Supporting Information

Neutral and Cationic Methallyl Nickel Complexes in Alkene Activation: A Combined DFT, ESI-MS and Chemometric Approach

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Experimental

All manipulations were performed under an inert atmosphere using standard glovebox and Schlenk-line techniques. All reagents were used as received from Aldrich, unless otherwise specified. Toluene and pentane were distilled from benzophenone ketyl, CH_2Cl_2 was distilled under nitrogen over calcium hydride and chlorobenzene was dried over 4Å molecular sieves, fractionally distilled under reduced pressure, and stored under a nitrogen atmosphere. Chemical shifts are given in parts per million relative to TMS [^{1}H and ^{13}C, $\delta(SiMe_4) = 0$] or an external standard [δ ($BF_3{\cdot}OEt_2$) = 0 for ^{11}B NMR, $\delta(C_6H_5CF_3) = 0$ for ^{19}F NMR]. NMR assignments were supported by additional 2D experiments. Infrared spectroscopy: Bruker Vector 22 FT-IR - infrared spectroscopy spectrometer. For X-ray crystal structure analysis, data sets were collected with a Bruker D8 Venture diffractometer by Dr. Constantin G. Daniliuc; full details can be found in the independently deposited crystallography information files (cif). Graphics show thermal ellipsoids at the 50% probability level. Results of the oligomerization reactions were assessed by GC for reaction mixture composition. Gas chromatography of oligomeric products was conducted on a GC Perkin Elmer equipment, model Clarus 680 with Phenomenex column model Zebron ZB-5MS and MS detector model Clarus SQ8T.

Electrospray Ionization Mass Spectrometry (ESI-MS) was applied to identify the catalytically active species, which are responsible for the alkene isomerization. The catalyst (1 equiv) and few drops of alkene of interest, in anhydrous and degassed toluene (5.0 mL), were mixed with anhydrous and degassed solution of $B(C_6F_5)_3$ (5-15 equiv) under Ar atmosphere using a dual-syringe pump operating at a flow rate of 1 μL-100 mL/min in an effective micromixer, that was coupled directly to the ion source of the mass spectrometer. The solution was fed continuously into the MS and the flow rate could be varied from 2.0 to 100 μL/min. By connecting the microreactor directly to the spray capillary, reaction times from 0.3 s to min could be covered. ESI-MS and ESI-MS/MS analyses were conducted in a Bruker Daltonics AmaZon SL ion trap mass spectrometer (Bruker Daltonics, Bremen, Germany). The ESI source and the mass spectrometer were operated in the positive-ion mode, and the capillary voltage and drying gas temperature set to +4.0 kV and 220 °C, respectively, with a scan range of *m/z* 70-2000. Drying gas flow and nebulizing gas pressure were set to 5.0 L/min and 8.0 psi, respectively. MS/MS experiments were carried out by mass selection of a specific ion in the ion trap, which was then submitted to collision-induced dissociation (CID) with helium (He) in the collision chamber.

Mass Spectrometry Experiments. MS/MS experiments were carried out by mass selection of a specific ion in the ion-trap, which was then submitted to collision-induced dissociation (CID) with helium (He) in the collision chamber.

Computational Methods

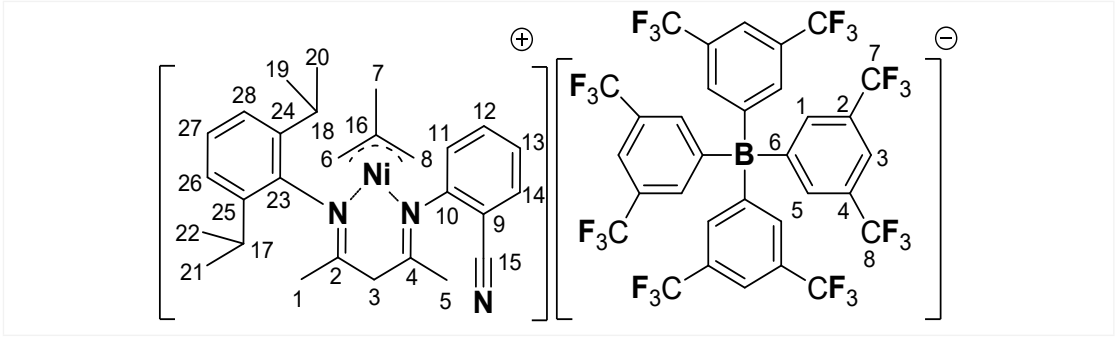
All geometry optimizations were performed with the Gaussian 09 software package[1] using the M06-L functional[2] and a mixed basis set of LANL2DZ[3] for Ni and 6-31G(d,p)[4] for other atoms. Dichloromethane was adopted as solvent (ε=8.93) using the PCM solvation model.[5] Frequency calculations were performed for each stationary point, confirming that each optimized structure is a local minimum or transition state. Gibb's free energy profile in the solution includes thermal corrections at standard conditions (298.15 K, 1 atm, and 1mol/L). Distortion-interaction/activation-strain model[6] and the second-generation energy decomposition analysis (EDA) based on absolutely localized molecular orbitals (ALMO-EDA)[7] calculations were performed in Q-Chem 5.2[8] to decompose the computed activation energy ($\Delta E^{\ddagger}$) of the rate-determining transition states of the cationic and neutral species. $\Delta E^{\ddagger}$ was decomposed into the distortion (ΔE_{dist}) and interaction (ΔE_{int}) energy terms between the reactive fragments of Ni-catalyst and the ethylene monomer using the distortion-interaction/activation-strain model ($\Delta E^{\ddagger} = \Delta E_{dist} + \Delta E_{int}$). ΔE_{dist} energy for each reactive fragment was calculated from the energy difference between the distorted fragment with their transition state geometry and the fully optimized ground state geometry of the same fragment. In contrast, ΔE_{int} is calculated from the differences between the activation energy and the distortion energy terms. Then, ΔE_{int} was further decomposed using the ALMO-EDA method ($\Delta E_{dist} = \Delta E_{PAULI} + \Delta E_{CT} + \Delta E_{ELEC} + \Delta E_{POL} + \Delta E_{DISP}$), in terms of Pauli repulsion (ΔE_{PAULI}), charge transfer (ΔE_{CT}), electrostatic (ΔE_{ELEC}), polarization (ΔE_{POL}), and dispersion (ΔE_{DISP}) energy differences. Specifically, in the overall activation energy, the sum between the distortion energy (ΔE_{dist}) and Pauli repulsion (ΔE_{PAULI}) corresponds to destabilizing terms and thus the description of steric effects. Charge transfer (ΔE_{CT}), electrostatic (ΔE_{ELEC}), and polarization (ΔE_{POL}) correspond to the contribution of stereoelectronic effects. Orbital interaction ($\Delta E_{CT} + \Delta E_{POL}$) is associated to the inter- fragment (ΔE_{CT}) and intra-fragment (ΔE_{POL}) interactions between the occupied and vacant orbitals of each reactive fragment, while the electrostatic contribution (ΔE_{ELEC}) is associated to Coulombic interactions between the reactive fragments. Therefore, the overall activation energy ($\Delta E^{\ddagger}$) is decomposed into contributions from steric, stereoelectronic and not least dispersive effects as shown in Figure S13 in the Supporting Information.

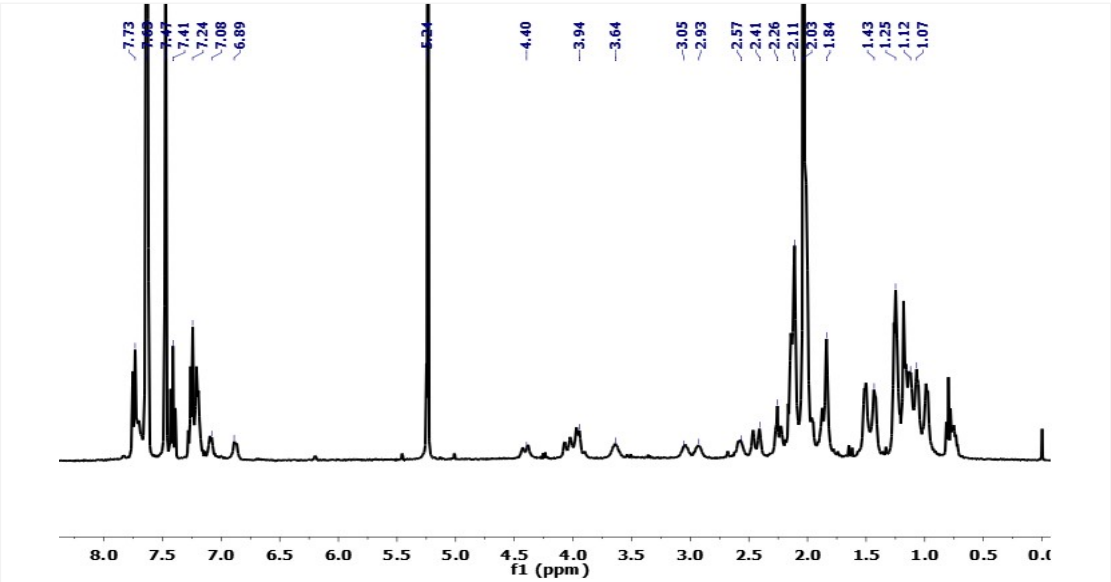
Chemometric analysis

134 descriptors were calculated using PaDEL-Descriptor software.[9] The most relevant descriptors were selected with the correlation-based method implemented in Weka[10] software and 9 of them were retained for clustering analysis. To explore and compare catalysts in catalyst map and show the contribution of selected descriptors, principal component analysis (PCA)[11] was conducted using the FactoMineR and factoextra packages in R environment (version 4.0.2).[12] In addition, a hierarchical clustering heatmap (HCH) was generated to visualize changes in the descriptors levels for each group of catalysts, using the Euclidean distance measure and the Ward clustering algorithm in the MetaboAnalyst 4.0 webserver.[13] In both PCA and HCH, data were scaled to unit variance.

[2-((4-((2,6-diisopropylphenyl)imino)pentan-2-ylidene)amino)benzonitrile κ^2N,N'] (η^3- methallyl)nickel (II) [tetrakis(3,5-bis(trifluoromethyl)phenyl)borate)] (1)

$Na[B(ArF)_4]$ (sodium-tetrakis(3,5-bis(trifluoromethyl)phenyl)borate (49 mg; 56 μmol)) and methallyl nickel chloride dimer (8.4 mg; 28 μmol) were dissolved in dry dichloromethane. The suspension was stirred and 2-((4-((2,6-diisopropylphenyl)imino)pentan-2-ylidene)amino)benzonitrile (20 mg; 56 μmol) was added. The mixture was stirred for 12 hours at room temperature. The resulting suspension was filtered through celite and dried in *vacuo*. The obtained yellow solid was washed with pentane and dried. Yield of **1**: 71 % (53 mg; 40 μmol). Single crystals for X-ray crystallography were grown by slow diffusion from dichloromethane-pentane at -30 °C.





^{1}H NMR (400 MHz, CD_2Cl_2, 299 K)

^{1}H NMR (400 MHz, 299 K, CD_2Cl_2) δ/ppm = 1.07 (m, 6H, CH_3 of iPr), 1.12 (m, 6H, CH_3 of iPr), 1.25 (m, 6H, CH_3 of iPr), 1.43 (m, 6H, CH_3 of iPr), 1.84 (m, 3H, allyl-CH_3), 2.03 (m, 9H, 2 × H_1, H_5), 2.11 (m, 6H, H_5, allyl-CH_3), 2.26 (m, 2H, =CH_2), 2.41 (m, 2H, =CH_2), 2.57 (bs, 1H, C*H* of iPr), 2.93 (bs, 1H, C*H* of iPr), 3.05 (bs, 1H, C*H* of iPr), 3.64 (bs, 1H, C*H* of iPr), 3.94 (m, 3H, 3 × H_3), 4.40 (d, 1H, H_3, $^{2}J_{HH}$ = 18 Hz), 6.89 (d, 1H, Ar-H_{11}, $^{3}J_{HH}$ = 7.4 Hz), 7.08 (d, 1H, Ar-H_{11}, $^{3}J_{HH}$ = 7.6 Hz), 7.24 (m, 2 × 3H, Ar-$H_{26\text{-}28}$), 7.41 (t, 2 ×1H, Ar-H_{12}, $^{3}J_{HH}$ = 7.5 Hz), 7.73 (m, 2 ×1H, Ar-H_{13}, 2 ×1H, Ar-H_{14}). Tetrakis (3,5-bis(trifluoromethyl) phenyl)borate: 7.47 (s, 16H, 2 × H_1, *p*-Ar), 7.63 (bs, 8H, 2 × H_1, *o*-Ar).

^{13}C {^{1}H} NMR (100.6 MHz, 299 K, CD_2Cl_2) δ/ppm = 23.08 (allyl-*C*H_3), 23.89 (*C*H_3 of iPr), 23.93 (*C*H_3 of iPr), 23.44 (*C*H_3 of iPr), 23.13 (*C*H_3 of iPr), 25.30 (allyl-*C*H_3), 28.82 (C_1, C_5), 31.21 (C_1, C_5), 48.37 (C_3), 60.94 (allyl=*C*H_2), 100.14 (Ar-*C*H), 123.79 (Ar-*C*), 125.04 (Ar-*C*H of Ph^{diiPr}), 126.53 (Ar-*C*), 128.14 (Ar-*C*H of Ph^{diiPr}), 128.88 (Ar-C_{12}), 129.30 (Ar-*C*), 214.96 (Ar-$C_{2,\ 4}$). Tetrakis (3, 5-bis(trifluoromethyl) phenyl)borate: 118.09 (Ar-C_3), 129.55 (Ar-*C*), 129.61 (Ar-*C*), 135.38 (Ar-$C_{1,\ 5}$).

GCOSY (400 MHz / 400 MHz, CD_2Cl_2, 299 K) δ (^{1}H)/ δ (^{1}H) /ppm = 1.07/ 2.57 (CH_3 of iPr/ C*H* of iPr), 1.12/ 2.93 (CH_3 of iPr/ C*H* of iPr), 1.25/ 3.05 (CH_3 of iPr/ C*H* of iPr), 1.43/ 3.64 (CH_3 of iPr/ C*H* of iPr), 2.57/ 1.07 (C*H* of iPr /CH_3 of iPr), 2.93/ 1.12 (C*H* of iPr/ CH_3 of iPr), 3.05/ 1.25 (C*H* of iPr/ CH_3 of iPr), 3.64/ 1.43 (C*H* of iPr/ CH_3 of iPr), 3.94/ 4.40 (H_3/ H_3), 4.40/ 3.94 (H_3/ H_3), 7.41/ 7.73 (Ar-H_{12}/ Ar-H_{13}), 7.73/ 7.41 (Ar-H_{13}/ Ar-H_{12}).

^{1}H, ^{13}C-HMQC (400 MHz / 100.6 MHz, CD_2Cl_2, 299 K): δ (^{1}H)/ δ (^{13}C) /ppm = 1.07/ 23.89 (CH_3 of iPr/ *C*H_3 of iPr), 1.12/ 23.93 (CH_3 of iPr/ *C*H_3 of iPr), 1.25/ 23.44 (CH_3 of iPr/ *C*H_3 of iPr), 1.43/ 23.13 (CH_3 of iPr/ *C*H_3 of iPr), 1.84/ 23.08

(allyl-CH_3/ CH_3 of iPr), 2.03/ 28.82, 31.21 (2 × H_1, H_5/ C_1, C_5), 2.11/ 25.30 (allyl-CH_3/ allyl-CH_3), 3.94/ 48.37 (3 × H_3/ C_3), 7.24/ 125.04, 128.14 (2 × 3H, Ar-$H_{26\text{-}28}$/ Ar-CH of Ph^{diiPr}), 7.41/ 128.88 (Ar-H_{12}/ Ar-C_{12}). Tetrakis (3,5-bis(trifluoromethyl) phenyl)borate: 7.47/ 135.38 (2 × H_1, *p*-Ar/ Ar-$C_{1,5}$), 7.63/ 118.09, (2 × H_1, *o*-Ar/ Ar-$C_{1,5}$),

^{1}H, ^{13}C-HMBC (400 MHz / 100.6 MHz, CD_2Cl_2, 299 K): δ (^{1}H)/ δ (^{13}C) /ppm = 2.03/ 214.96 (2 × H_1, H_5/ Ar-$C_{2,4}$), 6.89/ 128.88 (Ar-H_{11}/ Ar-C_{12}). Tetrakis (3,5-bis(trifluoromethyl) phenyl)borate: 7.47/ 135.38 (2 × H_1, *p*-Ar/ Ar-C_3), 7.63/ 118.09, 135.38 (2 × H_1, *o*-Ar/ Ar-C_3, Ar-$C_{1,5}$).

^{19}F NMR (470 MHz, CD_2Cl_2, 299 K): δ/ ppm = s, -62.9

^{11}B NMR (160 MHz, CD_2Cl_2, 299 K): δ/ ppm = s, -6.6

ESI-MS: *m/z* calculated (for $[C_{28}H_{36}N_3Ni]^+$) 472.2, found 472.5; *m/z* calculated (for $[C_{32}H_{12}BF_{24}]^-$) 863.1, found 863.3 (see Figure S1).

IR (KBr) $\tilde{\nu}$/cm^{-1}: 2231 (ν (C≡N), s) (see Figure S2).

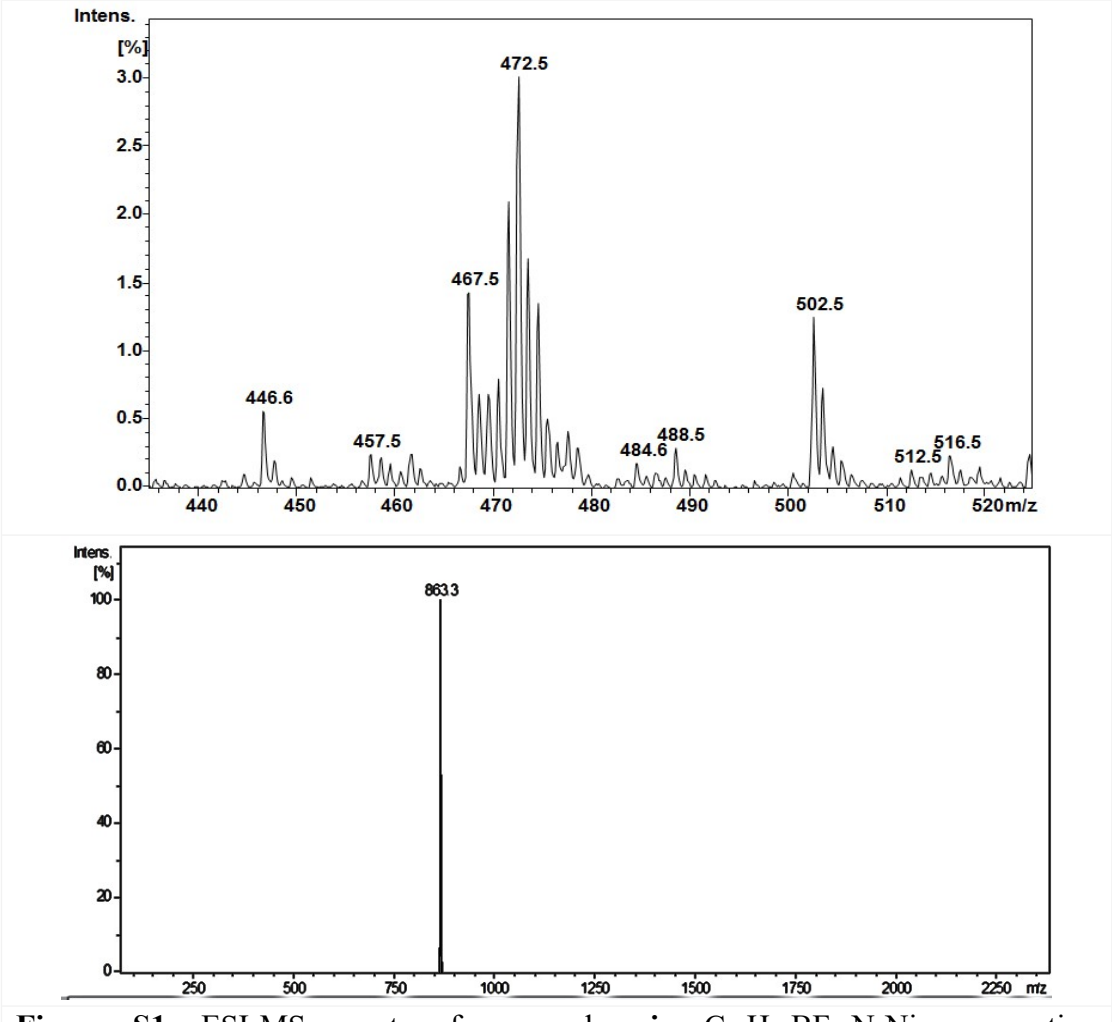


Figure S1. ESI-MS spectra for complex **i$_1$**, $C_{60}H_{48}BF_{24}N_3Ni$, see cation

$C_{28}H_{36}N_3Ni^+$ above (positive mode) and anion $C_{32}H_{12}BF_{24}^-$ below (negative mode).

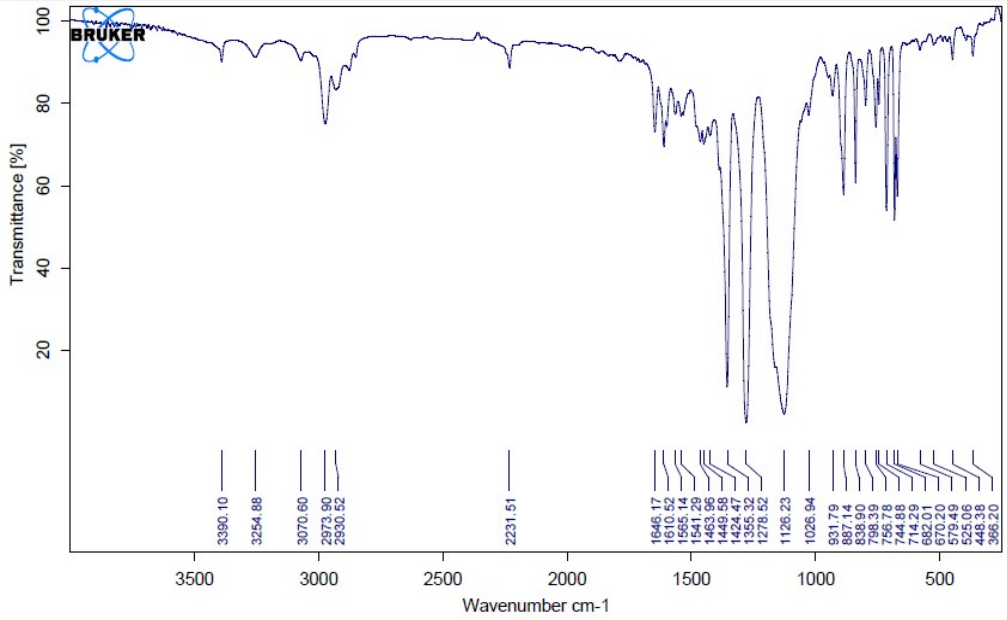


Figure S2. IR (KBr) spectra of nickel complex $\mathbf{i_1}$.

