Supporting Information

to the manuscript

POCN Ni(II) pincer complexes: synthesis, characterization and evaluation of catalytic hydrosilylation and hydroboration activity

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Experimental details

All manipulations were carried out using conventional inert atmosphere glove-box and Schlenk techniques. All protonated and deuterated solvents were dried by distillation from appropriate drying agents. NMR spectra were obtained with a Bruker Avance 300, 400 and 600 MHz and JEOL ECA-500 MHz instruments (^{1}H: 300, 400, 500 and 600 MHz; ^{13}C: 75.5, 125.8 and 151 MHz; ^{31}P: 121.5, 202.5 and 243 MHz; ^{29}Si: 99.4 and 119.2 MHz). ^{1}H and ^{13}C chemical shifts were referenced to residual proton and naturally abundant ^{13}C resonance of the deuterated solvent, respectively. ^{31}P NMR spectra were referenced to 85% H_3PO_4 externally. NMR analysis was done at room temperature unless specified. IR spectra were measured on an Nicolet iS10 FT-IR spectrometer. Elemental analyses were performed in the "Nazarbayev University Core Facilities" laboratories using Perkin Elmer 2400 Series II CHNS/O Elemental Analyzer. The preparation of iminophosphinite pincer ligands and the corresponding POCN bromide complexes of Ni(II), **1-^{t}Bu**, **1-Ph**, **1-Ar'**, and **1-Ar** was performed according to the literature procedures for analogous compounds.[1] $Ni(COD)_2$, 3-hydroxybenzaldehyde, $LiBHEt_3$ (1.0 M solution in THF), BF_3*Et_2O (45% in Et_2O), $AgBF_4$, $NaBPh_4$, $LiB(C_6F_5)_4$*Et_2O, L-Selectride (1.0 M solution in THF), MeLi (1.6 M solution in Et_2O), $LiBH_4$ (2.0 M solution in THF), $PhSiH_3$, $PhMeSiH_2$, Et_3SiH, tetramethylsilane, $Si(SiMe_3)_4$, HBPin, styrene, 1-octene, allylbenzene, benzaldehyde, acetone, cyclohexanone, acetophenone, benzophenone, EOAc, DMF, *N*-methylsuccinimide, acetamide, *N*-phenylpropionamide, *trans*-2-octene, cyclohexene, 4-octyne, 1-hexyne, nitrobenzene, and diisopropylamine were purchased from Sigma-Aldrich and used without further purification unless specified. Benzaldehyde, acetone, acetophenone, ethyl acetate, DMF were additionally dried over 3Å molecular sieves. *N*,*N*-diisopropylbenzamide was synthesized using literature procedure.[2] All catalytic reactions were done under nitrogen or argon atmosphere using NMR tubes equipped with Teflon valves. The yields for products and conversions of the substrates were determined by ^{1}H-NMR against tetrakis(trimethylsilyl)silane as an internal standard. Small amounts of Ph_2SiH_2, produced *via* redistribution of substituents in $PhSiH_3$, were observed in hydrosilylation reactions with $PhSiH_3$.[3]

Characterization of alcohol precursors to iminophosphinite POCN pincer ligands

1-(HO)-3-(CH=N^{t}Bu)-C$_6$H$_4$:[4]

^{1}H-NMR (500 MHz; $CDCl_3$; δ, ppm): 1.37 (s, 9H, 3 CH_3 of N^{t}Bu); 6.88 (m, 1H, C*H*); 7.21 (t, $^3J_{H\text{-}H}$ = 7.9 Hz, 1H, C*H*); 7.28 (m, 1H, C*H*); 8.24 (s, 1H, C*H*=N^{t}Bu); 8.58 (br s, O*H*). ^{13}C{^{1}H}-NMR (125.8 MHz; C_6D_6; δ, ppm): 29.7 (s, 3 CH_3 of N^t*Bu*); 57.3 (s, C_q of N^t*Bu*); 114.3 (s); 117.8 (s); 121.4 (s); 129.8 (s); 139.2 (s); 154.8 (s); 156.9 (s). NMR data are consistent with the previously published data.[4]

1-(HO)-3-(CH=NPh)-C$_6$H$_4$:[4]

