.540740	4.213781
H	-1.602573	0.777679	4.979321
H	-3.286222	1.039636	4.494047
H	-2.529892	-0.540369	4.236402
C	2.098482	4.560207	-1.913895
H	2.313691	5.046684	-2.864233
C	2.489678	5.173209	-0.720270
H	3.004697	6.131137	-0.743520
C	0.955414	2.603277	-3.136249
H	0.564466	3.282599	-3.907252
H	1.773084	2.035054	-3.605815
C	-2.036794	2.294925	-2.380648
H	-2.806133	1.717694	-1.855755
H	-1.946491	3.262335	-1.873668
H	-2.389584	2.479143	-3.405434
C	-0.502502	-0.128139	-3.531010
H	0.486089	-0.553310	-3.735253
H	-1.120315	-0.918975	-3.093331
H	-0.949050	0.150765	-4.496347
H	1.307833	2.879634	1.486820
H	2.503263	5.034960	1.434148

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B3LYP SCF energy: -1969.05113530 a.u.
B3LYP enthalpy: -1968.250158 a.u.
B3LYP free energy: -1968.376481 a.u.
M06 SCF energy in solution: -1969.96887529 a.u.
M06 enthalpy in solution: -1969.167898 a.u.
M06 free energy in solution: -1969.294221 a.u.
Three lowest frequencies (cm-1): 11.5698 18.5858 21.1732

Cartesian coordinates

ATOM	X	Y	Z
C	1.217970	-2.576985	0.300327
C	1.888465	-2.576866	1.542391
C	3.214790	-3.023014	1.558954
H	3.762157	-3.034572	2.495877
C	3.848901	-3.447827	0.393322
C	3.163379	-3.440915	-0.816866
C	1.832349	-3.009740	-0.892531
H	4.880999	-3.786068	0.430710
H	3.666387	-3.776520	-1.719319
C	-1.239400	-3.021413	0.354902
C	-2.355300	-2.271424	0.189874
H	-1.109553	-4.078142	0.528476
H	-3.399065	-2.541587	0.189083
C	-2.873545	0.108260	-0.270437
C	-3.617529	0.631543	0.809481
C	-4.576726	1.610898	0.523363
H	-5.166782	2.030502	1.332430
C	-4.781228	2.061987	-0.777562
C	-4.032665	1.531004	-1.822783
C	-3.071364	0.536783	-1.599002
H	-5.525494	2.828510	-0.976198
H	-4.201279	1.887505	-2.834899
N	-0.161729	-2.149994	0.249923
N	-1.934372	-0.958584	-0.011520
C	-0.563276	-0.854772	0.011739
Ni	0.776906	0.486601	-0.430324
C	2.903445	2.691482	-0.718429
C	2.147392	3.421338	0.215740
C	2.603548	4.673388	0.654884
C	3.805931	5.195152	0.174578
C	4.558632	4.464460	-0.752328
C	4.111261	3.220204	-1.199153
H	5.496858	4.869211	-1.126147
H	4.702006	2.658852	-1.921630
Si	0.602760	2.420450	0.654035
C	-3.300272	1.320145	3.246237
H	-4.236185	1.882439	3.342761
H	-3.050074	0.933251	4.240985
H	-2.515089	2.019441	2.945478
C	-3.431945	0.153817	2.248280
H	-2.499727	-0.418343	2.295122
C	-4.581994	-0.782351	2.676163
H	-4.424366	-1.140323	3.700490

H	-5.544445	-0.257616	2.647527
H	-4.662494	-1.657503	2.022413
C	-2.317125	-0.051268	-2.787812
H	-1.617485	-0.801876	-2.410490
C	-3.277756	-0.768139	-3.757737
H	-3.998269	-0.071718	-4.202272
H	-2.714616	-1.230293	-4.577171
H	-3.846105	-1.555352	-3.249072
C	-1.479279	1.016706	-3.515960
H	-2.109625	1.808695	-3.937268
H	-0.759671	1.477770	-2.831444
H	-0.922259	0.560290	-4.343204
C	0.964742	-4.482700	-2.760157
H	0.399105	-4.493268	-3.699278
H	1.943534	-4.935944	-2.955639
H	0.440145	-5.121364	-2.040334
C	1.791047	-2.134975	-3.276904
H	1.220723	-2.137235	-4.213489
H	1.859244	-1.102083	-2.920109
H	2.806719	-2.478091	-3.505789
C	1.105958	-3.040135	-2.234761
H	0.094721	-2.650308	-2.085223
C	1.198912	-2.148568	2.834532
H	0.351435	-1.511898	2.563026
C	0.643067	-3.375495	3.588362
H	1.451219	-4.059601	3.874383
H	0.126935	-3.061801	4.503526
H	-0.069935	-3.937656	2.975201
C	2.108845	-1.316138	3.754625
H	1.525821	-0.922657	4.594784
H	2.925093	-1.913366	4.177731
H	2.546794	-0.468298	3.219143
C	2.327054	1.358820	-1.140198
H	2.087621	1.365328	-2.222076
H	3.060968	0.543698	-0.980447
C	-0.936813	3.448881	0.179783
H	-0.922989	4.408764	0.715710
H	-0.940882	3.669601	-0.893706
H	-1.875617	2.939906	0.420101
C	0.562653	2.167049	2.552073
H	0.417583	3.127308	3.067487
H	-0.241597	1.491848	2.864995
H	1.510103	1.742940	2.902448
H	2.025094	5.247063	1.378282
H	4.160286	6.164305	0.518872

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B3LYP SCF energy: -2157.62863287 a.u.
B3LYP enthalpy: -2156.810077 a.u.
B3LYP free energy: -2156.940018 a.u.
M06 SCF energy in solution: -2158.53348889 a.u.
M06 enthalpy in solution: -2157.714933 a.u.
M06 free energy in solution: -2157.844874 a.u.
Three lowest frequencies (cm-1): 14.2893 25.0669 33.6718

Cartesian coordinates

ATOM	X	Y	Z
C	1.680663	-1.925486	0.753352
C	2.313129	-1.404592	1.904415
C	3.695913	-1.588216	2.018894
H	4.216257	-1.195867	2.885888
C	4.417728	-2.267338	1.041327
C	3.769468	-2.774305	-0.079930
C	2.388085	-2.616068	-0.255419
H	5.490396	-2.400204	1.154546
H	4.343869	-3.301395	-0.835121
C	-0.590573	-2.895697	0.966640
C	-1.856347	-2.483376	0.729269
H	-0.201203	-3.833782	1.327742
H	-2.802768	-2.987860	0.835951
C	-2.983853	-0.438613	-0.044502
C	-3.739669	0.098849	1.019550
C	-4.956218	0.716304	0.701510
H	-5.562996	1.141174	1.495299
C	-5.398399	0.799008	-0.614987
C	-4.639310	0.247576	-1.642987
C	-3.422602	-0.396956	-1.385124
H	-6.341545	1.289472	-0.840715
H	-5.003083	0.309093	-2.663254
C	1.534154	-0.714123	3.021586
H	0.638219	-0.269972	2.577078
C	1.709786	-3.219000	-1.484119
H	0.720091	-2.763967	-1.580977
C	-3.305368	-0.006621	2.481180
H	-2.248852	-0.292819	2.500593
N	0.238666	-1.828249	0.644978
N	-1.774920	-1.168638	0.275962
C	-2.671283	-1.097003	-2.515314
H	-1.622240	-1.189427	-2.222323
C	-0.474853	-0.734225	0.210374
Ni	0.625978	0.841292	-0.379421
C	2.215166	3.388612	-0.683907
C	2.123032	1.978694	-0.675702
C	3.299175	1.227046	-0.855663
C	4.540832	1.853698	-1.003539
C	4.621646	3.247838	-0.986394
C	3.462011	4.009877	-0.829377
H	5.584814	3.740460	-1.099254
H	3.526179	5.096592	-0.822245
C	0.342787	0.969193	-2.496114
O	-0.214944	1.928207	-2.936947
O	0.851078	-0.120060	-2.620017
C	0.916999	4.132560	-0.504031
H	1.030270	5.063713	0.068272
H	0.485030	4.404271	-1.477935
C	2.317656	0.431238	3.685560
H	3.160226	0.062230	4.282125
H	2.705056	1.132475	2.940043
H	1.659249	0.984195	4.364246
C	1.079718	-1.740261	4.081974
H	1.945169	-2.223999	4.550787
H	0.501475	-1.245059	4.871287

H	0.451348	-2.524757	3.646790
C	1.524688	-4.742694	-1.316523
H	1.010287	-5.161969	-2.189234
H	2.494483	-5.246437	-1.224424
H	0.935334	-4.992577	-0.427508
C	2.469599	-2.919257	-2.790075
H	1.884501	-3.277281	-3.644912
H	2.629598	-1.846506	-2.918160
H	3.439877	-3.428169	-2.825395
C	-2.697419	-0.321281	-3.844335
H	-2.342920	0.705428	-3.719376
H	-2.040512	-0.817163	-4.567607
H	-3.700592	-0.293047	-4.285848
C	-3.227242	-2.523620	-2.720186
H	-4.283073	-2.492325	-3.015528
H	-2.670041	-3.038396	-3.511751
H	-3.151045	-3.126087	-1.808494
C	-4.103478	-1.105079	3.215926
H	-3.769559	-1.189095	4.256888
H	-5.174471	-0.870220	3.223893
H	-3.981540	-2.085683	2.743961
C	-3.428851	1.327884	3.240777
H	-4.473907	1.636583	3.357127
H	-3.008554	1.222732	4.247769
H	-2.892681	2.133383	2.731879
Si	-0.194238	2.830297	0.341867
C	-0.006128	3.022949	2.229676
H	-0.476406	3.959125	2.561784
H	-0.466671	2.201384	2.788978
H	1.053099	3.063880	2.505905
C	-1.996729	3.154403	-0.163828
H	-2.106879	3.009003	-1.243000
H	-2.730264	2.521952	0.340667
H	-2.237828	4.203387	0.062758
H	3.257950	0.139611	-0.878659
H	5.440030	1.255131	-1.133472

9-TSa

B3LYP SCF energy: -2157.61852015 a.u.
B3LYP enthalpy: -2156.800743 a.u.
B3LYP free energy: -2156.927292 a.u.
M06 SCF energy in solution: -2158.52350399 a.u.
M06 enthalpy in solution: -2157.705727 a.u.
M06 free energy in solution: -2157.832276 a.u.
Three lowest frequencies (cm-1): -206.6846 15.3974 26.5202
Imaginary frequency: -206.6846 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	1.679305	-1.924238	0.697807
C	2.351344	-1.397018	1.822188
C	3.738773	-1.570298	1.883251
H	4.289325	-1.174201	2.729620
C	4.427133	-2.245085	0.878406
C	3.738682	-2.762174	-0.213779

C	2.350057	-2.616182	-0.334327
H	5.504452	-2.370075	0.949730
H	4.285726	-3.290556	-0.988390
C	-0.590191	-2.908225	0.910242
C	-1.855388	-2.507341	0.654128
H	-0.196022	-3.851025	1.253295
H	-2.796039	-3.028892	0.722184
C	-2.987097	-0.462772	-0.128356
C	-3.891691	-0.116716	0.898878
C	-5.101484	0.480901	0.522547
H	-5.819824	0.758400	1.288597
C	-5.394145	0.731419	-0.814085
C	-4.483490	0.378196	-1.806012
C	-3.263728	-0.235957	-1.494035
H	-6.336175	1.200705	-1.085041
H	-4.728713	0.572144	-2.844977
C	1.605780	-0.713899	2.965720
H	0.705029	-0.255840	2.546692
C	1.630910	-3.244155	-1.527209
H	0.613547	-2.843863	-1.562379
C	-3.617173	-0.380766	2.379809
H	-2.582666	-0.722756	2.480621
N	0.234650	-1.824451	0.632034
N	-1.784281	-1.178625	0.237507
C	-2.336856	-0.708025	-2.612576
H	-1.326784	-0.804733	-2.209199
C	-0.488309	-0.732852	0.209347
Ni	0.524270	0.776237	-0.452582
C	2.018674	3.341279	-0.443006
C	2.070320	1.977514	-0.840577
C	3.314682	1.320817	-0.874135
C	4.486165	1.978576	-0.488483
C	4.423361	3.310939	-0.081408
C	3.196499	3.984747	-0.056954
H	5.329910	3.833696	0.214925
H	3.156540	5.020318	0.274359
C	1.104442	1.379943	-2.421221
O	0.799475	2.310177	-3.124095
O	1.166503	0.136681	-2.442286
C	0.661728	3.970439	-0.352965
H	0.675770	4.936183	0.168182
H	0.263794	4.134917	-1.363770
C	2.414490	0.414167	3.628353
H	3.266483	0.029212	4.201239
H	2.793090	1.122921	2.884913
H	1.776374	0.963018	4.329318
C	1.164651	-1.750661	4.021492
H	2.035041	-2.248810	4.465534
H	0.606882	-1.261763	4.829287
H	0.520648	-2.523791	3.588471
C	1.532235	-4.775750	-1.357649
H	0.979817	-5.216596	-2.195751
H	2.528745	-5.233048	-1.335377
H	1.019292	-5.057309	-0.431104
C	2.293408	-2.897161	-2.873780
H	1.699284	-3.318804	-3.693226
H	2.346420	-1.815581	-3.014931

H	3.302040	-3.319307	-2.955192
C	-2.235179	0.282011	-3.785451
H	-1.921876	1.274598	-3.448589
H	-1.480380	-0.073301	-4.494478
H	-3.180388	0.380210	-4.332945
C	-2.780203	-2.100952	-3.110402
H	-3.789416	-2.063856	-3.538788
H	-2.095906	-2.461477	-3.887264
H	-2.788456	-2.837302	-2.298316
C	-4.533531	-1.495462	2.926219
H	-4.302946	-1.699470	3.978446
H	-5.588479	-1.203762	2.864633
H	-4.417675	-2.430909	2.367870
C	-3.756645	0.890032	3.240708
H	-4.785473	1.267324	3.247607
H	-3.481851	0.669673	4.278986
H	-3.106538	1.692574	2.880618
Si	-0.418313	2.632567	0.502602
C	-0.201650	2.823180	2.387282
H	-0.646853	3.767963	2.728772
H	-0.675989	2.009960	2.948286
H	0.860468	2.837053	2.654402
C	-2.225509	3.014515	0.049927
H	-2.393992	2.871741	-1.022546
H	-2.958774	2.407647	0.585045
H	-2.424619	4.070569	0.282709
H	3.362533	0.288714	-1.207788
H	5.438838	1.455649	-0.513509

9-TSa-SIPr

B3LYP SCF energy: -2158.82022511 a.u.
B3LYP enthalpy: -2157.978202 a.u.
B3LYP free energy: -2158.104082 a.u.
M06 SCF energy in solution: -2159.72725586 a.u.
M06 enthalpy in solution: -2158.885233 a.u.
M06 free energy in solution: -2159.011113 a.u.
Three lowest frequencies (cm-1): -204.9620 18.2121 32.2310
Imaginary frequency: -204.9620 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-1.717678	1.771302	0.871408
C	-2.488363	1.106042	1.853068
C	-3.875515	1.298792	1.839666
H	-4.489175	0.796881	2.581016
C	-4.482432	2.123453	0.898256
C	-3.706295	2.782025	-0.050209
C	-2.314609	2.630989	-0.083393
H	-5.560904	2.258483	0.907970
H	-4.187006	3.432912	-0.774430
C	0.509310	2.688639	1.622990
C	1.916735	2.418114	1.101810
H	0.151428	3.695232	1.399024
H	2.211775	3.111903	0.304586
C	2.980666	0.456224	-0.007610

C	3.942875	-0.054249	0.897853
C	5.153485	-0.529076	0.379934
H	5.903368	-0.926911	1.057730
C	5.409308	-0.507858	-0.987254
C	4.456083	0.004983	-1.859984
C	3.232450	0.510295	-1.399230
H	6.352569	-0.886640	-1.371812
H	4.669121	0.028765	-2.924050
C	-1.866929	0.238832	2.944146
H	-0.843350	-0.002688	2.642289
C	-1.509320	3.440520	-1.097900
H	-0.475932	3.080575	-1.073963
C	3.724668	-0.097286	2.410054
H	2.694444	0.214501	2.611396
N	-0.278253	1.671883	0.896751
N	1.787449	1.050576	0.540031
C	2.280248	1.155679	-2.403990
H	1.301215	1.273680	-1.934924
C	0.490987	0.695921	0.345674
Ni	-0.505424	-0.694679	-0.556042
C	-2.020136	-3.242316	-0.762800
C	-2.054162	-1.851285	-1.050451
C	-4.430307	-3.219186	-0.434828
C	-3.208745	-3.902826	-0.442841
H	-5.345213	-3.754839	-0.192147
H	-3.181426	-4.961469	-0.193008
C	-1.058425	-1.124104	-2.582075
O	-0.748892	-2.000848	-3.347447
O	-1.125716	0.113749	-2.500290
C	-0.672941	-3.897625	-0.726224
H	-0.697291	-4.888453	-0.254701
H	-0.297501	-4.021655	-1.751540
C	-2.610661	-1.096217	3.135359
H	-3.619779	-0.946726	3.536359
H	-2.698061	-1.643563	2.192253
H	-2.068361	-1.724334	3.850985
C	-1.803727	1.007858	4.281689
H	-2.811295	1.248286	4.641792
H	-1.308034	0.402740	5.050305
H	-1.255592	1.952269	4.187218
C	-1.503036	4.937894	-0.718079
H	-0.867171	5.504998	-1.408246
H	-2.513686	5.359565	-0.773015
H	-1.135638	5.108462	0.300672
C	-2.013301	3.263709	-2.542994
H	-1.364230	3.819951	-3.230290
H	-2.002969	2.212223	-2.836716
H	-3.029275	3.656673	-2.668948
C	2.054197	0.295959	-3.661367
H	1.702781	-0.707526	-3.407502
H	1.286679	0.760519	-4.288431
H	2.964909	0.202310	-4.265180
C	2.790335	2.558444	-2.800305
H	3.759871	2.495874	-3.309238
H	2.082092	3.041545	-3.483702
H	2.919267	3.210537	-1.928172
C	4.675073	0.873184	3.143970

H	4.452868	0.890902	4.217608
H	5.719636	0.562204	3.025802
H	4.597532	1.897853	2.763247
C	3.886156	-1.518444	2.986061
H	4.911852	-1.886229	2.868382
H	3.658259	-1.517923	4.058704
H	3.215590	-2.229632	2.496735
H	0.423826	2.523944	2.704760
H	2.676961	2.451584	1.883034
Si	0.466179	-2.635684	0.165228
C	2.230029	-2.992998	-0.452948
H	2.446073	-4.054845	-0.263797
H	2.299927	-2.830205	-1.533847
H	3.010103	-2.399105	0.026357
C	0.383381	-2.978891	2.039719
H	-0.655950	-3.101239	2.361696
H	0.922377	-3.904875	2.282868
H	0.822312	-2.170022	2.634683
C	-4.476029	-1.860099	-0.743485
H	-5.424074	-1.328265	-0.745650
C	-3.293182	-1.184456	-1.057311
H	-3.328213	-0.129712	-1.312006

9-TSa-ICy

B3LYP SCF energy: -1693.14103229 a.u.
B3LYP enthalpy: -1692.536277 a.u.
B3LYP free energy: -1692.633012 a.u.
M06 SCF energy in solution: -1694.27687945 a.u.
M06 enthalpy in solution: -1693.672124 a.u.
M06 free energy in solution: -1693.768859 a.u.
Three lowest frequencies (cm-1): -207.4095 18.3908 28.7804
Imaginary frequency: -207.4095 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ni	0.080553	0.585127	-0.273446
C	0.846687	3.297955	0.567827
C	0.698380	2.466667	-0.578685
C	1.500925	2.713610	-1.708083
C	2.454485	3.736083	-1.709388
C	2.600346	4.536144	-0.576886
C	1.805162	4.313339	0.554320
H	3.332856	5.339964	-0.568296
H	1.942748	4.932491	1.438298
C	-1.055750	2.020405	-1.299285
O	-1.902799	2.791867	-0.921087
O	-0.884505	1.112641	-2.136655
Si	0.338188	1.033453	1.922630
C	2.086633	0.733512	2.622673
H	2.848789	1.223138	2.006371
H	2.164954	1.138258	3.640916
H	2.328470	-0.334742	2.676123
C	-0.901893	0.240332	3.134101
H	-0.768909	-0.846266	3.199196
H	-0.767347	0.653257	4.143081

H	-1.937442	0.435324	2.832219
C	0.057277	2.931376	1.794584
H	0.364542	3.503284	2.679374
H	-1.011368	3.118470	1.621447
N	0.573741	-2.311306	-0.064299
N	-1.534817	-1.844806	-0.012819
C	-0.301113	-1.264963	-0.040112
C	-0.104981	-3.522345	-0.073347
C	-1.430056	-3.227477	-0.040855
C	-2.797465	-1.079893	-0.048521
C	-3.796465	-1.566894	1.012335
C	-5.066128	-0.698538	0.985507
C	-5.702829	-0.670395	-0.412827
C	-4.691891	-0.221681	-1.479184
C	-3.417772	-1.082117	-1.455945
C	2.034951	-2.148519	-0.149667
C	2.764965	-2.980624	0.916502
C	4.283845	-2.757278	0.832820
C	4.821519	-3.059492	-0.574531
C	4.076308	-2.246514	-1.644310
C	2.555971	-2.460761	-1.563494
H	0.398955	-4.475208	-0.096825
H	-2.289755	-3.877998	-0.030382
H	-2.501947	-0.054369	0.194509
H	-3.329508	-1.542140	2.004030
H	-4.074303	-2.611928	0.811660
H	-4.807212	0.326296	1.287631
H	-5.782531	-1.071650	1.727727
H	-6.576566	-0.006981	-0.414164
H	-6.072932	-1.676679	-0.661159
H	-4.411231	0.826649	-1.306852
H	-5.144831	-0.262850	-2.477090
H	-3.656874	-2.116826	-1.744429
H	-2.683763	-0.693305	-2.168414
H	2.202138	-1.085147	0.056231
H	2.550431	-4.048195	0.764328
H	2.387487	-2.718670	1.912254
H	4.789627	-3.381704	1.579165
H	4.509172	-1.713441	1.094227
H	4.702199	-4.132768	-0.785090
H	5.897147	-2.849750	-0.620916
H	4.433433	-2.512696	-2.646416
H	4.296932	-1.177892	-1.508676
H	2.034493	-1.826001	-2.289573
H	2.315408	-3.503734	-1.816543
H	1.357508	2.105104	-2.596719
H	3.068427	3.911950	-2.589119

9-TSa-SICy

B3LYP SCF energy:	-1694.34301429 a.u.
B3LYP enthalpy:	-1693.714095 a.u.
B3LYP free energy:	-1693.812338 a.u.
M06 SCF energy in solution:	-1695.47953676 a.u.
M06 enthalpy in solution:	-1694.850617 a.u.
M06 free energy in solution:	-1694.948860 a.u.