X-ray crystal structure of $\mathbf{i_1}$.

Crystals of $\mathbf{i_1}$ suitable for X-ray crystallography were grown from a solution (-30 °C), by layering pentane into dichloromethane under an inert atmosphere and the results of these studies are shown in Figure S3, Figure S4 and Figure S5. Analyzing the crystal structure of complex $\mathbf{i_1}$ it would be very interesting compare it with the structure of its isomer neutral nickel complex $\mathbf{g_1}$[14] (see Figure S3). The crystal structure of $\mathbf{i_1}$ confirms a four coordinate nickel, which adopts a slightly distorted square-planar geometry, the dihedral angle N1-C41A-C43-N2 is 4.4(1)º for nickel complex $\mathbf{g_1}$ the respective dihedral angle N1-C6-C8-N2 is -5.0(0)º, so for both complexes surrounding of Ni is almost square planar. Ni-N bond lengths in methallyl complex $\mathbf{i_1}$ are 1.922(6) and 1.941(5) Å and are within the range of typical bond lengths for *NN* coordination in methallyl nickel complexes.[15] Diketiminate ligand in complex $\mathbf{g_1}$ adopts a conformation with the vector of the cyano group *trans* with respect to the methyl group of methallyl see Figure S3, while in nickel complex $\mathbf{g_1}$ the vector of the cyano group remains *cis* with respect to the methyl group of methallyl (see Figure S4). Both aromatic rings of compound i**1** are rotated out of the central plane, thus dihedral angles Ni1-N2-C31-C32 and Ni1-N1-C11-C12 are -94.5(3) and 96.5(3)º respectively. Ni-N bond lengths are slightly larger for the cationic system $\mathbf{i_1}$ compared to the neutral nickel system $\mathbf{g_1}$, the values of these distances are 1.941(5) for Ni1-N1, 1.922(6) for Ni1-N2 and 1.913(3) for Ni1-N2, 1.903(2) for Ni1-N1 respectively (see Table S1). On the contrary the values of Ni-$C_{methallyl}$ bond lengths are larger for the neutral nickel system i**1** (see Table S1), but with the same trend of bond length rising from Ni-allyl*C*H_2 nearby $Ar_{diisopropyl}$ (see bond lengths for Ni-C41A and Ni1-C7 in Table S1) to Ni-allyl*C*H_2 nearby Ar-*CN* (see bond lengths for Ni1-C43 and Ni1-C8 in Table S1). In general, Ni-$C_{methallyl}$

bond lengths of $\mathbf{i_1}$ are within the range of 2.001(5) - 2.015(11) Å that is usual for η^3-methallyl ligated nickel complexes.[15]

Ni1-C2 distance is a bit larger for cationic methallyl nickel complex **1**, where is observed a deviation of the ligand from planarity to a boat-shaped arrangement (see Figures S3-S5).

It is worth to mention that in a case of compound $\mathbf{i_1}$ C2 carbon atom is sp^3 hybridized, while in nickel complex $\mathbf{g_1}$ atom C2 has sp^2 hybridization, which is represented in respective values of C5-C3-C2-C1 and C4-C1-C2-C3 dihedral angles, see Table S1. Thus, while in nickel complex $\mathbf{g_1}$ metal center lies in the same plane with diketiminate ligand core atoms; in cationic nickel complex $\mathbf{i_1}$ these atoms are out of the central plane forming the boat conformation (see Figure S4).

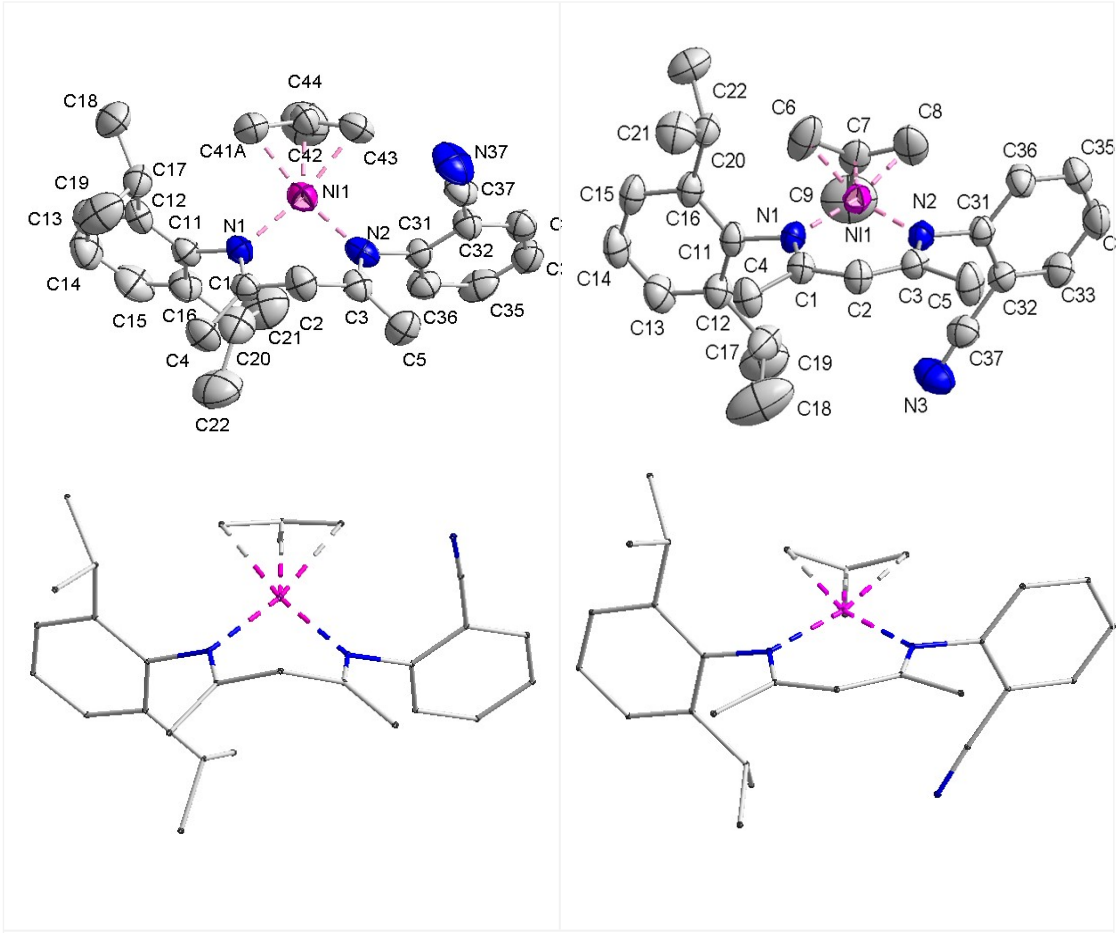


Figure S3. X-ray crystal structure of nickel complex $\mathbf{i_1}$ (left above) and nickel complex $\mathbf{g_1}$ (right above) with thermal ellipsoids drawn at the 50% probability level and their respective wire projections (see left below for $\mathbf{i_1}$ and right below for $\mathbf{g_1}$)

Table S1. Selected bond lengths, distances (Å) and angles (deg) for nickel complex $\mathbf{i_1}$ and $\mathbf{g_1}$.

Selected bond lengths (Å) and angles (deg)	Neutral Ni methallyl complex $\mathbf{g_1}$	Cationic Ni methallyl complex $\mathbf{i_1}$
Ni-N1	1.941(5)	1.903(2)
Ni-N2	1.922(6)	1.913(3)
Ni-C41A	2.001(14)	-
Ni-C42	2.004(12)	-
Ni-C43	2.015(11)	-
Ni-C2	3.0530(1)	3.2048(1)
Ni1-C7	-	2.008(3)
Ni1-C6	-	2.015(4)
Ni1-C8	-	2.029(4)
C5-C3-C2-C1	-131.4(2)	169.7(1)
C4-C1-C2-C3	124.2(3)	-174.4(1)

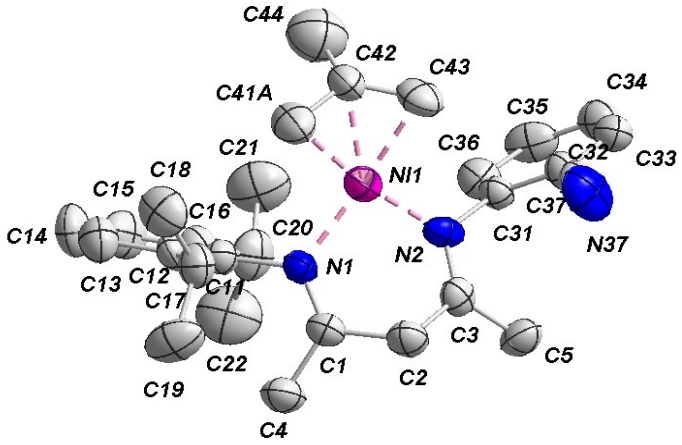


Figure S4. X-ray crystal structure of $\mathbf{i_1}$ with thermal ellipsoids drawn at the 50% probability level. Hydrogen atoms and the $[B(ArF)_4]^-$ counterion are omitted for clarity. Selected bond lengths (Å) and angles (deg): Ni1-N1 1.941(5), Ni1-N2 1.922(6), Ni1-C42 2.004(12), Ni1-C41A 2.001(14), Ni1-C43 2.015(11), N1-Ni1-N2 92.0(2), N1-C41A-C43-N2 4.4(1), N2-C31-C32 -94.5(3), Ni1-N1-C11-C12 96.5(3).

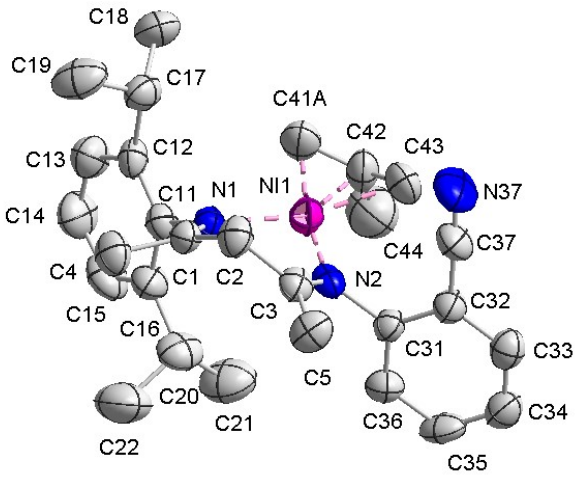


Figure S5. X-ray crystal structure of $\mathbf{g_1}$ with thermal ellipsoids drawn at the 50% probability level. Hydrogen atoms and the $[B(ArF)_4]^-$ counterion are omitted for clarity. Selected angles (deg): N2-C3-C2-C1 49.5(9), N1-C1-C2-C3 -55.6(9).

X-ray crystal structure analysis of $\mathbf{i_1}$: formula $C_{60}H_{48}BF_{24}N_3Ni$, M = 1336.53, orange crystal, 0.45 x 0.10 x 0.02 mm, a = 12.6058(3), b = 36.2340(8), c = 13.4322(4) Å, α = 90.000, β = 91.713(1), γ = 90.000°, V = 6132.50(3) Å^3, ρ_{calc} = 1.448 gcm^{-3}, μ = 0.430 mm^{-1}, Z = 4, monoclinic, space group P21/n (No. 14), λ = 0.71073 Å, T = -50 °C, 44301 reflections collected, data measured (±h, ±k, ±l), 10535 independent reflections and 5243 observed reflections, 1058 refined parameters, R = 0.092, Rw^2 = 0.187 internal consistency.

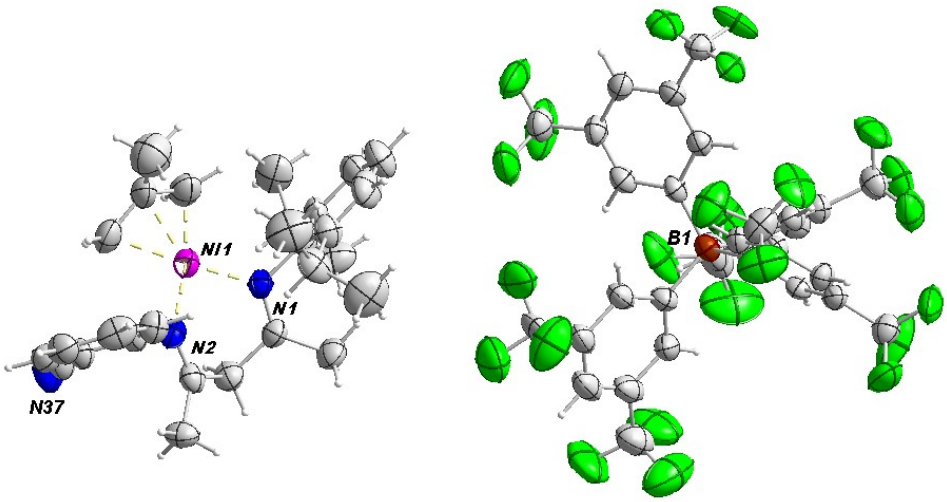


Figure S6. X-ray crystal structure of $\mathbf{i_1}$ with thermal ellipsoids drawn at the 50% probability level.

General procedure of ethylene oligomerization in a Parr Reactor.

Reactions were carried out in a Parr autoclave reactor (100 mL), loaded inside a glovebox with an appropriate amount ([Ni] = 3.4 x 10^{-4} M) of the catalyst and co-activator ($B(C_6F_5)_3$) and solvent such that the final volume of the solution was 22 mL. The reactor was sealed inside the glovebox. The reactor was attached to an ethylene line, and the gas was fed continuously into the reactor to the pressure of 12.5 bar. The pressurized reaction mixture was stirred at the corresponding temperature during 20 min. After that time, the reactor was cooled to -30 ºC, the ethylene gas was vented and the reaction mixture was analyzed through Gas Chromatography (GC).

Gas Chromatography (GC).

Instrument conditions:

Injection volume: 2.0 µl
Sampling rate: 12.5000 pts/s
Run time: 24.75 min
Initial temperature: 25 °C
Initial hold: 0.00 min
Ramp 1: 1.0/min to 35 °, hold for 5.00 min
Ramp 2: 20.0 0/min to 150 °, hold for 4.00 min
Maximum temperature: 300°C
Equilibration time: 0.5 min
Solvent: CH_2Cl_2
Column: ZB-5MS (0.25 mm-i.d. x 0.25 µm film thickness). Column length: 30 meter column length was used for measurements with heptane standard

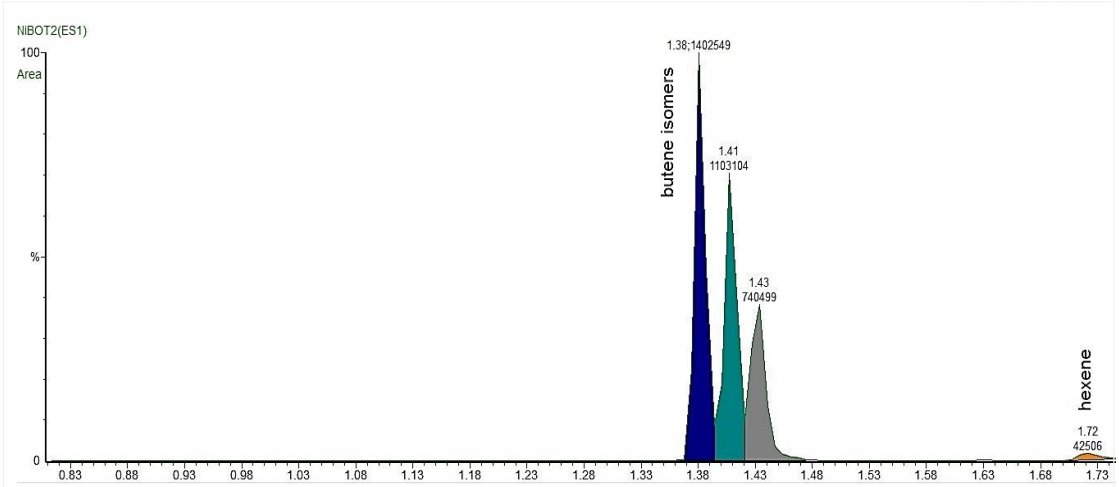


Figure S7. Representative GC spectrum of oligomer products (1.38-1.43 min butene isomers, 1.72 min hexene) formed during catalysis with nickel complex $\mathbf{i_1}$ and 4 equiv. of $B(C_6F_5)_3$ at 20 °C (column length 30 meters)

Table S2. Selected ethylene oligomerization reactions with complex $\mathbf{i_1}$.[a]

Entry [b]	$B(C_6F_5)_3$ co-activator (equiv)	T (°C)	Product (%)[c]		C_4 : 1-C_4H_8/ 2-trans/ 2-cis	TON (mol product /mol Ni)	TOF h^{-1}
			C_4	C_6			
1	1	20	100	n. d.	80/12/8	2	6
2	4	20	99	1	43/34/22	111	336

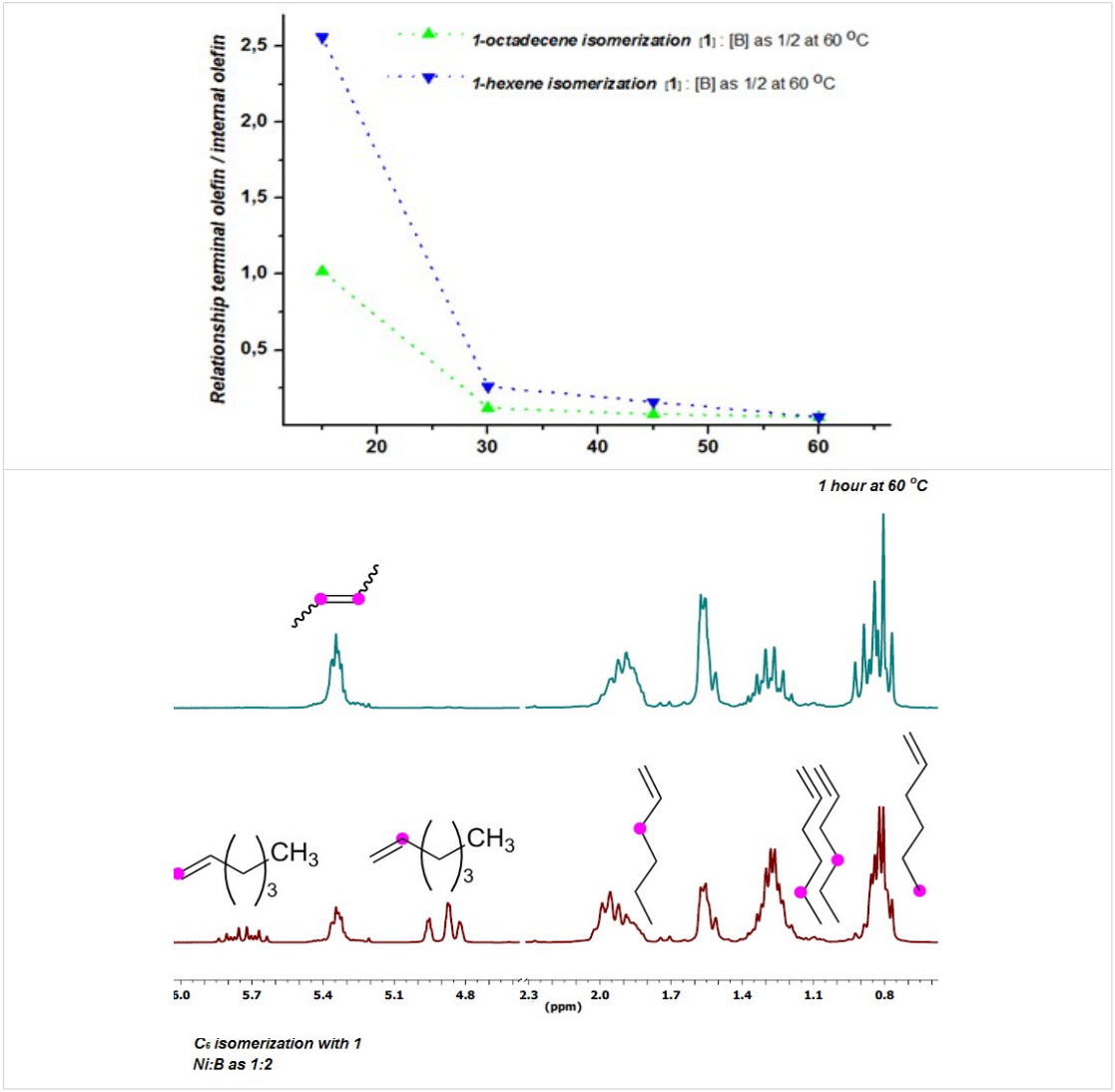
[a] Entries 1-2 were carried out in a Parr autoclave reactor in 22 mL of CH_2Cl_2 at an ethylene pressure of 12.5 bar, reaction time, 20 min. [b][Ni] = 3.4×10^{-4} M. [c]Determined by combined gas chromatography (GC).

^{1}H NMR studies of ethylene oligomerization (a) and of 1-hexene and 1-octadecene isomerization (b)

(a) Nickel complex (8 μmol from stock solution) (with 1 equiv. of $B(C_6F_5)_3$ (8 μmol) from stock solution) was dissolved in $CDCl_3$ and added into an NMR tube with J. Young valve inside a glovebox. The cell was brought out from the box and assembled on a Schlenk line. The cell was frozen, and the nitrogen gas was evacuated. Ethylene gas was charged through the Schlenk

line, and the J. Young valve was closed. NMR tube was brought out from the glove box and ^{1}H NMR spectra were recorded during that time.