^{1}H-NMR (500 MHz; C_6D_6; δ, ppm): 4.41 (br s, 1H, O*H*); 6.62 (br d, $^3J_{H\text{-}H}$ = 7.9 Hz, 1H); 6.99 (t, $^3J_{H\text{-}H}$ = 7.8 Hz, 1H); 7.04 (t, $^3J_{H\text{-}H}$ = 7.1 Hz, 1H); 7.17 (m, 4H); 7.26 (d, $^3J_{H\text{-}H}$ = 7.5 Hz, 1H); 7.3 (s, 1H); 8.07 (s, 1H, C*H*=NPh). ^{13}C{^{1}H}-NMR (125.8 MHz; C_6D_6; δ, ppm): 114.8 (s); 118.8 (s); 121.4 (s); 122.3 (s); 126.2 (s); 128.0 (s); 128.4 (s); 129.4 (s); 130.0 (s); 138.4 (s); 152.6 (s); 156.8 (s); 160.0 (s). NMR data are consistent with the previously published data.[4]

1-(HO)-3-(CH=NAr')-C$_6$H$_4$:

^{1}H-NMR (500 MHz; C_6D_6; δ, ppm): 2.12 (s, 6H, 2 CH_3, N*Ar'*); 4.22 (br s, O*H*); 6.61 (br d, $^3J_{H\text{-}H}$ = 8.4 Hz, 1H); 6.98 (m, 2H); 7.04 (m, 2H); 7.19 (d, $^3J_{H\text{-}H}$ = 7.6 Hz, 1H); 7.27 (s, 1H); 7.74 (s, C*H*=NAr'). ^{13}C{^{1}H}-NMR (125.8 MHz; C_6D_6; δ, ppm): 18.5 (s, 2 *CH_3*, N*Ar'*); 114.3 (s); 118.8 (s); 122.0 (s); 124.1 (s); 127.2 (s); 128.0 (s); 128.4 (s); 128.5 (s); 130.1 (s); 138.2 (s); 151.9 (s); 156.8 (s); 162.5 (s).

1-(HO)-3-(CH=NAr)-C$_6$H$_4$:

^{1}H-NMR (500 MHz; C_6D_6; δ, ppm): 1.18 (d, $^3J_{H\text{-}H}$ = 6.8 Hz, 12H, 4 CH_3, N*Ar*); 3.13 (sept, $^3J_{H\text{-}H}$ = 6.8 Hz, 2H, 2 CH, N*Ar*); 4.21 (br s, O*H*); 6.61 (br d, $^3J_{H\text{-}H}$ = 8.2 Hz, 1H); 6.98 (t, $^3J_{H\text{-}H}$ = 7.8 Hz, 1H); 7.13-7.19 (m, 3H); 7.24 (d, $^3J_{H\text{-}H}$ = 7.5 Hz, 1H); 7.26 (s, 1H); 7.95 (s, C*H*=NAr). ^{13}C{^{1}H}-NMR (125.8 MHz; C_6D_6; δ, ppm): 23.6 (s, 4 *CH_3*, N*Ar*); 28.5 (s, 2 *CH*, N*Ar*); 114.4 (s); 118.9 (s); 121.9 (s); 122.5 (s); 124.7 (s); 128.0 (s); 128.4 (s); 130.3 (s); 137.8 (s); 138.1 (s); 150.0 (s); 156.9 (s); 162.1 (s).

Characterization of iminophosphinite POCN pincer ligands

1-(^{i}Pr$_2$PO)-3-(CH=N^{t}Bu)-C$_6$H$_4$:

^{1}H-NMR (500 MHz; C_6D_6; δ, ppm): 0.95 (dd, J = 7.3 and 15.6 Hz, 6H, 2 CH_3 of $^{i}Pr_2$P); 1.11 (dd, J = 7.1 and 10.7 Hz, 6H, 2 CH_3 of $^{i}Pr_2$P); 1.21 (s, 9H, 3 CH_3 of N^{t}Bu); 1.75 (m, 2H, 2CH of $^{i}Pr_2$P); 7.11 (t, $^3J_{H\text{-}H}$ = 7.8 Hz, 1H, C*H*); 7.30 (br d, $^3J_{H\text{-}H}$ = 8.1 Hz, 1H, C*H*); 7.45 (br d, $^3J_{H\text{-}H}$ = 7.5 Hz, 1H, C*H*); 7.99 (br s, 1H, C*H*); 8.13 (s, C*H*=NPh). ^{13}C{^{1}H}-NMR (125.8 MHz; C_6D_6; δ, ppm): 17.1 (d, J = 8.6 Hz, 2 CH_3 of $^{i}Pr_2$P); 17.8 (d, J = 20.5 Hz, 2 CH_3 of $^{i}Pr_2$P); 28.6 (d, J = 18.7 Hz, 2 CH of $^{i}Pr_2$P); 29.8 (s, 3 CH_3 of N^{t}Bu); 57.3 (s, C_q of N^{t}Bu); 118.1 (d, J = 10.2 Hz); 120.5 (d, J = 10.7 Hz); 122.2 (s); 129.7 (s); 139.6 (s, C); 154.3 (s); 160.3 (d, J = 8.6 Hz). ^{31}P{^{1}H}-NMR (202.5 MHz; C_6D_6; δ, ppm): 147.7(s, OP^{i}Pr$_2$).

1-(^{i}Pr$_2$PO)-3-(CH=NPh)-C$_6$H$_4$:

^{1}H-NMR (500 MHz; C_6D_6; δ, ppm): 0.97 (dd, J = 7.2 and 16 Hz, 6H, 2 CH_3 of $^{i}Pr_2$P); 1.13 (dd, J = 7.0 and 10.7 Hz, 6H, 2 CH_3 of $^{i}Pr_2$P); 1.76 (m, 2H, 2CH of $^{i}Pr_2$P); 7.03 (m, 1H, C*H*); 7.09 (t, $^3J_{H\text{-}H}$ = 7.8 Hz, 1H, C*H*); 7.13 (m, 3H, 3C*H*); 7.17 (m, 1H, C*H*); 7.29 (br d, $^3J_{H\text{-}H}$ = 7.8 Hz, 1H, C*H*); 7.43 (d, $^3J_{H\text{-}H}$ = 7.5 Hz, 1H, C*H*); 8.06 (br s, 1H, C*H*); 8.10 (s, C*H*=NPh). ^{13}C{^{1}H}-NMR (125.8 MHz; C_6D_6; δ, ppm): 17.1 (d, J = 8.5 Hz, 2 CH_3 of $^{i}Pr_2$P); 17.8 (d, J = 20.6 Hz, 2 CH_3 of $^{i}Pr_2$P); 28.6 (d, J = 17.6 Hz, 2 CH of $^{i}Pr_2$P); 118.5 (d, J = 11.6 Hz); 121.4 (s, 2 *C*); 121.8 (d, J = 11.1 Hz); 122.1 (s); 126.1 (s); 129.3 (s, 2C); 130.0 (s); 138.6 (s); 152.8 (s); 159.8 (s); 160.4 (d, J = 9.3 Hz). ^{31}P{^{1}H}-NMR (202.5 MHz; C_6D_6; δ, ppm): 149.1 (s, OP^{i}Pr$_2$).

1-(^{i}Pr$_2$PO)-3-(CH=NAr')-C$_6$H$_4$:

^{1}H-NMR (500 MHz; C_6D_6; δ, ppm): 0.97 (dd, J = 7.2 and 16 Hz, 6H, 2 CH_3 of $^{i}Pr_2$P); 1.12 (dd, J = 6.9 and 10.5 Hz, 6H, 2 CH_3 of $^{i}Pr_2$P); 1.76 (m, 2H, 2CH of $^{i}Pr_2$P); 2.08 (s, 6H, 2 CH_3 of N*Ar'*); 6.95 (m, 1H, C*H*); 7.01 (m, 2H, 2 C*H*); 7.09 (t, $^3J_{H\text{-}H}$ = 7.8 Hz, 1H, C*H*); 7.32 (br d, $^3J_{H\text{-}H}$ = 8.1 Hz, 1H, C*H*); 7.4 (br d, $^3J_{H\text{-}H}$ = 7.5 Hz, 1H, C*H*); 7.76 (s, 1H, C*H*); 8.01 (s, C*H*=NPh). ^{13}C{^{1}H}-NMR (125.8 MHz; C_6D_6; δ, ppm): 17.1 (d, J = 8.5 Hz, 2 CH_3 of $^{i}Pr_2$P); 17.8 (d, J = 20.4 Hz, 2 CH_3 of $^{i}Pr_2$P); 18.5 (s, 2 CH_3 of N*Ar'*); 28.6 (d, J = 18.2 Hz, 2 CH of $^{i}Pr_2$P); 118.2 (d, J =