Three lowest frequencies (cm-1): -207.6749 20.8637 24.4157
Imaginary frequency: -207.6749 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ni	0.143237	0.543443	-0.226252
C	1.103775	3.216581	0.544097
C	0.977295	2.334750	-0.566682
C	1.888341	2.448031	-1.633149
C	2.921777	3.389691	-1.606756
C	3.041587	4.242505	-0.510555
C	2.141748	4.150429	0.558742
H	3.835814	4.984851	-0.481520
H	2.259444	4.807448	1.417938
C	-0.745334	2.001586	-1.437417
O	-1.533911	2.883836	-1.211221
O	-0.585821	1.012941	-2.181903
Si	0.306049	1.077620	1.961823
C	1.981649	0.661344	2.769266
H	2.814338	1.051709	2.173857
H	2.046168	1.104211	3.772482
H	2.120794	-0.420985	2.878644
C	-1.059627	0.462661	3.141495
H	-1.046381	-0.628924	3.245914
H	-0.919691	0.893892	4.141988
H	-2.055865	0.755777	2.791105
C	0.196028	2.982529	1.720620
H	0.482406	3.576140	2.598132
H	-0.838072	3.243541	1.456168
N	0.406571	-2.306281	0.229323
N	-1.691117	-1.670538	0.133824
C	-0.419226	-1.240470	0.112215
C	-0.327364	-3.582246	0.149042
C	-1.791793	-3.129472	0.305690
C	-2.864833	-0.805939	-0.056904
C	-3.980240	-1.110793	0.956946
C	-5.166503	-0.150282	0.764219
C	-5.699063	-0.191590	-0.676353
C	-4.581169	0.084768	-1.692711
C	-3.389756	-0.868893	-1.503783
C	1.852581	-2.213413	-0.012326
C	2.650013	-3.166519	0.892502
C	4.162485	-3.005776	0.661118
C	4.532840	-3.205209	-0.816190
C	3.725996	-2.264873	-1.724145
C	2.213259	-2.420333	-1.496620
H	-0.018281	-4.271385	0.939627
H	-2.191382	-3.370593	1.298271
H	-2.498520	0.210252	0.125134
H	-3.587374	-1.037465	1.978340
H	-4.333379	-2.143778	0.820415
H	-4.843255	0.873265	1.002249
H	-5.962909	-0.400061	1.476290
H	-6.511652	0.535522	-0.797684
H	-6.134272	-1.183357	-0.872415
H	-4.225480	1.118439	-1.579831
H	-4.964880	-0.001727	-2.716618

H	-3.699998	-1.899046	-1.737037
H	-2.576630	-0.599808	-2.185148
H	2.113236	-1.182774	0.258290
H	2.365438	-4.207250	0.677609
H	2.396951	-2.975890	1.943096
H	4.710507	-3.715163	1.293324
H	4.470283	-1.999776	0.980696
H	4.331987	-4.248402	-1.102961
H	5.608099	-3.042917	-0.960958
H	3.964359	-2.451363	-2.778380
H	4.015326	-1.223958	-1.518373
H	1.655234	-1.698697	-2.105443
H	1.901226	-3.425273	-1.817118
H	1.768839	1.800564	-2.497495
H	3.618318	3.462379	-2.438233
H	-2.453928	-3.573166	-0.443911
H	-0.149266	-4.070195	-0.818119

9-TSa-IMes

B3LYP SCF energy: -1921.76493838 a.u.
B3LYP enthalpy: -1921.127729 a.u.
B3LYP free energy: -1921.241545 a.u.
M06 SCF energy in solution: -1922.78072483 a.u.
M06 enthalpy in solution: -1922.143515 a.u.
M06 free energy in solution: -1922.257331 a.u.
Three lowest frequencies (cm-1): -196.3955 11.8760 20.7410
Imaginary frequency: -196.3955 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	1.829921	-2.191245	-0.172582
C	2.452515	-2.428100	1.063974
C	3.847048	-2.351129	1.119460
H	4.343175	-2.523309	2.072037
C	4.615996	-2.061063	-0.012297
C	3.957742	-1.873107	-1.231853
C	2.564774	-1.936786	-1.342878
H	4.542472	-1.674044	-2.127254
C	-0.291508	-3.473519	-0.422866
C	-1.609365	-3.165492	-0.445930
C	-2.983274	-1.111824	-0.242350
C	-3.723801	-1.150723	0.951081
C	-4.957274	-0.490508	0.979788
H	-5.533924	-0.500880	1.902220
C	-5.468081	0.168208	-0.141790
C	-4.732146	0.118403	-1.330303
C	-3.493344	-0.524822	-1.414568
H	-5.134505	0.586634	-2.225669
N	0.391105	-2.274175	-0.247819
N	-1.705610	-1.785461	-0.285075
C	-0.467348	-1.208133	-0.164247
Ni	0.187492	0.617346	-0.256904
C	1.190847	3.305360	0.544525
C	1.253116	2.302414	-0.462531
C	2.386872	2.249856	-1.295747

C	3.451474	3.140469	-1.128330
C	3.380435	4.114182	-0.133048
C	2.257768	4.191631	0.700154
H	4.197669	4.819618	-0.001298
H	2.220932	4.943071	1.486005
C	-0.268521	2.102879	-1.708580
O	-0.970826	3.076015	-1.695569
O	-0.037483	1.070006	-2.365456
Si	0.018546	1.349011	1.895927
C	1.558975	1.008303	2.968167
H	2.476758	1.270856	2.432472
H	1.515402	1.610581	3.886466
H	1.634254	-0.042215	3.267664
C	-1.498438	0.943160	2.975160
H	-1.448059	-0.062674	3.405484
H	-1.528901	1.654912	3.812047
H	-2.439697	1.033361	2.423396
C	0.030797	3.228675	1.492030
H	0.146439	3.885817	2.363356
H	-0.901510	3.498203	0.977832
C	1.889377	-1.753768	-2.681552
H	1.219001	-2.590978	-2.910922
H	1.285278	-0.841079	-2.708191
H	2.634895	-1.692988	-3.480022
C	6.118908	-1.939941	0.082759
H	6.520469	-2.549057	0.899436
H	6.606646	-2.251746	-0.847007
H	6.416479	-0.900479	0.273746
C	1.651819	-2.784120	2.294366
H	0.838016	-2.072801	2.466124
H	1.195793	-3.778484	2.204543
H	2.290896	-2.791537	3.181966
C	-3.262226	-1.936804	2.156569
H	-2.177471	-1.908865	2.279719
H	-3.718819	-1.547720	3.071048
H	-3.552645	-2.992701	2.068910
C	-2.774411	-0.621334	-2.738058
H	-1.848682	-0.037863	-2.747434
H	-2.508495	-1.660471	-2.969221
H	-3.415896	-0.252615	-3.543910
C	-6.780870	0.912913	-0.077274
H	-7.413954	0.542823	0.735898
H	-6.615888	1.984356	0.096334
H	-7.340439	0.820305	-1.014507
H	2.424862	1.513466	-2.093004
H	4.321539	3.080996	-1.777422
H	0.225464	-4.415655	-0.517078
H	-2.485603	-3.783619	-0.562461

9-TSa-SIMes

B3LYP SCF energy:	-1922.96697336 a.u.
B3LYP enthalpy:	-1922.305569 a.u.
B3LYP free energy:	-1922.420775 a.u.
M06 SCF energy in solution:	-1923.98351797 a.u.
M06 enthalpy in solution:	-1923.322114 a.u.

M06 free energy in solution: -1923.437320 a.u.
Three lowest frequencies (cm-1): -200.8737 14.1215 23.1353
Imaginary frequency: -200.8737 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	2.059588	-1.986161	-0.271001
C	2.956630	-2.330575	0.756855
C	4.326926	-2.158154	0.532312
H	5.022859	-2.412330	1.329164
C	4.822071	-1.663657	-0.676418
C	3.905380	-1.361577	-1.688846
C	2.527398	-1.521986	-1.517448
H	4.271990	-0.998689	-2.646751
C	0.115045	-3.578889	-0.234302
C	-1.382621	-3.367056	0.014678
C	-2.815780	-1.298008	-0.091442
C	-3.553232	-1.099230	1.088028
C	-4.825257	-0.523336	0.987878
H	-5.391882	-0.347312	1.900114
C	-5.385184	-0.177956	-0.242987
C	-4.654631	-0.461727	-1.402189
C	-3.378765	-1.027099	-1.355859
H	-5.088720	-0.234395	-2.373356
N	0.655095	-2.210475	-0.072699
N	-1.506490	-1.894028	-0.030552
C	-0.312161	-1.258341	-0.032424
Ni	0.006525	0.642000	-0.150561
C	0.756732	3.388685	0.727227
C	0.593416	2.554476	-0.415198
C	1.308294	2.870495	-1.587417
C	2.179099	3.963094	-1.636905
C	2.327356	4.771167	-0.510952
C	1.623327	4.480709	0.664447
H	2.992016	5.631498	-0.540945
H	1.765991	5.103659	1.544896
C	-1.199913	2.146118	-1.080092
O	-2.005486	2.942702	-0.685509
O	-1.049369	1.229558	-1.909447
Si	0.662281	1.070159	1.997210
C	2.550653	1.052473	2.258329
H	3.053028	1.681853	1.516608
H	2.795206	1.441355	3.256880
H	2.973085	0.046251	2.176959
C	-0.094411	0.180732	3.507534
H	0.101979	-0.898130	3.521644
H	0.347292	0.603248	4.420598
H	-1.177087	0.328714	3.564410
C	0.116853	2.917077	1.999708
H	0.433493	3.496497	2.876222
H	-0.977404	2.973346	1.924757
C	1.587869	-1.223155	-2.662854
H	0.892936	-2.051578	-2.846301
H	0.976125	-0.334752	-2.473299
H	2.152548	-1.051626	-3.584285
C	6.302742	-1.444577	-0.880779
H	6.600412	-1.651429	-1.914647

H	6.579678	-0.404025	-0.665859
H	6.898244	-2.083971	-0.220791
C	2.480158	-2.885774	2.079508
H	1.542051	-2.423959	2.399269
H	2.312100	-3.970415	2.026268
H	3.226626	-2.716944	2.861515
C	-3.047094	-1.548756	2.437421
H	-1.958065	-1.583616	2.478147
H	-3.393934	-0.878872	3.230688
H	-3.424981	-2.552424	2.678764
C	-2.649561	-1.350000	-2.638041
H	-1.789935	-0.689364	-2.770857
H	-2.290987	-2.386953	-2.655887
H	-3.314430	-1.215653	-3.496676
C	-6.737751	0.489043	-0.326038
H	-6.630300	1.576602	-0.430083
H	-7.307569	0.135765	-1.192766
H	-7.334285	0.302593	0.573108
H	0.328978	-3.944658	-1.246695
H	-2.016221	-3.827958	-0.748231
H	-1.702168	-3.740339	0.995365
H	0.572739	-4.267980	0.480051
H	1.158701	2.265780	-2.477212
H	2.724823	4.187097	-2.550017

9-TSb

B3LYP SCF energy: -2005.18051362 a.u.
B3LYP enthalpy: -2004.389322 a.u.
B3LYP free energy: -2004.511602 a.u.
M06 SCF energy in solution: -2006.16553898 a.u.
M06 enthalpy in solution: -2005.374347 a.u.
M06 free energy in solution: -2005.496627 a.u.
Three lowest frequencies (cm-1): -275.1453 14.3464 20.0251
Imaginary frequency: -275.1453 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Si	0.997383	-2.517731	0.788252
C	2.450540	0.997267	-0.449589
C	3.508940	0.391386	-1.162862
C	4.805636	0.540059	-0.652568
H	5.638383	0.084984	-1.179857
C	5.045178	1.252470	0.517056
C	3.986915	1.852547	1.192586
C	2.670795	1.755141	0.724150
H	6.058235	1.348079	0.898450
H	4.187657	2.422957	2.093502
C	0.754020	1.624137	-2.144538
C	-0.574629	1.444088	-2.314624
H	1.475144	2.181617	-2.718994
H	-1.250085	1.804762	-3.073272
C	-2.438055	0.444908	-1.033019
C	-3.034379	-0.761795	-1.451268
C	-4.417536	-0.894676	-1.277976
H	-4.907536	-1.812972	-1.583227

C	-5.177668	0.130521	-0.724791
C	-4.567189	1.318862	-0.339590
C	-3.187542	1.508208	-0.483282
H	-6.249287	0.003295	-0.596815
H	-5.170260	2.114621	0.086170
N	1.110825	0.925280	-0.992508
N	-1.017369	0.656611	-1.256029
C	0.019969	0.313451	-0.422296
Ni	-0.142701	-0.594278	1.269302
C	4.009914	-1.756028	-2.454213
H	3.708377	-2.353300	-1.590160
H	3.749893	-2.313855	-3.361322
H	5.101297	-1.658220	-2.434457
C	3.314309	-0.380362	-2.468340
H	2.242852	-0.558336	-2.603922
C	3.813306	0.439805	-3.677601
H	4.891141	0.626644	-3.604503
H	3.629635	-0.105079	-4.610994
H	3.317012	1.413254	-3.752586
C	1.565601	2.541786	1.428428
H	0.601822	2.098950	1.169373
C	1.661817	2.494245	2.963371
H	2.537270	3.033593	3.343578
H	0.773497	2.963059	3.400016
H	1.709399	1.463051	3.328097
C	1.558028	4.001949	0.926436
H	0.741452	4.562699	1.396572
H	2.500546	4.507240	1.170286
H	1.422172	4.052865	-0.159867
C	-2.272715	-1.686179	-3.670330
H	-1.675691	-2.463620	-4.162092
H	-3.299470	-1.757442	-4.049017
H	-1.871498	-0.712281	-3.972192
C	-2.238924	-1.867059	-2.137272
H	-1.198382	-1.777730	-1.815035
C	-2.714139	-3.279370	-1.754498
H	-3.716955	-3.495555	-2.140160
H	-2.039856	-4.028510	-2.184380
H	-2.731371	-3.415113	-0.668098
C	-2.904185	3.927432	-1.153978
H	-3.986211	4.091468	-1.221681
H	-2.436149	4.882637	-0.887379
H	-2.549680	3.645538	-2.151510
C	-2.576507	2.853242	-0.094256
H	-1.489173	2.737460	-0.061959
C	-3.020265	3.331545	1.301119
H	-2.471374	4.242459	1.569941
H	-4.087819	3.579966	1.326618
H	-2.820545	2.565638	2.053185
C	0.064832	-3.660879	1.997967
H	0.542398	-4.643990	2.121333
H	-0.929785	-3.845558	1.569326
C	-1.844962	-0.663858	2.460993
O	-2.695759	-1.468829	2.713580
O	-1.655089	0.535289	2.195871
C	-0.098726	-2.922882	3.345621
H	0.690433	-3.238815	4.044338

H	-1.051099	-3.194009	3.814034
C	-0.048996	-1.400526	3.186499
H	-0.437594	-0.887038	4.075095
C	2.825098	-2.434602	1.344957
H	3.420126	-1.714472	0.774861
H	2.903879	-2.159629	2.403149
H	3.289581	-3.424015	1.227104
C	0.979260	-3.306017	-0.951309
H	1.703146	-4.131483	-0.989619
H	-0.005949	-3.725977	-1.175999
H	1.235249	-2.606361	-1.753887
H	0.983597	-1.013275	3.100214

9-TSc

B3LYP SCF energy: -2196.92740524 a.u.
B3LYP enthalpy: -2196.079167 a.u.
B3LYP free energy: -2196.206452 a.u.
M06 SCF energy in solution: -2197.81523479 a.u.
M06 enthalpy in solution: -2196.966997 a.u.
M06 free energy in solution: -2197.094282 a.u.
Three lowest frequencies (cm-1): -208.7451 19.0797 22.4933
Imaginary frequency: -208.7451 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	2.326529	-1.594310	-0.319697
C	3.332212	-1.843841	0.639818
C	4.663574	-1.611289	0.265500
H	5.455198	-1.788300	0.986741
C	4.988217	-1.160311	-1.006931
C	3.983406	-0.968793	-1.951240
C	2.637293	-1.198452	-1.644605
H	6.025786	-0.975544	-1.271945
H	4.253464	-0.648868	-2.951288
C	0.455014	-3.152637	0.166627
C	-0.882907	-3.056078	0.331242
H	1.105586	-4.010695	0.127644
H	-1.637669	-3.811780	0.476369
C	-2.586372	-1.261326	0.197133
C	-3.253470	-0.865686	1.374521
C	-4.596588	-0.483792	1.264300
H	-5.135217	-0.166641	2.151208
C	-5.255775	-0.511049	0.040238
C	-4.587578	-0.946100	-1.099299
C	-3.244729	-1.339902	-1.052017
H	-6.296182	-0.203878	-0.023888
H	-5.118579	-0.983657	-2.044888
C	3.055897	-2.411705	2.030988
H	1.981120	-2.344633	2.222093
C	1.585042	-1.126754	-2.752367
H	0.656968	-0.739468	-2.326025
C	-2.590676	-0.926853	2.745231
H	-1.509208	-0.904379	2.594563
N	0.940544	-1.853326	0.022632
N	-1.202786	-1.702640	0.271904

C	-2.589500	-1.908768	-2.309437
H	-1.505421	-1.884723	-2.170020
C	-0.077773	-0.930333	0.097230
Ni	-0.048641	0.986025	-0.158829
C	-0.040303	4.061274	0.213351
C	0.168263	2.933518	-0.623192
C	1.014642	3.090696	-1.740714
C	1.675746	4.293681	-2.006080
C	1.467112	5.385178	-1.165507
C	0.607700	5.264489	-0.066794
H	1.958827	6.334029	-1.366532
H	0.445179	6.121774	0.583848
C	-1.519214	2.105414	-1.424601
O	-1.124226	1.078236	-1.981936
O	-2.443185	2.846999	-1.283926
Si	0.834703	1.578305	1.854831
C	3.775823	-1.631997	3.148489
H	3.567358	-0.560834	3.092074
H	3.443475	-1.993015	4.128516
H	4.862078	-1.770180	3.102014
C	3.451036	-3.903248	2.101784
H	4.526939	-4.030161	1.934279
H	3.213459	-4.314099	3.090098
H	2.929793	-4.507630	1.351281
C	1.304771	-2.541424	-3.308445
H	0.536893	-2.496555	-4.090039
H	2.213025	-2.968757	-3.750795
H	0.952886	-3.227393	-2.531645
C	1.960474	-0.188420	-3.911975
H	1.090717	-0.049511	-4.562597
H	2.274989	0.797129	-3.555078
H	2.767698	-0.598848	-4.530601
C	-2.898932	-1.100701	-3.583081
H	-2.635122	-0.049415	-3.453383
H	-2.317115	-1.502718	-4.421489
H	-3.955764	-1.168747	-3.866044
C	-3.008625	-3.382252	-2.511353
H	-4.091650	-3.460580	-2.664459
H	-2.512727	-3.802094	-3.394710
H	-2.749299	-4.008426	-1.651151
C	-2.934711	-2.256941	3.450296
H	-2.432122	-2.315945	4.423101
H	-4.014608	-2.343037	3.620895
H	-2.620642	-3.122416	2.856198
C	-2.955272	0.265226	3.646819
H	-4.012448	0.255048	3.935399
H	-2.371292	0.226063	4.573398
H	-2.747669	1.219743	3.152600
H	2.327702	4.381842	-2.871795
H	1.135000	2.260839	-2.430510
C	-0.098822	3.125668	2.532495
H	0.650440	3.788350	2.991474
H	-0.777300	2.820400	3.340531
C	-0.882707	3.908374	1.456259
C	0.804821	0.358556	3.335784
H	-0.174924	0.351974	3.822589
H	1.048828	-0.672393	3.066974

H	1.534854	0.684408	4.089396
C	2.670863	2.052652	1.612034
H	3.263697	1.213998	1.229271
H	2.770030	2.878183	0.899423
H	3.114744	2.371154	2.566089
H	-1.191189	4.893265	1.831402
H	-1.796346	3.361472	1.197292