(b) Nickel complex (8 µmol) (with 2 equiv. of $B(C_6F_5)_3$ or $BF_3{*}OEt_2$, 16 µmol) was dissolved in $CDCl_3$ (600 µl) and added into an NMR tube with J. Young valve inside a glovebox. 1-hexene (50 µl, 404 µmol) or 1-octadecene (50 µl, 156 µmol) was added dropwise by microsyringe into the NMR tube. NMR tube was brought out from the box and heated during 1 hour in oil bath at 60^o C. ^{1}H NMR spectra were recorded during that time.



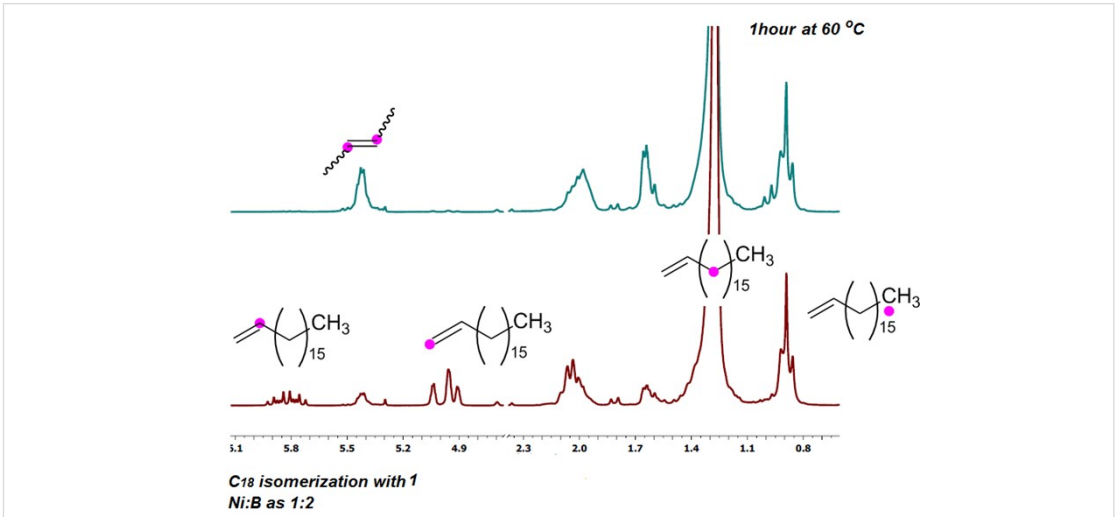
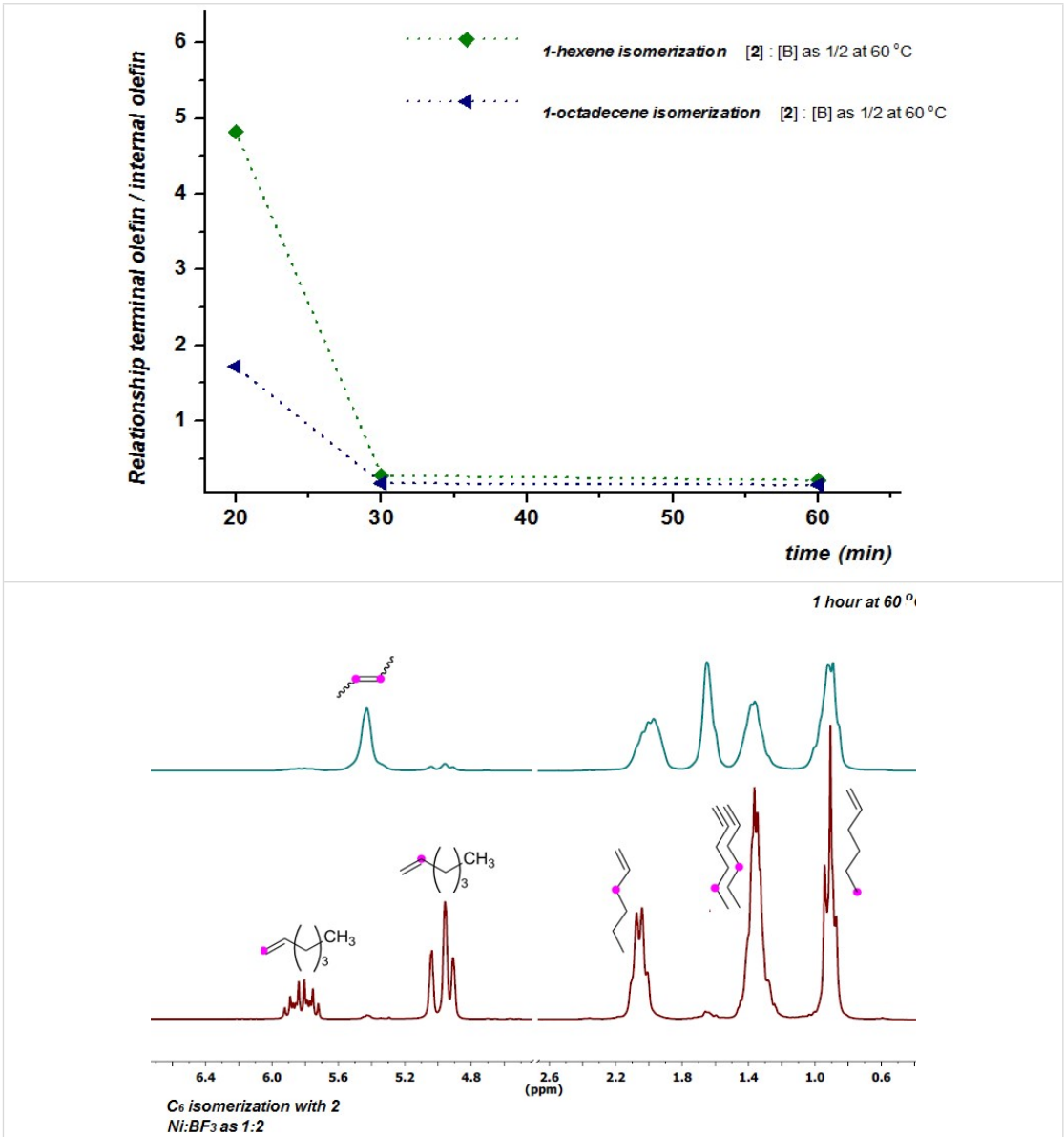


Figure S8. 1-hexene and 1-octadecene isomerization by $\mathbf{i_1}$ (as **1**)



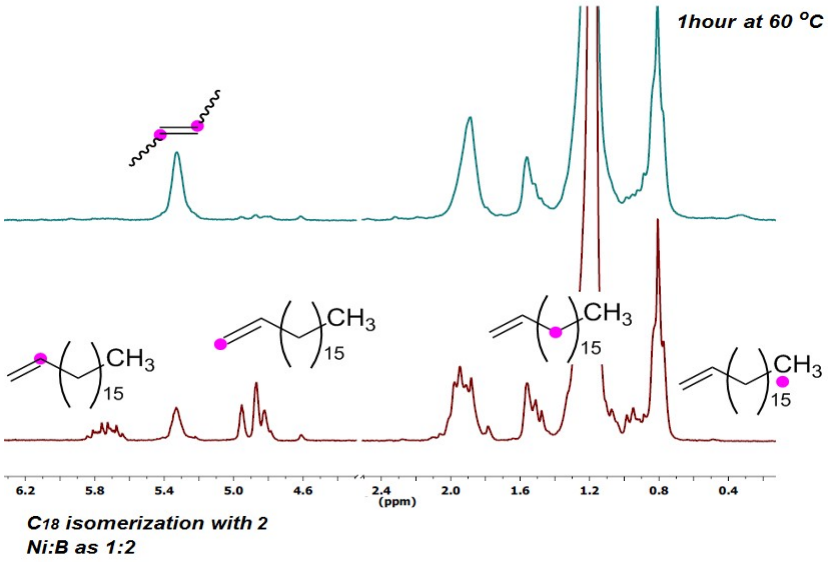


Figure S9. 1-hexene and 1-octadecene isomerization by $\mathbf{g_1}$ (as **2**)

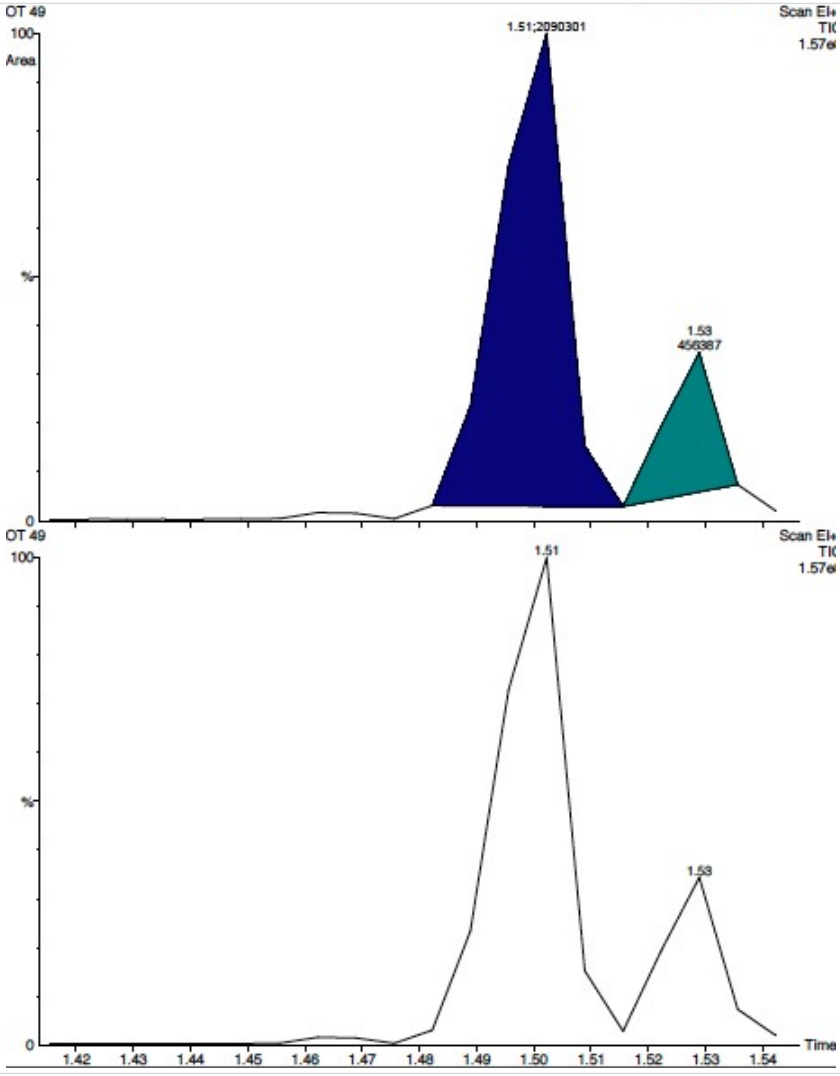


Figure S10. Representative GC spectrum of hexene isomers (1.51-1.53 min) formed during catalysis with nickel complex $\mathbf{g_1}$ and 2 equiv. of BF_3 at 60 °C (for isomerization conditions see page S13).

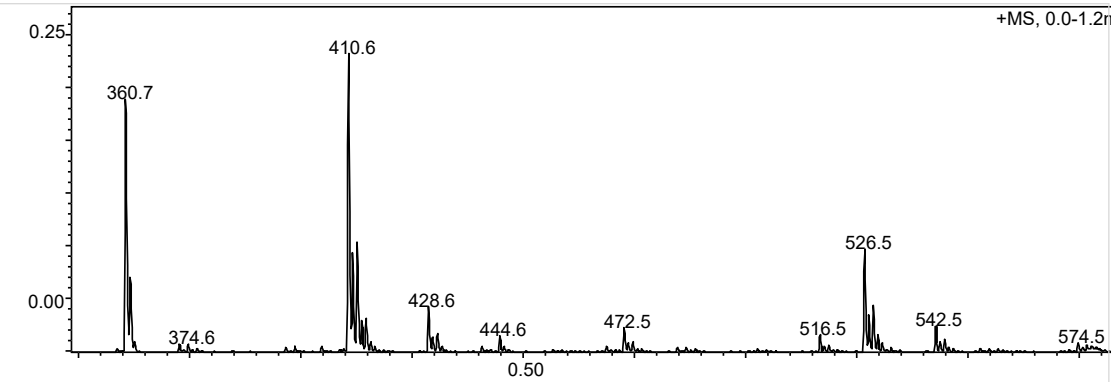


Figure S11. *In situ* ESI-MS monitoring of 1-hexene isomerization: $\mathbf{g_1}/B(C_6F_5)_3$ heated for several minutes at 60 °C.

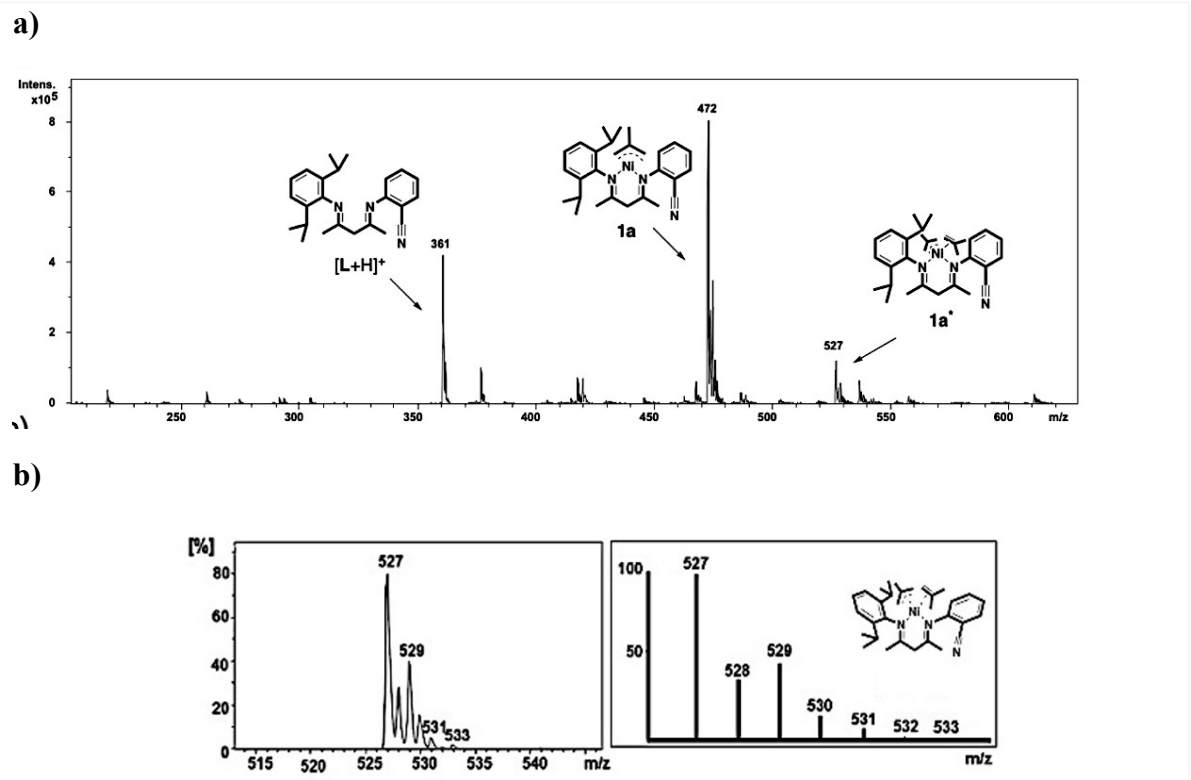


Figure S12. *In situ* ESI-MS monitoring of 1-hexene isomerization: $\mathbf{i_1}/B(C_6F_5)_3$, seconds (**a**); theoretical isotopic pattern for the ion of m/z 527 that matched for the suggested species **1a*** (**b**).

Table S3. List of 9 relevant descriptors used in PCA

Descriptor	Description
nN	Number of nitrogen atoms
Mse	Mean atomic Sanderson electronegativities (scaled on carbon atom)
Mpe	Mean atomic Pauling electronegativities (scaled on carbon atom)
Mare	Mean atomic Allred-Rochow electronegativities (scaled on carbon atom)
Mi	Mean first ionization potentials (scaled on carbon atom)
nAtomLAC	Number of atoms in the longest aliphatic chain
nTRing	Number of rings (includes counts from fused rings)
RotBFrac	Fraction of rotatable bonds, excluding terminal bonds
RotBtFrac	Fraction of rotatable bonds, including terminal bonds

Energy decomposition analysis of the rate-determining transition states in the $\mathbf{i_1}$/B(C_6F_5)$_3$ and $\mathbf{g_1}$/B(C_6F_5)$_3$ species

Our DFT calculations indicated that in the $\mathbf{i_1}$ and $\mathbf{g_1}$ catalysts co-catalyzed by B(C_6F_5)$_3$, the first ethylene insertion rate-determining step is the first. To further explore the nature of the transition states' reactivity associated with the first ethylene insertion into each species, we performed the distortion-interaction/activation-strain analysis shown in Figure S13. The results indicate that activation energies are mainly associated with the distortion energy (ΔE_{dist}) since the interaction energy (ΔE_{int}) between the Ni-catalyst catalyst and the ethylene monomer is almost the same for both catalysts. Interestingly, both transition state structures differ in the arrangement of the six-membered diketiminate chelate ring. $\mathbf{i_1}$**-TS** adopts a destabilizing energy boat conformation.

In contrast, $\mathbf{g_1}$**-TS** adopts a slightly distorted square-planar geometry. As a result, the aromatic rings with $Ar_{diisopropyl}$ and Ar_{CN} substituents in each transition state of the structure adopt different orientations and create distinct steric environments around the nickel center. For example, in $\mathbf{i_1}$**-TS**, both aromatic rings with $Ar_{diisopropyl}$ and Ar_{CN} substituents are placed close to the nickel center (Figure S13a). In contrast, in the geometry of the $\mathbf{g_1}$**-TS**, the aromatic ring with $Ar_{diisopropyl}$ substituents placed to the nickel center, while the aromatic ring with Ar_{CN} substituent is placed in proximity from the nickel center (Figure S13b). For more in-depth, we applied the energy decomposition analysis to decompose the interaction energy according to Figure S13 in terms of Pauli repulsion (ΔE_{PAULI}), charge transfer (ΔE_{CT}), electrostatic (ΔE_{ELEC}), polarization (ΔE_{POL}), and dispersion (ΔE_{DISP}) energy differences. We found that the $\mathbf{i_1}$**-TS** is the disfavored geometry mainly attributed to the Pauli repulsion (ΔE_{PAULI}) but is compensated by more substantial attractive stereoelectronic effects ($\Delta E_{ELEC} + \Delta E_{CT} + \Delta E_{POL}$). However, the sum of the stabilizing effects (stereoelectronic and dispersion effects) into the activation energy is lower than the destabilizing or steric effects (see Figure S13),

thus indicating that these factors are not determinant rationalizing the different reactivity between both catalysts. Therefore, the significant positive steric effects represent the major factor between the Ni-catalyst and the ethylene interaction for both rate-determining transition states' reactivity. This reactivity trend was successfully reproduced by the percent buried volume descriptor ($\%V_{bur}$)[16] to compare both catalytic species' ligand steric properties. The $\%V_{Bur}$ indicates the fraction of a sphere's volume centered on the metal of a catalytic species occupied by their ligands. **i_1-TS** has a more significant $\%V_{Bur}$ than the **g_1-TS** (49% versus 46%), which indicates that the nickel center in the cationic catalytic species is more hindered than in the neutral one.

DFT calculations suggest that the origin of both species' catalytic activity is mainly attributed to steric repulsion effects. In addition, the chelate ring conformation might affect the complex's symmetry, providing a suitable explanation for these complexes' different experimental activities and selectivities.

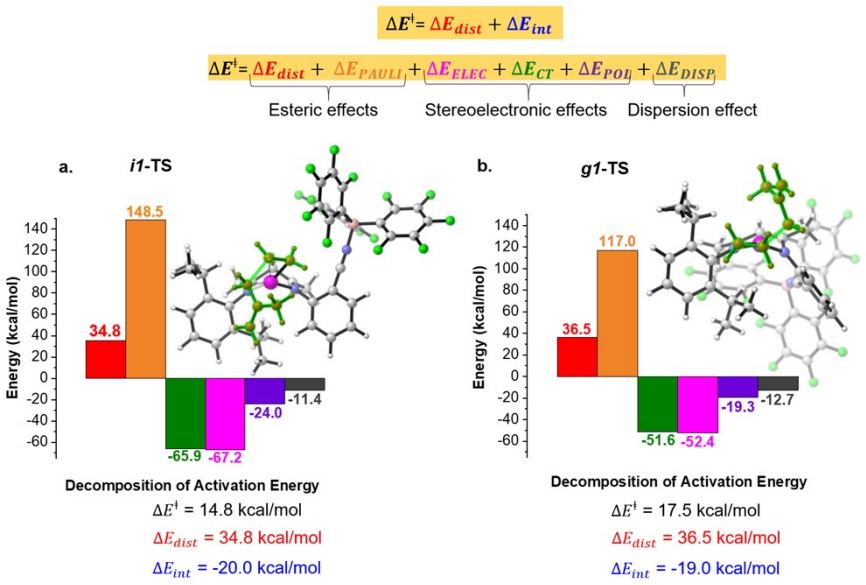


Figure S13. Decomposition of the activation energy of the cationic the **i_1**/$B(C_6F_5)_3$ (a) and neutral the **g_1**/$B(C_6F_5)_3$. (b) rate-determining transition states in terms of the distortion-interaction/activation-strain and ALMO-EDA energy decomposition analysis. The activation energy is decomposed in steric, stereoelectronic, and dispersion effects between the Ni-catalyst and the ethylene monomer in each catalytic species.

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Cartesian coordinates of located key structures

1a

SCF energy: -3630.1188089 a.u.
Enthalpy: -3629.31743 a.u.
Gibbs free energy: -3629.472987 a.u.

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I-1b

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Enthalpy: -3707. 846325 a.u.

Gibbs free energy: -3708. 011728 a.u.