9-TSd

B3LYP SCF energy: -2044.49070338 a.u.
B3LYP enthalpy: -2043.669362 a.u.
B3LYP free energy: -2043.792735 a.u.
M06 SCF energy in solution: -2045.45572383 a.u.
M06 enthalpy in solution: -2044.634382 a.u.
M06 free energy in solution: -2044.757755 a.u.
Three lowest frequencies (cm-1): -309.0719 19.1790 27.6610
Imaginary frequency: -309.0719 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Si	-0.969895	2.530368	-0.133358
C	-2.461036	-1.165593	-0.140774
C	-3.553569	-0.840559	-0.976653
C	-4.832548	-0.836357	-0.403508
H	-5.689863	-0.588136	-1.021742
C	-5.024558	-1.138676	0.939634
C	-3.935662	-1.481249	1.734858
C	-2.634711	-1.521234	1.217720
H	-6.024615	-1.120402	1.364450
H	-4.099565	-1.741873	2.775335
C	-0.788658	-2.251029	-1.614101
C	0.536121	-2.129409	-1.849518
H	-1.514637	-2.955258	-1.985010
H	1.202197	-2.697728	-2.477984
C	2.419468	-0.818032	-0.936980
C	3.026604	0.207088	-1.688889
C	4.414056	0.363057	-1.575433
H	4.909557	1.146171	-2.139876
C	5.169475	-0.472117	-0.760487
C	4.549286	-1.493071	-0.048168
C	3.166208	-1.696100	-0.117937
H	6.244322	-0.331248	-0.684566
H	5.149317	-2.145991	0.577603
N	-1.133928	-1.241223	-0.717063
N	0.992276	-1.064777	-1.077698
C	-0.037288	-0.485534	-0.373880
Ni	0.158307	0.875545	0.972150
C	-4.143334	0.758511	-2.880732
H	-3.830038	1.607405	-2.268152
H	-3.920439	0.992962	-3.928025
H	-5.231245	0.660046	-2.793469
C	-3.419295	-0.538611	-2.469244
H	-2.357787	-0.405787	-2.698656
C	-3.941081	-1.716270	-3.320845
H	-5.010523	-1.881164	-3.145225

H	-3.804285	-1.505980	-4.388052
H	-3.424742	-2.655245	-3.093487
C	-1.500748	-2.047327	2.096449
H	-0.549555	-1.710734	1.682139
C	-1.547482	-1.519337	3.541004
H	-2.403734	-1.911877	4.102137
H	-0.639215	-1.825827	4.070435
H	-1.594120	-0.425988	3.564465
C	-1.498825	-3.591374	2.080170
H	-0.663687	-3.976779	2.677001
H	-2.429267	-3.991622	2.501060
H	-1.396305	-3.983350	1.061764
C	2.378091	0.535137	-4.100102
H	1.785920	1.140021	-4.797246
H	3.422493	0.558757	-4.433813
H	2.028632	-0.501304	-4.171472
C	2.244516	1.079919	-2.661993
H	1.189539	1.025641	-2.385704
C	2.658340	2.560696	-2.601668
H	3.686814	2.715525	-2.946859
H	2.010008	3.158700	-3.252143
H	2.579623	2.954211	-1.582890
C	2.838075	-4.200873	-0.104216
H	3.916049	-4.396865	-0.148076
H	2.365339	-5.040308	0.419551
H	2.461693	-4.191256	-1.132709
C	2.551986	-2.875506	0.635397
H	1.467947	-2.734402	0.666690
C	3.033492	-2.975735	2.095206
H	2.484697	-3.774860	2.608552
H	4.098957	-3.225835	2.158799
H	2.859760	-2.037294	2.625087
C	1.863502	1.056996	2.183496
O	2.822134	1.768883	2.276840
O	1.522861	-0.139802	2.167673
C	0.190832	2.134446	2.678312
H	0.430001	1.651821	3.634391
C	-2.781914	2.622180	0.481910
H	-2.837601	2.725710	1.571567
H	-3.278271	3.500417	0.044515
H	-3.364947	1.737358	0.209325
C	-1.054558	2.541625	-2.045116
H	-1.830373	3.249907	-2.366503
H	-0.109542	2.884043	-2.477467
H	-1.291896	1.569260	-2.487032
H	-0.894475	1.954631	2.578504
C	-0.242271	4.559930	1.819812
H	-1.295591	4.582198	2.135357
H	0.136171	5.580734	1.976717
C	0.548185	3.619066	2.740374
H	1.619987	3.717533	2.527564
H	0.415846	3.970701	3.774732
C	-0.161811	4.199261	0.328083
H	-0.663743	4.980049	-0.265247
H	0.889417	4.198748	0.004614

9-TSe

B3LYP SCF energy: -2236.23207109 a.u.
B3LYP enthalpy: -2235.354057 a.u.
B3LYP free energy: -2235.483975 a.u.
M06 SCF energy in solution: -2237.10039795 a.u.
M06 enthalpy in solution: -2236.222384 a.u.
M06 free energy in solution: -2236.352302 a.u.
Three lowest frequencies (cm-1): -219.0558 18.2430 21.6107
Imaginary frequency: -219.0558 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	1.981704	-4.896104	-0.359221
C	0.944933	-3.963769	-0.218035
C	1.250117	-2.644941	0.214686
C	2.598847	-2.360485	0.540232
C	3.622824	-3.296825	0.395609
C	3.308290	-4.575494	-0.064159
H	1.742908	-5.901736	-0.701530
H	2.853843	-1.368738	0.910569
H	4.648711	-3.034825	0.643545
H	4.086729	-5.325558	-0.182787
C	-1.511390	-3.457146	-0.972829
H	-2.453145	-4.009726	-1.106143
H	-1.711200	-2.706222	-0.197757
C	-1.126837	-2.745802	-2.280905
H	-2.019622	-2.241189	-2.677575
H	-0.840030	-3.488770	-3.041933
C	-0.470112	-4.460643	-0.463167
H	-0.417737	-5.301248	-1.169452
H	-0.838229	-4.884234	0.482497
Si	0.246712	-1.400425	-2.149000
C	-2.797241	0.759723	0.286438
C	-3.145547	0.216968	1.546872
C	-4.344608	-0.500805	1.634627
H	-4.627147	-0.946965	2.581802
C	-5.189825	-0.638517	0.537859
C	-4.868514	-0.019983	-0.664085
C	-3.677207	0.702776	-0.816331
H	-6.112775	-1.204826	0.629988
H	-5.556196	-0.091350	-1.500726
C	-1.513249	2.882549	0.285127
C	-0.212993	3.249274	0.244311
H	-2.412291	3.466896	0.393227
H	0.254005	4.218234	0.311940
C	1.982000	2.095781	0.144953
C	2.617326	1.941749	1.399092
C	4.017072	1.988851	1.426713
H	4.533412	1.864613	2.372750
C	4.757326	2.206096	0.269357
C	4.106480	2.405444	-0.943169
C	2.709023	2.364973	-1.035330
H	5.842750	2.236487	0.315415
H	4.692965	2.600224	-1.834786
N	-1.549343	1.494973	0.162991
N	0.530724	2.081539	0.096566

C	1.889310	4.214399	-2.545828
H	2.872349	4.700275	-2.554923
H	1.391439	4.440846	-3.496205
H	1.300174	4.668758	-1.742768
C	2.033661	2.686933	-2.365312
H	1.028821	2.256264	-2.346505
C	1.678017	3.220859	3.354830
H	1.101623	3.144413	4.284568
H	2.653898	3.658581	3.597631
H	1.153999	3.917216	2.691653
C	1.845130	1.826276	2.711308
H	0.850085	1.437938	2.487052
C	2.487637	0.856451	3.718649
H	2.669202	-0.123684	3.270808
H	3.434367	1.241803	4.115456
H	1.813616	0.714413	4.570488
C	-2.398435	-0.638549	3.853687
H	-2.158832	-1.612763	3.419324
H	-1.672543	-0.440197	4.649758
H	-3.384948	-0.707563	4.328053
C	-2.339410	0.494442	2.814230
H	-1.291979	0.614748	2.533142
C	-2.817585	1.814317	3.461448
H	-3.872844	1.743860	3.752011
H	-2.232579	2.028490	4.364066
H	-2.711217	2.667502	2.783905
C	-3.443722	1.469770	-2.115264
H	-2.391402	1.764236	-2.153649
C	-4.287158	2.764028	-2.132569
H	-4.095949	3.332290	-3.050634
H	-5.357997	2.531986	-2.095407
H	-4.060765	3.413704	-1.280276
C	-0.280251	0.969716	0.039721
Ni	0.340476	-0.870555	0.069677
C	-0.245471	-0.056555	-3.429395
H	-0.976297	0.668099	-3.065777
H	0.634624	0.496019	-3.770175
H	-0.674984	-0.546826	-4.314323
C	1.883181	-2.033997	-2.912317
H	2.232040	-2.968714	-2.466818
H	1.746721	-2.194979	-3.991221
H	2.682197	-1.291908	-2.789974
C	-3.744912	0.636846	-3.375094
H	-3.424835	1.182815	-4.269635
H	-3.221585	-0.322895	-3.360059
H	-4.817416	0.438400	-3.482022
C	2.770716	2.091417	-3.578737
H	2.958996	1.020827	-3.454052
H	2.167352	2.227744	-4.483094
H	3.732098	2.586967	-3.757243
C	0.171971	-2.198069	2.045795
O	0.447206	-1.027570	2.228354
O	-0.328196	-3.204373	2.427041

9-TSf

B3LYP SCF energy: -2083.78663643 a.u.
B3LYP enthalpy: -2082.934692 a.u.
B3LYP free energy: -2083.062352 a.u.
M06 SCF energy in solution: -2084.73331994 a.u.
M06 enthalpy in solution: -2083.881376 a.u.
M06 free energy in solution: -2084.009036 a.u.
Three lowest frequencies (cm-1): -244.3312 11.1938 15.5285
Imaginary frequency: -244.3312 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-0.954188	-4.747540	-0.638549
H	-0.838926	-5.840331	-0.663603
H	-0.308628	-4.352344	-1.427788
C	-0.514161	-4.203876	0.736575
H	0.282934	-4.846575	1.144206
H	-1.336074	-4.269774	1.463475
C	-2.417081	-4.420943	-0.987211
H	-3.072558	-5.124271	-0.452629
H	-2.581440	-4.595239	-2.058517
Si	0.307786	-2.467458	0.764018
C	2.751454	0.771196	-0.033238
C	3.076411	0.740333	-1.408747
C	4.365684	0.315978	-1.754845
H	4.641981	0.267102	-2.802270
C	5.303135	-0.029383	-0.786694
C	4.969148	0.047353	0.560243
C	3.690604	0.446502	0.971158
H	6.297878	-0.351183	-1.083254
H	5.711003	-0.211239	1.309427
C	1.337187	2.566389	0.883614
C	0.023352	2.797097	1.099434
H	2.202891	3.190677	1.030993
H	-0.496985	3.662461	1.477053
C	-2.099272	1.590767	0.653062
C	-2.742276	2.131782	-0.482813
C	-4.143180	2.106661	-0.502782
H	-4.668504	2.511633	-1.361896
C	-4.872030	1.580323	0.558422
C	-4.212426	1.077234	1.676575
C	-2.814549	1.074875	1.755150
H	-5.958075	1.570548	0.519565
H	-4.794193	0.684589	2.503927
N	1.450390	1.273790	0.372352
N	-0.651388	1.645541	0.712019
C	-2.031280	1.730716	4.061291
H	-3.031833	2.070063	4.355116
H	-1.511539	1.387520	4.963739
H	-1.486457	2.595961	3.668212
C	-2.119158	0.590738	3.023431
H	-1.098525	0.303008	2.757290
C	-2.089259	4.331939	-1.520037
H	-1.511245	4.811234	-2.318699
H	-3.130222	4.664332	-1.612075
H	-1.707489	4.698164	-0.560273
C	-1.988049	2.795198	-1.633948

H	-0.931567	2.524652	-1.554747
C	-2.466051	2.324182	-3.019805
H	-2.352273	1.242996	-3.124941
H	-3.510056	2.598727	-3.210419
H	-1.858233	2.801716	-3.797164
C	2.249618	0.448263	-3.817781
H	2.157648	-0.629518	-3.656278
H	1.439187	0.746238	-4.489648
H	3.197715	0.648847	-4.332348
C	2.123891	1.227247	-2.497761
H	1.099389	1.072371	-2.157687
C	2.330790	2.738644	-2.740838
H	3.348048	2.943345	-3.097080
H	1.628105	3.099078	-3.501539
H	2.170918	3.326070	-1.829371
C	3.396388	0.533931	2.468198
H	2.316702	0.656100	2.600065
C	4.086840	1.760430	3.102676
H	3.851004	1.821007	4.171760
H	5.176237	1.690326	3.002272
H	3.772819	2.700037	2.635811
C	0.216572	0.680037	0.252847
Ni	-0.577280	-0.844204	-0.604627
C	3.812247	-0.744718	3.222550
H	3.458864	-0.699434	4.259116
H	3.392596	-1.640610	2.757946
H	4.901756	-0.858320	3.254479
C	-2.792015	-0.644726	3.646587
H	-2.910020	-1.449835	2.913616
H	-2.180580	-1.022337	4.473464
H	-3.780982	-0.412665	4.058289
C	-0.773463	-1.643840	-2.524950
O	-0.408266	-2.667073	-3.056871
O	-0.656103	-0.406471	-2.707062
C	-2.885803	-3.008364	-0.613195
H	-2.723535	-2.848276	0.458242
H	-3.978561	-2.975639	-0.753149
C	-2.314531	-1.822043	-1.393206
H	-2.788063	-1.799516	-2.382130
H	-2.640714	-0.871227	-0.936966
C	2.025021	-2.789423	-0.008685
H	1.908444	-3.112966	-1.049236
H	2.680490	-1.916646	-0.003386
H	2.528303	-3.598563	0.540560
C	0.501517	-2.091703	2.626523
H	-0.471459	-2.131325	3.127756
H	1.140385	-2.851498	3.097028
H	0.943722	-1.111863	2.828350

10-TSa

B3LYP SCF energy:	-2157.61185011 a.u.
B3LYP enthalpy:	-2156.794607 a.u.
B3LYP free energy:	-2156.923785 a.u.
M06 SCF energy in solution:	-2158.51559934 a.u.
M06 enthalpy in solution:	-2157.698356 a.u.

M06 free energy in solution: -2157.827534 a.u.
Three lowest frequencies (cm-1): -174.5973 18.4156 24.0349
Imaginary frequency: -174.5973 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-2.889499	-0.668944	0.357809
C	-3.592718	-0.645820	-0.864557
C	-4.829600	0.010995	-0.877559
H	-5.397451	0.054676	-1.801099
C	-5.347294	0.604204	0.270956
C	-4.639090	0.548073	1.467397
C	-3.395174	-0.091723	1.540875
H	-6.309333	1.108313	0.233320
H	-5.055464	1.008363	2.358965
C	-1.590884	-2.714311	0.860140
C	-0.282590	-3.061234	0.915638
H	-2.487094	-3.269217	1.086993
H	0.200122	-3.983147	1.197604
C	1.887677	-1.915593	0.493818
C	2.558352	-2.474890	-0.614649
C	3.958378	-2.483591	-0.579126
H	4.507829	-2.906285	-1.414344
C	4.658064	-1.961142	0.504606
C	3.969504	-1.421078	1.586505
C	2.570218	-1.388309	1.611214
H	5.744735	-1.977228	0.507303
H	4.526334	-1.021288	2.428304
C	-3.086857	-1.365036	-2.112981
H	-2.005200	-1.493685	-2.016264
C	-2.659496	-0.157386	2.877909
H	-1.717460	-0.691820	2.725072
C	1.821782	-3.100895	-1.796530
H	0.785747	-2.752453	-1.772427
N	-1.637166	-1.389574	0.436438
N	0.439625	-1.943259	0.519512
C	1.848804	-0.847910	2.843631
H	0.795946	-0.700908	2.585370
C	-0.383242	-0.886725	0.222006
Ni	0.434355	0.821794	-0.382255
Si	-0.439154	3.076210	-0.638713
C	1.953365	3.175545	0.322519
C	1.836856	2.102773	-0.593510
C	2.968412	1.686220	-1.314802
C	4.206890	2.299578	-1.097017
C	4.321264	3.337631	-0.167998
C	3.197440	3.781460	0.534995
H	5.283839	3.817416	-0.006058
H	3.286473	4.610329	1.234762
C	-2.301058	1.243595	3.410140
H	-1.752983	1.159823	4.356254
H	-1.672196	1.788642	2.698916
H	-3.196666	1.846918	3.597938
C	-3.469273	-0.953015	3.921316
H	-2.905716	-1.037626	4.857913
H	-4.422356	-0.462091	4.149506
H	-3.693636	-1.965597	3.567143

C	-3.720987	-2.769858	-2.211056
H	-4.811139	-2.701226	-2.310610
H	-3.334183	-3.300799	-3.088702
H	-3.504018	-3.379145	-1.326404
C	-3.324737	-0.575175	-3.412079
H	-2.845885	-1.098112	-4.247353
H	-4.391447	-0.487946	-3.651866
H	-2.891366	0.426486	-3.350196
C	1.815706	-4.640180	-1.676684
H	1.257025	-5.085279	-2.508386
H	2.836471	-5.040171	-1.704804
H	1.353760	-4.978234	-0.742176
C	2.397853	-2.671088	-3.157439
H	3.419876	-3.038418	-3.308549
H	1.780415	-3.084706	-3.962894
H	2.389507	-1.583819	-3.258622
C	1.902998	-1.873510	3.995332
H	2.937816	-2.062967	4.304604
H	1.353916	-1.500491	4.868236
H	1.461505	-2.832727	3.701734
C	2.392057	0.518732	3.300492
H	2.382291	1.247050	2.483472
H	1.775440	0.908703	4.119039
H	3.419703	0.446208	3.674682
C	-0.143172	0.745612	-2.191864
O	-0.961245	1.677514	-2.364994
O	0.336030	-0.161178	-2.842131
C	0.628283	3.641963	0.875739
H	0.359342	3.130339	1.811298
H	0.595548	4.722493	1.074233
C	-0.068611	4.352452	-1.988746
H	-0.129118	5.361394	-1.558361
H	0.930157	4.230647	-2.416742
H	-0.798922	4.274052	-2.799283
C	-2.283086	3.130615	-0.208043
H	-2.894822	3.084733	-1.113417
H	-2.596984	2.318346	0.451100
H	-2.485674	4.079207	0.309678
H	2.886840	0.886048	-2.046083
H	5.079978	1.974952	-1.658713

10-TSb

B3LYP SCF energy: -2005.17598984 a.u.
B3LYP enthalpy: -2004.385587 a.u.
B3LYP free energy: -2004.510116 a.u.
M06 SCF energy in solution: -2006.15455898 a.u.
M06 enthalpy in solution: -2005.364156 a.u.
M06 free energy in solution: -2005.488685 a.u.
Three lowest frequencies (cm-1): -182.7035 19.6471 25.4116
Imaginary frequency: -182.7035 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Si	-1.247792	2.872344	-1.169916
C	-2.268049	-1.215948	0.680766

C	-3.003158	-1.658798	-0.438385
C	-4.389088	-1.457422	-0.412951
H	-4.986944	-1.778595	-1.259542
C	-5.014891	-0.858767	0.677007
C	-4.265129	-0.448407	1.775115
C	-2.875106	-0.617908	1.804498
H	-6.092135	-0.715149	0.671625
H	-4.764455	0.010057	2.623898
C	-0.323647	-2.604937	1.329010
C	1.025698	-2.489903	1.290207
H	-0.962778	-3.377290	1.725986
H	1.807474	-3.140849	1.647507
C	2.643167	-0.773115	0.480820
C	3.393898	-1.209471	-0.632445
C	4.700913	-0.720870	-0.754553
H	5.306410	-1.032456	-1.599410
C	5.237874	0.157548	0.182603
C	4.478071	0.561770	1.276086
C	3.166842	0.103343	1.454895
H	6.253941	0.524029	0.062469
H	4.909897	1.238997	2.007200
N	-0.842264	-1.461257	0.729165
N	1.299776	-1.280527	0.664716
C	0.150659	-0.618833	0.310489
Ni	0.316869	1.105559	-0.676402
C	-2.911005	-1.973464	-2.978720
H	-2.836975	-0.891766	-3.117913
H	-2.327637	-2.455286	-3.771002
H	-3.956040	-2.278969	-3.111650
C	-2.354072	-2.395819	-1.607525
H	-1.288343	-2.152139	-1.615114
C	-2.488312	-3.922371	-1.416687
H	-3.542613	-4.224850	-1.405467
H	-1.993783	-4.452465	-2.239079
H	-2.034146	-4.259415	-0.477918
C	-2.090483	-0.192869	3.044194
H	-1.025333	-0.335925	2.840684
C	-2.287261	1.297554	3.380238
H	-3.331120	1.525127	3.624858
H	-1.678121	1.570996	4.250123
H	-1.991278	1.936626	2.542446
C	-2.448538	-1.080664	4.253618
H	-1.847771	-0.799576	5.126719
H	-3.505095	-0.975208	4.526216
H	-2.264298	-2.140015	4.041734
C	3.356906	-3.633816	-1.328698
H	2.942411	-4.354066	-2.043814
H	4.450630	-3.687620	-1.392366
H	3.067396	-3.956303	-0.322072
C	2.852880	-2.210116	-1.650526
H	1.762378	-2.207266	-1.580126
C	3.198006	-1.835313	-3.102454
H	4.274399	-1.900550	-3.302120
H	2.696302	-2.528608	-3.786469
H	2.849948	-0.827520	-3.339345
C	2.971492	-0.141592	3.960087
H	4.006485	0.175669	4.133409

H	2.384017	0.130887	4.844898
H	2.968309	-1.234060	3.873501
C	2.386955	0.524691	2.697637
H	1.356633	0.173647	2.590533
C	2.324954	2.054854	2.860626
H	1.705056	2.316388	3.726247
H	3.317970	2.488817	3.024710
H	1.891737	2.532100	1.975524
C	1.294380	2.674349	-1.351665
H	1.392597	2.777018	-2.436920
H	2.213684	2.163954	-1.007020
C	1.078804	4.028666	-0.628433
H	1.108683	4.852968	-1.351838
H	1.891719	4.221117	0.085452
C	-0.303022	4.005430	0.063699
H	-0.224354	3.518089	1.047128
H	-0.734483	5.004121	0.231143
C	-0.338197	0.485357	-2.337394
O	-1.412221	1.090336	-2.571998
O	0.330723	-0.374832	-2.876784
C	-2.987343	2.475939	-0.531500
H	-3.614463	2.074006	-1.332586
H	-2.990188	1.753771	0.288878
H	-3.441051	3.405782	-0.159343
C	-1.383592	3.900909	-2.759605
H	-2.182713	3.508565	-3.395752
H	-1.617237	4.943676	-2.505385
H	-0.462183	3.899478	-3.349793

10-TSc

B3LYP SCF energy: -2196.91409853 a.u.
B3LYP enthalpy: -2196.066464 a.u.
B3LYP free energy: -2196.194718 a.u.
M06 SCF energy in solution: -2197.80242756 a.u.
M06 enthalpy in solution: -2196.954793 a.u.
M06 free energy in solution: -2197.083047 a.u.
Three lowest frequencies (cm-1): -228.9504 18.9678 25.4382
Imaginary frequency: -228.9504 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	4.082753	3.399690	-0.578448
C	4.972819	2.401594	-0.969650
C	4.483861	1.123599	-1.229942
C	3.117385	0.873230	-1.085201
C	2.200293	1.854942	-0.651336
C	2.708722	3.155476	-0.419795
H	4.458259	4.405379	-0.395078
H	6.029674	2.627885	-1.090149
H	5.149114	0.330802	-1.564266
H	2.761716	-0.123344	-1.334939
C	1.847470	4.328344	0.017415
H	1.755590	4.326305	1.114443
H	2.376524	5.259345	-0.226654
C	0.446471	4.340879	-0.602830

H	-0.106306	5.220988	-0.238908
H	0.507492	4.429167	-1.693105
Ni	0.614028	0.817616	-0.289931
Si	-0.576609	2.825644	-0.133144
C	-0.456694	2.691889	1.792461
H	-0.857616	3.615255	2.239603
H	-1.045801	1.855804	2.180664
H	0.572819	2.568136	2.143146
C	-0.476049	-0.785151	0.287990
C	-0.560819	-2.929729	1.091045
C	-1.832782	-2.534691	0.857770
H	-0.155591	-3.858617	1.459082
H	-2.771812	-3.049919	0.975260
N	0.252067	-1.862018	0.736325
N	-1.772422	-1.228840	0.377928
C	-3.004299	-0.548480	0.024386
C	-3.807481	-0.031764	1.065299
C	-3.422426	-0.557548	-1.324275
C	-5.053333	0.503844	0.715166
C	-4.673493	0.003417	-1.612069
C	-5.482502	0.525786	-0.607824
H	-5.694624	0.911508	1.490216
H	-5.021742	0.021924	-2.639251
H	-6.451212	0.950555	-0.857217
C	1.695940	-1.969885	0.768671
C	2.405009	-1.398124	1.846940
C	2.327661	-2.717199	-0.248689
C	3.790838	-1.590715	1.878835
C	3.716421	-2.878567	-0.159630
C	4.441392	-2.322746	0.889324
H	4.369941	-1.161695	2.689707
H	4.234709	-3.447196	-0.925994
H	5.518447	-2.459062	0.937080
C	-2.610322	-1.213959	-2.438295
H	-1.562789	-1.245564	-2.130164
C	-2.650605	-0.430472	-3.762383
H	-2.364218	0.614169	-3.613829
H	-1.939197	-0.873432	-4.466758
H	-3.641694	-0.463131	-4.231106
C	-3.082865	-2.668204	-2.656208
H	-2.992723	-3.268675	-1.743870
H	-4.132403	-2.696170	-2.973771
H	-2.481363	-3.148310	-3.436967
C	-3.395119	-0.067798	2.536708
H	-2.315658	-0.248090	2.582356
C	-3.671780	1.262852	3.264005
H	-3.220558	1.241799	4.262671
H	-3.258425	2.116625	2.720703
H	-4.745745	1.435143	3.398260
C	-4.097653	-1.220126	3.286981
H	-5.186236	-1.091404	3.262917
H	-3.867777	-2.197589	2.851583
H	-3.783849	-1.238763	4.337410
C	1.569937	-3.369042	-1.404482
H	0.528292	-3.038316	-1.363477
C	1.576526	-4.905793	-1.263604
H	1.151303	-5.230147	-0.306574

H	0.989094	-5.363987	-2.067673
H	2.595506	-5.305669	-1.324657
C	2.115627	-2.942101	-2.780856
H	2.028062	-1.861771	-2.920620
H	3.163799	-3.234292	-2.913678
H	1.536300	-3.430016	-3.573673
C	1.708668	-0.643718	2.976994
H	0.748119	-0.280588	2.598898
C	1.415233	-1.590926	4.159733
H	0.790230	-2.437336	3.853420
H	2.345659	-1.994292	4.577274
H	0.890584	-1.054776	4.959518
C	2.496007	0.591415	3.449971
H	2.755514	1.243412	2.609678
H	1.889690	1.167333	4.158254
H	3.422692	0.316338	3.966785
C	-2.415718	3.139615	-0.464079
H	-2.529723	3.665468	-1.417716
H	-3.007561	2.224061	-0.523600
H	-2.837602	3.763907	0.334950
C	0.141714	1.018701	-2.130434
O	-0.598743	2.027856	-2.227631
O	0.539300	0.132565	-2.855599

10-TSd

B3LYP SCF energy: -2044.49527973 a.u.
B3LYP enthalpy: -2043.674354 a.u.
B3LYP free energy: -2043.798113 a.u.
M06 SCF energy in solution: -2045.45385847 a.u.
M06 enthalpy in solution: -2044.632933 a.u.
M06 free energy in solution: -2044.756692 a.u.
Three lowest frequencies (cm-1): -209.3327 21.5732 28.1029
Imaginary frequency: -209.3327 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	0.838984	4.972993	0.909977
H	1.216070	4.808073	1.930242
H	0.974408	6.044612	0.705347
C	-0.652152	4.605101	0.844195
H	-1.195844	5.100502	1.663266
H	-1.088695	4.973230	-0.091901
Ni	0.509855	1.155714	0.094923
Si	-1.010618	2.749092	0.978369
C	-0.495445	2.255507	2.781538
H	-1.191626	2.727377	3.491895
H	-0.538171	1.174023	2.956484
H	0.516459	2.595095	3.027816
C	0.054829	-0.788635	-0.091513
C	0.730731	-2.945818	-0.442575
C	-0.621876	-2.926572	-0.513105
H	1.440034	-3.751734	-0.542253
H	-1.337636	-3.712594	-0.692582
N	1.127309	-1.639768	-0.189077
N	-1.020411	-1.610355	-0.296490

C	-2.426239	-1.261661	-0.252418
C	-3.117279	-1.438900	0.965245
C	-3.070143	-0.864278	-1.442748
C	-4.496996	-1.199712	0.966493
C	-4.450002	-0.630866	-1.376961
C	-5.157703	-0.798088	-0.190619
H	-5.059484	-1.326943	1.886379
H	-4.977084	-0.316592	-2.271784
H	-6.228430	-0.613487	-0.167353
C	2.510465	-1.250678	-0.010161
C	3.047452	-1.269022	1.294785
C	3.279735	-0.918933	-1.147196
C	4.395879	-0.921084	1.444111
C	4.622803	-0.583765	-0.934424
C	5.175662	-0.579780	0.343576
H	4.840714	-0.924353	2.434879
H	5.244857	-0.320060	-1.783316
H	6.220340	-0.313470	0.480919
C	-2.337898	-0.744543	-2.776773
H	-1.270852	-0.627035	-2.572735
C	-2.765308	0.490241	-3.590600
H	-2.670639	1.405712	-3.000596
H	-2.116038	0.589145	-4.466808
H	-3.797316	0.407619	-3.952912
C	-2.522680	-2.032364	-3.608223
H	-2.151587	-2.917729	-3.079268
H	-3.581245	-2.201137	-3.840915
H	-1.977197	-1.953533	-4.555933
C	-2.430250	-1.911186	2.244806
H	-1.349344	-1.809129	2.105790
C	-2.808836	-1.058108	3.470097
H	-2.212845	-1.365276	4.337470
H	-2.626116	0.005122	3.289152
H	-3.863626	-1.178787	3.742139
C	-2.728767	-3.401119	2.513089
H	-3.802998	-3.564650	2.659713
H	-2.405562	-4.035701	1.680685
H	-2.209840	-3.740260	3.417604
C	2.713758	-0.964244	-2.564720
H	1.626618	-0.872710	-2.498235
C	3.047899	-2.314652	-3.234666
H	2.654498	-3.164146	-2.665247
H	2.615872	-2.356219	-4.241287
H	4.132595	-2.449067	-3.327027
C	3.193182	0.203386	-3.444447
H	2.968313	1.166205	-2.979334
H	4.268040	0.150035	-3.655497
H	2.668702	0.173067	-4.405406
C	2.239112	-1.697205	2.516894
H	1.190142	-1.786449	2.219236
C	2.696320	-3.084750	3.012324
H	2.605511	-3.841637	2.225020
H	3.743858	-3.064330	3.335149
H	2.087737	-3.407112	3.865459
C	2.297939	-0.661248	3.654897
H	1.956320	0.321917	3.316382
H	1.653871	-0.977426	4.483769

H	3.312741	-0.548706	4.053230
C	-2.880296	2.420346	0.962746
H	-3.363700	3.007837	0.175911
H	-3.118836	1.369081	0.779071
H	-3.317547	2.697663	1.931211
C	-0.184273	1.853209	-1.506076
O	-1.151004	2.607923	-1.200247
O	0.318419	1.473991	-2.545762
C	1.691173	4.151466	-0.066394
H	1.325369	4.306149	-1.090400
H	2.719745	4.545844	-0.047838
C	1.728604	2.655327	0.252079
H	2.442970	2.163232	-0.432144
H	2.101268	2.494815	1.279186

10-TSe

B3LYP SCF energy: -2236.22440761 a.u.
B3LYP enthalpy: -2235.346286 a.u.
B3LYP free energy: -2235.477208 a.u.
M06 SCF energy in solution: -2237.09113908 a.u.
M06 enthalpy in solution: -2236.213017 a.u.
M06 free energy in solution: -2236.343939 a.u.
Three lowest frequencies (cm-1): -203.6758 23.5106 27.6301
Imaginary frequency: -203.6758 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-4.239207	2.914774	-0.307333
C	-2.859134	2.818991	-0.064047
C	-2.158665	1.675454	-0.521662
C	-2.889680	0.698645	-1.229565
C	-4.264194	0.800249	-1.456835
C	-4.944768	1.922368	-0.987433
H	-4.770606	3.795107	0.049722
H	-2.381827	-0.188659	-1.611778
H	-4.789608	0.013264	-1.992400
H	-6.014102	2.029291	-1.152980
C	-2.172246	3.972187	0.636411
H	-2.932311	4.593936	1.124697
H	-1.537113	3.587920	1.435744
C	-1.513562	-2.338570	0.524780
C	-1.917318	-3.015304	-0.646287
C	-3.278474	-3.314367	-0.783176
H	-3.623119	-3.833869	-1.672849
C	-4.193436	-2.964879	0.205763
C	-3.763900	-2.307958	1.355296
C	-2.416187	-1.977544	1.546605
H	-5.245440	-3.207920	0.081707
H	-4.487775	-2.042622	2.118852
C	0.776636	-3.020106	1.198270
C	2.015814	-2.481397	1.111872
H	0.436369	-3.979086	1.555059
H	2.984022	-2.872400	1.379806
C	3.040390	-0.421207	0.234263
C	3.609998	-0.586962	-1.047824

C	4.801160	0.096756	-1.319063
H	5.265825	-0.006770	-2.294710
C	5.401276	0.906241	-0.358799
C	4.824183	1.040826	0.899265
C	3.636124	0.376231	1.232909
H	6.324064	1.430830	-0.591920
H	5.305435	1.669280	1.641675
N	-0.101095	-2.067909	0.698323
N	1.868712	-1.210489	0.564568
C	3.064057	1.934456	3.173760
H	2.543299	2.601007	2.481475
H	2.536876	1.968491	4.133116
H	4.076667	2.321626	3.340381
C	3.871239	-0.426446	3.611217
H	4.926083	-0.129473	3.658507
H	3.456455	-0.360296	4.623820
H	3.835369	-1.477441	3.301851
C	3.080082	0.486385	2.649854
H	2.041976	0.147051	2.638548
C	3.777093	-2.854683	-2.147623
H	3.328676	-3.528950	-2.887237
H	4.825913	-2.698237	-2.426684
H	3.761181	-3.360380	-1.176115
C	3.013608	-1.513972	-2.104837
H	1.979203	-1.730161	-1.821075
C	2.968869	-0.877193	-3.506277
H	2.456813	0.089360	-3.492147
H	3.972067	-0.722891	-3.919713
H	2.432414	-1.537673	-4.197580
C	-1.289653	-2.861078	-3.111120
H	-1.302006	-1.766391	-3.084283
H	-0.547809	-3.172131	-3.856248
H	-2.271234	-3.199397	-3.462467
C	-0.938696	-3.454916	-1.733476
H	0.056910	-3.086163	-1.469767
C	-0.848889	-4.993018	-1.805901
H	-1.810127	-5.436399	-2.090657
H	-0.105392	-5.298580	-2.551488
H	-0.558077	-5.422463	-0.840601
C	-2.908184	-0.168584	3.280569
H	-2.463251	0.362422	4.128353
H	-3.061679	0.556229	2.475907
H	-3.886969	-0.545685	3.601676
C	-1.964973	-1.301077	2.837180
H	-0.993528	-0.835239	2.659208
C	-1.800178	-2.345366	3.961529
H	-1.447989	-1.861072	4.879701
H	-2.753895	-2.839753	4.184208
H	-1.075884	-3.123173	3.692314
C	0.553167	-0.927234	0.303606
Ni	-0.558589	0.665682	-0.157603
C	-0.284091	1.640276	-3.158399
H	-1.362118	1.562790	-3.325430
H	0.157194	2.210120	-3.989880
H	0.140792	0.629692	-3.202247
C	2.010433	2.839782	-1.702704
H	2.347133	3.649594	-1.048656

H	2.600662	1.953129	-1.456025
H	2.233396	3.108487	-2.744543
C	-0.805596	4.202988	-1.587666
H	-1.650452	4.033149	-2.267711
H	-0.136037	4.907301	-2.105082
C	-1.319717	4.877780	-0.302740
H	-1.923716	5.747255	-0.596588
H	-0.474021	5.267723	0.273713
Si	0.139267	2.551938	-1.508150
C	0.085888	1.784068	1.204962
O	-0.083734	1.419228	2.352903
O	0.626621	2.779674	0.652535

10-TSf

B3LYP SCF energy: -2083.79679236 a.u.
B3LYP enthalpy: -2082.945711 a.u.
B3LYP free energy: -2083.073415 a.u.
M06 SCF energy in solution: -2084.73678590 a.u.
M06 enthalpy in solution: -2083.885705 a.u.
M06 free energy in solution: -2084.013409 a.u.
Three lowest frequencies (cm-1): -207.2737 15.1887 23.7673
Imaginary frequency: -207.2737 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-2.411132	-1.525388	0.065520
C	-2.901940	-1.682118	-1.247750
C	-4.261131	-1.423096	-1.465873
H	-4.669371	-1.529532	-2.466593
C	-5.095769	-1.037590	-0.421466
C	-4.587322	-0.907649	0.868518
C	-3.236144	-1.147147	1.147556
H	-6.147728	-0.841724	-0.611517
H	-5.250641	-0.611915	1.674642
C	-0.550753	-3.050937	0.722521
C	0.795831	-2.944196	0.820691
H	-1.215979	-3.881393	0.896991
H	1.549391	-3.661946	1.102357
C	2.511223	-1.219030	0.406742
C	3.235566	-1.490937	-0.773540
C	4.598363	-1.169275	-0.784616
H	5.185176	-1.364352	-1.677122
C	5.211745	-0.602341	0.328553
C	4.473286	-0.351138	1.480846
C	3.108416	-0.658598	1.554717
H	6.269808	-0.356082	0.298111
H	4.964462	0.088598	2.342682
N	-1.013103	-1.806666	0.316121
N	1.125447	-1.638579	0.467950
C	2.674013	0.897222	3.537681
H	2.519950	1.735035	2.852399
H	2.009781	1.041646	4.396263
H	3.705218	0.930184	3.909993
C	2.606851	-1.619567	3.829237
H	3.669691	-1.684115	4.092732

H	2.037253	-1.479969	4.755437
H	2.311702	-2.581495	3.394461
C	2.346774	-0.445862	2.860300
H	1.277732	-0.427141	2.635038
C	3.023161	-3.632263	-2.100823
H	2.545954	-4.107024	-2.966470
H	4.108932	-3.725611	-2.221966
H	2.738010	-4.196768	-1.206206
C	2.604361	-2.150687	-1.997673
H	1.517169	-2.122878	-1.874881
C	2.929049	-1.406326	-3.306355
H	2.656123	-0.348865	-3.243478
H	3.994114	-1.465623	-3.557454
H	2.373497	-1.854105	-4.138761
C	-2.049800	-1.152297	-3.585965
H	-1.736478	-0.153377	-3.266352
H	-1.366124	-1.486388	-4.375184
H	-3.048490	-1.066702	-4.029476
C	-2.030301	-2.148062	-2.410813
H	-0.996166	-2.211085	-2.059895
C	-2.442316	-3.559454	-2.876474
H	-3.470094	-3.569235	-3.257858
H	-1.783221	-3.903789	-3.682163
H	-2.384357	-4.284603	-2.056820
C	-3.273161	0.170989	3.339408
H	-2.778989	0.248019	4.313817
H	-3.075757	1.098108	2.796213
H	-4.350931	0.087461	3.524270
C	-2.716991	-1.045949	2.579659
H	-1.632983	-0.913920	2.536966
C	-3.018878	-2.346606	3.355058
H	-2.619012	-2.283200	4.373840
H	-4.099847	-2.518422	3.427038
H	-2.573975	-3.224853	2.874020
C	0.012256	-0.908727	0.147962
Ni	-0.523806	0.972703	-0.286723
C	0.549634	1.994912	-3.021606
H	-0.445214	2.261615	-3.393470
H	1.292276	2.438896	-3.701621
H	0.653739	0.905530	-3.099800
C	2.785720	2.335145	-1.102719
H	3.221229	2.917146	-0.285198
H	3.027330	1.283719	-0.924522
H	3.270424	2.629980	-2.043516
C	0.657409	4.530076	-1.263187
H	1.076500	4.858202	-2.228092
H	1.335815	4.918279	-0.491122
C	-0.721875	5.189984	-1.064040
H	-1.379587	4.973593	-1.918399
H	-0.580576	6.279904	-1.072765
Si	0.912864	2.641637	-1.227810
C	0.052012	1.840487	1.270609
O	-0.455982	1.493734	2.319929
O	0.946768	2.674667	0.946618
C	-1.782603	2.387771	-0.741133
H	-2.541118	1.574950	-0.736892
H	-1.723150	2.722664	-1.781396

C	-2.305043	3.524892	0.143526
H	-2.510174	3.150520	1.153809
H	-3.280530	3.834816	-0.268428
C	-1.418957	4.784153	0.249118
H	-2.052654	5.610403	0.598481
H	-0.653645	4.635417	1.019416

11-TSa

B3LYP SCF energy: -2157.60953219 a.u.
B3LYP enthalpy: -2156.792172 a.u.
B3LYP free energy: -2156.919116 a.u.
M06 SCF energy in solution: -2158.51633670 a.u.
M06 enthalpy in solution: -2157.698977 a.u.
M06 free energy in solution: -2157.825921 a.u.
Three lowest frequencies (cm-1): -271.2454 17.8907 21.9573
Imaginary frequency: -271.2454 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-2.274126	4.426876	-0.448767
C	-3.420973	5.024351	0.088901
C	-1.634929	3.373355	0.213323
C	-3.926288	4.570556	1.306898
C	-3.285741	3.533152	1.991564
C	-2.141423	2.931764	1.457192
H	-4.822252	5.021497	1.726996
H	-3.685216	3.184192	2.941209
C	2.945195	-0.071400	0.060408
C	3.167102	-0.151759	1.454866
C	4.247108	0.568943	1.980265
H	4.439104	0.530288	3.047736
C	5.092359	1.311876	1.162660
C	4.873516	1.345863	-0.209959
C	3.798803	0.662979	-0.794575
H	5.927448	1.856776	1.594565
H	5.545179	1.917936	-0.842607
C	2.133292	-1.968880	-1.311000
C	0.939361	-2.534172	-1.595141
H	3.136667	-2.254273	-1.579862
H	0.684385	-3.407894	-2.172415
C	-1.409908	-2.237263	-0.892928
C	-1.701923	-3.294076	-0.000539
C	-3.009411	-3.792565	0.003034
H	-3.267229	-4.599915	0.681233
C	-3.984932	-3.271756	-0.840870
C	-3.666252	-2.242092	-1.718600
C	-2.374025	-1.703580	-1.770357
H	-4.995116	-3.671396	-0.815820
H	-4.432532	-1.850897	-2.379727
N	1.872491	-0.848389	-0.523670
N	-0.034869	-1.768695	-0.962210
C	0.524725	-0.704436	-0.296224
Ni	-0.445917	0.501353	0.832449
O	-3.439410	0.105570	1.688788
Si	-0.095235	2.426012	-0.358403