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H	0.56857700	4.04734400	0.15368900

H	-0.25212100	3.45645700	1.68520000
C	1.84554500	2.95543100	1.49861200
H	1.95364600	2.65115700	2.53616300
H	2.76796000	3.19434100	0.97465800
C	-0.86347407	2.98536259	3.39346774
N	-0.02755327	3.66516821	3.70723939
B	0.80553490	4.94162205	4.16973408
H	-5.29380914	1.57521327	2.89207621
C	2.32530442	4.64903219	3.70155494
C	2.90690212	3.41676009	3.99323479
C	3.15871264	5.56831187	3.06986032
C	4.21369793	3.08539205	3.66145812
C	4.47547854	5.28244337	2.72579512
C	5.00487131	4.03064423	3.01850031
C	0.74776639	5.05418592	5.77944224
C	1.50372640	6.07276622	6.35907491
C	0.07836253	4.23139124	6.67711120
C	1.62092649	6.26232810	7.72899813
C	0.17337674	4.37846116	8.05731137
C	0.95022066	5.39924852	8.58818694
C	-0.01304798	6.08678221	3.34954788
C	-0.89862602	6.99959843	3.92041945
C	0.04565850	6.12180398	1.95363957
C	-1.62592784	7.92012044	3.17041006
C	-0.66411828	7.01940392	1.16872661
C	-1.51300669	7.93129353	1.78795105
F	6.25905165	3.73771932	2.68812211
F	5.22852698	6.19654647	2.11444469
F	4.70940652	1.88052862	3.95024220
F	2.17774388	2.47465918	4.63258297
F	2.71028761	6.79461807	2.76499229
F	0.80471371	5.22161675	1.30078054
F	-0.57019727	6.99539815	-0.16116010
F	-2.23311331	8.78032917	1.06027929
F	-2.49708938	8.74066098	3.77095985
F	-1.14131768	7.00752516	5.24249652
F	2.14307366	6.94206102	5.55949132
F	2.35916138	7.25316007	8.22295304
F	1.04227134	5.55381182	9.90652427
F	-0.47989883	3.54989153	8.88182105
F	-0.72733165	3.22657646	6.23889185
H	2.49084700	0.85552300	3.17243800
C	-0.35977300	0.47857900	-1.19408700
H	-1.40558000	0.18027100	-1.16131600

H	0.37654500	-0.31337000	-1.28094900
H	-1.22926900	2.83316500	-2.85038800
H	-3.61363075	3.10808360	3.85425316

TS-1b

SCF energy: -3708. 6790102 a.u.

Enthalpy: -3707. 819401 a.u.

Gibbs free energy: -3707. 978867 a.u.

Ni	0.77112900	1.59653700	1.10133400
N	0.02808900	0.54740500	2.56780400
N	2.11573500	-0.00776400	0.75978300
C	-1.46884300	2.95996000	-1.05490800
H	-2.37194200	2.52507600	-1.49241100
H	-1.66940400	3.15562700	0.00654600
C	0.46594400	-1.08401100	4.39565700
H	1.15669200	-1.93114800	4.33162500
H	-0.55428000	-1.45344900	4.28788600
H	0.58304800	-0.67650000	5.40654100
C	0.83500200	-0.07148100	3.36937700
C	2.29626400	0.20143600	3.14147100
H	2.90235200	-0.19040600	3.96163600
C	2.72229300	-0.41452700	1.81912400
C	3.78134600	-1.45948100	1.88652800
H	3.51892000	-2.22103300	2.62921400
H	4.71699300	-1.00963800	2.23886900
H	3.95826400	-1.94095200	0.92430400
C	-1.38754900	0.47020900	2.63802700
C	-2.01999660	1.23719229	3.61420060
C	-3.40527654	1.13611326	3.78090005
C	-3.52138087	-0.51455868	2.04308163
H	-4.09161486	-1.21277708	1.43979372
C	-2.14153875	-0.42381545	1.86818684
C	2.40169000	-0.63467700	-0.49885700
C	1.52595900	-1.65819400	-0.91870100
C	1.79866600	-2.28768400	-2.13186900
H	1.14580300	-3.08341800	-2.47908200
C	2.88312400	-1.89986500	-2.91378200
C	3.69826400	-0.85614800	-2.50108000
H	4.53032800	-0.54369300	-3.12744500
C	3.47706400	-0.19460700	-1.28795700
C	-0.29079600	2.05407300	-1.24817400
C	1.04397300	2.50351700	-0.77768300
H	1.38869600	3.41147700	-1.27142200

H	1.83320500	1.75950500	-0.92013800
C	0.31615700	-2.02464500	-0.08200700
H	0.01001500	-1.09824400	0.42882400
C	4.38809600	0.94779400	-0.87722100
H	3.95368600	1.43015700	0.01227400
C	-0.87187600	-2.51286200	-0.90153800
H	-0.68306500	-3.48994800	-1.35772200
H	-1.75079600	-2.63187100	-0.26332000
H	-1.13626900	-1.81785700	-1.70593200
C	0.65416300	-3.05004000	1.00176500
H	-0.22726700	-3.27415300	1.61264100
C	4.49353400	2.00777000	-1.97441900
H	5.01052600	1.61643800	-2.85614100
C	-4.17086713	0.26567624	2.98925101
H	3.51242700	2.36059000	-2.30623700
H	5.06717400	2.87039700	-1.62321100
C	5.78510200	0.44230700	-0.51256900
H	6.42575700	1.26520600	-0.18262300
H	0.99202000	-3.99071600	0.55487800
H	1.45040700	-2.70695300	1.67059200
H	5.76514500	-0.30986800	0.28080100
H	6.26478200	-0.01917600	-1.38206300
H	3.07936500	-2.40285700	-3.85558800
H	-1.64597002	-1.07367760	1.15345337
C	0.25016300	3.22827900	1.97115400
H	-0.82668700	3.38092100	2.05201100
H	0.77338400	3.19248700	2.92705200
C	0.93065900	3.72185700	0.81618800
H	1.97423700	4.01593400	0.91115800
H	0.36035300	4.39949100	0.18836800
C	-1.62485578	2.19345942	4.58673180
N	-1.30314691	2.97201634	5.37853030
B	-0.77755946	4.04089837	6.43132816
H	-5.24412422	0.20277262	3.13170686
C	-2.05107899	4.44292645	7.34740769
C	-3.29279067	4.68303909	6.76083188
C	-1.99435234	4.66138595	8.72312201
C	-4.41967932	5.07588311	7.47032531
C	-3.09593630	5.06321945	9.47196129
C	-4.31892214	5.26606702	8.84306830
C	-0.28575858	5.34321321	5.59833907
C	0.38309987	6.33846483	6.31114779
C	-0.49570476	5.62684710	4.25329738
C	0.84594652	7.51680171	5.74317998

C	-0.03989597	6.78910987	3.63794121
C	0.63391836	7.74295554	4.38649773
C	0.40290363	3.17688459	7.15390058
C	1.76406017	3.29573305	6.87468215
C	0.08046247	2.13783014	8.03237653
C	2.73915583	2.47509512	7.43542445
C	1.02104083	1.31261216	8.63583583
C	2.36681516	1.48232778	8.33079236
F	-5.38336558	5.63689960	9.54856633
F	-2.98970490	5.24801474	10.78720212
F	-5.58492387	5.26932546	6.84828499
F	-3.44307049	4.52861058	5.42441314
F	-0.84956326	4.47724051	9.39706783
F	-1.20731641	1.87740394	8.31273225
F	0.64497673	0.34153649	9.46901425
F	3.28257806	0.66904405	8.85285089
F	4.01920040	2.61208112	7.08359958
F	2.21711014	4.19570591	5.98023774
F	0.62906939	6.14424260	7.61779199
F	1.49514488	8.42017141	6.47512404
F	1.07604523	8.85839652	3.81119572
F	-0.24408332	6.98285071	2.33010948
F	-1.15737474	4.76335470	3.44671959
H	2.45222900	1.28713800	3.08553100
C	-0.41210100	0.88507800	-1.90521800
H	-1.36412800	0.57047300	-2.32606700
H	0.44506300	0.24798400	-2.09883500
H	-1.31045800	3.93607800	-1.53046400
H	-3.88990778	1.73293069	4.52510535

βH-1b

SCF energy: -3708. 7102423 a.u.

Enthalpy: -3707.852608 a.u.

Gibbs free energy: -3708. 019473 a.u.

Ni	0.60456000	1.20528000	2.25519600
N	-0.09633300	-0.25809600	3.28826400
N	1.94603600	0.06680300	1.40006300
C	-1.51153000	5.26332900	-1.06228400
H	-2.15191200	6.14473800	-1.00128200
H	-0.69603700	5.48617900	-1.76059700
C	0.29713700	-2.13487500	4.83715300
H	0.49007000	-3.15628500	4.49355100
H	-0.74654700	-2.05321500	5.13785800

H	0.93140300	-1.98598100	5.72086200
C	0.70758500	-1.13525900	3.81423800
C	2.16169400	-1.17742500	3.42481500
H	2.57763000	-2.13047100	3.76281100
C	2.45014400	-0.97369100	1.95894300
C	3.27371700	-2.00212700	1.26782500
H	2.70675800	-2.93971900	1.20352500
H	4.17715200	-2.22933800	1.84227800
H	3.55194500	-1.69670400	0.25812900
C	-1.50672400	-0.44423700	3.42956400
C	-2.29163800	0.32430500	4.31224800
C	-3.68514200	0.15124000	4.37195500
C	-3.51972800	-1.56773200	2.70172100
H	-3.99121100	-2.31493500	2.07072400
C	-2.13880400	-1.39812200	2.63809200
C	2.11887400	0.36045000	0.00427400
C	1.23324100	-0.21386200	-0.92328600
C	1.36667300	0.16463200	-2.26162900
H	0.69395900	-0.26074100	-3.00189800
C	2.33244000	1.07963700	-2.65682300
C	3.17616800	1.65362900	-1.71210300
H	3.91773100	2.38031100	-2.03036800
C	3.08325000	1.31931100	-0.36024300
C	-0.98319600	4.86643400	0.27943200
C	-0.10173600	3.64491600	0.26339500
H	0.73596000	3.80985200	-0.42949500
H	-0.65888200	2.79814100	-0.16809800
C	0.09941900	-1.12904500	-0.50457400
H	0.30768400	-1.49802200	0.51073200
C	3.99139100	1.94533300	0.67999400
H	3.43520700	1.97200900	1.62975700
C	-1.20439900	-0.32848000	-0.44242400
H	-1.40302100	0.16434100	-1.39998500
H	-2.06220700	-0.97053500	-0.21727400
H	-1.15647500	0.45338600	0.33007500
C	-0.04413900	-2.34866200	-1.40991600
H	-0.80745100	-3.02964200	-1.02091800
C	4.38729700	3.37848500	0.34684500
H	5.02459900	3.43206300	-0.54086200
C	-4.29617400	-0.79129900	3.56077900
H	3.51307800	4.01449200	0.17193500
H	4.95466100	3.81170700	1.17311300
C	5.23625900	1.08858600	0.91761600
H	5.88355000	1.55080100	1.66787900

H	-0.35318700	-2.07147600	-2.42213900
H	0.89456500	-2.90435400	-1.49369500
H	4.98434600	0.08416000	1.27317600
H	5.81367900	0.97758400	-0.00613600
H	2.42216600	1.35605300	-3.70287700
H	-1.53651400	-1.99563200	1.95862700
C	-0.58039400	2.66316300	2.56744700
H	-1.58516000	2.49570200	2.16764800
H	-0.58767600	3.05707900	3.58174100
C	0.41027400	3.25574100	1.64088100
H	1.28074900	2.50404600	1.43376400
H	1.00215900	4.04850500	2.11303100
C	-1.69831500	1.28912400	5.14704800
N	-1.26680800	2.13171100	5.81103600
B	-0.51287000	3.40488400	6.39518700
H	-5.37158800	-0.92291000	3.60035700
C	-0.73545800	3.38630700	7.98956200
C	-2.03190400	3.25114200	8.48081100
C	0.25632200	3.56678600	8.94848200
C	-2.34603700	3.27599000	9.83219500
C	-0.01313500	3.60493200	10.31327300
C	-1.32234700	3.45531500	10.75687800
C	-1.21046900	4.71336000	5.74251500
C	-0.63878200	5.94446800	6.06506500
C	-2.34565800	4.78134000	4.93891800
C	-1.11656300	7.16133500	5.60125300
C	-2.86032300	5.97863100	4.45094900
C	-2.24033700	7.17517100	4.77972300
C	0.98606800	3.04602600	5.84546700
C	1.68194900	3.71992700	4.84414700
C	1.56366200	1.83799100	6.24165100
C	2.84494200	3.22682200	4.25320800
C	2.72918200	1.32286700	5.69668900
C	3.36817200	2.01297900	4.67273900
F	-1.59891200	3.48334800	12.05673100
F	0.97202600	3.77917000	11.19331400
F	-3.60403700	3.12809900	10.24808000
F	-3.05261100	3.08460300	7.60925600
F	1.53852700	3.71672900	8.57776700
F	0.94464000	1.06605200	7.15301300
F	3.20259900	0.12863300	6.08939600
F	4.44800200	1.49094200	4.08213000
F	3.43520500	3.90599300	3.26478000
F	1.23271800	4.87566400	4.32733100

F	0.46532300	5.95688800	6.83333000
F	-0.51718900	8.30518400	5.92341500
F	-2.70737600	8.32379000	4.30054000
F	-3.92378800	5.97766400	3.64373000
F	-3.01006200	3.66569300	4.55490900
H	2.71859400	-0.41658600	3.98310000
C	-1.26938900	5.55275500	1.39142000
H	-1.91193500	6.42774800	1.35460900
H	-0.88019300	5.28997500	2.37223900
H	-2.09195600	4.45209600	-1.51810100
H	-4.26007400	0.76595200	5.05737300

$TS_{\beta H}$-1b

SCF energy: -3708.6959339 a.u.

Enthalpy: -3707. 844073 a.u.

Gibbs free energy: -3708. 0098 a.u.

Ni	0.64484600	1.27633500	2.19301300
N	-0.10190400	-0.21067900	3.24268200
N	1.96006300	0.09991300	1.37212600
C	-1.43175700	5.22171000	-1.19755600
H	-2.09450100	6.08859700	-1.20154200
H	-0.55956500	5.46035100	-1.81747100
C	0.28856900	-2.06634000	4.82285500
H	0.47998600	-3.08849200	4.47991800
H	-0.75483800	-1.98498000	5.12469700
H	0.92600300	-1.91826600	5.70409200
C	0.69815000	-1.07310700	3.79319000
C	2.15742700	-1.10896800	3.42021500
H	2.58197400	-2.04888900	3.78280200
C	2.45324900	-0.93367400	1.95414600
C	3.26763000	-1.98321600	1.28367600
H	2.68940000	-2.91488400	1.23558200
H	4.16613000	-2.21012500	1.86579700
H	3.55251700	-1.70134800	0.26920400
C	-1.51135100	-0.39458500	3.39574300
C	-2.28356100	0.34263700	4.31668900
C	-3.67748700	0.17206000	4.38635100
C	-3.53807700	-1.48444800	2.65294500
H	-4.01909000	-2.20789700	2.00178000
C	-2.15746800	-1.31668300	2.57859700
C	2.15573500	0.36531900	-0.02849000
C	1.26655900	-0.20260500	-0.95483400
C	1.42065500	0.15390500	-2.29725400
H	0.74440800	-0.26607900	-3.03747200

C	2.41220400	1.03896200	-2.69641500
C	3.26389300	1.60261800	-1.75239600
H	4.02933900	2.30314800	-2.07359000
C	3.15012900	1.29058700	-0.39703800
C	-1.02250600	4.84472400	0.19042500
C	-0.13595600	3.62309500	0.26626400
H	0.73937400	3.76243600	-0.38315500
H	-0.67350400	2.76196600	-0.15933000
C	0.11180200	-1.09086600	-0.53488000
H	0.30122600	-1.44365400	0.48982100
C	4.06864900	1.90547700	0.64034700
H	3.52196000	1.92745300	1.59428200
C	-1.18107400	-0.27127800	-0.50502100
H	-1.35263900	0.21925600	-1.46894300
H	-2.05317900	-0.89907000	-0.29486200
H	-1.13779900	0.51315600	0.26494000
C	-0.03693700	-2.32517500	-1.41946600
H	-0.81835200	-2.98606600	-1.03131400
C	4.46286700	3.34138900	0.31724800
H	5.09246700	3.40576100	-0.57527600
C	-4.30180200	-0.73757100	3.54890000
H	3.58633200	3.97834300	0.15702600
H	5.03597400	3.76614900	1.14459800
C	5.31248600	1.04232600	0.85805200
H	5.96087300	1.48480700	1.61929400
H	-0.32315200	-2.06237600	-2.44215000
H	0.89360100	-2.89775800	-1.47612700
H	5.05884700	0.02878200	1.18568200
H	5.89094800	0.95253000	-0.06752700
H	2.51826300	1.29788700	-3.74546200
H	-1.56545800	-1.89408900	1.87339600
C	-0.62997500	2.68446600	2.58128000
H	-1.62196300	2.42011400	2.20658400
H	-0.59653300	2.99627800	3.62105000
C	0.28708700	3.31640200	1.68014700
H	1.40273400	2.36771500	1.50044800
H	0.95298600	4.06085100	2.12489000
C	-1.68098900	1.28507400	5.17081000
N	-1.24004700	2.12070300	5.83791700
B	-0.49021100	3.40392100	6.41197100
H	-5.37710500	-0.86711200	3.59677700
C	-0.69162700	3.37900500	8.00935200
C	-1.98013300	3.22724900	8.51671700
C	0.31007900	3.56218000	8.95743700

C	-2.27757400	3.23686300	9.87218800
C	0.05748700	3.58549400	10.32558400
C	-1.24400200	3.41802200	10.78538300
C	-1.20834600	4.70714800	5.76974900
C	-0.65255600	5.94174200	6.10737100
C	-2.34169200	4.77138000	4.96364700
C	-1.14887300	7.15857000	5.66390600
C	-2.87182500	5.96848700	4.49073000
C	-2.27255300	7.16930700	4.84233700
C	1.00573700	3.06681500	5.84203900
C	1.68175500	3.75528300	4.83657500
C	1.60715200	1.86827400	6.23014900
C	2.84871000	3.28436600	4.23547500
C	2.78004900	1.37762300	5.67860500
C	3.40015500	2.08251200	4.65269500
F	-1.50229800	3.43040800	12.08925300
F	1.05232000	3.76172500	11.19414900
F	-3.52908200	3.07204200	10.30122500
F	-3.01080600	3.05796000	7.65734300
F	1.58636200	3.72839800	8.57359500
F	1.00826000	1.08447600	7.14523100
F	3.27582400	0.18983200	6.06251900
F	4.48531900	1.58285900	4.05331200
F	3.41020100	3.96808200	3.23367300
F	1.20667500	4.90337300	4.32543800
F	0.45445500	5.95945700	6.87116700
F	-0.56619200	8.30549900	6.00438400
F	-2.76132000	8.31939700	4.39013500
F	-3.93238300	5.96353700	3.67933200
F	-2.99055300	3.65195400	4.56206300
H	2.69644100	-0.32728000	3.96676200
C	-1.41531000	5.53266800	1.26780400
H	-2.06495200	6.39807500	1.17384500
H	-1.10897200	5.27621300	2.27922100
H	-1.94910300	4.39544600	-1.69977300
H	-4.24195300	0.76371100	5.10022800

$P_{\beta H}$-1b

SCF energy: -3708. 7027557 a.u.

Enthalpy: -3707. 848294 a.u.

Gibbs free energy: -3708.011494 a.u.

Ni	0.33045000	1.38311600	2.31636800
N	-0.15123200	-0.33123900	3.40755900
N	1.80167200	0.29397400	1.39833000

C	0.01229300	5.15333100	-1.69850100
H	-0.01414500	6.21705500	-1.94138800
H	0.92708400	4.72565900	-2.12916700
C	0.46349900	-2.31562800	4.73819500
H	0.64037800	-3.27738400	4.24458100
H	-0.54781400	-2.30759500	5.14332600
H	1.18132800	-2.26444100	5.56546500
C	0.73674000	-1.18311400	3.80979700
C	2.17085100	-1.06193200	3.35680600
H	2.68028900	-1.99850900	3.59904100
C	2.39000400	-0.73285600	1.90164100
C	3.28896800	-1.65851100	1.15574300
H	2.82559800	-2.65060000	1.09088400
H	4.22606500	-1.79743700	1.70490700
H	3.50893300	-1.30773000	0.14720500
C	-1.53228200	-0.61126900	3.58238100
C	-2.35679500	0.19216500	4.39835800
C	-3.74205200	-0.03439600	4.46905400
C	-3.49734100	-1.85777600	2.92189700
H	-3.93710100	-2.66162200	2.33961200
C	-2.12442800	-1.63977500	2.85082300
C	1.90931600	0.56908400	-0.00858100
C	1.06279800	-0.11177300	-0.90100800
C	1.15274000	0.21976800	-2.25596200
H	0.50913700	-0.29261700	-2.96760300
C	2.04604500	1.18239600	-2.70577600
C	2.84896400	1.86144400	-1.79564400
H	3.52591100	2.63328700	-2.15027100
C	2.78408700	1.58703800	-0.42817800
C	-0.04651600	4.91487700	-0.22341300
C	-0.05963900	3.45561500	0.17156100
H	0.67880800	2.93056100	-0.44789400
H	-1.02946100	3.00601800	-0.09256800
C	0.04357200	-1.14348400	-0.45499400
H	0.13038600	-1.26975500	0.63390600
C	3.59896600	2.37078500	0.57924000
H	3.03720800	2.35227500	1.52546400
C	-1.37865600	-0.66146500	-0.74260800
H	-1.53529900	-0.50551000	-1.81473500
H	-2.12092900	-1.39222900	-0.40467000
H	-1.59429600	0.29249500	-0.24410200
C	0.28912200	-2.50340300	-1.10737700
H	-0.41284700	-3.25287600	-0.72765000
C	3.77769900	3.83244600	0.18308900

H	4.39296900	3.93891200	-0.71558200
C	-4.30916400	-1.05724500	3.72558900
H	2.81779500	4.32696600	-0.00713500
H	4.28325400	4.38251200	0.97927300
C	4.95089600	1.71002100	0.85054700
H	5.51394800	2.27580100	1.59839000
H	0.15039500	-2.45220300	-2.19184400
H	1.30521000	-2.86788600	-0.92978800
H	4.83993400	0.68667500	1.22548100
H	5.55251600	1.66417700	-0.06316400
H	2.10869100	1.41427000	-3.76441900
H	-1.49852300	-2.25282100	2.20685900
C	-0.78172200	2.99159800	2.57946000
H	-1.82156700	2.91059600	2.26464800
H	-0.63655700	3.28257000	3.61706400
C	0.22860400	3.24453800	1.62437000
H	-0.68986600	1.08584600	1.39498500
H	1.16303500	3.69643400	1.97731800
C	-1.78885500	1.23802000	5.15094900
N	-1.34090000	2.12256500	5.74666000
B	-0.54064400	3.35401900	6.34388000
H	-5.37832900	-1.23022000	3.77133900
C	-0.71070500	3.29680400	7.94570800
C	-1.98502400	3.15012600	8.48968800
C	0.31963900	3.47506300	8.86405100
C	-2.24185700	3.15886100	9.85388300
C	0.10833800	3.49597600	10.23870800
C	-1.18009600	3.33357300	10.73591000
C	-1.20021200	4.71600100	5.77469400
C	-0.57415700	5.90995300	6.13279600
C	-2.37595500	4.85880900	5.04392400
C	-1.04655100	7.16418300	5.77625300
C	-2.88760700	6.09559800	4.66164500
C	-2.22021900	7.25571200	5.03252900
C	0.94452400	2.97454100	5.77242300
C	1.66505300	3.66490400	4.79836100
C	1.52403700	1.77317000	6.18429600
C	2.87149300	3.20348600	4.26723600
C	2.72945500	1.28991300	5.69993200
C	3.40226400	1.99971800	4.71132100
F	-1.39669500	3.34554700	12.04685100
F	1.12737400	3.66498000	11.07969200
F	-3.48096700	3.00395300	10.32029300
F	-3.04003000	2.99332100	7.65941400

F	1.58507900	3.63836900	8.44199400
F	0.87853700	0.98719700	7.06266000
F	3.20512400	0.10215600	6.10481300
F	4.52040600	1.50652800	4.17639300
F	3.51198400	3.91262200	3.33490400
F	1.21564800	4.81433600	4.27354100
F	0.57057800	5.84812000	6.83671400
F	-0.39655300	8.26978800	6.13244100
F	-2.69489800	8.44432600	4.67607500
F	-4.01072400	6.17043500	3.94587100
F	-3.08617100	3.77705700	4.64437400
H	2.68584900	-0.31088800	3.96281900
C	-0.07637500	5.90613200	0.67323400
H	-0.06212400	6.94499300	0.35913400
H	-0.12361100	5.72562500	1.74505300
H	-0.82407000	4.66632800	-2.21421900
H	-4.34627700	0.60297500	5.10663400

1c

SCF energy: -3474.0590581 a.u.