O	-1.382091	-0.874504	2.103405
C	1.421453	3.393743	0.293359
H	1.446609	4.389173	-0.171435
H	1.350719	3.542472	1.377230
H	2.375275	2.898219	0.089092
C	-2.263977	-0.040665	1.841303
C	-0.004893	2.444814	-2.262534
H	0.313669	3.435694	-2.612867
H	0.707023	1.712999	-2.658092
H	-0.982387	2.237774	-2.706501
C	-3.114811	0.468868	-2.882271
H	-2.803476	1.243534	-3.592276
H	-4.077208	0.082033	-3.235367
H	-3.275569	0.940790	-1.907609
C	-1.818062	-1.277040	-4.189250
H	-2.727682	-1.776788	-4.543483
H	-1.542019	-0.514615	-4.927556
H	-1.017074	-2.024901	-4.160093
C	-2.043252	-0.633578	-2.804396
H	-1.106454	-0.155795	-2.507171
C	-0.212974	-5.307730	0.339802
H	0.560352	-5.753209	0.976951
H	-1.057720	-6.005563	0.299416
H	0.193972	-5.222148	-0.673670
C	-0.656949	-3.941979	0.907143
H	0.221536	-3.290701	0.937091
C	-1.142733	-4.106029	2.359867
H	-1.961598	-4.830807	2.437774
H	-0.320943	-4.480514	2.982546
H	-1.481713	-3.150235	2.764486
C	4.715552	-0.114653	-3.025032
H	4.558309	-0.100913	-4.109894
H	5.714646	0.290175	-2.825617
H	4.715885	-1.159917	-2.697602
C	3.654254	2.166064	-2.856637
H	4.640404	2.629340	-2.737693
H	3.422769	2.163171	-3.928056
H	2.920564	2.799989	-2.352563
C	3.631336	0.723326	-2.313257
H	2.656771	0.296274	-2.569235
C	3.131901	-2.369648	2.640886
H	4.081721	-2.174436	3.153412
H	2.539294	-3.042872	3.271489
H	3.358577	-2.893149	1.704980
C	2.359513	-1.058012	2.383154
H	1.421677	-1.319125	1.890193
C	1.974643	-0.381109	3.710922
H	1.460572	0.569886	3.538561
H	1.294637	-1.031961	4.270744
H	2.845860	-0.188491	4.347731
C	-1.426484	1.816289	2.149521
H	-0.367139	2.054203	2.363440
H	-1.842950	1.603536	3.140056
H	-1.894871	4.779339	-1.406893
H	-3.921118	5.827845	-0.446539

12-TSa

B3LYP SCF energy:	-2157.60804086 a.u.
B3LYP enthalpy:	-2156.791514 a.u.
B3LYP free energy:	-2156.919978 a.u.
M06 SCF energy in solution:	-2158.50752793 a.u.
M06 enthalpy in solution:	-2157.691001 a.u.
M06 free energy in solution:	-2157.819465 a.u.
Three lowest frequencies (cm-1):	-217.5936 18.6963 24.0220
Imaginary frequency:	-217.5936 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	3.429551	4.158529	-0.693645
C	4.780179	4.329887	-0.377815
C	2.835853	2.896202	-0.582028
C	5.535459	3.235574	0.052223
C	4.950329	1.971186	0.159120
C	3.598531	1.790510	-0.160446
H	6.583916	3.368755	0.309113
H	5.544974	1.124497	0.497380
C	-2.794406	0.756787	0.220091
C	-3.316182	1.214879	-1.009864
C	-4.041975	2.412449	-0.997334
H	-4.457021	2.795532	-1.924086
C	-4.241149	3.120901	0.184419
C	-3.721145	2.641620	1.381928
C	-2.990869	1.446807	1.434236
H	-4.805213	4.049730	0.170878
H	-3.885515	3.202273	2.296149
C	-2.840886	-1.708710	0.418994
C	-1.951173	-2.727789	0.346035
H	-3.907071	-1.704785	0.577648
H	-2.080938	-3.795695	0.420444
C	0.510177	-2.907507	-0.051370
C	0.862343	-3.297833	-1.361490
C	2.028612	-4.056744	-1.518693
H	2.328940	-4.372938	-2.513185
C	2.804252	-4.417803	-0.421096
C	2.424660	-4.031619	0.861508
C	1.270067	-3.270142	1.082669
H	3.705893	-5.007297	-0.564757
H	3.035513	-4.325815	1.708611
N	-2.122827	-0.528546	0.244878
N	-0.708560	-2.146563	0.132275
C	-0.788836	-0.778644	0.067046
Ni	0.961650	0.180517	-0.017465
O	0.667817	2.344051	1.312983
Si	1.073167	2.366054	-0.915740
O	0.913276	0.474615	2.625954
C	0.856096	1.137991	1.609941
C	2.889185	0.461523	-0.088585
H	3.084561	-0.133890	-1.001488
H	3.238028	-0.139500	0.764237
C	-1.894248	2.011142	3.673332
H	-1.118302	2.570232	3.144162
H	-2.655724	2.714902	4.031104

H	-1.434480	1.549419	4.553460
C	-2.500188	0.914536	2.778065
H	-1.704789	0.189258	2.589007
C	-3.643102	0.185969	3.517754
H	-3.282091	-0.214021	4.472468
H	-4.471594	0.872375	3.731029
H	-4.044207	-0.649797	2.933162
C	-4.407332	-0.436378	-2.586096
H	-5.300823	0.189972	-2.694345
H	-4.280945	-1.007405	-3.513758
H	-4.593597	-1.148682	-1.775828
C	-3.161006	0.433267	-2.313299
H	-2.303430	-0.238682	-2.201807
C	-2.874658	1.336307	-3.527392
H	-2.040008	2.017140	-3.336764
H	-2.620959	0.719958	-4.397495
H	-3.747364	1.939040	-3.803710
C	-0.734803	-4.234608	-3.075748
H	-1.379964	-3.992272	-3.928504
H	-0.025507	-5.005760	-3.398540
H	-1.361865	-4.668074	-2.288459
C	0.002451	-2.973065	-2.580302
H	-0.758224	-2.247503	-2.277533
C	0.811856	-2.327609	-3.719986
H	1.566240	-3.011218	-4.125681
H	0.144310	-2.051114	-4.544386
H	1.323479	-1.421799	-3.380432
C	2.026381	-2.494728	3.400401
H	2.591077	-1.673818	2.951404
H	1.644034	-2.141084	4.363625
H	2.708890	-3.328732	3.603513
C	0.846770	-2.911631	2.505146
H	0.180697	-2.047154	2.454110
C	0.071015	-4.083319	3.145181
H	0.701950	-4.977343	3.222103
H	-0.257352	-3.814089	4.155834
H	-0.818238	-4.352453	2.564020
C	1.017557	1.657145	-2.710032
H	0.085008	1.128543	-2.935216
H	1.105504	2.493126	-3.420607
H	1.852533	0.972676	-2.893262
C	-0.226811	3.740211	-0.925681
H	-1.242081	3.338641	-0.841422
H	-0.072916	4.426975	-0.088692
H	-0.169397	4.302333	-1.867365
H	2.840362	5.018149	-1.008072
H	5.238820	5.312851	-0.453386

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B3LYP SCF energy:	-2157.62544572 a.u.
B3LYP enthalpy:	-2156.805680 a.u.
B3LYP free energy:	-2156.933526 a.u.
M06 SCF energy in solution:	-2158.52828488 a.u.
M06 enthalpy in solution:	-2157.708519 a.u.
M06 free energy in solution:	-2157.836365 a.u.

Three lowest frequencies (cm-1): 18.9730 21.6679 29.6284

Cartesian coordinates

ATOM	X	Y	Z
C	-1.784819	1.813620	0.650388
C	-2.442757	1.301935	1.789884
C	-3.836793	1.415622	1.833938
H	-4.376695	1.033558	2.693781
C	-4.545047	2.014399	0.794738
C	-3.870327	2.511971	-0.314839
C	-2.475094	2.426731	-0.417221
H	-5.627427	2.095624	0.853209
H	-4.432667	2.980332	-1.116948
C	0.435795	2.911945	0.853043
C	1.718859	2.566787	0.607036
H	-0.004903	3.843278	1.170319
H	2.633250	3.134184	0.662354
C	2.956197	0.559200	-0.116043
C	3.874784	0.304392	0.926135
C	5.117683	-0.238033	0.575538
H	5.847930	-0.444317	1.352707
C	5.429246	-0.521822	-0.750215
C	4.503469	-0.260198	-1.756390
C	3.248582	0.294409	-1.471914
H	6.397870	-0.945862	-1.001430
H	4.761743	-0.480785	-2.786690
C	-1.676459	0.695062	2.962388
H	-0.747228	0.274483	2.566543
C	-1.773505	3.038554	-1.628329
H	-0.723471	2.733878	-1.606656
C	3.580746	0.608555	2.396103
H	2.530996	0.905112	2.481879
N	-0.336954	1.783080	0.603279
N	1.716943	1.225488	0.222565
C	2.297707	0.659494	-2.609903
H	1.277043	0.681610	-2.223914
C	0.442582	0.722716	0.205127
Ni	-0.449966	-0.775434	-0.479165
C	-1.836942	-3.254609	-0.442870
C	-2.084609	-2.101011	-1.238674
C	-3.322176	-1.430687	-1.112451
C	-4.323503	-1.909037	-0.275139
C	-4.087895	-3.062748	0.479934
C	-2.854189	-3.708977	0.410456
H	-4.863731	-3.454475	1.133568
H	-2.668514	-4.585189	1.027553
C	-1.211881	-1.653893	-2.463934
O	-0.859680	-2.495079	-3.286211
O	-0.982941	-0.379169	-2.444693
C	-0.456044	-3.845347	-0.391025
H	-0.447659	-4.827831	0.097220
H	-0.050561	-3.950254	-1.403320
C	-2.432076	-0.456552	3.647604
H	-3.309413	-0.101831	4.201430
H	-2.765706	-1.203592	2.919998
H	-1.773903	-0.951791	4.369852
C	-1.304246	1.782671	3.992824

H	-2.204824	2.249057	4.410319
H	-0.734823	1.346232	4.822331
H	-0.693387	2.574396	3.545592
C	-1.819309	4.580048	-1.555777
H	-1.269957	5.016512	-2.397996
H	-2.851797	4.946140	-1.603882
H	-1.376444	4.962334	-0.628711
C	-2.350837	2.538923	-2.965892
H	-1.801562	2.999381	-3.795907
H	-2.241149	1.454900	-3.049282
H	-3.406520	2.810830	-3.084444
C	2.282899	-0.367468	-3.754797
H	2.053637	-1.373069	-3.389943
H	1.493890	-0.101404	-4.464139
H	3.232224	-0.398549	-4.304033
C	2.635435	2.068326	-3.144406
H	3.647797	2.098029	-3.566514
H	1.930399	2.350579	-3.934792
H	2.580073	2.827389	-2.355047
C	4.441222	1.783585	2.905809
H	4.193038	2.016567	3.947998
H	5.508828	1.538552	2.862327
H	4.288026	2.691009	2.311413
C	3.774100	-0.622231	3.303450
H	4.817637	-0.956169	3.321867
H	3.491044	-0.375039	4.333462
H	3.157526	-1.464156	2.975286
Si	0.581582	-2.538268	0.581100
C	0.309110	-2.812377	2.445341
H	0.788077	-3.745866	2.771576
H	0.729371	-1.996207	3.044383
H	-0.758309	-2.880302	2.680656
C	2.400145	-2.893687	0.164588
H	2.603890	-2.706553	-0.894188
H	3.113965	-2.310245	0.749646
H	2.590463	-3.958604	0.360783
H	-3.483189	-0.538357	-1.708460
H	-5.277243	-1.393215	-0.211237

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B3LYP SCF energy: -2157.66175205 a.u.
B3LYP enthalpy: -2156.841526 a.u.
B3LYP free energy: -2156.971480 a.u.
M06 SCF energy in solution: -2158.55423802 a.u.
M06 enthalpy in solution: -2157.734012 a.u.
M06 free energy in solution: -2157.863966 a.u.
Three lowest frequencies (cm-1): 11.4967 19.5520 23.1612

Cartesian coordinates

ATOM	X	Y	Z
C	5.587484	-1.165280	0.908031
C	6.585836	-1.830306	0.197021
C	4.405918	-0.754629	0.280808
C	6.411163	-2.061998	-1.167038
C	5.254453	-1.611434	-1.805412

C	4.232261	-0.952271	-1.106774
H	7.178271	-2.577224	-1.740010
H	5.144369	-1.761380	-2.877650
C	-0.788094	2.829858	-0.017566
C	-0.625897	3.502767	-1.247275
C	0.155039	4.665068	-1.249652
H	0.300872	5.208134	-2.178045
C	0.755588	5.133231	-0.084808
C	0.579449	4.450133	1.113995
C	-0.200090	3.288535	1.181707
H	1.364259	6.033021	-0.112081
H	1.053076	4.824239	2.015677
C	-3.022871	1.729049	0.146860
C	-3.474176	0.457003	0.265301
H	-3.547231	2.670952	0.144790
H	-4.471468	0.066169	0.386439
C	-2.436006	-1.807962	0.406274
C	-2.889564	-2.612652	-0.662262
C	-2.979077	-3.992995	-0.442614
H	-3.323278	-4.638389	-1.244618
C	-2.632200	-4.553257	0.783187
C	-2.208057	-3.735878	1.825270
C	-2.110078	-2.347185	1.669775
H	-2.701557	-5.627920	0.928515
H	-1.956908	-4.179856	2.783747
N	-1.638882	1.656933	0.028851
N	-2.358886	-0.374004	0.217738
C	-1.202207	0.356935	0.087467
Ni	0.558010	-0.179392	0.412484
O	3.612194	0.780990	1.926892
C	3.341133	-0.126454	1.148847
O	2.164673	-0.714454	1.061591
Si	1.281842	-1.087070	-1.507986
C	0.291306	-0.624215	-3.071625
H	0.612685	-1.244915	-3.919838
H	-0.786354	-0.760310	-2.946829
H	0.465496	0.421538	-3.344929
C	1.309327	-2.975030	-1.319867
H	0.304721	-3.381091	-1.155637
H	1.728004	-3.449557	-2.218129
H	1.931500	-3.250385	-0.462749
C	3.043528	-0.407405	-1.867572
H	3.215483	-0.554591	-2.943603
H	2.983895	0.682082	-1.726435
C	-0.340566	3.123810	-3.755153
H	-0.159401	4.163682	-4.050300
H	0.629771	2.660986	-3.550298
H	-0.787558	2.615607	-4.616986
C	-1.283637	3.027736	-2.540657
H	-1.546791	1.972217	-2.415557
C	-2.584441	3.808750	-2.826255
H	-2.377444	4.879172	-2.942595
H	-3.049546	3.452177	-3.753023
H	-3.316246	3.697627	-2.019218
C	-1.518086	3.388297	3.323096
H	-1.721607	2.889064	4.277849
H	-1.187705	4.410723	3.541934

H	-2.460300	3.453357	2.766429
C	-0.437209	2.618973	2.533211
H	-0.824796	1.612495	2.348965
C	0.845654	2.458254	3.370026
H	0.614433	1.894111	4.281791
H	1.633748	1.922119	2.830641
H	1.246874	3.427617	3.688655
C	-2.878606	-1.491984	3.911028
H	-3.053693	-2.497752	4.310744
H	-2.630915	-0.835363	4.753268
H	-3.818508	-1.140029	3.470176
C	-1.733323	-1.492103	2.876587
H	-1.605275	-0.460125	2.539612
C	-0.403140	-1.924970	3.522580
H	-0.157554	-1.252378	4.352776
H	-0.461517	-2.940918	3.930424
H	0.423654	-1.888155	2.806354
C	-4.859597	-1.959530	-2.109640
H	-5.159654	-1.519794	-3.068150
H	-5.305591	-2.958857	-2.042619
H	-5.292757	-1.350158	-1.309366
C	-3.320888	-2.037384	-2.009568
H	-2.932513	-1.015944	-2.080459
C	-2.758387	-2.830082	-3.205165
H	-2.975111	-2.300000	-4.139682
H	-1.675018	-2.960125	-3.130924
H	-3.213554	-3.823823	-3.283916
H	5.706074	-0.960228	1.968078
H	7.490392	-2.159027	0.702044

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B3LYP SCF energy: -2157.66062629 a.u.
B3LYP enthalpy: -2156.842167 a.u.
B3LYP free energy: -2156.973802 a.u.
M06 SCF energy in solution: -2158.54897367 a.u.
M06 enthalpy in solution: -2157.730514 a.u.
M06 free energy in solution: -2157.862149 a.u.
Three lowest frequencies (cm-1): 12.6516 20.5715 25.6726

Cartesian coordinates

ATOM	X	Y	Z
C	2.038943	1.204579	-2.874788
C	3.187384	1.628678	-3.553229
C	1.905744	1.352022	-1.481954
C	4.215885	2.247700	-2.842403
C	4.085291	2.446472	-1.465551
C	2.941504	2.013680	-0.779296
H	5.111010	2.589765	-3.356805
H	4.882407	2.947007	-0.917422
C	1.269835	-2.385868	0.836196
C	1.862919	-2.138088	2.092782
C	3.227874	-2.417013	2.230017
H	3.715728	-2.238171	3.183576
C	3.970443	-2.920512	1.165236
C	3.358344	-3.165248	-0.060414

C	1.995086	-2.908639	-0.255657
H	5.029724	-3.126944	1.292573
H	3.947031	-3.564956	-0.879991
C	-1.141704	-3.024026	1.033397
C	-2.319127	-2.413664	0.753960
H	-0.920795	-3.995150	1.447384
H	-3.339051	-2.743373	0.872977
C	-3.049225	-0.238179	-0.180682
C	-3.631698	0.595078	0.794541
C	-4.692767	1.414492	0.392247
H	-5.165542	2.069134	1.118506
C	-5.148042	1.408939	-0.922863
C	-4.544751	0.583925	-1.866556
C	-3.481571	-0.257903	-1.520021
H	-5.971203	2.055818	-1.214479
H	-4.898173	0.598359	-2.893421
N	-0.142392	-2.125738	0.677421
N	-2.012247	-1.160874	0.231442
C	-0.660194	-0.959359	0.169327
Ni	0.513743	0.405254	-0.610853
O	-0.106408	2.917985	0.322203
Si	1.336953	3.506824	0.994884
C	-0.361365	2.014719	-0.679311
O	-1.225478	2.238668	-1.494182
C	-2.831955	2.045558	2.723377
H	-3.724456	2.681668	2.752915
H	-2.419461	2.014182	3.739324
H	-2.097814	2.519347	2.065178
C	-3.163348	0.618641	2.246727
H	-2.237611	0.038228	2.312715
C	-4.197324	-0.048741	3.176204
H	-3.837047	-0.053736	4.212045
H	-5.152264	0.489720	3.156339
H	-4.394823	-1.085975	2.881604
C	-3.826147	-2.196991	-3.116841
H	-4.689512	-1.729167	-3.604597
H	-3.334537	-2.839639	-3.856970
H	-4.205059	-2.836041	-2.310470
C	-2.252917	-0.290600	-3.731000
H	-1.691999	-0.928949	-4.425056
H	-3.044092	0.205859	-4.305543
H	-1.590283	0.484636	-3.335902
C	-2.839054	-1.139419	-2.585363
H	-2.004973	-1.676338	-2.123466
C	1.719788	-0.411689	3.966574
H	1.874070	0.404006	3.253356
H	1.077307	-0.041381	4.773973
H	2.690841	-0.660763	4.409516
C	0.834017	-2.761127	4.313039
H	1.785100	-3.126027	4.718869
H	0.225689	-2.402279	5.151626
H	0.316796	-3.614422	3.860148
C	1.064300	-1.629077	3.290082
H	0.083232	-1.305414	2.929861
C	2.145636	-2.756003	-2.802414
H	1.583521	-2.946726	-3.724104
H	2.343567	-1.681330	-2.739320

H	3.106854	-3.274623	-2.895852
C	1.337726	-3.253631	-1.589852
H	0.364445	-2.754905	-1.627068
C	1.084011	-4.773031	-1.685802
H	0.582024	-5.018665	-2.629026
H	2.027315	-5.331082	-1.650128
H	0.453207	-5.129894	-0.863668
C	2.772349	2.302342	0.698325
H	2.579377	1.375324	1.253958
H	3.686528	2.742401	1.121727
C	1.698655	5.165861	0.182466
H	0.836012	5.836940	0.263008
H	2.558026	5.661419	0.652190
H	1.925751	5.035280	-0.881377
C	0.982771	3.727952	2.832968
H	0.129749	4.398898	2.987920
H	0.746939	2.772948	3.316138
H	1.847202	4.162828	3.350410
H	1.229144	0.752905	-3.445790
H	3.271611	1.488725	-4.628882

16-TS

B3LYP SCF energy: -2157.65758573 a.u.
B3LYP enthalpy: -2156.838754 a.u.
B3LYP free energy: -2156.968113 a.u.
M06 SCF energy in solution: -2158.54570956 a.u.
M06 enthalpy in solution: -2157.726878 a.u.
M06 free energy in solution: -2157.856237 a.u.
Three lowest frequencies (cm-1): -56.3963 9.7545 17.5999
Imaginary frequency: -56.3963 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Si	2.030914	0.754168	-1.365898
C	-1.840552	2.390348	0.469162
C	-1.954258	3.292768	-0.611047
C	-1.591122	4.626479	-0.384544
H	-1.668341	5.345512	-1.194181
C	-1.128453	5.047424	0.859363
C	-1.032395	4.139491	1.908800
C	-1.392845	2.795933	1.743891
H	-0.846392	6.086029	1.010757
H	-0.677256	4.478148	2.877803
C	-3.581198	0.612813	0.362795
C	-3.589997	-0.734531	0.223281
H	-4.383893	1.315085	0.521576
H	-4.402086	-1.444153	0.229837
C	-1.863907	-2.509953	-0.072721
C	-1.925449	-3.115702	-1.345839
C	-1.580505	-4.469326	-1.437331
H	-1.619122	-4.966703	-2.401777
C	-1.185004	-5.189755	-0.313232
C	-1.132404	-4.567990	0.930131
C	-1.474325	-3.218043	1.082778
H	-0.917539	-6.238951	-0.407657

H	-0.823675	-5.139268	1.800583
N	-2.251403	1.018748	0.280512
N	-2.265748	-1.128686	0.058806
C	-1.402922	-0.055045	0.105731
Ni	0.440863	-0.148112	0.233757
C	-1.668803	3.459716	-3.145815
H	-0.599737	3.258100	-3.031849
H	-1.999882	3.017430	-4.092521
H	-1.801991	4.544297	-3.231786
C	-2.485677	2.872151	-1.979522
H	-2.411646	1.781543	-2.046570
C	-3.973372	3.253097	-2.135960
H	-4.105933	4.339264	-2.063791
H	-4.351882	2.930799	-3.113385
H	-4.596673	2.789301	-1.364501
C	-1.323036	1.853176	2.941472
H	-1.610905	0.853728	2.605622
C	0.106008	1.741421	3.505738
H	0.473984	2.706208	3.874762
H	0.126008	1.035515	4.344629
H	0.798796	1.377355	2.739812
C	-2.323994	2.276087	4.035875
H	-2.302298	1.561051	4.866751
H	-2.082653	3.265396	4.442275
H	-3.348660	2.315903	3.648450
C	-3.845533	-2.681584	-2.934317
H	-3.968120	-3.748980	-3.153829
H	-4.519990	-2.432180	-2.108032
H	-4.169253	-2.116101	-3.816420
C	-2.377230	-2.355385	-2.589934
H	-2.316108	-1.285343	-2.367704
C	-1.471327	-2.617000	-3.806968
H	-1.561229	-3.646516	-4.172641
H	-1.752237	-1.952951	-4.632534
H	-0.419433	-2.434749	-3.566277
C	-2.564412	-3.180408	3.359141
H	-2.419207	-4.255499	3.518891
H	-2.568466	-2.694439	4.342076
H	-3.553520	-3.041117	2.907242
C	-1.448618	-2.589529	2.473025
H	-1.649979	-1.520124	2.365870
C	-0.071398	-2.723728	3.149858
H	-0.085264	-2.217741	4.122970
H	0.189845	-3.773055	3.331702
H	0.725777	-2.276478	2.547544
C	3.668895	0.002845	-2.025902
H	3.967945	0.513287	-2.950573
H	3.423165	-1.028569	-2.328822
C	3.318081	-0.750720	0.863770
O	2.294187	-0.081849	0.283770
O	3.144376	-1.465135	1.831456
C	0.923092	0.553394	-2.919790
H	0.802484	-0.506518	-3.166995
H	-0.072697	0.974826	-2.766518
H	1.392713	1.049839	-3.783800
C	2.257762	2.589616	-0.970698
H	1.298522	3.081564	-0.779517

H	2.889397	2.727458	-0.086528
H	2.741182	3.101793	-1.814176
C	4.659551	-0.452648	0.279735
C	4.826957	-0.038108	-1.060406
C	6.125707	0.279743	-1.484160
H	6.276946	0.599422	-2.512663
C	5.765836	-0.581986	1.131563
H	5.593758	-0.926972	2.146091
C	7.044937	-0.261422	0.687834
H	7.895411	-0.351912	1.357789
C	7.220548	0.180443	-0.625871
H	8.212919	0.439180	-0.986957

17-TS

B3LYP SCF energy: -2157.65347462 a.u.
B3LYP enthalpy: -2156.836349 a.u.
B3LYP free energy: -2156.966029 a.u.
M06 SCF energy in solution: -2158.54787380 a.u.
M06 enthalpy in solution: -2157.730748 a.u.
M06 free energy in solution: -2157.860428 a.u.
Three lowest frequencies (cm-1): -239.8761 15.0450 20.8819
Imaginary frequency: -239.8761 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	1.453168	3.190472	-0.817279
C	2.047145	4.347192	-0.316057
C	0.249428	2.702278	-0.278682
C	1.415070	5.052681	0.711848
C	0.199326	4.601655	1.228612
C	-0.403308	3.428962	0.749517
H	1.859424	5.965770	1.100730
H	-0.291992	5.165266	2.019450
C	2.905169	-0.998851	0.133032
C	3.446885	-0.471306	1.322509
C	4.660222	0.221614	1.230317
H	5.101322	0.645102	2.128225
C	5.308681	0.377033	0.008161
C	4.755717	-0.163948	-1.149522
C	3.543582	-0.864474	-1.117105
H	6.249532	0.918945	-0.041879
H	5.270953	-0.039396	-2.097748
C	1.562132	-3.102337	0.297043
C	0.239870	-3.399662	0.284326
H	2.434636	-3.733252	0.363127
H	-0.278062	-4.344085	0.339938
C	-1.885682	-2.120279	0.167770
C	-2.570190	-2.142663	1.399536
C	-3.970539	-2.172279	1.364034
H	-4.527596	-2.196516	2.296667
C	-4.657295	-2.175681	0.153116
C	-3.955095	-2.137723	-1.048913
C	-2.555225	-2.107972	-1.073849
H	-5.743865	-2.202677	0.145635
H	-4.502799	-2.132313	-1.985866

C	2.765250	-0.628259	2.678366
H	1.858055	-1.222456	2.534161
C	2.976289	-1.455035	-2.405054
H	2.025507	-1.940829	-2.167111
C	-1.847468	-2.148880	2.744099
H	-0.775478	-2.044826	2.553464
N	1.655961	-1.719115	0.196739
N	-0.443521	-2.190118	0.182920
C	-2.422256	-1.168383	-3.448965
H	-1.786434	-1.147750	-4.341007
H	-3.419316	-1.497415	-3.766918
H	-2.489663	-0.146875	-3.066338
C	-2.264491	-0.954584	3.623202
H	-1.684895	-0.947889	4.554039
H	-2.087879	-0.005690	3.105757
H	-3.325630	-0.998904	3.894548
C	-2.058331	-3.482181	3.488648
H	-1.503989	-3.485617	4.434698
H	-3.117124	-3.646973	3.720688
H	-1.713166	-4.333193	2.890658
C	2.330159	0.735168	3.250265
H	1.657976	1.254690	2.558397
H	1.805178	0.598137	4.203514
H	3.192582	1.386730	3.433486
C	3.657504	-1.393022	3.675571
H	3.937878	-2.378583	3.286518
H	4.581967	-0.845713	3.893641
H	3.128240	-1.540016	4.624555
C	2.675752	-0.367607	-3.455299
H	1.919839	0.337455	-3.095738
H	3.580276	0.191274	-3.725138
H	2.291086	-0.832233	-4.371434
C	3.914437	-2.539020	-2.973819
H	4.102904	-3.333893	-2.242363
H	3.469780	-2.996429	-3.865423
H	4.884542	-2.118927	-3.264782
C	-1.709470	-3.553852	-2.956968
H	-2.706688	-3.965368	-3.156116
H	-1.146900	-3.563701	-3.898030
H	-1.204102	-4.226681	-2.254593
C	-1.806612	-2.115940	-2.404250
H	-0.791019	-1.755754	-2.217985
C	0.418769	-1.123956	0.124237
Ni	0.185765	0.755142	-0.086312
C	-1.745531	2.973783	1.277847
H	-1.653289	2.011072	1.797069
H	-2.144789	3.696291	2.000986
O	-2.052838	1.875050	-1.347355
Si	-2.924711	2.740114	-0.188849
C	-0.685439	1.665083	-1.456837
O	-0.204801	1.516716	-2.574230
C	-4.453069	1.744507	0.262728
H	-5.062159	2.278760	1.003285
H	-5.079872	1.570181	-0.619718
H	-4.186463	0.767223	0.678112
C	-3.400447	4.404282	-0.931089
H	-3.964835	4.270021	-1.861107

H	-4.022906	4.988600	-0.241304
H	-2.508339	4.996297	-1.165246
H	1.896821	2.659310	-1.653788
H	2.984669	4.706860	-0.732604

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B3LYP SCF energy: -2157.67686299 a.u.
B3LYP enthalpy: -2156.857341 a.u.
B3LYP free energy: -2156.991803 a.u.
M06 SCF energy in solution: -2158.55688967 a.u.
M06 enthalpy in solution: -2157.737368 a.u.
M06 free energy in solution: -2157.871830 a.u.
Three lowest frequencies (cm-1): 7.8454 10.3782 14.2251

Cartesian coordinates

ATOM	X	Y	Z
Si	4.500219	0.412841	1.612527
C	-2.233518	-2.408692	0.485632
C	-1.728775	-2.924532	1.697055
C	-1.365418	-4.276409	1.730285
H	-0.965716	-4.698657	2.648126
C	-1.503163	-5.087228	0.606788
C	-2.009907	-4.556570	-0.576365
C	-2.387573	-3.210896	-0.663543
H	-1.214542	-6.134319	0.653368
H	-2.109167	-5.195626	-1.449449
C	-3.914837	-0.575571	0.718193
C	-3.905487	0.768214	0.552841
H	-4.704241	-1.250327	1.011295
H	-4.685076	1.504639	0.672444
C	-2.195620	2.468801	-0.100803
C	-1.700145	3.250228	0.963267
C	-1.311408	4.565646	0.681945
H	-0.918864	5.187887	1.481640
C	-1.413563	5.087310	-0.605024
C	-1.910953	4.297902	-1.638342
C	-2.314458	2.976322	-1.410849
H	-1.105075	6.110816	-0.802934
H	-1.983605	4.711715	-2.640383
N	-2.627122	-1.026213	0.427600
N	-2.612268	1.117478	0.164539
C	-1.779754	0.012407	0.074286
Ni	-0.025586	-0.051005	-0.404093
C	-0.040735	-1.796574	3.195509
H	0.416814	-1.308960	2.327341
H	0.087812	-1.144104	4.068607
H	0.495504	-2.733494	3.392579
C	-1.538167	-2.055093	2.935718
H	-2.000676	-1.084038	2.737505
C	-2.230825	-2.648486	4.176856
H	-1.788686	-3.607143	4.472621
H	-2.131876	-1.964954	5.028638
H	-3.299320	-2.815443	3.997970
C	-2.908521	-2.651809	-1.983358
H	-3.244771	-1.626679	-1.803786

C	-1.778014	-2.579556	-3.028603
H	-1.382559	-3.576958	-3.257646
H	-2.148519	-2.140909	-3.963581
H	-0.956703	-1.957941	-2.655221
C	-4.117746	-3.444344	-2.514696
H	-4.506604	-2.975720	-3.426669
H	-3.851094	-4.477903	-2.765533
H	-4.929245	-3.479024	-1.778509
C	-2.277671	3.564412	3.420509
H	-1.849379	4.571454	3.487991
H	-3.341498	3.670898	3.178400
H	-2.199613	3.107009	4.414123
C	-1.547630	2.698299	2.376878
H	-2.005530	1.705464	2.400402
C	-0.059298	2.516443	2.734412
H	0.472420	3.476171	2.723293
H	0.041791	2.087452	3.739606
H	0.424679	1.843079	2.018613
C	-4.018155	2.792823	-3.290509
H	-3.732203	3.738098	-3.766600
H	-4.400760	2.131640	-4.077241
H	-4.839380	3.004727	-2.595966
C	-2.828979	2.129567	-2.570529
H	-3.185111	1.180430	-2.160194
C	-1.688493	1.796456	-3.552381
H	-2.059000	1.161537	-4.366965
H	-1.267140	2.705612	-3.998935
H	-0.885693	1.261541	-3.033075
C	5.660913	0.942525	0.226295
H	6.720836	0.853601	0.491878
H	5.480066	2.012507	0.038956
C	2.864410	-0.012105	-0.530229
O	3.019520	0.316926	0.768427
O	1.720762	-0.143292	-0.984947
C	4.261379	1.707331	2.946846
H	3.997941	2.677432	2.511339
H	3.454705	1.418748	3.630365
H	5.173868	1.837459	3.541786
C	4.920036	-1.275040	2.322678
H	4.124298	-1.624657	2.990493
H	5.043392	-2.020637	1.529227
H	5.852209	-1.240994	2.900512
C	4.051018	-0.246573	-1.386321
C	5.367805	0.147178	-1.032655
C	6.414587	-0.185153	-1.902184
H	7.426813	0.109991	-1.635564
C	3.830785	-0.918094	-2.605655
H	2.814118	-1.199408	-2.857163
C	4.885351	-1.226345	-3.454742
H	4.695853	-1.751579	-4.386587
C	6.187860	-0.864951	-3.097787
H	7.023345	-1.107071	-3.749209

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B3LYP SCF energy:	-828.32861103 a.u.
B3LYP enthalpy:	-828.117033 a.u.
B3LYP free energy:	-828.170342 a.u.
M06 SCF energy in solution:	-828.10257604 a.u.
M06 enthalpy in solution:	-827.890998 a.u.
M06 free energy in solution:	-827.944307 a.u.
Three lowest frequencies (cm-1):	45.9726 73.4818 122.6535

Cartesian coordinates

ATOM	X	Y	Z
C	-3.433747	0.051495	0.285366
C	-2.388573	0.964109	0.202870
C	-3.183921	-1.300054	0.038481
C	-1.086568	0.547110	-0.116441
C	-0.830970	-0.816517	-0.390541
C	-1.898802	-1.720156	-0.298319
H	-3.989305	-2.027090	0.103347
H	-1.713454	-2.771469	-0.505651
Si	1.882107	-0.323894	0.070442
C	3.528250	-0.323758	-0.825804
H	4.231458	0.370752	-0.352276
H	3.985966	-1.320642	-0.815247
H	3.408397	-0.016808	-1.870523
C	2.063931	-0.788134	1.881280
H	2.500699	-1.788533	1.991399
H	2.717814	-0.079398	2.402239
H	1.094430	-0.787092	2.391806
O	1.263746	1.256996	-0.050085
C	-0.041071	1.630648	-0.127064
O	-0.327468	2.805610	-0.171316
C	0.540628	-1.312003	-0.809526
H	0.620663	-2.392224	-0.641229
H	0.673424	-1.159695	-1.891690
H	-2.550935	2.020244	0.389217
H	-4.433830	0.389178	0.541820

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B3LYP SCF energy:	-1988.30826000 a.u.
B3LYP enthalpy:	-1987.492507 a.u.
B3LYP free energy:	-1987.613529 a.u.
M06 SCF energy in solution:	-1987.51684408 a.u.
M06 enthalpy in solution:	-1986.701091 a.u.
M06 free energy in solution:	-1986.822113 a.u.
Three lowest frequencies (cm-1):	-137.6038 21.3340 24.0740
Imaginary frequency:	-137.6038 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	5.690203	-1.953405	-0.550281
C	4.509631	-1.995325	0.145095
C	5.636099	-1.949139	-1.976619
C	3.238142	-2.052333	-0.504150
C	3.170138	-2.200052	-1.960336
C	4.445328	-2.048636	-2.638745

H	6.560963	-1.880410	-2.547522
H	4.432706	-2.077342	-3.726913
Si	0.367257	-0.445976	-1.292277
C	1.640222	0.816113	-1.842258
H	2.527272	0.778925	-1.203033
H	1.961123	0.527409	-2.846244
H	1.268912	1.843521	-1.863411
O	0.852174	-1.702332	-0.316582
C	2.105084	-1.827012	0.340896
O	2.085073	-1.683225	1.566146
C	2.033119	-2.443152	-2.718685
H	2.148433	-2.542471	-3.796928
H	1.149136	-2.901296	-2.296794
H	4.503981	-1.955323	1.230268
H	6.644390	-1.902679	-0.033447
C	0.399021	2.649132	0.551545
C	-0.030547	3.680981	-0.308287
C	0.856182	4.741214	-0.530005
H	0.563391	5.550632	-1.192234
C	2.103245	4.774970	0.086658
C	2.486552	3.751338	0.947567
C	1.645579	2.661755	1.209193
H	2.778031	5.605663	-0.101372
H	3.459076	3.792894	1.426057
C	-1.435803	1.682905	1.883391
C	-2.231392	0.588338	1.837504
H	-1.422047	2.530829	2.548492
H	-3.052765	0.276666	2.461513
C	-2.519269	-1.395920	0.393840
C	-3.627612	-1.275976	-0.475290
C	-4.334973	-2.445065	-0.775954
H	-5.187521	-2.396054	-1.445322
C	-3.966816	-3.669926	-0.226440
C	-2.894162	-3.746874	0.653909
C	-2.145721	-2.612928	1.000050
H	-4.527256	-4.566294	-0.478303
H	-2.627329	-4.704555	1.087632
N	-0.534275	1.570600	0.836332
N	-1.809265	-0.177310	0.763631
C	-0.749582	0.418435	0.136406
C	-0.189576	-3.998904	1.880686
H	0.151686	-4.117275	0.848960
H	0.698233	-3.917834	2.513525
H	-0.736979	-4.902634	2.176532
C	-1.628950	-2.654469	3.464675
H	-2.316400	-3.489120	3.649994
H	-0.823490	-2.708409	4.205608
H	-2.182257	-1.724329	3.640620
C	-1.036503	-2.724257	2.040250
H	-0.345029	-1.889519	1.912502
C	-5.249573	0.632508	-0.149457
H	-5.579311	1.606029	-0.531248
H	-6.113907	-0.041623	-0.151812
H	-4.935397	0.767846	0.890414
C	-4.112659	0.064259	-1.026884
H	-3.278443	0.773019	-0.984556
C	-4.574073	-0.007029	-2.494433

H	-3.817374	-0.464652	-3.138132
H	-5.501044	-0.581066	-2.602038
H	-4.776926	1.002865	-2.868730
C	-1.313922	3.794856	-2.506221
H	-0.721584	2.974313	-2.924401
H	-2.315972	3.750693	-2.948456
H	-0.853661	4.735650	-2.827758
C	-1.406360	3.701228	-0.970995
H	-1.916249	2.761201	-0.737498
C	-2.275528	4.841027	-0.402092
H	-1.835648	5.821708	-0.615992
H	-3.276418	4.818591	-0.848675
H	-2.386498	4.756375	0.684713
C	3.555528	1.196955	2.078548
H	3.745385	0.319048	2.701410
H	3.824575	0.926999	1.053270
H	4.221306	2.002128	2.412922
C	2.070770	1.581724	2.199980
H	1.505218	0.667999	1.997126
C	1.755748	2.023025	3.645903
H	2.039007	1.230682	4.347361
H	2.314609	2.928695	3.911935
H	0.690332	2.234090	3.792578
C	-0.873890	-0.886170	-2.630488
H	-1.591460	-0.072785	-2.790879
H	-0.331874	-1.064759	-3.562328
H	-1.431811	-1.794076	-2.384622

cat1

B3LYP SCF energy: -793.39808630 a.u.
B3LYP enthalpy: -793.015645 a.u.
B3LYP free energy: -793.075386 a.u.
M06 SCF energy in solution: -794.75267035 a.u.
M06 enthalpy in solution: -794.370229 a.u.
M06 free energy in solution: -794.429970 a.u.
Three lowest frequencies (cm-1): 72.7870 90.4372 104.7306

Cartesian coordinates

ATOM	X	Y	Z
Ni	-0.000068	-0.000913	-0.001177
C	-1.537510	-0.471006	1.481755
H	-1.002892	-0.535147	2.426452
C	-1.395232	-1.538149	0.614947
H	-0.781616	-2.370186	0.956772
C	-2.246521	-1.836365	-0.602642
H	-3.155566	-2.392768	-0.318310
H	-1.674552	-2.513474	-1.249998
C	-2.637096	-0.582225	-1.420255
H	-2.887178	-0.893646	-2.442024
H	-3.553779	-0.139541	-1.016939
C	-1.538069	0.471239	-1.481122
H	-1.004591	0.535206	-2.426502
C	-1.394038	1.538281	-0.614295
H	-0.780018	2.369739	-0.956910
C	-2.244157	1.837411	0.603845

H	-3.152872	2.394661	0.320181
H	-1.671116	2.514003	1.250808
C	-2.635392	0.583621	1.421724
H	-2.884417	0.895213	2.443708
H	-3.552819	0.141894	1.019047
C	1.537224	-0.471171	-1.481243
H	1.003296	-0.535799	-2.426329
C	1.394477	-1.538338	-0.614171
H	0.781505	-2.370713	-0.956494
C	2.245722	-1.836736	0.603418
H	3.154504	-2.393609	0.319209
H	1.673493	-2.513466	1.250967
C	2.636941	-0.582620	1.420746
H	2.886989	-0.893886	2.442580
H	3.553753	-0.140380	1.017242
C	1.538484	0.471314	1.481557
H	1.003853	0.534555	2.426326
C	1.394810	1.538206	0.614907
H	0.780223	2.369480	0.956893
C	2.245032	1.836937	-0.603280
H	3.154001	2.393756	-0.319564
H	1.672280	2.513810	-1.250182
C	2.635627	0.583001	-1.421238
H	2.884711	0.894600	-2.443200
H	3.552906	0.140870	-1.018687

cat2

B3LYP SCF energy: -1641.38895118 a.u.
B3LYP enthalpy: -1640.592765 a.u.
B3LYP free energy: -1640.710299 a.u.
M06 SCF energy in solution: -1642.33765083 a.u.
M06 enthalpy in solution: -1641.541465 a.u.
M06 free energy in solution: -1641.658999 a.u.
Three lowest frequencies (cm-1): 13.5061 16.4007 22.7186

Cartesian coordinates

ATOM	X	Y	Z
Ni	0.184972	-0.561472	1.219643
C	0.331574	-2.685114	1.792711
H	0.651467	-3.159349	0.865644
C	1.329949	-2.735031	2.929296
H	2.334975	-2.746168	2.486934
H	1.244491	-3.675493	3.499368
C	1.230250	-1.528485	3.900680
H	0.486089	-1.730609	4.677844
H	2.187430	-1.428569	4.428793
C	0.912480	-0.221972	3.192443
H	1.769647	0.426956	3.007443
C	-0.344369	0.343194	3.040964
H	-0.409403	1.408519	2.827961
C	-1.653014	-0.322319	3.417592
H	-2.452854	0.168191	2.849521
H	-1.892204	-0.156311	4.481410
C	-1.711072	-1.853451	3.129995
H	-1.319035	-2.408327	3.988110