Enthalpy: -3473.327587 a.u.

Gibbs free energy: -3473.501757 a.u.

Ni	-3.07807938	1.73848927	0.56277806
N	-3.58533038	0.24567527	-0.53166394
N	-1.86468738	2.55574727	-0.75295894
C	-3.63043238	-1.15641573	-2.54817794
H	-3.78802638	-0.89947773	-3.59886094
H	-4.52683438	-1.63166373	-2.14958994
H	-2.82668838	-1.90348573	-2.52675394
C	-3.22773438	0.05097127	-1.75982994
C	-2.41965638	1.02892927	-2.55566794
H	-3.10968038	1.45264527	-3.30418894
C	-1.67327938	2.18236027	-1.97524994
C	-4.46851638	-0.70568673	0.10410606
C	-5.82509438	-0.34756673	0.21428106
C	-6.67460738	-1.22522873	0.89010006
H	-7.72762138	-0.97770573	0.98749306
C	-6.19060038	-2.40166673	1.44768706
H	-6.86422938	-3.07132373	1.97424206
C	-4.84402338	-2.72215673	1.33433406
H	-4.47997738	-3.64418673	1.77564306
C	-3.94822238	-1.88731473	0.65906106
C	-6.34080438	0.94637727	-0.38380394
H	-5.53781838	1.69407627	-0.27377394

C	-7.57071138	1.49356327	0.33037706
H	-7.81039438	2.49216527	-0.04540094
H	-7.42076438	1.56535927	1.41227806
H	-8.45195538	0.86698127	0.15827206
C	-6.62709538	0.79415527	-1.87919794
H	-6.98093438	1.73818627	-2.30473294
H	-7.40290838	0.03933027	-2.04662494
H	-5.74418338	0.48432227	-2.44586594
C	-2.47190038	-2.23431973	0.58105006
H	-2.11186138	-1.96084773	-0.42176194
C	-2.20753738	-3.72444673	0.76323706
H	-1.16358438	-3.95246473	0.54836306
H	-2.82993838	-4.32856673	0.09602306
H	-2.40715638	-4.04441973	1.79104206
C	-1.65248138	-1.41259073	1.57974706
H	-0.59890138	-1.70149173	1.53793306
H	-2.00477238	-1.57290673	2.60621506
H	-1.71476338	-0.33668473	1.36774206
C	-1.13296438	3.65345027	-0.21876094
C	-1.69867838	4.92303627	-0.15956594
C	-1.01324438	5.96325727	0.46146906
H	-1.46621238	6.94880227	0.49433006
C	0.82042662	4.50020727	0.99481606
H	1.79274262	4.30994327	1.43722506
C	0.23970662	5.75544527	1.04194506
H	-2.67775938	5.08309527	-0.59931894
C	0.13536462	3.44446127	0.36397206
C	0.74671762	2.17523527	0.33310706
N	1.31050862	1.16304327	0.34214206
C	-0.72513938	2.85929027	-2.90600894
H	-0.60522138	3.91772827	-2.67042194
H	0.26542562	2.39435227	-2.84144594
H	-1.05267238	2.75283227	-3.94190594
H	0.75993662	6.57157027	1.52943906
B	2.20153962	-0.13538673	0.17024906
H	-2.86170600	2.84908900	1.47821000
C	2.16961062	-0.99862873	1.54066306
C	1.58482962	-0.63560973	2.74980206
C	2.86100462	-2.20918573	1.56269306
C	1.63458062	-1.42999673	3.89103506
C	2.93866862	-3.03223273	2.67583606
C	2.31865162	-2.63512773	3.85550906
C	3.71093362	0.43075127	-0.05387994
C	4.22248662	1.39270127	0.81651706

C	4.59891562	-0.01149073	-1.03244294
C	5.50634662	1.91154127	0.72396606
C	5.89463562	0.47937927	-1.15864094
C	6.35187362	1.44750427	-0.27491494
C	1.49680662	-0.81282473	-1.13831394
C	1.45358462	-0.08984773	-2.33142994
C	0.78458462	-2.00891373	-1.16769594
C	0.75203562	-0.48524573	-3.46037794
C	0.05387862	-2.44143273	-2.27298994
C	0.03480462	-1.67426773	-3.42799494
F	4.23345862	-0.95186173	-1.92025194
F	6.70099262	0.03174227	-2.12678194
F	7.59050562	1.92939227	-0.38199294
F	5.93355162	2.84443627	1.58037606
F	3.44816762	1.86943227	1.81645806
F	1.03011762	-1.03533473	5.01789706
F	0.90106962	0.51994027	2.87868006
F	2.38244762	-3.40658873	4.94097606
F	3.59547862	-4.19524673	2.63044506
F	3.46221662	-2.63407673	0.43497406
F	0.74354462	-2.81700573	-0.09499294
F	-0.66718338	-3.56632173	-2.21407294
F	-0.70062338	-2.04553373	-4.47588094
F	0.70083862	0.29322927	-4.54771094
F	2.08219262	1.10359027	-2.41254294
H	-1.72393238	0.46414627	-3.19134094

I-1d

SCF energy: -3552. 6859691 a.u.

Enthalpy: -3551. 923592 a.u.

Gibbs free energy: -3552. 079709 a.u.

Ni	-2.50001321	1.31273492	1.15080756
N	-3.48015808	0.40722517	-0.40351385
N	-1.66838111	2.65753139	-0.00527637
C	-3.95181514	-0.09812461	-2.76742665
H	-3.17832886	-0.63630434	-3.32987206
H	-4.43057687	0.57666499	-3.48346382
H	-4.68735275	-0.81651863	-2.40804648
C	-3.31003688	0.66825835	-1.65456932
C	-2.47157001	1.80361358	-2.15362833
H	-3.13727504	2.41414358	-2.78297929
C	-1.72049204	2.75880023	-1.29537839
C	-4.47461696	-0.56541292	-0.02212958
C	-5.79442283	-0.08910114	0.15892905

C	-6.72128642	-0.96687888	0.72240750
H	-7.74276850	-0.63372094	0.87684945
C	-6.36595694	-2.26639394	1.07265165
H	-7.10099123	-2.92690117	1.52175816
C	-5.09047325	-2.73086445	0.79646532
H	-4.83833116	-3.76754337	1.00511282
C	-4.11731202	-1.90109568	0.22707053
C	-6.20689123	1.30519261	-0.29559478
H	-5.70806291	1.48866777	-1.26027722
C	-5.76097956	2.42026795	0.65346439
H	-4.67073784	2.46227409	0.77707516
H	-6.20285650	2.28942267	1.64737662
H	-6.08979950	3.39347064	0.27580062
C	-7.70529086	1.42411096	-0.55154714
H	-7.93115205	2.38298685	-1.02521537
H	-8.27846153	1.38704171	0.38018868
H	-8.07471603	0.62879708	-1.20443285
C	-2.80337886	-2.51355357	-0.23117956
H	-2.11913831	-1.70823280	-0.53908053
C	-3.09717050	-3.40185518	-1.44743957
H	-2.19718540	-3.91096086	-1.79680974
H	-3.51744937	-2.84047139	-2.28689159
H	-3.82243990	-4.17773788	-1.18103762
C	-2.08784094	-3.34494212	0.83271434
H	-1.14044110	-3.72205331	0.43223801
H	-2.67962985	-4.21811191	1.12463225
H	-1.85430608	-2.78112014	1.73815408
C	-0.91023171	3.63395298	0.72064074
C	-1.48952248	4.81486451	1.16493370
C	-0.72823251	5.72641839	1.89342732
H	-1.18931910	6.64805375	2.23445604
C	1.20335945	4.29621115	1.75460592
H	2.24260046	4.07001726	1.97152468
C	0.61216448	5.47269882	2.18767410
H	-2.53448409	5.01015872	0.94159644
C	0.44156076	3.37351817	1.01935571
C	1.00996294	2.15398384	0.59562042
N	1.45854894	1.14606388	0.24526292
C	-1.01789343	3.82720346	-2.06953104
H	-0.15027847	3.38537303	-2.57065627
H	-1.66301290	4.21763676	-2.86033761
H	-0.67328477	4.65513520	-1.45270129
H	1.19241310	6.19050648	2.75647990
B	2.18138525	-0.23647028	-0.11701314

H	-1.77087899	1.94149841	2.22230312
C	-3.74789290	0.76898267	2.73368868
H	-4.70593133	0.53122492	2.27851224
H	-3.72726548	1.60957976	3.42249475
C	-2.69793492	-0.11464258	2.65435404
H	-1.81998913	-0.01502449	3.28271855
H	-2.80743567	-1.05594938	2.12348861
C	2.16430835	-1.01098681	1.30759516
C	0.94102544	-1.22767279	1.93707738
C	3.27039386	-1.52835916	1.97844156
C	0.79097399	-1.89812190	3.13927929
C	3.16812810	-2.21005550	3.18987919
C	1.92237040	-2.39588237	3.77614689
C	3.62182059	0.22110231	-0.68373924
C	4.40214766	1.13321544	0.02770373
C	4.18228932	-0.23200658	-1.87682608
C	5.64137624	1.58726083	-0.39703126
C	5.42608082	0.19113207	-2.33886151
C	6.15916392	1.10728403	-1.59625667
C	1.22066815	-0.94700503	-1.21711767
C	0.57601674	-0.24063847	-2.22651062
C	1.02379952	-2.32676253	-1.25928995
C	-0.22278082	-0.83360792	-3.19468243
C	0.23747641	-2.96217733	-2.21526296
C	-0.41152175	-2.20809641	-3.18386499
F	4.25497947	-2.68293416	3.79304585
F	4.50320518	-1.40764305	1.47233717
F	1.81132258	-3.03843805	4.93269751
F	-0.42080046	-2.07342369	3.68881975
F	-0.19730446	-0.78013829	1.33746343
F	1.61391425	-3.12938438	-0.36421413
F	0.08054071	-4.28580780	-2.18420816
F	-1.20792958	-2.78195653	-4.08243152
F	-0.83138322	-0.08598147	-4.13767472
F	0.73091530	1.10571296	-2.32822831
F	3.53837314	-1.12501881	-2.64725854
F	5.91489005	-0.27487218	-3.48641444
F	7.34520607	1.52307397	-2.02621382
F	6.33235905	2.47025294	0.32446699
F	3.94953819	1.60898226	1.21143654
H	-1.76041406	1.41346381	-2.89590147

TS-1d

SCF energy: -3552. 6652315 a.u.

Enthalpy: -3551.904115 a.u.
Gibbs free energy: -3552.054271 a.u.

Ni	-2.31800100	1.17271900	0.92372400
N	-3.29628100	0.32637700	-0.52469400
N	-1.54602100	2.59662500	-0.19318600
C	-3.93725100	-0.10821900	-2.85907300
H	-3.23857400	-0.44841800	-3.63259800
H	-4.63401000	0.57915000	-3.35218800
H	-4.50290800	-0.95934500	-2.48424100
C	-3.18463700	0.60439100	-1.78140400
C	-2.30662300	1.68917800	-2.32023500
H	-2.91347300	2.25832900	-3.04131800
C	-1.59171800	2.68709500	-1.48324900
C	-4.29990500	-0.63507500	-0.11504700
C	-5.58232500	-0.13217400	0.18334600
C	-6.51048100	-1.02101600	0.72830700
H	-7.50759200	-0.66529700	0.97047700
C	-6.18602300	-2.35386100	0.95539800
H	-6.92178400	-3.02678000	1.38438000
C	-4.93111100	-2.82701900	0.60496800
H	-4.69465400	-3.87881000	0.74657500
C	-3.95753200	-1.98423900	0.05851200
C	-5.94887100	1.32387600	-0.05419800
H	-5.38411400	1.67471700	-0.93031200
C	-5.54274100	2.20787100	1.12740200
H	-5.82848500	3.24997900	0.95156000
H	-4.45842300	2.18372600	1.30719400
H	-6.03821400	1.87694600	2.04713500
C	-7.42670200	1.52075500	-0.37451800
H	-7.61284500	2.55113200	-0.68924700
H	-8.06090800	1.33797600	0.49831700
H	-7.76232500	0.85556000	-1.17510900
C	-2.63666200	-2.58064100	-0.39536100
H	-1.95260000	-1.76503600	-0.67622100
C	-2.88518000	-3.46160500	-1.62513100
H	-1.97560400	-3.97730100	-1.93919500
H	-3.26080800	-2.89282500	-2.48121500
H	-3.62795400	-4.23278700	-1.39594700
C	-1.94594800	-3.40492200	0.69061700
H	-0.97715600	-3.76888200	0.33193700
H	-2.53555900	-4.28664000	0.96032200
H	-1.76738000	-2.83487500	1.60535100
C	-0.84633600	3.61001100	0.52910900
C	-1.46203500	4.79592500	0.90842300

C	-0.75181700	5.73730300	1.65165400
H	-1.24213500	6.66132100	1.94201800
C	1.20401800	4.33182500	1.65553700
H	2.23475700	4.12748800	1.92862500
C	0.57456900	5.51197000	2.02194700
H	-2.49587200	4.97221500	0.62496700
C	0.49159900	3.37696000	0.91281500
C	1.09004800	2.15445400	0.54037900
N	1.55016600	1.14044300	0.22497600
C	-0.94306400	3.78866100	-2.25875200
H	-1.63370700	4.63363700	-2.36155800
H	-0.04017600	4.16601800	-1.77599900
H	-0.68954400	3.45395100	-3.26629700
H	1.11511700	6.25577300	2.59648300
B	2.26682300	-0.25249200	-0.09092600
H	-1.53348200	1.83891700	2.13019200
C	-2.11780800	0.93268000	3.06442400
H	-2.61373400	1.67710700	3.68724200
H	-1.17245400	0.57911400	3.47399500
C	-2.92912400	-0.00165400	2.34099100
H	-2.53481100	-1.00056700	2.17044800
H	-4.01270200	0.06149400	2.42561000
C	2.19065200	-1.00579200	1.34577200
C	0.94918100	-1.18156200	1.95031700
C	3.26510200	-1.54294400	2.05260400
C	0.75073900	-1.82636300	3.15983700
C	3.11485100	-2.20110200	3.27219100
C	1.85120700	-2.34516400	3.83226700
C	3.73498200	0.17823100	-0.60621800
C	4.50359500	1.07754000	0.13388600
C	4.33736300	-0.29509300	-1.77046200
C	5.77430300	1.49369500	-0.23176800
C	5.61277700	0.09160800	-2.17439200
C	6.33501600	0.99212500	-1.40269800
C	1.34544400	-0.97556800	-1.21440700
C	0.72877000	-0.29113500	-2.25682600
C	1.18576400	-2.36026800	-1.25408700
C	-0.01211600	-0.91351800	-3.25352900
C	0.46093500	-3.02283000	-2.23953400
C	-0.16073600	-2.29292300	-3.24398800
F	4.17416700	-2.68936900	3.91033200
F	4.51239400	-1.46371100	1.57531800
F	1.69662400	-2.96479200	4.99618700
F	-0.48099100	-1.94567100	3.67968400

F	-0.16869400	-0.71006000	1.32590500
F	1.76501700	-3.13966000	-0.33092400
F	0.33551000	-4.34966200	-2.20569600
F	-0.89016000	-2.89613700	-4.17799300
F	-0.59728900	-0.18929400	-4.22878500
F	0.85286800	1.05796800	-2.36375800
F	3.70759500	-1.17343500	-2.56855600
F	6.14248400	-0.39521300	-3.29451700
F	7.55165800	1.37159300	-1.77728700
F	6.45457100	2.36040700	0.51912200
F	4.00453300	1.57621800	1.28955900
H	-1.55626900	1.23178300	-2.98032800

P-1d

SCF energy: -3552.6734169 a.u.
enthalpy: -3551.908071 a.u.
Gibbs free energy: -3552.062907 a.u.

Ni	-3.11483700	1.54982000	0.40726400
N	-3.62208800	0.05700600	-0.68717800
N	-1.90144500	2.36707800	-0.90847300
C	-3.66719000	-1.34508500	-2.70369200
H	-3.82478400	-1.08814700	-3.75437500
H	-4.56359200	-1.82033300	-2.30510400
H	-2.86344600	-2.09215500	-2.68226800
C	-3.26449200	-0.13769800	-1.91534400
C	-2.45641400	0.84026000	-2.71118200
H	-3.14643800	1.26397600	-3.45970300
C	-1.71003700	1.99369100	-2.13076400
C	-4.50527400	-0.89435600	-0.05140800
C	-5.86185200	-0.53623600	0.05876700
C	-6.71136500	-1.41389800	0.73458600
H	-7.76437900	-1.16637500	0.83197900
C	-6.22735800	-2.59033600	1.29217300
H	-6.90098700	-3.25999300	1.81872800
C	-4.88078100	-2.91082600	1.17882000
H	-4.51673500	-3.83285600	1.62012900
C	-3.98498000	-2.07598400	0.50354700
C	-6.37756200	0.75770800	-0.53931800
H	-5.57457600	1.50540700	-0.42928800
C	-7.60746900	1.30489400	0.17486300
H	-7.84715200	2.30349600	-0.20091500
H	-7.45752200	1.37669000	1.25676400
H	-8.48871300	0.67831200	0.00275800
C	-6.66385300	0.60548600	-2.03471200

H	-7.01769200	1.54951700	-2.46024700
H	-7.43966600	-0.14933900	-2.20213900
H	-5.78094100	0.29565300	-2.60138000
C	-2.50865800	-2.42298900	0.42553600
H	-2.14861900	-2.14951700	-0.57727600
C	-2.24429500	-3.91311600	0.60772300
H	-1.20034200	-4.14113400	0.39284900
H	-2.86669600	-4.51723600	-0.05949100
H	-2.44391400	-4.23308900	1.63552800
C	-1.68923900	-1.60126000	1.42423300
H	-0.63565900	-1.89016100	1.38241900
H	-2.04153000	-1.76157600	2.45070100
H	-1.75152100	-0.52535400	1.21222800
C	-1.16972200	3.46478100	-0.37427500
C	-1.73543600	4.73436700	-0.31508000
C	-1.05000200	5.77458800	0.30595500
H	-1.50297000	6.76013300	0.33881600
C	0.78366900	4.31153800	0.83930200
H	1.75598500	4.12127400	1.28171100
C	0.20294900	5.56677600	0.88643100
H	-2.71451700	4.89442600	-0.75483300
C	0.09860700	3.25579200	0.20845800
C	0.70996000	1.98656600	0.17759300
N	1.27375100	0.97437400	0.18662800
C	-0.76189700	2.67062100	-3.06152300
H	-0.64197900	3.72905900	-2.82593600
H	0.22866800	2.20568300	-2.99696000
H	-1.08943000	2.56416300	-4.09742000
H	0.72317900	6.38290100	1.37392500
B	2.16478200	-0.32405600	0.01473500
C	2.13285300	-1.18729800	1.38514900
C	1.54807200	-0.82427900	2.59428800
C	2.82424700	-2.39785500	1.40717900
C	1.59782300	-1.61866600	3.73552100
C	2.90191100	-3.22090200	2.52032200
C	2.28189400	-2.82379700	3.69999500
C	3.67417600	0.24208200	-0.20939400
C	4.18572900	1.20403200	0.66100300
C	4.56215800	-0.20016000	-1.18795700
C	5.46958900	1.72287200	0.56845200
C	5.85787800	0.29071000	-1.31415500
C	6.31511600	1.25883500	-0.43042900
C	1.46004900	-1.00149400	-1.29382800
C	1.41682700	-0.27851700	-2.48694400

C	0.74782700	-2.19758300	-1.32321000
C	0.71527800	-0.67391500	-3.61589200
C	0.01712100	-2.63010200	-2.42850400
C	-0.00195300	-1.86293700	-3.58350900
F	4.19670100	-1.14053100	-2.07576600
F	6.66423500	-0.15692700	-2.28229600
F	7.55374800	1.74072300	-0.53750700
F	5.89679400	2.65576700	1.42486200
F	3.41141000	1.68076300	1.66094400
F	0.99336000	-1.22400400	4.86238300
F	0.86431200	0.33127100	2.72316600
F	2.34569000	-3.59525800	4.78546200
F	3.55872100	-4.38391600	2.47493100
F	3.42545900	-2.82274600	0.27946000
F	0.70678700	-3.00567500	-0.25050700
F	-0.70394100	-3.75499100	-2.36958700
F	-0.73738100	-2.23420300	-4.63139500
F	0.66408100	0.10456000	-4.70322500
F	2.04543500	0.91492100	-2.56805700
H	-1.76069000	0.27547700	-3.34685500
C	-4.00252416	1.10981908	2.05189487
H	-5.02829070	1.40885665	1.99462756
H	-3.94745754	0.05383354	2.21548640
C	-3.31744080	1.84634092	3.21799794
H	-3.43654213	2.90221222	3.09209848
H	-3.76443747	1.54467617	4.14216911
H	-2.27534346	1.60387334	3.22994035

I-1e

SCF energy: -3631.2864918 a.u.