H	-2.765560	-2.143513	3.043076
C	-0.979531	-2.272039	1.866747
H	-1.603568	-2.426602	0.989811
C	-2.445269	0.431627	-0.914862
C	-3.065542	1.449766	-0.157197
C	-4.418044	1.287726	0.167368
H	-4.924565	2.051713	0.748685
C	-5.129915	0.164801	-0.248782
C	-4.500020	-0.821228	-1.001785
C	-3.146904	-0.712888	-1.349617
H	-6.179975	0.060938	0.012433
H	-5.067565	-1.688875	-1.325125
C	-0.671587	1.114287	-2.529848
C	0.680147	1.092323	-2.549688
H	-1.385773	1.450004	-3.265083
H	1.384526	1.410424	-3.302486
C	2.468018	0.434556	-0.933510
C	3.105040	1.549680	-0.349756
C	4.457770	1.424976	-0.006745
H	4.974575	2.269282	0.441245
C	5.150218	0.239581	-0.233430
C	4.500206	-0.849550	-0.810457
C	3.149212	-0.779363	-1.171366
H	6.200063	0.162942	0.037897
H	5.053804	-1.767207	-0.983455
N	-1.066840	0.587493	-1.296543
N	1.090356	0.554329	-1.329272
C	0.017956	0.227250	-0.509512
C	2.895567	-3.324085	-1.265877
H	2.802646	-3.345071	-0.175145
H	2.265305	-4.121197	-1.677126
H	3.932965	-3.569844	-1.522377
C	2.680938	-1.935906	-3.368987
H	3.748146	-2.010958	-3.611414
H	2.165773	-2.777174	-3.848661
H	2.299111	-1.010833	-3.813478
C	2.460333	-1.965075	-1.841705
H	1.386581	-1.866060	-1.654710
C	2.922215	3.970059	-1.057559
H	2.369101	4.905882	-0.913047
H	3.982446	4.174788	-0.865834
H	2.824743	3.678364	-2.109450
C	2.382681	2.873430	-0.116962
H	1.326110	2.724733	-0.354261
C	2.453254	3.325216	1.353339
H	2.024924	2.565903	2.014885
H	3.483815	3.516370	1.675005
H	1.888103	4.255159	1.490027
C	-2.724568	3.264772	1.623962
H	-2.666718	2.495457	2.400384
H	-2.055438	4.084707	1.909463
H	-3.744041	3.668834	1.621261
C	-2.312714	2.715634	0.246897
H	-1.251294	2.456800	0.308398
C	-2.477173	3.812105	-0.827743
H	-3.531852	4.092971	-0.938744
H	-1.915969	4.711951	-0.547371

H	-2.111929	3.479939	-1.804729
C	-2.819661	-3.219155	-1.759365
H	-2.248202	-3.939899	-2.356000
H	-2.566302	-3.376897	-0.706245
H	-3.881142	-3.459861	-1.890544
C	-2.490529	-1.785776	-2.215673
H	-1.406659	-1.660574	-2.133490
C	-2.875672	-1.600962	-3.698962
H	-2.380379	-2.355664	-4.321731
H	-3.958500	-1.705762	-3.838461
H	-2.585082	-0.613069	-4.071547

cat3

B3LYP SCF energy: -1641.39489881 a.u.
B3LYP enthalpy: -1640.597722 a.u.
B3LYP free energy: -1640.717183 a.u.
M06 SCF energy in solution: -1642.34146982 a.u.
M06 enthalpy in solution: -1641.544293 a.u.
M06 free energy in solution: -1641.663754 a.u.
Three lowest frequencies (cm-1): 9.9647 20.5379 22.7231

Cartesian coordinates

ATOM	X	Y	Z
Ni	0.052938	0.782589	-0.675617
C	0.123340	5.663807	-1.376680
H	0.001040	6.581964	-1.955079
C	-1.180944	4.945059	-1.129928
H	-1.737786	4.931804	-2.079739
H	-1.795261	5.560251	-0.450920
C	-1.124041	3.504095	-0.579840
H	-0.657116	3.504026	0.407570
H	-2.158258	3.172528	-0.415173
C	-0.461363	2.511327	-1.518422
H	-1.110525	2.218198	-2.349544
C	0.906052	2.262869	-1.709227
H	1.150338	1.764494	-2.652013
C	2.124674	2.917943	-1.073372
H	2.816697	3.190307	-1.885193
H	2.667333	2.180313	-0.463618
C	1.893747	4.182181	-0.215579
H	1.245266	3.943661	0.631686
H	2.860887	4.462333	0.222387
C	1.374727	5.366798	-1.002038
H	2.149938	6.059841	-1.332804
C	2.309271	-1.469419	0.454261
C	2.991747	-0.802675	1.492496
C	4.353893	-0.535328	1.307370
H	4.905223	-0.013274	2.084154
C	5.012607	-0.924957	0.143880
C	4.319253	-1.598011	-0.858175
C	2.955483	-1.888401	-0.726196
H	6.070036	-0.706256	0.019690
H	4.843367	-1.900828	-1.760297
C	0.400502	-2.909287	1.187349
C	-0.949356	-2.799473	1.169442

H	1.047044	-3.693790	1.548599
H	-1.723067	-3.468380	1.512914
C	-2.583212	-1.080647	0.381985
C	-3.205952	-0.361588	1.422399
C	-4.507164	0.106278	1.200800
H	-5.010796	0.671101	1.980348
C	-5.164391	-0.136802	-0.002333
C	-4.531845	-0.862239	-1.008402
C	-3.231789	-1.354522	-0.839351
H	-6.173489	0.237150	-0.155126
H	-5.055355	-1.049080	-1.941884
N	0.903283	-1.743303	0.612394
N	-1.242589	-1.569469	0.582885
C	-0.102234	-0.884956	0.222240
C	-2.287776	-1.249973	-3.183859
H	-1.637566	-0.414555	-2.903006
H	-1.789360	-1.826392	-3.972982
H	-3.215942	-0.841392	-3.601577
C	-3.391361	-3.387243	-2.352622
H	-4.366059	-3.112646	-2.772668
H	-2.858419	-3.971227	-3.112280
H	-3.571789	-4.037346	-1.488759
C	-2.566990	-2.145789	-1.961516
H	-1.598808	-2.499908	-1.595732
C	-3.316798	-0.594963	3.950021
H	-2.763218	-0.426300	4.881279
H	-4.283580	-0.087101	4.045017
H	-3.512758	-1.669769	3.861332
C	-2.509430	-0.068901	2.747793
H	-1.549688	-0.593370	2.748101
C	-2.203473	1.434464	2.891682
H	-1.574271	1.778657	2.064581
H	-3.123511	2.031316	2.893501
H	-1.675156	1.629079	3.833117
C	2.112771	1.180282	2.785052
H	1.535306	1.504621	1.912363
H	1.579707	1.495263	3.690613
H	3.081627	1.694167	2.768298
C	2.291729	-0.350365	2.770434
H	1.290369	-0.791065	2.778394
C	3.014843	-0.844105	4.037627
H	4.013685	-0.403747	4.137800
H	2.443194	-0.564740	4.930495
H	3.129533	-1.934170	4.034764
C	2.108106	-1.732534	-3.103319
H	1.559744	-2.260012	-3.893510
H	1.572073	-0.806674	-2.869685
H	3.096405	-1.468547	-3.498918
C	2.222880	-2.618235	-1.847516
H	1.204147	-2.824345	-1.506625
C	2.877303	-3.974398	-2.174655
H	2.291954	-4.502668	-2.936530
H	3.893913	-3.853274	-2.566599
H	2.936974	-4.615043	-1.287237

cat4

B3LYP SCF energy:	-1953.41500139 a.u.
B3LYP enthalpy:	-1952.425702 a.u.
B3LYP free energy:	-1952.558528 a.u.
M06 SCF energy in solution:	-1954.21827391 a.u.
M06 enthalpy in solution:	-1953.228975 a.u.
M06 free energy in solution:	-1953.361801 a.u.
Three lowest frequencies (cm-1):	13.8917 18.6504 27.3890

Cartesian coordinates

ATOM	X	Y	Z
Ni	-0.052973	-0.749017	0.649080
C	-2.940282	-4.761313	-0.219983
H	-3.905265	-5.204564	0.031857
C	-3.033403	-3.576483	-1.156585
H	-3.997364	-3.089177	-0.959059
H	-3.112135	-3.941251	-2.195587
C	-1.925279	-2.488989	-1.100074
H	-1.005398	-2.870405	-1.545689
H	-2.253846	-1.673500	-1.759576
C	-1.661135	-1.942681	0.290216
H	-2.508450	-1.385663	0.699262
C	-0.818488	-2.538118	1.256005
H	-1.130567	-2.387937	2.289419
C	0.063968	-3.780245	1.076923
H	0.185785	-4.236102	2.067893
H	1.078660	-3.513146	0.751240
C	-0.424229	-4.900123	0.114791
H	-0.269194	-4.589603	-0.922347
H	0.233938	-5.767076	0.264493
C	-1.854379	-5.327318	0.318919
H	-2.009643	-6.171363	0.992265
C	-2.350545	1.804631	0.575706
C	-2.040301	2.337388	1.848912
C	-3.077755	2.437902	2.783343
H	-2.869194	2.832832	3.771780
C	-4.378136	2.054611	2.466189
C	-4.667023	1.569330	1.196489
C	-3.666452	1.434679	0.224188
H	-5.167637	2.145099	3.207672
H	-5.686828	1.288314	0.952904
C	-1.227881	2.740652	-1.411330
C	-0.137198	2.459560	-2.153845
H	-1.942463	3.544903	-1.476141
H	0.288828	2.960272	-3.008194
C	1.715919	0.843055	-2.097189
C	2.874404	1.577244	-1.752150
C	4.097381	1.162192	-2.296401
H	5.002488	1.709056	-2.049405
C	4.173120	0.066431	-3.148956
C	3.016711	-0.629737	-3.489411
C	1.765618	-0.253904	-2.984677
H	5.132567	-0.240699	-3.557005
H	3.086702	-1.472656	-4.168705
N	-1.316271	1.749807	-0.433627
N	0.436386	1.309208	-1.609472
C	-0.289399	0.821402	-0.531546

C	0.706264	-2.459805	-3.740472
H	1.170998	-2.973622	-2.891911
H	-0.260713	-2.935713	-3.936510
H	1.332377	-2.629488	-4.624565
C	-0.084418	-0.260994	-4.698571
H	0.625430	-0.292111	-5.534360
H	-1.006957	-0.759515	-5.019689
H	-0.322993	0.788496	-4.496916
C	0.499424	-0.963387	-3.453131
H	-0.236774	-0.885004	-2.649953
C	3.000983	4.103244	-1.717824
H	2.936960	4.995223	-1.083301
H	3.974625	4.118370	-2.221928
H	2.227399	4.182127	-2.488253
C	2.842341	2.824090	-0.867401
H	1.864105	2.869559	-0.379324
C	3.909658	2.809396	0.245244
H	3.841456	1.912715	0.867796
H	4.925630	2.861320	-0.162657
H	3.777507	3.683025	0.894424
C	-0.301012	2.771502	3.686556
H	-0.492813	1.769967	4.084873
H	0.760925	2.997877	3.833378
H	-0.869908	3.489523	4.289353
C	-0.650124	2.871877	2.191036
H	0.080197	2.268611	1.643853
C	-0.500465	4.337075	1.724016
H	-1.230543	4.980643	2.229977
H	0.502181	4.712892	1.962313
H	-0.649817	4.438952	0.644848
C	-4.989761	-0.271312	-1.135705
H	-5.098048	-0.692025	-2.142004
H	-4.610333	-1.055363	-0.475763
H	-5.993132	0.004709	-0.790689
C	-4.042614	0.942352	-1.171479
H	-3.122909	0.629346	-1.675455
C	-4.685723	2.069835	-2.008097
H	-4.938581	1.704012	-3.010510
H	-5.610011	2.424585	-1.536432
H	-4.020351	2.930849	-2.124562
C	4.428397	-1.360429	2.840769
H	5.461099	-1.029184	2.722951
C	3.846434	-2.091517	1.652159
H	3.241963	-2.940106	1.981510
H	4.669520	-2.526583	1.069893
C	3.020682	-1.200419	0.684889
H	3.717639	-0.552080	0.140990
H	2.581593	-1.855361	-0.080743
C	1.952445	-0.308683	1.301013
H	2.002489	0.728246	0.988952
C	1.172130	-0.572895	2.412428
H	0.644106	0.288721	2.823419
C	1.346999	-1.683551	3.424310
H	1.574913	-2.636352	2.950139
H	0.400180	-1.834912	3.958858
C	2.424787	-1.343186	4.481052
H	2.087510	-0.461671	5.047141

H	2.459701	-2.158184	5.223402
C	3.830924	-1.058654	4.001489
H	4.439328	-0.528694	4.736913

cat5

B3LYP SCF energy: -1517.95004456 a.u.
B3LYP enthalpy: -1517.327023 a.u.
B3LYP free energy: -1517.433503 a.u.
M06 SCF energy in solution: -1519.01829204 a.u.
M06 enthalpy in solution: -1518.395270 a.u.
M06 free energy in solution: -1518.501750 a.u.
Three lowest frequencies (cm-1): 16.8007 22.7740 25.8232

Cartesian coordinates

ATOM	X	Y	Z
C	2.555919	-0.032298	-0.529276
C	3.163771	-1.292296	-0.352014
C	4.481291	-1.312401	0.121555
H	4.976022	-2.266525	0.277926
C	5.163906	-0.132132	0.404123
C	4.540206	1.098189	0.216759
C	3.224272	1.178554	-0.255746
H	6.184961	-0.171532	0.774049
H	5.081253	2.012160	0.444649
C	0.829044	0.025908	-2.349795
C	-0.526343	0.062058	-2.379006
H	1.560264	0.004926	-3.142668
H	-1.220453	0.081092	-3.204306
C	-2.355128	0.136689	-0.682393
C	-3.077192	-1.068171	-0.574621
C	-4.438069	-0.977809	-0.258842
H	-5.023300	-1.887533	-0.165254
C	-5.048890	0.254684	-0.047748
C	-4.307872	1.428473	-0.151297
C	-2.946040	1.398683	-0.474817
H	-6.104897	0.300356	0.204744
H	-4.792367	2.384598	0.024704
N	1.194585	0.018186	-1.007778
N	-0.959708	0.078738	-1.056558
C	0.096808	0.051836	-0.186379
C	-2.032338	3.371256	0.813507
H	-1.546494	2.695645	1.525598
H	-1.433545	4.287515	0.741933
H	-3.013609	3.642711	1.220177
C	-2.775052	3.670509	-1.602104
H	-3.782525	3.989331	-1.311365
H	-2.157153	4.571820	-1.691480
H	-2.845379	3.206893	-2.592769
C	-2.162348	2.704100	-0.570184
H	-1.149092	2.469232	-0.910307
C	-2.891203	-3.041138	-2.144781
H	-2.404574	-4.009499	-2.312363
H	-3.975437	-3.204984	-2.156111
H	-2.645038	-2.387886	-2.990248
C	-2.436323	-2.433581	-0.802144

H	-1.352537	-2.290749	-0.854013
C	-2.706183	-3.402061	0.365234
H	-2.420796	-2.952505	1.320299
H	-3.765038	-3.681123	0.423370
H	-2.133386	-4.326344	0.222082
C	2.127872	-3.341154	0.699213
H	1.528573	-2.713879	1.367681
H	1.568906	-4.263445	0.501105
H	3.051414	-3.612989	1.224009
C	2.431522	-2.603704	-0.620460
H	1.470664	-2.367438	-1.087601
C	3.202498	-3.506668	-1.602157
H	4.163600	-3.832200	-1.188008
H	2.618411	-4.407392	-1.823499
H	3.404289	-2.991422	-2.548284
C	2.345081	3.236755	0.922574
H	1.836124	4.197784	0.782758
H	1.728706	2.619795	1.586866
H	3.296620	3.431036	1.431257
C	2.564094	2.542096	-0.436217
H	1.577089	2.385245	-0.881591
C	3.360004	3.442406	-1.400668
H	2.831449	4.390005	-1.556667
H	4.354753	3.680780	-1.007007
H	3.493590	2.963031	-2.377050
Ni	0.161985	0.093298	1.685573
C	-1.037702	-0.611620	2.914175
O	-0.087168	-0.071116	3.548614
O	-2.064637	-1.218922	3.046730

cat6

B3LYP SCF energy: -1969.03620881 a.u.
B3LYP enthalpy: -1968.235208 a.u.
B3LYP free energy: -1968.360284 a.u.
M06 SCF energy in solution: -1969.95733210 a.u.
M06 enthalpy in solution: -1969.156331 a.u.
M06 free energy in solution: -1969.281407 a.u.
Three lowest frequencies (cm-1): 14.0826 21.1842 25.0810

Cartesian coordinates

ATOM	X	Y	Z
C	-1.774400	-1.907268	0.659262
C	-2.563699	-2.447738	-0.378185
C	-3.954163	-2.447231	-0.206079
H	-4.588546	-2.857925	-0.986353
C	-4.535616	-1.930647	0.948288
C	-3.733470	-1.412680	1.962382
C	-2.337978	-1.392398	1.846116
H	-5.616642	-1.937413	1.061505
H	-4.198786	-1.024832	2.863396
C	0.436823	-3.059773	0.726206
C	1.716376	-2.711999	0.453939
H	0.007578	-3.996390	1.045577
H	2.630636	-3.283813	0.483631
C	2.878440	-0.625248	-0.266741

C	3.207592	-0.473949	-1.629343
C	4.358949	0.259670	-1.942089
H	4.632238	0.402530	-2.983895
C	5.163246	0.800480	-0.942562
C	4.830897	0.612646	0.396523
C	3.683073	-0.100019	0.765325
H	6.055013	1.362730	-1.207473
H	5.471036	1.028382	1.169479
C	-1.953413	-3.060673	-1.636749
H	-0.890301	-2.803784	-1.654504
C	-1.475220	-0.898538	3.004428
H	-0.478756	-0.684659	2.609172
C	2.372367	-1.084763	-2.750586
H	1.576227	-1.678608	-2.292753
N	-0.341407	-1.922615	0.514566
N	1.696325	-1.368231	0.085960
C	3.359188	-0.306288	2.242442
H	2.370658	-0.769418	2.308713
C	0.420060	-0.839723	0.116349
Ni	-0.104989	0.936921	-0.229192
Si	-2.543357	2.881631	-1.412647
C	-2.992558	3.199113	0.435445
H	-3.514283	4.125966	0.701071
H	-3.495516	2.367293	0.943729
C	-2.571660	-2.505249	-2.932732
H	-2.055409	-2.927207	-3.803311
H	-3.632859	-2.763943	-3.025587
H	-2.484755	-1.415892	-2.978549
C	-2.061247	-4.599627	-1.602647
H	-3.109572	-4.921275	-1.587751
H	-1.587616	-5.037985	-2.489237
H	-1.572935	-5.019625	-0.716167
C	-1.334782	-2.003508	4.072749
H	-0.684093	-1.667019	4.888899
H	-2.309972	-2.261890	4.503485
H	-0.902691	-2.917973	3.650659
C	-1.990402	0.407525	3.632374
H	-2.971518	0.283457	4.106125
H	-1.294668	0.741403	4.411162
H	-2.061204	1.202828	2.884282
C	4.369095	-1.271004	2.897179
H	5.385262	-0.859181	2.873598
H	4.104438	-1.449682	3.946262
H	4.391960	-2.239380	2.384120
C	3.286249	1.022216	3.017846
H	2.999735	0.832666	4.059414
H	4.253282	1.539212	3.032961
H	2.545072	1.693621	2.574246
C	3.208986	-2.038732	-3.625548
H	2.571417	-2.519471	-4.377017
H	4.005908	-1.508702	-4.160379
H	3.677961	-2.825787	-3.023874
C	1.687586	0.001126	-3.601823
H	2.421206	0.665527	-4.074725
H	1.090203	-0.459666	-4.398342
H	1.021631	0.605684	-2.977153
C	-3.294984	1.376676	-2.272842

H	-3.252868	0.492904	-1.628537
H	-4.344312	1.559152	-2.539180
H	-2.752708	1.146993	-3.198872
C	-2.765657	4.401354	-2.523921
H	-2.376703	5.303760	-2.039086
H	-2.230165	4.275885	-3.473460
H	-3.823513	4.571457	-2.761404
C	-1.482086	3.233683	0.674158
C	-0.872831	2.778117	-0.554261
C	0.552714	2.794735	-0.672354
C	1.303970	3.317341	0.425708
C	0.681384	3.778079	1.575848
C	-0.729632	3.748015	1.714619
H	1.285798	4.188851	2.381853
H	-1.201598	4.149560	2.608901
H	1.051353	2.688994	-1.635088
H	2.386438	3.379627	0.338872

cat7

B3LYP SCF energy: -1969.03733520 a.u.
B3LYP enthalpy: -1968.236667 a.u.
B3LYP free energy: -1968.362957 a.u.
M06 SCF energy in solution: -1969.95635402 a.u.
M06 enthalpy in solution: -1969.155686 a.u.
M06 free energy in solution: -1969.281976 a.u.
Three lowest frequencies (cm-1): 12.6775 22.2131 22.4342

Cartesian coordinates

ATOM	X	Y	Z
C	-3.152603	-0.125100	0.107488
C	-3.509395	-1.066143	1.094888
C	-4.484709	-2.016119	0.766792
H	-4.780452	-2.753089	1.508065
C	-5.081012	-2.031582	-0.491513
C	-4.715815	-1.086579	-1.446584
C	-3.750304	-0.110759	-1.169132
H	-5.834899	-2.778506	-0.726650
H	-5.190217	-1.102766	-2.423971
C	-2.483528	2.099923	1.018026
C	-1.316575	2.770570	1.166076
H	-3.496800	2.370520	1.271024
H	-1.102282	3.745393	1.575783
C	1.079798	2.311182	0.674419
C	1.854669	2.001084	1.811002
C	3.195751	2.405004	1.813520
H	3.818972	2.178030	2.673858
C	3.743671	3.090747	0.732294
C	2.956990	3.384263	-0.378051
C	1.609392	3.006501	-0.431560
H	4.786878	3.394936	0.754685
H	3.395471	3.915705	-1.217929
C	-2.892891	-1.059735	2.490727
H	-2.080105	-0.328195	2.494184
C	-3.389578	0.921422	-2.233312
H	-2.637121	1.592599	-1.810053