Enthalpy: -3630.462207 a.u.

Gibbs free energy: -3630.622563 a.u.

Ni	-1.91835800	-2.57104700	-0.78515700
N	-1.92011600	-2.87029100	1.29870000
N	0.13704300	-2.80319800	-0.83069900
C	-0.97839300	-2.70081200	3.57281600
H	-0.06627500	-3.06871800	4.04900900
H	-1.83984500	-3.23954100	3.97071600
H	-1.09332500	-1.65340200	3.87714400
C	-0.89361600	-2.80350300	2.07746900
C	0.51685000	-2.84637700	1.58973800
H	1.00072400	-3.68138800	2.11722200
C	0.95114900	-2.92775600	0.16884600
C	-3.20859900	-2.86561600	1.94615700

C	-3.86454300	-4.10025900	2.09320400
C	-5.11820500	-4.10074800	2.70824600
H	-5.64812100	-5.04023800	2.83801700
C	-5.69876700	-2.91626100	3.14377700
H	-6.67395500	-2.93347900	3.62069600
C	-5.03715900	-1.70736600	2.96344000
H	-5.50389200	-0.78805700	3.30361500
C	-3.77671700	-1.64951700	2.36409300
C	-3.22221900	-5.37679100	1.58360700
H	-2.59215700	-5.09133800	0.72542300
C	-4.23818700	-6.40221500	1.09263500
H	-3.73089300	-7.23491200	0.59729500
H	-4.95011900	-5.96860500	0.38334000
H	-4.81387300	-6.83079700	1.91872000
C	-2.29914700	-5.99944300	2.63257300
H	-1.84957800	-6.92458300	2.25926900
H	-2.85735100	-6.24524400	3.54201000
H	-1.48434400	-5.32683400	2.92105300
C	-3.07819600	-0.32265600	2.12858100
H	-2.00232000	-0.46156500	2.30017900
C	-3.53754800	0.78253300	3.07057300
H	-2.89125000	1.65601000	2.96708500
H	-3.50199100	0.46256300	4.11624200
H	-4.56085600	1.10313100	2.85165700
C	-3.23607800	0.10565000	0.67025000
H	-2.72723500	1.05393800	0.47193400
H	-4.29406600	0.21630200	0.40499100
H	-2.81407000	-0.64683200	-0.01316100
C	0.67975500	-2.90798100	-2.14258900
C	0.48847600	-4.06572300	-2.88840500
C	0.95745300	-4.13720000	-4.19721300
H	0.81033000	-5.05121300	-4.76423800
C	1.79838700	-1.88524000	-4.06687500
H	2.28698500	-1.02160900	-4.50646000
C	1.60541600	-3.05106700	-4.78937700
H	-0.03042000	-4.90417100	-2.43340400
C	1.34125400	-1.81293700	-2.73957100
C	1.47332000	-0.62019800	-1.99867800
N	1.51702000	0.35426500	-1.37567200
C	2.42972300	-3.12077600	0.01813200
H	2.70226700	-3.61926900	-0.91266000
H	2.93173300	-2.14412400	0.03168900
H	2.84161500	-3.68318700	0.85842000
H	1.95470400	-3.11471500	-5.81384200

B	1.45437600	1.67474800	-0.50012000
C	-3.06614400	-0.71131900	-2.86923500
H	-3.75983500	-1.36786400	-3.40276800
H	-3.61466000	-0.18688500	-2.08127000
C	-1.84686300	-1.42325900	-2.37274900
H	-1.34395100	-1.97619100	-3.17007100
H	-1.13934700	-0.73793600	-1.88222400
C	-3.88921100	-3.05365500	-1.08387900
H	-4.42361000	-2.20379800	-1.49499400
H	-4.27242000	-3.43682000	-0.14400200
C	-3.05975300	-3.83562600	-1.88111000
H	-2.75166300	-4.82722300	-1.54709300
H	-2.93622200	-3.64160600	-2.94446600
C	0.12150600	2.49088600	-0.93884800
C	-0.69983600	2.25954800	-2.03871500
C	-0.20476800	3.62851000	-0.19733500
C	-1.80639800	3.04467500	-2.34785200
C	-1.29542000	4.44322500	-0.46865800
C	-2.11029500	4.14372100	-1.55717700
C	2.76753300	2.54524600	-0.87558300
C	3.08269200	2.77320600	-2.21468100
C	3.59192200	3.18918500	0.04557300
C	4.13834400	3.56996800	-2.63495800
C	4.66046000	3.99724100	-0.33046300
C	4.93586100	4.18903400	-1.67902100
C	1.46199400	1.03341800	1.00590600
C	2.57573200	0.29317300	1.40885100
C	0.45257400	1.11778800	1.96329600
C	2.72107000	-0.29677700	2.65787000
C	0.55354500	0.54657400	3.23157500
C	1.69224000	-0.16448500	3.58722600
F	3.38215600	3.05356800	1.36550800
F	5.42170600	4.58560300	0.59026600
F	5.95287300	4.95741600	-2.05236300
F	4.38926200	3.74413700	-3.93252300
F	2.32998900	2.19932400	-3.18026800
F	-2.56716500	2.74978700	-3.40688900
F	-0.46810600	1.23514800	-2.89629900
F	-3.16378800	4.90363900	-1.83629400
F	-1.56586200	5.50081900	0.29292200
F	0.55933100	3.94703900	0.86151000
F	-0.70001400	1.75734200	1.71269700
F	-0.46510600	0.63845300	4.09556200
F	1.77393000	-0.75565700	4.77611100

F	3.79990000	-1.02462800	2.94879200
F	3.59177400	0.10076900	0.54242900
H	-2.74572900	0.05729500	-3.58464500
H	1.03948000	-1.97789300	2.02249000

TS-1e

SCF energy: -3631.2692988 a.u.

Enthalpy: -3630.445156 a.u.

Gibbs free energy: -3630.602134 a.u.

Ni	-2.80808200	1.25677000	0.82919100
N	-3.42044500	-0.05993100	-0.51467000
N	-1.64780300	2.26428700	-0.54334800
C	-3.32158800	-1.40892400	-2.57025800
H	-3.03133300	-1.24249900	-3.61009300
H	-4.39126700	-1.62224400	-2.52016000
H	-2.80875800	-2.31761300	-2.23455100
C	-2.94419000	-0.24364700	-1.70206800
C	-1.97347000	0.67757700	-2.36306800
H	-2.40903500	0.93759100	-3.33913200
C	-1.43340200	1.93233500	-1.77529600
C	-4.41370200	-1.01212600	-0.06890100
C	-5.76398300	-0.63528600	-0.17655500
C	-6.72569800	-1.54967000	0.25866900
H	-7.77822100	-1.29031800	0.19045900
C	-6.35585500	-2.78124400	0.78329300
H	-7.11716500	-3.47989100	1.11630300
C	-5.01262800	-3.12163000	0.88275900
H	-4.73633900	-4.08967700	1.28989100
C	-4.00666600	-2.25178400	0.45461000
C	-6.16112600	0.71665500	-0.74601100
H	-5.34741000	1.42119200	-0.50475300
C	-7.44206200	1.26787500	-0.12738800
H	-7.60399300	2.30154900	-0.44510700
H	-7.41306300	1.25020400	0.96697000
H	-8.32299700	0.69980800	-0.44140700
C	-6.28721200	0.67888600	-2.27013800
H	-6.61218500	1.64896500	-2.65830600
H	-7.02703600	-0.06672300	-2.57998900
H	-5.34192700	0.42727800	-2.76162700
C	-2.54087400	-2.62355800	0.58853000
H	-2.00160900	-2.20203100	-0.26994900
C	-2.29313000	-4.12660400	0.57024200
H	-1.22184100	-4.32705000	0.50152700
H	-2.77869600	-4.60864400	-0.28393800

H	-2.65802800	-4.61048100	1.48165900
C	-1.93477900	-1.98703600	1.83944600
H	-0.88622200	-2.27428600	1.96120100
H	-2.47999500	-2.29524200	2.73913700
H	-1.97668700	-0.89204100	1.78161900
C	-1.05228700	3.45310100	-0.04549300
C	-1.81909900	4.58449800	0.21404600
C	-1.22987800	5.70859000	0.78711200
H	-1.83742000	6.58850200	0.97431800
C	0.90596000	4.60028300	0.88356600
H	1.95873300	4.57348100	1.14597400
C	0.12476100	5.71809500	1.12821800
H	-2.87424200	4.57510900	-0.04325800
C	0.31906300	3.46905000	0.29189500
C	1.07520000	2.30023000	0.07313600
N	1.65035100	1.30751900	-0.07768500
C	-0.59750300	2.73318200	-2.72457600
H	-0.56891600	3.79324500	-2.46936900
H	0.43498400	2.36004000	-2.71897600
H	-0.95211300	2.62196400	-3.75159700
H	0.56722500	6.59651900	1.58464800
B	2.37790500	-0.09201300	-0.18592800
C	-1.56794800	1.09310000	3.76816700
H	-2.04090800	1.66335300	4.57192200
H	-2.03646100	0.10613000	3.73424200
C	-1.60596700	1.79961800	2.44201400
H	-1.26497200	2.83539300	2.48889700
H	-0.97958100	1.25140900	1.71298100
C	-4.22953500	1.01170200	2.13923500
H	-4.09131500	0.21532900	2.86959900
H	-5.15585000	0.95262900	1.57651100
C	-3.62050000	2.28310200	2.37353500
H	-3.94524100	3.12141500	1.75000100
H	-3.37064200	2.61846500	3.37539500
C	2.28364300	-0.81405000	1.26301700
C	1.86576900	-0.26781300	2.47164800
C	2.79628200	-2.10876700	1.35325300
C	1.90220500	-0.96168300	3.67758600
C	2.85488500	-2.83934800	2.53126300
C	2.39837700	-2.25727800	3.71074000
C	3.93319900	0.22658600	-0.50526600
C	4.61020500	1.20158800	0.22638700
C	4.71456600	-0.48436200	-1.41375600
C	5.96032500	1.48323400	0.06954900

C	6.07220900	-0.24270200	-1.59664000
C	6.69894400	0.75081100	-0.85433200
C	1.54311600	-0.79269000	-1.40367200
C	1.59824500	-0.22449400	-2.67808600
C	0.72664300	-1.91782100	-1.30856400
C	0.93353900	-0.72406000	-3.79154300
C	0.03940400	-2.45633600	-2.39552700
C	0.14136300	-1.86110500	-3.64666700
F	4.17680200	-1.45930000	-2.16448000
F	6.77157100	-0.95491800	-2.47791300
F	7.99341300	0.99764500	-1.02178400
F	6.54698300	2.43799100	0.79209100
F	3.93679000	1.92665300	1.15141300
F	1.46683500	-0.38001100	4.80113100
F	1.38538700	0.99963200	2.54615400
F	2.44370500	-2.93118600	4.85451800
F	3.34617000	-4.07592400	2.54819400
F	3.24491700	-2.70143600	0.23402100
F	0.54353500	-2.55196900	-0.13996600
F	-0.74814800	-3.52559100	-2.23214900
F	-0.54875500	-2.34205300	-4.67732100
F	1.00689500	-0.10236700	-4.96856600
F	2.31656300	0.90144500	-2.86832900
H	-0.52312800	0.93418500	4.05153500
H	-1.10189500	0.07369600	-2.66354000

βH-1e

SCF energy: -3631.3179162 a.u.

Enthalpy: -3630.491072 a.u.

Gibbs free energy: -3630.648698 a.u.

Ni	2.93226200	1.29390200	-0.71307200
N	3.40691800	0.06629000	0.68155900
N	1.76413300	2.42738700	0.39089100
C	3.42943400	-0.86691200	2.95306600
H	3.49932700	-0.40800000	3.94271300
H	4.37197300	-1.35867700	2.70838500
H	2.66556600	-1.65136300	3.02687800
C	3.03745700	0.14231800	1.91870700
C	2.23761800	1.28094400	2.47797300
H	2.92583300	1.82909100	3.14458600
C	1.54215900	2.31662300	1.66086700
C	4.30185500	-0.99842300	0.28300000
C	5.65668800	-0.65395600	0.11862200
C	6.52840600	-1.65330800	-0.31535500

H	7.58107100	-1.42091800	-0.44681600
C	6.06763100	-2.93442700	-0.58810900
H	6.75944800	-3.69999100	-0.92556400
C	4.72095100	-3.23734700	-0.43541600
H	4.37412000	-4.24145400	-0.65698800
C	3.80011900	-2.27995900	0.00200100
C	6.14903000	0.75209000	0.40505100
H	5.33764200	1.44318100	0.11494400
C	7.38036600	1.13570600	-0.40726900
H	7.60250300	2.19875900	-0.28092600
H	7.24622300	0.94235500	-1.47629400
H	8.26984500	0.58690900	-0.08272400
C	6.41761700	0.96065500	1.89675900
H	6.76550200	1.97936600	2.09380600
H	7.19238400	0.27162600	2.24882800
H	5.52826900	0.78742500	2.51135300
C	2.32079900	-2.60937400	0.10668000
H	1.92644800	-2.11867400	1.00821500
C	2.05235600	-4.10158500	0.25830300
H	0.99745500	-4.27275500	0.47520900
H	2.63811100	-4.53808000	1.07292100
H	2.28992700	-4.65008300	-0.65862900
C	1.54298900	-2.03805600	-1.08311400
H	0.49386100	-2.34106100	-1.03955300
H	1.95720200	-2.39547000	-2.03353600
H	1.57073800	-0.93970300	-1.09578400
C	1.09924700	3.44109300	-0.35788000
C	1.74972800	4.63259600	-0.66556200
C	1.12905100	5.57386500	-1.48208900
H	1.64522000	6.50176600	-1.70826200
C	-0.80379600	4.15815400	-1.72034700
H	-1.79162900	3.94552000	-2.11764800
C	-0.14025400	5.33858300	-2.01411900
H	2.74287800	4.81038900	-0.26349400
C	-0.18583700	3.20679200	-0.88846300
C	-0.86110600	2.00364300	-0.59207800
N	-1.44733100	1.03088500	-0.36940100
C	0.61880100	3.21499100	2.41414700
H	0.63110800	4.23270700	2.01817400
H	-0.41224200	2.84894800	2.33885000
H	0.86232800	3.23493600	3.47770800
H	-0.60982200	6.07569100	-2.65588600
B	-2.34045200	-0.21238200	0.06026900
C	1.76601400	0.11297300	-4.61046500

H	2.23304800	0.61510500	-5.46289600
H	2.38067300	-0.75918300	-4.36608000
C	1.62245800	1.04172600	-3.41975700
H	1.01322200	1.91313900	-3.69145800
H	1.06891400	0.52725200	-2.62554400
C	3.81009900	0.49708000	-2.20365100
H	3.54774600	-0.55368700	-2.33152800
H	4.88732700	0.67254500	-2.18688500
C	2.95578200	1.51293200	-2.84998100
H	2.69814300	2.32275700	-2.04243400
H	3.51244000	2.18448400	-3.51812400
C	-2.31196900	-1.30913700	-1.12506300
C	-1.79800400	-1.15142800	-2.40761400
C	-2.94782800	-2.52791000	-0.89040500
C	-1.84869300	-2.14726300	-3.37800600
C	-3.02229800	-3.55078200	-1.82492500
C	-2.46377900	-3.35705500	-3.08559400
C	-3.83790900	0.38624000	0.21519200
C	-4.36824100	1.23315700	-0.75688200
C	-4.70420900	0.05830800	1.25635100
C	-5.65467000	1.75204700	-0.70539900
C	-6.00538300	0.54353000	1.34059800
C	-6.48204800	1.40116900	0.35615500
C	-1.59869700	-0.61843900	1.46059400
C	-1.55200900	0.32146700	2.49178100
C	-0.88703200	-1.78781100	1.71814900
C	-0.85110200	0.15136500	3.67647900
C	-0.15430600	-1.99758700	2.88591700
C	-0.13019700	-1.02176800	3.87057300
F	-4.30167700	-0.75591800	2.24462900
F	-6.79253100	0.20067500	2.35843600
F	-7.71728800	1.88560200	0.42767400
F	-6.09624000	2.57888000	-1.65398900
F	-3.60504400	1.59461600	-1.81738600
F	-1.31259700	-1.94063700	-4.58523500
F	-1.19694100	0.00192600	-2.78143800
F	-2.51881400	-4.32008400	-3.99948500
F	-3.61519200	-4.70576600	-1.53114600
F	-3.49462800	-2.74720000	0.31735300
F	-0.83724500	-2.78573500	0.82432100
F	0.58087500	-3.10486800	3.03554300
F	0.62980800	-1.17170500	4.95563700
F	-0.78693100	1.13035000	4.58701900
F	-2.17925800	1.50957500	2.33883300

H	0.78731100	-0.25457800	-4.92695000
H	1.51086100	0.87451400	3.19421800

$TS_{\beta H}$-1e

SCF energy: -3631.3018911 a.u.

Enthalpy: -3630.481433 a.u.

Gibbs free energy: -3630.642618 a.u.

Ni	2.93060600	1.43074200	-0.77103800
N	3.41868700	0.17108100	0.64438000
N	1.76513200	2.52729600	0.36388600
C	3.47058200	-0.74901700	2.92612600
H	3.62826000	-0.26954000	3.89595700
H	4.36254300	-1.30863500	2.64407100
H	2.65989700	-1.47381400	3.07136000
C	3.07981700	0.25749700	1.88870800
C	2.32336700	1.42086600	2.45798600
H	3.05841200	1.98491300	3.05874300
C	1.59163500	2.43483000	1.64395900
C	4.29161300	-0.91148900	0.24356000
C	5.65043500	-0.59280000	0.06592900
C	6.50035800	-1.60766700	-0.37708400
H	7.55585000	-1.39544200	-0.51810900
C	6.01336000	-2.87930900	-0.64870400
H	6.68726100	-3.65675100	-0.99475700
C	4.66304500	-3.15822700	-0.48096400
H	4.29746400	-4.15594800	-0.69914600
C	3.76517600	-2.18555600	-0.02977900
C	6.17045200	0.80459200	0.34730900
H	5.36268600	1.50860400	0.08004100
C	7.38924700	1.17375500	-0.49066100
H	7.62892700	2.23312800	-0.36659500
H	7.23091400	0.98526400	-1.55728300
H	8.27731200	0.61128700	-0.18632300
C	6.47779000	1.00153900	1.83324200
H	6.84632400	2.01367200	2.02588200
H	7.24996300	0.29900800	2.16339300
H	5.60134700	0.83922000	2.46869100
C	2.28388100	-2.49289100	0.11101400
H	1.93541800	-2.04064300	1.05154100
C	1.99074000	-3.98567100	0.19610800
H	0.94206900	-4.15048000	0.44256900
H	2.59610100	-4.47427600	0.96508400
H	2.18527900	-4.48862300	-0.75641800
C	1.46966900	-1.84591300	-1.01317300

H	0.41572200	-2.12552700	-0.93702700
H	1.82786100	-2.16706900	-1.99930200
H	1.52744400	-0.74934800	-0.97452000
C	1.05066100	3.52967900	-0.36262100
C	1.62406300	4.77404100	-0.60830200
C	0.95090100	5.71097400	-1.38711900
H	1.40892700	6.67883700	-1.56489400
C	-0.88515400	4.18920800	-1.70635400
H	-1.85625800	3.93599400	-2.12006200
C	-0.29736600	5.42080400	-1.94174200
H	2.60262000	4.99469100	-0.19252200
C	-0.21508600	3.24060700	-0.91080900
C	-0.84279200	2.00043600	-0.66498800
N	-1.42225600	1.01413900	-0.48571600
C	0.68677500	3.33460300	2.41812100
H	0.63252300	4.33478700	1.98560800
H	-0.33039800	2.92637700	2.43015800
H	1.00112500	3.40566200	3.46080600
H	-0.80962400	6.15511600	-2.55306200
B	-2.34182100	-0.20932000	-0.03721300
C	1.81338900	0.11823100	-4.69819100
H	2.26750600	0.63140100	-5.55049500
H	2.43376300	-0.75321000	-4.46708000
C	1.67662200	1.03335400	-3.49017600
H	1.06796800	1.90899000	-3.74408100
H	1.13682300	0.50372800	-2.69925100
C	3.84218100	0.53938600	-2.24127800
H	3.54704000	-0.50960600	-2.23525100
H	4.91729800	0.71087400	-2.19498700
C	3.01884200	1.47417700	-2.95111400
H	2.66481800	2.51721800	-1.92600500
H	3.53780200	2.24392900	-3.53074400
C	-2.35895500	-1.32165600	-1.20598500
C	-1.80157500	-1.22062700	-2.47571700
C	-3.10080500	-2.48045300	-0.97729200
C	-1.91906500	-2.21328900	-3.44304700
C	-3.25000200	-3.49620200	-1.91069200
C	-2.65027700	-3.35932800	-3.16002500
C	-3.82298500	0.42958500	0.11118600
C	-4.34877900	1.22523700	-0.90550700
C	-4.68864700	0.16706600	1.17100900
C	-5.63392200	1.74934100	-0.88697100
C	-5.98749600	0.66318300	1.22689900
C	-6.46192400	1.46268900	0.19318800

C	-1.60744600	-0.61160500	1.36445700
C	-1.49664600	0.36047800	2.36006500
C	-0.95395500	-1.80733700	1.65254500
C	-0.77185000	0.20047300	3.53056200
C	-0.19919000	-2.00871400	2.80856000
C	-0.09872900	-0.99524000	3.74946800
F	-4.29171700	-0.59646000	2.20083800
F	-6.77547100	0.38270200	2.26288400
F	-7.69664900	1.95092500	0.23631300
F	-6.07481200	2.51721100	-1.88444600
F	-3.58212200	1.52174500	-1.98295100
F	-1.33806900	-2.06482700	-4.63823400
F	-1.08853300	-0.12807300	-2.83706200
F	-2.77494600	-4.31793600	-4.07155100
F	-3.95370100	-4.58993000	-1.62792200
F	-3.68488800	-2.64281500	0.22220200
F	-0.98238600	-2.83941600	0.79709200
F	0.47740600	-3.14581400	2.99130100
F	0.68203900	-1.13701600	4.82187700
F	-0.63810200	1.20710800	4.40606700
F	-2.08287000	1.56624100	2.18163400
H	0.83090900	-0.24786800	-5.00486500
H	1.63842100	1.05209900	3.23312700

$P_{\beta H}$-1e

SCF energy: -3631.3054635 a.u.

Enthalpy: -3630.486434 a.u.

Gibbs free energy: -3630.646746 a.u.

Ni	3.09846800	1.10700800	-1.01311800
N	3.56405500	0.11816500	0.66910500
N	1.68020000	2.27456600	-0.01616400
C	3.32111700	-0.75479900	2.95108100
H	2.43686300	-1.32365600	3.25853600
H	3.62905600	-0.17635500	3.82877900
H	4.11407900	-1.45640400	2.69155500
C	2.99595700	0.16735000	1.82003800
C	1.86302700	1.10818300	2.11518100
H	1.94552700	1.44848400	3.15457400
C	1.44891700	2.26378200	1.25502600
C	4.44979900	-0.93939200	0.28884500
C	5.82527400	-0.67487200	0.14497600
C	6.62490500	-1.69324700	-0.37651300
H	7.69029500	-1.52419200	-0.49761000
C	6.07967800	-2.91727800	-0.74125900

H	6.71928700	-3.69805600	-1.14065700
C	4.71625200	-3.14942000	-0.59419300
H	4.30948100	-4.11258900	-0.88310500
C	3.86372100	-2.17005500	-0.08188600
C	6.40273300	0.65853000	0.56079000
H	5.66182000	1.42599700	0.26804100
C	7.71342400	1.00141700	-0.13314900
H	8.00440700	2.03026900	0.09332900
H	7.64336300	0.90080300	-1.22027900
H	8.53177200	0.35962900	0.20859800
C	6.56241100	0.74863100	2.07987800
H	6.95008500	1.72817800	2.37401600
H	7.26686300	-0.00986000	2.43672900
H	5.61704000	0.59088600	2.60678700
C	2.36380800	-2.40432600	0.02939100
H	2.03352000	-2.07410200	1.02604300
C	1.97819300	-3.87451300	-0.08817300
H	0.91667500	-4.00196500	0.12754700
H	2.54018000	-4.49591300	0.61384000
H	2.15649200	-4.25980300	-1.09721800
C	1.57945300	-1.58717400	-1.00488400
H	0.51974500	-1.86247700	-1.00140800
H	1.96631900	-1.75579100	-2.01554600
H	1.59603000	-0.50118700	-0.79829900
C	1.11759000	3.27277300	-0.84594100
C	1.88368600	4.31066100	-1.37020600
C	1.30862800	5.22316700	-2.24985500
H	1.91380200	6.03644900	-2.63805800
C	-0.80429500	4.07310400	-2.14630100
H	-1.84190800	3.94839600	-2.43986100
C	-0.02799900	5.10709900	-2.64250100
H	2.92745200	4.39159400	-1.08092000
C	-0.23481800	3.15810200	-1.24293700
C	-0.99955000	2.08549900	-0.74224700
N	-1.60636500	1.17910900	-0.35448200
C	0.68009300	3.31566500	1.98440900
H	0.34243400	4.12565500	1.33891700
H	-0.19125300	2.87964600	2.48609900
H	1.30345400	3.73869000	2.77896500
H	-0.45769700	5.82013100	-3.33694100
B	-2.44344800	-0.07168500	0.13634600
C	0.95172100	1.57434200	-4.62210700
H	0.81580800	2.64135500	-4.41425000
H	1.58264000	1.48806000	-5.51051900

C	1.57171900	0.85853300	-3.43121000
H	0.87117400	0.93266800	-2.58514700
H	1.65398500	-0.21723700	-3.63102100
C	4.03000000	0.62751100	-2.71086700
H	3.98583800	-0.46275600	-2.77171500
H	5.03108600	1.05080900	-2.72624200
C	2.91453400	1.41216100	-3.04336800
H	4.20900100	1.94919800	-0.62562000
H	3.07762900	2.47239100	-3.25011900
C	-2.38677200	-1.20696600	-1.01796800
C	-1.85602300	-1.09776000	-2.29847000
C	-3.01056900	-2.42517800	-0.74571700
C	-1.87612500	-2.13117500	-3.22991200
C	-3.06423700	-3.48263500	-1.64266900
C	-2.48738400	-3.33344800	-2.90181800
C	-3.96733500	0.45184400	0.29023900
C	-4.55509000	1.19442700	-0.73324600
C	-4.80871800	0.13497400	1.35465800
C	-5.87608100	1.62057300	-0.71484800
C	-6.14011400	0.53480700	1.41201300
C	-6.67631200	1.28579900	0.37224400
C	-1.67949200	-0.42530200	1.53858100
C	-1.68605400	0.51912400	2.56833100
C	-0.93546100	-1.57005100	1.81678500
C	-1.03322000	0.36073500	3.78412700
C	-0.25415700	-1.77007200	3.01727300
C	-0.30224800	-0.80155800	4.01113600
F	-4.35405900	-0.58997500	2.38991800
F	-6.90142800	0.20672000	2.45387200
F	-7.94406400	1.68011400	0.41491300
F	-6.37797800	2.33849700	-1.72019900
F	-3.81946600	1.53061300	-1.81976700
F	-1.31122400	-1.96206100	-4.42949300
F	-1.25709900	0.04318800	-2.71551100
F	-2.51907800	-4.33335700	-3.77611400
F	-3.65288900	-4.63037600	-1.31488500
F	-3.55802500	-2.60929100	0.46790100
F	-0.80660200	-2.55830600	0.91744400
F	0.49774900	-2.86329600	3.19055200
F	0.40310500	-0.95069600	5.13004400
F	-1.02907000	1.34142900	4.68974600
F	-2.32164000	1.69327000	2.38457200
H	-0.02583800	1.14797600	-4.85728300
H	0.97219000	0.45476100	2.14340300

TScw-1f

SCF energy: -3631. 2953734 a.u.

enthalpy: -3630.47471 a.u.

Gibbs free energy: -3630.636278 a.u.

Ni	2.47845300	0.93544200	-0.98495900
N	3.25553800	-0.15808400	0.48433600
N	1.71670800	2.27482600	0.28649400
C	3.59263400	-0.62339900	2.89585300
H	2.92623900	-1.27875500	3.46913100
H	3.85619200	0.19896400	3.57194300
H	4.49740300	-1.16953000	2.63238000
C	2.87211900	-0.06590400	1.71384100
C	1.58969000	0.63616100	2.04344400
H	1.44092700	0.64109600	3.12585300
C	1.37786300	2.01794800	1.50907600
C	4.43394200	-0.92638400	0.18770400
C	5.59092200	-0.22827500	-0.20131800
C	6.71814300	-0.97867800	-0.54006900
H	7.62944300	-0.47126000	-0.84058400
C	6.68147800	-2.36662000	-0.51915500
H	7.56247100	-2.93679200	-0.79713700
C	5.52064800	-3.03047600	-0.13878200
H	5.51444600	-4.11527300	-0.12109100
C	4.36795300	-2.33483300	0.23911100
C	5.59947400	1.28778300	-0.26151900
H	4.62300700	1.59328800	-0.69067800
C	6.68357800	1.85633300	-1.16793200
H	6.54403200	2.93332500	-1.29649000
H	6.67737600	1.39405200	-2.15955900
H	7.68197300	1.71523400	-0.74167200
C	5.70012500	1.91536700	1.13022400
H	5.72114600	3.00807500	1.06527100
H	6.62108400	1.59813900	1.62995100
H	4.86275600	1.63720700	1.77726800
C	3.11529200	-3.08188300	0.68080100
H	2.72801100	-2.58787600	1.58296600
C	3.38619700	-4.52936700	1.07328400
H	2.48879300	-4.96340900	1.52112900
H	4.20065800	-4.61738600	1.79801400
H	3.63993700	-5.14532600	0.20450500
C	1.99121100	-3.02314900	-0.35666400
H	1.15066900	-3.64740800	-0.04110900
H	2.33328900	-3.38888300	-1.33237400

H	1.60511500	-2.00883000	-0.48651600
C	1.27655900	3.49151500	-0.30631500
C	2.14164600	4.54237700	-0.58190500
C	1.66070500	5.68234600	-1.22292600
H	2.34168300	6.50324300	-1.42424300
C	-0.55298900	4.73979800	-1.35358800
H	-1.59632400	4.78799400	-1.64960100
C	0.32298800	5.78320100	-1.61061500
H	3.18496900	4.45927300	-0.29171400
C	-0.07946200	3.59202600	-0.69693600
C	-0.94205600	2.50191500	-0.43776300
N	-1.62304300	1.58955300	-0.21819800
C	0.71406700	2.97815200	2.43350400
H	0.60620500	3.97886700	2.01649400
H	-0.27574200	2.60952200	2.72579200
H	1.29211700	3.04148800	3.36127800
H	-0.03345700	6.67419200	-2.11498400
B	-2.57573800	0.30080700	0.00842700
C	4.05690500	-1.28129700	-4.42731800
H	3.41191700	-2.16585800	-4.42171700
H	3.63342600	-0.57105800	-5.14396200
C	4.16307600	-0.67451000	-3.02729900
H	4.64708000	-1.39651300	-2.36470000
H	4.80435700	0.21774400	-3.05072100
C	2.07945900	0.76509000	-3.06334200
H	2.57388500	1.39455700	-3.80397500
H	0.99808200	0.71171900	-3.16806200
C	2.79562500	-0.33051100	-2.51383800
H	2.12065100	1.98840900	-2.01760000
H	2.18603700	-1.17425400	-2.19875000
C	-2.43324400	-0.53907900	-1.37019500
C	-1.17518100	-0.85180500	-1.87832000
C	-3.50089000	-1.03849600	-2.11700700
C	-0.95382000	-1.60791400	-3.01609300
C	-3.32875900	-1.79271300	-3.27808900
C	-2.04907500	-2.07762800	-3.73385900
C	-4.03848800	0.93118900	0.26042700
C	-4.53510300	1.93575700	-0.56861900
C	-4.92043900	0.48724300	1.24276800
C	-5.80207100	2.48642700	-0.44081300
C	-6.20076900	1.00611600	1.40672500
C	-6.64412800	2.01544300	0.56070100
C	-1.88469100	-0.39873900	1.31240100
C	-1.77856800	0.33852100	2.49311400

C	-1.29512600	-1.66345800	1.36783700
C	-1.12491600	-0.09934000	3.63570400
C	-0.60528400	-2.13617000	2.48638500
C	-0.51627000	-1.34943100	3.62645600
F	-4.56278300	-0.49763000	2.08510900
F	-7.00098500	0.54384700	2.36512800
F	-7.86195700	2.52520000	0.70428400
F	-6.21469700	3.45041500	-1.26449100
F	-3.76805100	2.40701600	-1.58106300
F	0.28949900	-1.89218300	-3.43202200
F	-0.06683300	-0.43923200	-1.19214500
F	-1.86662500	-2.79538400	-4.83554000
F	-4.38389800	-2.24254500	-3.94968600
F	-4.76808700	-0.83626100	-1.73962800
F	-1.34211200	-2.50635000	0.32765500
F	-0.00039300	-3.32640100	2.45378900
F	0.20622000	-1.75148100	4.67112200
F	-0.97749700	0.70698700	4.69141300
F	-2.29062300	1.58768500	2.53953400
H	5.03934800	-1.58603700	-4.79526700
H	0.76837800	0.02834800	1.62578800

Pcw-1f

SCF energy: -3631.3171064 a.u.

enthalpy: -3630.493151 a.u.

Gibbs free energy: -3630. 653783 a.u.

Ni	2.47610300	1.10659800	-0.92222000
N	3.16909700	-0.05893500	0.44918500
N	1.72684000	2.44822500	0.36947400
C	3.43834900	-0.83592900	2.78323400
H	2.65623100	-1.40522800	3.30146000
H	3.88034200	-0.17422600	3.53690400
H	4.20119900	-1.52630500	2.42861700
C	2.82719700	-0.01043000	1.69673000
C	1.70961900	0.85964100	2.18349200
H	1.76563900	0.93476000	3.27379600
C	1.44866900	2.21226100	1.61070300
C	4.21559800	-0.97253600	0.07069400
C	5.47910200	-0.43458200	-0.23015400
C	6.48574900	-1.32740200	-0.60386600
H	7.47519000	-0.94882600	-0.84046500
C	6.23549600	-2.69077900	-0.69425500
H	7.03022000	-3.36889200	-0.98939500
C	4.96875100	-3.18985400	-0.41287200

H	4.78562300	-4.25709200	-0.49177000
C	3.92671200	-2.34744500	-0.01673000
C	5.71905900	1.06294200	-0.18054600
H	4.81664600	1.53616200	-0.61779900
C	6.91590300	1.51229900	-1.00973100
H	6.94945000	2.60362600	-1.06701400
H	6.88333500	1.12128900	-2.03123400
H	7.86122800	1.18991100	-0.56147700
C	5.85968600	1.58570300	1.25093100
H	6.04814500	2.66405400	1.25208300
H	6.70217400	1.10315700	1.75695100
H	4.96609200	1.40709300	1.85620100
C	2.53561100	-2.89836200	0.24736900
H	2.08773900	-2.33277800	1.07572600
C	2.52510400	-4.35960400	0.67661100
H	1.51838400	-4.63487600	1.00298100
H	3.21235100	-4.54863700	1.50710400
H	2.79429700	-5.03225000	-0.14385500
C	1.63433600	-2.67959600	-0.97191000
H	0.71012100	-3.25493700	-0.88315600
H	2.13631800	-2.98668200	-1.89745500
H	1.35609100	-1.62468800	-1.06759600
C	1.23253500	3.63127400	-0.24004100
C	2.06374600	4.68426300	-0.60293400
C	1.53230900	5.78360700	-1.27465200
H	2.18625300	6.60767400	-1.54192400
C	-0.66418300	4.79085300	-1.27279600
H	-1.71662700	4.80337800	-1.53716700
C	0.17816900	5.83908300	-1.61112500
H	3.11903600	4.63574500	-0.35020000
C	-0.14058500	3.68580100	-0.58345600
C	-0.93717400	2.56385700	-0.26440900
N	-1.49583300	1.57884700	-0.02247200
C	0.77131400	3.16958500	2.53241800
H	0.61494600	4.15392700	2.09214200
H	-0.19964100	2.77299400	2.85280800
H	1.36345700	3.28307300	3.44573800
H	-0.21708500	6.69768500	-2.14203400
B	-2.24837000	0.18552700	0.17492900
C	4.01130500	-0.66098000	-4.58297400
H	3.18615200	-1.34854500	-4.79596800
H	3.83703100	0.25068100	-5.16324200
C	4.10079300	-0.36604800	-3.08379300
H	4.33965300	-1.29375600	-2.55324900

H	4.92503400	0.33380400	-2.88687500
C	2.40205400	1.55174300	-3.02951700
H	3.22246700	2.14749500	-3.43793000
H	1.53097800	1.55769600	-3.69171200
C	2.80384700	0.19058100	-2.58347500
H	1.97833000	2.18806700	-2.17584000
H	1.98694300	-0.53202000	-2.64657000
C	-1.89321800	-0.73811800	-1.11282500
C	-0.99576000	-0.47775300	-2.14035100
C	-2.59408600	-1.93826700	-1.24902600
C	-0.79131000	-1.32423600	-3.22419000
C	-2.42574800	-2.81807300	-2.31035200
C	-1.51341700	-2.50540300	-3.31506600
C	-3.81684000	0.57895600	0.17722700
C	-4.33092200	1.37247000	-0.84785100
C	-4.74891800	0.13744300	1.11364200
C	-5.66910000	1.72733500	-0.94944200
C	-6.09987900	0.46322200	1.04833900
C	-6.56236600	1.26536700	0.01110800
C	-1.64042100	-0.34300700	1.59433800
C	-1.71290500	0.49196400	2.71293800
C	-0.94787000	-1.53600200	1.81222300
C	-1.12112300	0.21742800	3.93863100
C	-0.33146300	-1.85061200	3.02452700
C	-0.40846300	-0.96764600	4.09245900
F	-4.36869600	-0.64846800	2.13337600
F	-6.95049100	0.01413700	1.96870300
F	-7.84807800	1.58935400	-0.06315700
F	-6.09908100	2.50016600	-1.94722200
F	-3.49885200	1.84223900	-1.80761800
F	0.11233800	-1.00903100	-4.16416400
F	-0.21933700	0.64354400	-2.13467300
F	-1.32847500	-3.33143600	-4.33843300
F	-3.11542400	-3.95343400	-2.37167400
F	-3.44962900	-2.29985000	-0.28076100
F	-0.80231700	-2.45446900	0.84792600
F	0.38782200	-2.97104600	3.14328000
F	0.24201500	-1.22356000	5.22392500
F	-1.16301900	1.10840300	4.93089600
F	-2.34573600	1.67867000	2.60955900
H	4.93379400	-1.11867300	-4.94761900
H	0.77875800	0.29681800	1.99671200

βH-1f

SCF energy: -3631.3208111 a.u.
enthalpy: -3630.499894 a.u.
Gibbs free energy: -3630.656519 a.u.

Ni	3.32241600	2.02167500	-0.50503800
N	3.71130700	0.87696300	1.05183300
N	2.16652600	3.22911300	0.43222100
C	3.73913500	0.21737800	3.42524200
H	4.45574100	-0.55546600	3.14629300
H	2.83474200	-0.27162600	3.80836200
H	4.14182200	0.80044800	4.25941300
C	3.38726000	1.10474300	2.27574200
C	2.64924000	2.34775800	2.67359100
H	3.36515700	2.96314500	3.24552900
C	1.96376100	3.26622800	1.71498300
C	4.56523800	-0.23298300	0.70257900
C	5.91436100	0.07324700	0.43211600
C	6.74565500	-0.97035600	0.02258000
H	7.79233500	-0.76884100	-0.18448800
C	6.25196100	-2.26030500	-0.12642800
H	6.91341300	-3.06142400	-0.44115200
C	4.91014500	-2.52572300	0.11549900
H	4.53744400	-3.53565300	-0.01828900
C	4.02982400	-1.52085200	0.52707200
C	6.44233300	1.48726700	0.59103700
H	5.62222200	2.17519800	0.30928500
C	7.62433200	1.79944300	-0.31895400
H	7.86574700	2.86522400	-0.27648100
H	7.42244800	1.53851600	-1.36265700
H	8.52594800	1.26012600	-0.01308300
C	6.80253900	1.78633100	2.04743700
H	7.15808800	2.81482100	2.16187900
H	7.59995100	1.11860300	2.38913300
H	5.95300800	1.64644300	2.72312300
C	2.54527400	-1.78696900	0.68642100
H	2.18779200	-1.23669300	1.57255300
C	2.21641900	-3.26001000	0.89172800
H	1.14742100	-3.39678900	1.05669000
H	2.74781100	-3.68622300	1.74775800
H	2.47056300	-3.85262000	0.00753100
C	1.78383900	-1.24227200	-0.52494300
H	0.71351100	-1.45134600	-0.44105800
H	2.13750000	-1.71182000	-1.44975900
H	1.90096800	-0.15444200	-0.63597100
C	1.43699900	4.12327900	-0.40708300

C	1.84141300	5.43376400	-0.62517300
C	1.13133600	6.24054300	-1.51348900
H	1.45951800	7.26183400	-1.67929300
C	-0.42995900	4.46008100	-1.95241600
H	-1.32148600	4.06746900	-2.43043200
C	0.00665000	5.75683800	-2.18155300
H	2.71411500	5.81446600	-0.10288700
C	0.28784900	3.64053200	-1.06520700
C	-0.20153400	2.35205700	-0.76006200
N	-0.70073300	1.34498800	-0.48177400
C	1.06354400	4.26598500	2.36894600
H	0.59135000	3.84023100	3.25504700
H	1.65279900	5.13141100	2.69487800
H	0.28576600	4.63408100	1.69991200
H	-0.53801200	6.39466100	-2.86850200
B	-1.71100700	0.22469600	0.04292000
C	3.22479000	0.50880700	-3.32142200
H	3.60350400	-0.51400800	-3.25560000
H	2.17486900	0.49847900	-3.01747100
C	4.04070200	1.46493400	-2.47121600
H	4.19207300	0.92610000	-1.44894500
H	5.09914800	1.49797700	-2.76417900
C	4.44882500	3.97436400	-2.24776100
H	5.36624900	3.73928000	-1.69533700
H	4.75281800	4.22895800	-3.27235800
C	3.48635800	2.82351800	-2.24305700
H	4.01534400	4.88195200	-1.82020500
H	2.52543000	3.01810700	-2.73087400
C	-1.94805300	-0.85032400	-1.13722200
C	-1.27048700	-0.92851500	-2.34920700
C	-2.99582200	-1.75913500	-0.98583000
C	-1.58904400	-1.84614700	-3.34519800
C	-3.34940300	-2.69339900	-1.94872200
C	-2.63880200	-2.73280200	-3.14506000
C	-3.07157600	1.09178900	0.27739600
C	-3.56418900	1.90295300	-0.74591700
C	-3.85983000	1.05270900	1.42684700
C	-4.73352000	2.64494200	-0.65312800
C	-5.04427500	1.77182400	1.56042900
C	-5.48316700	2.57641100	0.51581500
C	-1.01824000	-0.32323000	1.41196700
C	-0.60460700	0.57950200	2.39082000
C	-0.83408000	-1.66245600	1.75684900
C	-0.05400600	0.21035600	3.60815500

C	-0.28710600	-2.08064900	2.97036900
C	0.12175400	-1.13604700	3.90066500
F	-3.50953700	0.29008600	2.47442700
F	-5.75782700	1.69696000	2.68217200
F	-6.60651100	3.27550300	0.63241200
F	-5.13610400	3.41556000	-1.66513400
F	-2.87904500	2.00230600	-1.91256000
F	-0.89627900	-1.87471000	-4.48611800
F	-0.23586100	-0.09653500	-2.62014400
F	-2.95612800	-3.61797500	-4.08390300
F	-4.35044800	-3.54603800	-1.74234800
F	-3.68865300	-1.76338500	0.16648500
F	-1.14934600	-2.64883200	0.90581600
F	-0.12441100	-3.37646400	3.22628200
F	0.69169000	-1.50253000	5.04600000
F	0.32804900	1.14150900	4.50436800
F	-0.76108700	1.91162600	2.18926700
H	3.26835700	0.81608100	-4.36885700
H	1.91388600	2.07648200	3.43914600

$TS_{\beta Htrans}$-1g

SCF energy: -3631.3047056 a.u.