C	1.290729	1.226796	2.998441
H	0.210662	1.131173	2.855169
N	-2.169695	0.878016	0.427254
N	-0.312845	1.943191	0.664084
C	0.778192	3.325737	-1.669902
H	-0.261792	3.065054	-1.453461
C	-0.815029	0.748029	0.188684
Ni	0.033618	-0.690328	-0.677960
Si	4.149157	-2.209642	-0.836612
C	3.570088	-3.387105	0.575143
H	3.931171	-4.423434	0.552042
H	3.672646	-3.019454	1.604732
C	-2.272555	-2.419396	2.862108
H	-1.803760	-2.359959	3.851803
H	-3.025843	-3.215283	2.903113
H	-1.505408	-2.709182	2.137501
C	-3.924221	-0.613388	3.546769
H	-4.768295	-1.311435	3.601169
H	-3.461738	-0.569758	4.540164
H	-4.328461	0.379318	3.317456
C	-4.609063	1.780971	-2.620984
H	-4.316159	2.552977	-3.342486
H	-5.398783	1.177419	-3.083899
H	-5.041434	2.280211	-1.746209
C	-2.756736	0.260993	-3.472844
H	-3.446084	-0.444777	-3.951797
H	-2.490566	1.023399	-4.215255
H	-1.845985	-0.279101	-3.194491
C	0.809715	4.824679	-2.023366
H	1.814480	5.156729	-2.309675
H	0.144047	5.026662	-2.870793
H	0.481986	5.442527	-1.179405
C	1.222178	2.456862	-2.863230
H	0.602489	2.669193	-3.743227
H	2.267544	2.652643	-3.131652
H	1.121470	1.393871	-2.617921
C	1.510417	1.963379	4.333207
H	1.028334	1.414402	5.150658
H	2.574551	2.051867	4.581292
H	1.088151	2.974557	4.307877
C	1.869126	-0.201695	3.043737
H	2.957044	-0.184868	3.183817
H	1.432169	-0.764389	3.877928
H	1.649479	-0.737976	2.114510
C	4.953979	-0.571171	-0.343009
H	4.376445	-0.060677	0.434339
H	5.973613	-0.729668	0.031506
H	5.018450	0.107186	-1.203034
C	5.192331	-3.028624	-2.190379
H	4.778470	-4.002370	-2.475048
H	5.229792	-2.404926	-3.092326
H	6.225245	-3.184375	-1.853926
C	2.173317	-3.192515	-0.016896
C	2.289629	-2.277695	-1.074050
C	1.158552	-1.908400	-1.855593
C	-0.100678	-2.511121	-1.534014
C	-0.180599	-3.441955	-0.452947

C	0.931628	-3.789692	0.300238
H	-1.141379	-3.907336	-0.243625
H	0.847925	-4.515668	1.106276
H	1.289040	-1.378781	-2.798655
H	-0.939848	-2.450870	-2.224575

cat8

B3LYP SCF energy: -1969.03644950 a.u.
B3LYP enthalpy: -1968.235908 a.u.
B3LYP free energy: -1968.363715 a.u.
M06 SCF energy in solution: -1969.95431916 a.u.
M06 enthalpy in solution: -1969.153778 a.u.
M06 free energy in solution: -1969.281585 a.u.
Three lowest frequencies (cm-1): 14.4654 19.1243 22.5791

Cartesian coordinates

ATOM	X	Y	Z
C	1.320500	2.494995	0.724538
C	0.292339	3.073813	1.495571
C	-0.047165	4.406613	1.232410
H	-0.842150	4.876468	1.804703
C	0.613868	5.137475	0.248737
C	1.635815	4.546743	-0.489538
C	2.015008	3.217101	-0.267008
H	0.334031	6.170592	0.059260
H	2.147395	5.126462	-1.252966
C	2.664393	0.759602	1.908561
C	2.742299	-0.591968	1.875500
H	3.198426	1.489229	2.497268
H	3.358588	-1.283479	2.428737
C	1.618404	-2.407970	0.586397
C	0.670276	-3.156457	1.312497
C	0.506842	-4.505308	0.972680
H	-0.218929	-5.106331	1.513619
C	1.256038	-5.087570	-0.045907
C	2.194303	-4.329032	-0.741207
C	2.401936	-2.977736	-0.438262
H	1.111751	-6.135557	-0.295839
H	2.776894	-4.792986	-1.532213
C	-0.459226	2.295852	2.570714
H	0.021860	1.319316	2.677018
C	3.136761	2.599289	-1.095900
H	3.320107	1.590268	-0.715914
C	-0.163982	-2.552949	2.437702
H	0.099217	-1.494868	2.522147
N	1.693463	1.127257	0.978756
N	1.818942	-1.022358	0.924982
C	3.439816	-2.176337	-1.217891
H	3.513533	-1.185926	-0.759709
C	1.143193	0.032130	0.341332
Ni	-0.121806	-0.041419	-1.048778
Si	-5.064147	-0.309508	-0.595685
C	-4.553103	1.499668	-1.029334
H	-5.164205	2.029849	-1.770815
H	-4.382289	2.182393	-0.187167

C	-1.917351	2.036931	2.144957
H	-2.436208	1.440055	2.905537
H	-2.470409	2.976232	2.021680
H	-1.948170	1.493927	1.194890
C	-0.389001	2.992549	3.942897
H	-0.894039	3.965592	3.932300
H	-0.878944	2.376299	4.706058
H	0.648395	3.158920	4.255319
C	4.453474	3.387176	-0.956759
H	5.255458	2.886474	-1.512151
H	4.363345	4.405012	-1.353877
H	4.764017	3.465415	0.091515
C	2.721380	2.454399	-2.572616
H	2.499023	3.428297	-3.025209
H	3.528486	1.990462	-3.152909
H	1.830287	1.823320	-2.654865
C	4.837800	-2.819931	-1.143345
H	4.860899	-3.802458	-1.628987
H	5.574213	-2.185213	-1.650337
H	5.162210	-2.953765	-0.104946
C	2.995574	-1.965022	-2.678239
H	3.740860	-1.372271	-3.222947
H	2.876158	-2.920294	-3.203791
H	2.039989	-1.430683	-2.708969
C	0.153521	-3.218342	3.791387
H	-0.419773	-2.741177	4.595219
H	-0.104853	-4.284007	3.786298
H	1.218240	-3.135483	4.038577
C	-1.670112	-2.618709	2.122026
H	-2.020714	-3.654638	2.038020
H	-2.246609	-2.137541	2.921435
H	-1.891089	-2.104592	1.181365
C	-5.228352	-0.711219	1.247280
H	-4.390988	-0.292574	1.816251
H	-6.158746	-0.299172	1.658267
H	-5.241251	-1.794679	1.418863
C	-6.561565	-0.999371	-1.527334
H	-6.513837	-0.747482	-2.592582
H	-6.611787	-2.092265	-1.444622
H	-7.498587	-0.594021	-1.124842
C	-3.274074	0.881848	-1.600957
C	-3.382171	-0.530093	-1.396592
C	-2.381211	-1.384287	-1.837662
C	-1.252127	-0.848451	-2.521926
C	-1.140738	0.567246	-2.704193
C	-2.169222	1.433857	-2.228570
H	-0.394167	0.968118	-3.387488
H	-2.090038	2.505828	-2.398947
H	-2.457996	-2.463013	-1.714089
H	-0.590633	-1.524714	-3.060623

cat9

B3LYP SCF energy:	-1969.03787564 a.u.
B3LYP enthalpy:	-1968.237195 a.u.
B3LYP free energy:	-1968.364874 a.u.

M06 SCF energy in solution: -1969.95603756 a.u.
M06 enthalpy in solution: -1969.155357 a.u.
M06 free energy in solution: -1969.283036 a.u.
Three lowest frequencies (cm-1): 10.0459 17.6872 20.5961

Cartesian coordinates

ATOM	X	Y	Z
C	0.288497	2.811084	0.582928
C	-0.814191	3.010901	1.438449
C	-1.677113	4.075437	1.150011
H	-2.541274	4.247570	1.785349
C	-1.447507	4.913449	0.061874
C	-0.340892	4.705328	-0.757036
C	0.553299	3.655156	-0.514281
H	-2.130546	5.733008	-0.146054
H	-0.167657	5.366724	-1.601294
C	2.281253	1.808867	1.708428
C	2.865223	0.586847	1.724229
H	2.533892	2.725894	2.217659
H	3.733582	0.219674	2.248724
C	2.419557	-1.615053	0.642699
C	1.806492	-2.594314	1.449932
C	2.145548	-3.933178	1.218386
H	1.687243	-4.710262	1.823738
C	3.058695	-4.285077	0.228112
C	3.653605	-3.297978	-0.553124
C	3.349819	-1.944014	-0.364053
H	3.308352	-5.330486	0.065793
H	4.365478	-3.581738	-1.323461
C	-1.098235	2.100321	2.628877
H	-0.240749	1.432807	2.754639
C	1.753137	3.451121	-1.433764
H	2.363069	2.644799	-1.016268
C	0.812389	-2.244622	2.552701
H	0.648747	-1.163890	2.528454
N	1.184919	1.715954	0.853366
N	2.113530	-0.227307	0.879522
C	4.020650	-0.888132	-1.237045
H	3.637174	0.091063	-0.936687
C	1.052706	0.451761	0.314723
Ni	-0.195788	-0.150731	-0.962096
Si	-4.791643	-1.454771	-0.614520
C	-4.103094	0.195200	-1.334509
H	-4.603931	0.600615	-2.223860
H	-3.932035	1.024801	-0.638184
C	-2.328232	1.211893	2.359163
H	-2.506521	0.538107	3.206575
H	-3.231846	1.816787	2.215285
H	-2.173529	0.604669	1.460841
C	-1.253816	2.891328	3.941529
H	-2.129025	3.550967	3.920473
H	-1.382721	2.202348	4.784596
H	-0.373004	3.512230	4.141654
C	2.641274	4.707989	-1.506320
H	3.527737	4.510092	-2.120543
H	2.111715	5.555662	-1.956616
H	2.979776	5.017455	-0.510801

C	1.305511	2.997873	-2.836897
H	0.670909	3.751771	-3.318594
H	2.177921	2.831353	-3.480857
H	0.740988	2.061564	-2.769293
C	5.547797	-0.870145	-1.029352
H	6.006768	-1.818748	-1.332295
H	6.005673	-0.073352	-1.627619
H	5.806471	-0.696646	0.021573
C	3.661827	-1.075269	-2.723364
H	4.115972	-0.280725	-3.327822
H	4.022762	-2.035808	-3.110031
H	2.576972	-1.036449	-2.863526
C	1.374995	-2.596563	3.944206
H	0.668447	-2.299149	4.728396
H	1.551155	-3.674087	4.046321
H	2.325954	-2.084939	4.133071
C	-0.555758	-2.910217	2.315222
H	-0.485865	-4.004101	2.353787
H	-1.267810	-2.596725	3.088382
H	-0.959613	-2.627093	1.338308
C	-5.180125	-1.504557	1.239016
H	-4.374519	-1.053951	1.828541
H	-6.107819	-0.961667	1.460780
H	-5.312252	-2.537308	1.585663
C	-6.246919	-2.210981	-1.563527
H	-6.078882	-2.167102	-2.645359
H	-6.394496	-3.263566	-1.291106
H	-7.181518	-1.679392	-1.343688
C	-2.847562	-0.619810	-1.652129
C	-3.073510	-1.924749	-1.187378
C	-2.106246	-2.937089	-1.393375
C	-0.932515	-2.618516	-2.056132
C	-0.684930	-1.298140	-2.547577
C	-1.661707	-0.266188	-2.355955
H	0.123639	-1.157931	-3.263391
H	-1.617133	0.665724	-2.918241
H	-2.276557	-3.955974	-1.051811
H	-0.184698	-3.387636	-2.237432

cat10

B3LYP SCF energy: -1969.03406420 a.u.
B3LYP enthalpy: -1968.233379 a.u.
B3LYP free energy: -1968.360004 a.u.
M06 SCF energy in solution: -1969.95510500 a.u.
M06 enthalpy in solution: -1969.154420 a.u.
M06 free energy in solution: -1969.281045 a.u.
Three lowest frequencies (cm-1): 10.3009 21.3155 28.1422

Cartesian coordinates

ATOM	X	Y	Z
C	-3.039775	0.245005	0.251692
C	-3.420997	-0.130788	1.555839
C	-4.484639	-1.032437	1.688161
H	-4.794892	-1.348329	2.680398
C	-5.153264	-1.527328	0.571498

C	-4.772902	-1.120942	-0.704979
C	-3.711337	-0.227432	-0.894784
H	-5.977619	-2.224738	0.696602
H	-5.308221	-1.503324	-1.569747
C	-2.109546	2.542495	-0.033317
C	-0.873296	3.068955	-0.197075
H	-3.081473	3.008653	0.011697
H	-0.545452	4.088498	-0.326850
C	1.443005	2.183219	-0.333436
C	2.212668	2.522944	0.798378
C	3.577688	2.771571	0.607533
H	4.195654	3.039240	1.460135
C	4.156173	2.680653	-0.656023
C	3.376252	2.333910	-1.755864
C	2.005121	2.080900	-1.622515
H	5.217488	2.877902	-0.782813
H	3.837180	2.262088	-2.737057
C	-2.727172	0.411405	2.801763
H	-1.978744	1.140748	2.479351
C	-3.339659	0.220412	-2.305470
H	-2.441789	0.840819	-2.236412
C	1.607981	2.636484	2.194453
H	0.564770	2.314027	2.135787
N	-1.944307	1.164530	0.083392
N	0.023555	2.001373	-0.175604
C	1.175197	1.729841	-2.852836
H	0.156102	1.514562	-2.520423
C	-0.615675	0.788841	-0.000268
Ni	0.043094	-0.962126	0.148075
Si	3.459678	-2.694298	0.620237
C	1.967298	-2.597584	1.836509
H	1.860169	-3.464990	2.502730
H	1.829171	-1.692155	2.436167
C	-1.975754	-0.699369	3.559082
H	-1.473923	-0.286215	4.442799
H	-2.658015	-1.487801	3.899781
H	-1.216666	-1.151749	2.912487
C	-3.716522	1.149733	3.724735
H	-4.479839	0.473869	4.128108
H	-3.183953	1.590817	4.575717
H	-4.234225	1.956350	3.192899
C	-4.456792	1.088726	-2.919296
H	-4.162121	1.445741	-3.913405
H	-5.388345	0.520854	-3.030543
H	-4.673882	1.963552	-2.295487
C	-2.995423	-0.967639	-3.222837
H	-3.851751	-1.639255	-3.357977
H	-2.702499	-0.604009	-4.215263
H	-2.164310	-1.547920	-2.811119
C	1.105127	2.916891	-3.833960
H	2.097602	3.176736	-4.221388
H	0.467825	2.667721	-4.690850
H	0.691374	3.810443	-3.352241
C	1.696651	0.458207	-3.547984
H	1.054289	0.204032	-4.399919
H	2.715657	0.593207	-3.930664
H	1.697696	-0.389989	-2.856226

C	1.616652	4.095324	2.692937
H	1.145073	4.166070	3.680413
H	2.639043	4.481754	2.782217
H	1.070266	4.755062	2.009175
C	2.309455	1.703125	3.198756
H	3.360423	1.977857	3.347431
H	1.812853	1.755800	4.175057
H	2.275615	0.664783	2.853296
C	4.579681	-1.179356	0.474933
H	5.229299	-1.089574	1.355260
H	5.228055	-1.253448	-0.407334
H	3.995530	-0.258280	0.385586
C	4.528741	-4.249807	0.787953
H	3.908770	-5.146343	0.899137
H	5.164504	-4.390378	-0.095188
H	5.188317	-4.183355	1.662586
C	1.079541	-2.693357	0.582781
C	1.980481	-2.854882	-0.529090
C	1.516863	-3.243272	-1.778934
C	0.131680	-3.458452	-1.954490
C	-0.757619	-3.296194	-0.894930
C	-0.318934	-2.921349	0.410347
H	-1.814867	-3.498549	-1.049198
H	-0.999425	-3.028508	1.253350
H	2.198238	-3.408046	-2.611237
H	-0.247500	-3.766543	-2.926305

CO_2

B3LYP SCF energy: -188.58094022 a.u.
B3LYP enthalpy: -188.565756 a.u.
B3LYP free energy: -188.590066 a.u.
M06 SCF energy in solution: -188.55865811 a.u.
M06 enthalpy in solution: -188.543474 a.u.
M06 free energy in solution: -188.567784 a.u.
Three lowest frequencies (cm-1): 640.0427 640.0427 1372.1017

Cartesian coordinates

ATOM	X	Y	Z
C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.169156
O	0.000000	0.000000	-1.169156

COD

B3LYP SCF energy: -312.02446468 a.u.
B3LYP enthalpy: -311.834904 a.u.
B3LYP free energy: -311.874798 a.u.
M06 SCF energy in solution: -311.86103147 a.u.
M06 enthalpy in solution: -311.671471 a.u.
M06 free energy in solution: -311.711365 a.u.
Three lowest frequencies (cm-1): 80.8844 228.6030 232.0403

Cartesian coordinates

ATOM	X	Y	Z

C	-1.214729	-1.236579	-0.495271
C	-1.923470	0.010237	-0.024405
C	-1.083733	1.107214	0.665448
C	-0.008736	1.704735	-0.218177
C	1.214772	1.236540	-0.495266
C	1.923467	-0.010289	-0.024368
C	1.083669	-1.107145	0.665602
C	0.008768	-1.704736	-0.218082
H	-1.821285	-1.842463	-1.170789
H	-2.425290	0.454962	-0.896781
H	-2.741458	-0.284451	0.653084
H	-0.666727	0.724176	1.600272
H	-1.772563	1.909322	0.959155
H	-0.292398	2.634953	-0.711658
H	1.821400	1.842428	-1.170719
H	2.425203	-0.455107	-0.896745
H	2.741518	0.284414	0.653040
H	0.666579	-0.723938	1.600316
H	1.772442	-1.909231	0.959505
H	0.292531	-2.634927	-0.711559

IPr

B3LYP SCF energy: -1160.03537450 a.u.
B3LYP enthalpy: -1159.432198 a.u.
B3LYP free energy: -1159.526495 a.u.
M06 SCF energy in solution: -1159.44812458 a.u.
M06 enthalpy in solution: -1158.844948 a.u.
M06 free energy in solution: -1158.939245 a.u.
Three lowest frequencies (cm-1): 9.9835 25.1019 32.2087

Cartesian coordinates

ATOM	X	Y	Z
C	-2.436669	-0.152485	0.106559
C	-2.972602	-1.413626	-0.228276
C	-4.311818	-1.464914	-0.631354
H	-4.753237	-2.419256	-0.901315
C	-5.091194	-0.311949	-0.691844
C	-4.539344	0.919834	-0.356868
C	-3.201573	1.027993	0.044942
H	-6.130316	-0.375323	-1.004646
H	-5.152618	1.815116	-0.413838
C	-0.675751	-0.045846	1.875018
C	0.675724	0.046424	1.875026
H	-1.385868	-0.094097	2.686710
H	1.385809	0.095014	2.686725
C	2.436702	0.152503	0.106586
C	3.201520	-1.028031	0.045011
C	4.539311	-0.919970	-0.356763
H	5.152518	-1.815299	-0.413727
C	5.091277	0.311775	-0.691686
C	4.311990	1.464803	-0.631214
C	2.972746	1.413608	-0.228226
H	6.130422	0.375075	-1.004427
H	4.753503	2.419121	-0.901108
N	-1.062626	-0.071573	0.532563

N	1.062643	0.071710	0.532578
C	0.000024	-0.000088	-0.337185
C	1.506888	2.927917	-1.603283
H	0.905486	2.068735	-1.916124
H	0.864699	3.817441	-1.586588
H	2.294622	3.093151	-2.348791
C	2.867862	3.916402	0.303428
H	3.652439	4.241072	-0.390013
H	2.169994	4.754480	0.413087
H	3.334611	3.733744	1.278073
C	2.116221	2.675727	-0.208288
H	1.283459	2.498396	0.480761
C	3.335097	-3.051215	1.572762
H	2.867417	-4.011427	1.820982
H	4.392642	-3.243312	1.356142
H	3.288816	-2.411711	2.461564
C	2.619408	-2.399108	0.374386
H	1.571088	-2.262373	0.653558
C	2.640903	-3.323903	-0.857940
H	2.093516	-2.874493	-1.692741
H	3.664992	-3.525555	-1.194000
H	2.173186	-4.287024	-0.620258
C	-1.507060	-2.928177	-1.603374
H	-0.905817	-2.069000	-1.916538
H	-0.864777	-3.817631	-1.586642
H	-2.294964	-3.093651	-2.348648
C	-2.116022	-2.675699	-0.208271
H	-1.283062	-2.498148	0.480477
C	-2.867457	-3.916258	0.304021
H	-3.652252	-4.241172	-0.389057
H	-2.169527	-4.754283	0.413708
H	-3.333897	-3.733326	1.278764
C	-2.641442	3.324076	-0.857845
H	-2.173780	4.287215	-0.620127
H	-2.094179	2.874846	-1.692827
H	-3.665616	3.525676	-1.193674
C	-2.619568	2.399118	0.374342
H	-1.571164	2.262487	0.653256
C	-3.335092	3.050947	1.572969
H	-2.867546	4.011223	1.821197
H	-4.392728	3.242846	1.356622
H	-3.288468	2.411344	2.461682