Enthalpy: -3630.486863 a.u.

Gibbs free energy: -3630.645413 a.u.

Ni	3.21856300	1.77316100	-0.64341300
N	3.66051100	0.60044600	0.88189300
N	2.24948600	3.09832400	0.44038700
C	3.71730700	-0.18733100	3.21890600
H	2.87173000	-0.82899400	3.49928000
H	3.99018900	0.37333200	4.11752900
H	4.54559800	-0.83590100	2.93358900
C	3.31159100	0.73705100	2.11440700
C	2.43616700	1.85882500	2.56312000
H	2.91700000	2.32174600	3.43781600
C	1.95725900	2.97515100	1.70136700
C	4.56870800	-0.46555100	0.51746500
C	5.89896400	-0.10397900	0.22921700
C	6.77281800	-1.11763800	-0.16622000
H	7.80756000	-0.87322900	-0.38684000
C	6.33819400	-2.43281100	-0.28273300
H	7.03338100	-3.20851800	-0.58836600
C	5.01355700	-2.75426700	-0.01729700
H	4.68024000	-3.78203500	-0.12529100
C	4.09487600	-1.78136100	0.38644700

C	6.36366000	1.33260400	0.37160300
H	5.51652500	1.97870800	0.07251100
C	7.53970300	1.68272100	-0.53174500
H	7.73940800	2.75755900	-0.49741900
H	7.35573800	1.40431000	-1.57430200
H	8.45937900	1.18190100	-0.21404300
C	6.69481600	1.66509300	1.82776900
H	7.01215200	2.70720000	1.93157000
H	7.51088800	1.03122100	2.18951300
H	5.84106300	1.50656900	2.49466700
C	2.62866600	-2.12098000	0.56054600
H	2.19957800	-1.44853100	1.31531300
C	2.38657200	-3.54393100	1.04767800
H	1.32983700	-3.68201600	1.28533500
H	2.96626600	-3.76686000	1.94901700
H	2.64726900	-4.28737700	0.28817900
C	1.89028600	-1.85051000	-0.75313400
H	0.84433900	-2.15528600	-0.68214700
H	2.34992600	-2.40576600	-1.57905800
H	1.90981100	-0.78274100	-1.01547300
C	1.65028800	4.19756100	-0.24839700
C	2.31955300	5.40145800	-0.43102300
C	1.71857100	6.43177000	-1.15250100
H	2.25442800	7.36629300	-1.28600700
C	-0.25612400	5.10074700	-1.49562100
H	-1.26054500	4.96178500	-1.88302900
C	0.44482300	6.27915900	-1.70069800
H	3.30800600	5.52662200	0.00018100
C	0.34068600	4.06522400	-0.75761100
C	-0.39445100	2.90237100	-0.45005900
N	-1.00038000	1.96265800	-0.15397700
C	1.07044900	3.94172400	2.42609700
H	1.27228500	4.97639800	2.14183500
H	0.01647200	3.74583200	2.19506600
H	1.17408900	3.84072000	3.50750000
H	-0.00640300	7.08399400	-2.26981300
B	-1.85774700	0.69720200	0.25816400
C	2.86626700	0.42383600	-3.55627300
H	3.15383900	-0.62420500	-3.45018600
H	1.80846600	0.51643700	-3.31622900
C	3.72366200	1.33591200	-2.72266000
H	3.79537100	0.59109800	-1.44481000
H	4.79962100	1.21866200	-2.89383600
C	4.38534100	3.73904400	-2.40165400

H	5.32996100	3.36199800	-1.99408700
H	4.58934200	4.06406300	-3.43026200
C	3.32189100	2.67866400	-2.38873900
H	4.10790000	4.63477100	-1.84528900
H	2.32089500	2.97716300	-2.71752500
C	-1.65848600	-0.43567700	-0.87912200
C	-0.88551100	-0.35481000	-2.03050000
C	-2.38635200	-1.61805900	-0.74194100
C	-0.80418500	-1.37360900	-2.97366900
C	-2.34134400	-2.66178300	-1.65590700
C	-1.54013300	-2.53596700	-2.78838700
C	-3.39268700	1.21413200	0.25157800
C	-3.87989800	1.95158400	-0.82669100
C	-4.33045000	0.90726100	1.23534600
C	-5.19617100	2.37949800	-0.93484800
C	-5.66071300	1.30848600	1.16488400
C	-6.09574500	2.05246500	0.07396300
C	-1.23668700	0.36408300	1.73139900
C	-1.30269300	1.33984200	2.72800900
C	-0.57221000	-0.80034400	2.10969900
C	-0.75581600	1.20600500	3.99796900
C	0.01270000	-0.97334100	3.36372400
C	-0.07832000	0.03114100	4.31796200
F	-3.97544800	0.18840600	2.31216100
F	-6.51705900	0.98947100	2.13322700
F	-7.36125300	2.44818600	-0.00551200
F	-5.59868900	3.09444100	-1.98628600
F	-3.04500700	2.28545900	-1.84012200
F	-0.00387000	-1.24652100	-4.03820000
F	-0.11650500	0.73713700	-2.27980400
F	-1.47186000	-3.52272800	-3.67560800
F	-3.04583700	-3.77374200	-1.46171500
F	-3.14614200	-1.78280600	0.35356600
F	-0.44053800	-1.83691800	1.26989600
F	0.70014800	-2.08733700	3.63862800
F	0.51223200	-0.10922900	5.50148700
F	-0.82405900	2.20192900	4.88393300
F	-1.90951500	2.51576500	2.45877300
H	2.99699500	0.69484500	-4.60850900
H	1.53203800	1.41605600	3.01339900

$TS_{\beta Hcis}$-1g

SCF energy: -3631.3085533 a.u.

Enthalpy: -3630.490683 a.u.

Gibbs free energy: -3630.651575 a.u.

Ni	2.95759600	1.64768300	-0.63321900
N	3.59117700	0.53770400	0.84598000
N	2.30299300	3.08552500	0.53211100
C	3.77298500	-0.26181300	3.17167600
H	2.92370700	-0.78297700	3.63204900
H	4.24696500	0.31765600	3.97047900
H	4.48010600	-1.00529900	2.80507000
C	3.27780700	0.63970200	2.08918600
C	2.31066900	1.68056500	2.55096200
H	2.58708600	1.97737400	3.57003300
C	1.99351100	2.92181900	1.78422400
C	4.54822100	-0.44969200	0.40754100
C	5.84358500	0.00257000	0.08755900
C	6.75815900	-0.94127300	-0.38170000
H	7.76826900	-0.62833100	-0.62809600
C	6.39359500	-2.27303500	-0.55130100
H	7.12018300	-2.99102600	-0.91870700
C	5.09776500	-2.67988200	-0.26483200
H	4.81062700	-3.71713600	-0.42000500
C	4.14276700	-1.78067300	0.21891600
C	6.22103700	1.46341900	0.25564400
H	5.33701300	2.05821300	-0.04395100
C	7.38377400	1.89833500	-0.62866400
H	7.51078000	2.98359800	-0.58198900
H	7.23816400	1.62060400	-1.67761300
H	8.32919100	1.45532600	-0.30018600
C	6.52517900	1.80458500	1.71596500
H	6.79403200	2.85990900	1.82387400
H	7.36787900	1.20863200	2.08107200
H	5.67587300	1.60778700	2.37698400
C	2.71554600	-2.23846500	0.43972300
H	2.15553200	-1.42726600	0.92023400
C	2.62181700	-3.46087300	1.34906200
H	1.57530700	-3.72388800	1.52344700
H	3.08880800	-3.28539600	2.32306700
H	3.10977700	-4.33245000	0.90154800
C	2.04368600	-2.51502100	-0.90686700
H	0.99250600	-2.78531300	-0.76897900
H	2.53835800	-3.34078800	-1.42946600
H	2.08030100	-1.64118100	-1.56873400
C	1.81557200	4.26272400	-0.10728200
C	2.60059700	5.39742900	-0.26503400
C	2.08492800	6.51005800	-0.92842400

H	2.70534800	7.39370800	-1.04062500
C	-0.01044700	5.38102700	-1.29677100
H	-1.02237900	5.35048800	-1.68765200
C	0.79164300	6.50157500	-1.45273600
H	3.61265800	5.39911600	0.12904400
C	0.49640300	4.26436700	-0.61378000
C	-0.29563400	3.11758300	-0.39047900
N	-0.89374900	2.15286900	-0.16381800
C	1.19217700	3.92244800	2.55968100
H	1.42264500	4.94981000	2.27293300
H	0.12022700	3.77015600	2.37920300
H	1.34335100	3.80847500	3.63405100
H	0.40867000	7.37024900	-1.97615900
B	-1.73253200	0.84765100	0.17743100
C	4.50465600	0.58450000	-3.17414900
H	4.63932100	0.84881500	-4.22827800
H	5.32779500	1.03203700	-2.61104700
C	3.15907900	1.07393000	-2.70758600
H	3.02030000	0.33293400	-1.43304300
H	2.30767400	0.53687400	-3.12925300
C	4.01278600	3.46842900	-2.61481900
H	4.92325200	3.20590900	-2.06236700
H	4.30168200	3.52852300	-3.67299800
C	2.91013100	2.46770600	-2.42257200
H	3.71003400	4.47176600	-2.31384600
H	1.90030200	2.81804000	-2.64657300
C	-1.44027800	-0.26193800	-0.96317500
C	-0.57497100	-0.16296900	-2.04346500
C	-2.17252800	-1.44890400	-0.90784900
C	-0.41926700	-1.16091900	-2.99839300
C	-2.05834300	-2.47111500	-1.84044200
C	-1.16841100	-2.32458000	-2.90230400
C	-3.27874100	1.32160300	0.09404600
C	-3.72367700	2.03848900	-1.01603400
C	-4.26096400	0.99899700	1.02768200
C	-5.04130900	2.43583600	-1.19900300
C	-5.59368200	1.37068000	0.88279600
C	-5.98584700	2.09675200	-0.23611000
C	-1.18739100	0.48278800	1.67280300
C	-1.32782500	1.42524800	2.69422400
C	-0.54465200	-0.69364500	2.05822100
C	-0.87739500	1.24858100	3.99640300
C	-0.06622000	-0.91291600	3.35049600
C	-0.23365800	0.05928700	4.32878900

F	-3.95046700	0.29039100	2.12516700
F	-6.49416200	1.03846700	1.80541400
F	-7.25391800	2.46286800	-0.38507000
F	-5.40232100	3.13149100	-2.27790900
F	-2.84170000	2.38004000	-1.98472900
F	0.47619200	-1.01270800	-3.98472800
F	0.20323500	0.93717300	-2.21829400
F	-1.02700000	-3.29296700	-3.80067600
F	-2.77723000	-3.58471200	-1.72684100
F	-3.00984500	-1.64136400	0.12406600
F	-0.32756400	-1.69379600	1.19076300
F	0.59508200	-2.03650300	3.64404400
F	0.25989000	-0.12475100	5.54919400
F	-1.00920300	2.21642500	4.90421900
F	-1.91226600	2.61095200	2.41966700
H	4.59160000	-0.50083200	-3.08577200
H	1.34014100	1.17948000	2.70328700

$P_{\beta Htrans}$-1g

SCF energy: -3631.3080818 a.u.

Enthalpy: -3630.499258 a.u.

Gibbs free energy: -3630.652036 a.u.

Ni	3.04320700	1.71503500	-0.63093700
N	3.58814700	0.52641800	0.90891300
N	2.26548300	3.10905300	0.73447600
C	3.76971500	-0.33847600	3.20822500
H	2.93437000	-0.91463800	3.62670200
H	4.20080200	0.22770500	4.04004900
H	4.51421600	-1.03743500	2.82738600
C	3.26527600	0.58958700	2.15205000
C	2.27313900	1.59594700	2.65205700
H	2.49591400	1.81653100	3.70355300
C	1.95757400	2.88678400	1.96889900
C	4.51234300	-0.44521500	0.41116100
C	5.73619000	0.05860500	-0.07970800
C	6.63075600	-0.84105500	-0.65360200
H	7.58505700	-0.48600100	-1.03044800
C	6.31131200	-2.19295200	-0.75954100
H	7.01688700	-2.88128800	-1.21385300
C	5.08840600	-2.65620400	-0.29772400
H	4.83788100	-3.70898100	-0.40377000
C	4.15439300	-1.79893100	0.29618200
C	6.06370600	1.53706700	0.05036500
H	5.12808900	2.11527500	-0.14246500

C	7.08691700	2.03390500	-0.96150000
H	7.18548800	3.12144700	-0.90399100
H	6.81996900	1.77038300	-1.99016200
H	8.07752300	1.61508900	-0.76118000
C	6.49752700	1.89307100	1.47215700
H	6.70074400	2.96407000	1.56768200
H	7.41530100	1.35557900	1.72973300
H	5.74173700	1.62264200	2.21542600
C	2.80157200	-2.34511700	0.71217500
H	2.25229400	-1.56562900	1.25381900
C	2.92599500	-3.54667400	1.64736200
H	1.93652500	-3.84664000	2.00295700
H	3.54664100	-3.32903100	2.52236400
H	3.36710300	-4.40955500	1.13866100
C	1.96900100	-2.70887200	-0.52090000
H	1.05920800	-3.23855900	-0.22930600
H	2.53316100	-3.36109300	-1.19644000
H	1.66795800	-1.81890500	-1.08438000
C	1.82019800	4.29698800	0.10634000
C	2.58727900	5.45605600	0.06850500
C	2.13197300	6.56451900	-0.64250300
H	2.73606800	7.46621800	-0.66143400
C	0.13345800	5.38804200	-1.29726200
H	-0.82153000	5.34113900	-1.81078200
C	0.91854700	6.53102100	-1.33263100
H	3.54161700	5.47741100	0.58699400
C	0.57891800	4.27222400	-0.57176600
C	-0.20856900	3.10782900	-0.44480300
N	-0.81727500	2.13795100	-0.27352800
C	1.21665600	3.86412400	2.82637400
H	0.54937200	4.50822100	2.25212800
H	0.63885200	3.36094000	3.60431800
H	1.93719500	4.51376400	3.33733100
H	0.58281100	7.39858200	-1.88926400
B	-1.70234600	0.87129300	0.07874500
C	3.09753500	-0.20726600	-2.95941100
H	3.42361100	-1.06213200	-2.35998200
H	2.00889000	-0.20667700	-3.02561200
C	3.62887100	1.07733000	-2.42090800
H	1.80965300	1.06852100	-0.88499400
H	4.71978400	1.10267000	-2.30437700
C	3.76194100	3.60799900	-2.62811500
H	4.64348400	3.61400100	-1.97237100
H	4.14046300	3.72751200	-3.65153300

C	2.97821700	2.33379600	-2.51505000
H	3.16228500	4.49248500	-2.40442900
H	1.96714200	2.34145100	-2.92413000
C	-1.49261000	-0.26470400	-1.05332200
C	-0.77775400	-0.16429300	-2.24037300
C	-2.19894400	-1.45762800	-0.89404900
C	-0.72782900	-1.17788100	-3.19291200
C	-2.17611300	-2.49892700	-1.81071700
C	-1.42829800	-2.35670500	-2.97659800
C	-3.23425400	1.39946200	0.00557500
C	-3.65877000	2.13602700	-1.09996500
C	-4.22746900	1.09659700	0.93472100
C	-4.96455000	2.57060100	-1.28232100
C	-5.54946100	1.50556400	0.78968300
C	-5.92010300	2.25031900	-0.32393300
C	-1.17234200	0.50237500	1.58110700
C	-1.33686400	1.43533100	2.60864800
C	-0.55321300	-0.68330300	1.97621200
C	-0.96853100	1.21592200	3.93046800
C	-0.14720600	-0.93823100	3.28658600
C	-0.36023200	0.01263700	4.27614000
F	-3.94116800	0.37510000	2.03079100
F	-6.45995900	1.19227800	1.70934200
F	-7.17768700	2.65187100	-0.47195100
F	-5.30417900	3.28339000	-2.35702000
F	-2.76745000	2.45775900	-2.06642000
F	-0.00474900	-1.02146600	-4.30685000
F	-0.06958700	0.95479900	-2.53739400
F	-1.38685600	-3.33701600	-3.87261200
F	-2.85453300	-3.62237400	-1.58914100
F	-2.92586300	-1.63057000	0.22378200
F	-0.28698500	-1.66174200	1.10037100
F	0.49572100	-2.07251100	3.58434600
F	0.05957200	-0.20123300	5.51884600
F	-1.12565100	2.17244700	4.85103000
F	-1.87115800	2.63899500	2.32936500
H	3.48886700	-0.36553000	-3.97169000
H	1.30427900	1.07449700	2.71681800

$P_{\beta Hcis}$-1g

SCF energy: -3631.3094784 a.u.

Enthalpy: -3630.499276 a.u.

Gibbs free energy: -3630.653703 a.u.

Ni	2.98161500	1.52818700	-0.64543600

N	3.56788500	0.46545900	0.90551800
N	2.41297100	3.10592900	0.69811200
C	3.78870800	-0.25851100	3.24738700
H	2.97430800	-0.83367100	3.70736000
H	4.19991900	0.37559600	4.03955100
H	4.55625000	-0.95281200	2.90656300
C	3.23713300	0.57959200	2.14354900
C	2.17573400	1.55068600	2.55893800
H	2.22292100	1.69039300	3.64360300
C	1.99608300	2.88551300	1.90041000
C	4.58185400	-0.45139300	0.47929100
C	5.82028700	0.10501700	0.10333500
C	6.81436900	-0.76651500	-0.33688400
H	7.78564300	-0.37480700	-0.62345500
C	6.56923500	-2.13346500	-0.43802700
H	7.35287300	-2.79778600	-0.78854700
C	5.31824500	-2.64520200	-0.11811500
H	5.12696000	-3.70877000	-0.23405700
C	4.29005400	-1.81857500	0.34524300
C	6.03693700	1.60872200	0.16023900
H	5.09096200	2.09413100	-0.17394900
C	7.12908500	2.10387000	-0.77915100
H	7.13650200	3.19699600	-0.81360800
H	7.00324000	1.73169100	-1.80101900
H	8.11958900	1.79063000	-0.43551200
C	6.30053000	2.10566800	1.58151600
H	6.43075700	3.19227600	1.59935900
H	7.21668200	1.65411200	1.97478400
H	5.48953300	1.85334700	2.27031800
C	2.89610100	-2.36835400	0.56916200
H	2.32428100	-1.64909500	1.16797200
C	2.87804500	-3.69324900	1.32253200
H	1.84566600	-3.99267700	1.52198700
H	3.39947000	-3.62561800	2.28245900
H	3.34280500	-4.49940700	0.74654100
C	2.18687100	-2.49287100	-0.78315900
H	1.18442000	-2.91150200	-0.66383700
H	2.74937900	-3.14779400	-1.45773800
H	2.08598400	-1.51532800	-1.27001400
C	1.98448500	4.27122800	0.02511700
C	2.80706600	5.37691200	-0.16184400
C	2.34892100	6.46376100	-0.90360400
H	2.99491500	7.32661300	-1.03267500
C	0.24571300	5.36292900	-1.31657200

H	-0.74506500	5.33225200	-1.75882900
C	1.08021100	6.45692800	-1.48754300
H	3.80145500	5.37458500	0.27582600
C	0.69076500	4.27204900	-0.55220400
C	-0.13469400	3.14341000	-0.34753100
N	-0.78421300	2.20173400	-0.16173100
C	1.18760700	3.85808300	2.69925900
H	0.13121600	3.56119400	2.70003300
H	1.50188000	3.85714700	3.74578000
H	1.24855900	4.87399600	2.30854100
H	0.74377100	7.30529400	-2.07255300
B	-1.69339500	0.92117300	0.10296100
C	4.31581900	0.17984500	-2.86462400
H	4.40396200	0.05539500	-3.95214500
H	5.18415600	0.75725600	-2.53377400
C	3.01398700	0.84165200	-2.55094000
H	1.74945600	0.82142000	-0.68962200
H	2.12842800	0.23639800	-2.73344400
C	3.90470500	3.23116900	-2.74000900
H	4.85796800	2.94223300	-2.28047100
H	4.10250900	3.31647400	-3.81670600
C	2.80833900	2.23876600	-2.49123300
H	3.64236300	4.22947100	-2.38345400
H	1.78983800	2.59102200	-2.64748200
C	-1.45587800	-0.14778200	-1.08884700
C	-0.71990700	0.01735400	-2.25536800
C	-2.12731200	-1.36736900	-0.99001600
C	-0.59513800	-0.96779700	-3.22995400
C	-2.04302600	-2.37680000	-1.93861700
C	-1.26044000	-2.17564800	-3.07302300
C	-3.22029700	1.45751700	0.04001100
C	-3.63027900	2.26499200	-1.02058300
C	-4.22650100	1.09499800	0.93347600
C	-4.93380900	2.71058800	-1.19217300
C	-5.54661500	1.51274000	0.79752800
C	-5.90236300	2.32843800	-0.27031700
C	-1.17814400	0.44911600	1.58252000
C	-1.35414700	1.31567000	2.66472600
C	-0.50697200	-0.73313500	1.90053300
C	-0.91715200	1.06173400	3.95867800
C	-0.04945800	-1.03158700	3.18458700
C	-0.25176100	-0.13160000	4.22189200
F	-3.95418800	0.30521600	1.98503100
F	-6.46926000	1.14012600	1.68211500

F	-7.15799700	2.73859900	-0.40982300
F	-5.25936300	3.49131900	-2.22312000
F	-2.72653700	2.65039800	-1.95195800
F	0.16865000	-0.75391300	-4.30729200
F	-0.06363900	1.17629600	-2.51191100
F	-1.15107700	-3.12803600	-3.99304900
F	-2.69034200	-3.52779100	-1.77298700
F	-2.87077500	-1.60486900	0.10422000
F	-0.21973900	-1.65584600	0.97046500
F	0.64700100	-2.15147500	3.40775700
F	0.24759800	-0.37693000	5.42972700
F	-1.06746900	1.97215700	4.92152900
F	-1.94337800	2.51220400	2.46116500
H	4.38472400	-0.81799500	-2.42099800
H	1.20851000	1.04766900	2.39796600