10.9 Hz); 121.8 (d, J = 11.1 Hz); 122.6 (s); 124.0 (s); 127.2 (s); 128.0 (s); 128.35 (s); 128.42 (s); 130.0 (s); 138.4 (s); 152.0 (s); 160.4 (d, J = 8.9 Hz); 162.3 (s). $^{31}P\{^{1}H\}$-NMR (202.5 MHz; C_6D_6; δ, ppm): 149.0 (s, O$P^{i}Pr_2$).

1-(^{i}Pr$_2$PO)-3-(CH=NAr)-C$_6$H$_4$:

^{1}H-NMR (500 MHz; C_6D_6; δ, ppm): 0.95 (dd, J = 7.3 and 15.8 Hz, 6H, 2 CH_3 of $^{i}Pr_2$P); 1.10 (dd, J = 6.9 and 10.6 Hz, 6H, 2 CH_3 of $^{i}Pr_2$P); 1.15 (d, $^{3}J_{H\text{-}H}$ = 6.9 Hz, 12H, 4 CH_3 of N*Ar*); 1.74 (m, 2H, 2CH of $^{i}Pr_2$P); 3.12 (sept, $^{3}J_{H\text{-}H}$ = 6.9 Hz, 2H, 2 CH of N*Ar*); 7.09 (t, $^{3}J_{H\text{-}H}$ = 7.8 Hz, 1H, C*H*); 7.11-7.18 (m, 3H, C*H*); 7.33 (m, 1H, C*H*); 7.41 (m, 1H, C*H*); 7.99 (s, 1H, C*H*); 8.07 (br s, 1H, C*H*=NAr). $^{13}C\{^{1}H\}$-NMR (125.8 MHz; C_6D_6; δ, ppm): 17.1 (d, J = 8.5 Hz, 2 CH_3 of $^{i}Pr_2$P); 17.8 (d, J = 20.2 Hz, 2 CH_3 of $^{i}Pr_2$P); 23.6 (s, 4 CH_3 of N*Ar*); 28.5 (s, 2 CH of N*Ar*); 28.6 (d, J = 18.1 Hz, 2 CH of $^{i}Pr_2$P); 118.1 (d, J = 10.8 Hz); 121.8 (d, J = 11.7 Hz); 122.8 (s); 123.4 (s, 2C); 124.6 (s); 128.4 (s); 130.2 (s); 137.7 (s); 138.3 (s); 150.1 (s); 160.6 (d, J = 8.8 Hz); 161.9 (s). $^{31}P\{^{1}H\}$-NMR (202.5 MHz; C_6D_6; δ, ppm): 149.1 (s, O$P^{i}Pr_2$).

Characterization of POCN nickel bromide precursors

($^{i\text{-}Pr}$POCN$^{t\text{-}Bu}$)NiBr (1-^{t}Bu): 53% yield

^{1}H-NMR (500 MHz; C_6D_6; δ, ppm): 1.17 (dd, J = 7.0 and 15.0 Hz, 6H, 2 CH_3 of $^{i}Pr_2$P); 1.43 (s, 9H, 3 CH_3 of N^{t}*Bu*); 1.49 (dd, J = 7.3 and 17.5 Hz, 6H, 2 CH_3 of $^{i}Pr_2$P); 2.35 (m, 2H, 2CH of $^{i}Pr_2$P); 6.62 (m, 2H, *m*-C*H*); 6.81 (t, $^{3}J_{H\text{-}H}$ = 7.7 Hz, 1H, *p*-C*H*); 7.55 (br s, 1H, C*H*=NAr). $^{13}C\{^{1}H\}$-NMR (125.8 MHz; C_6D_6; δ, ppm): 16.6 (s, 2 CH_3 of $^{i}Pr_2$P); 18.3 (s, 2 CH_3 of $^{i}Pr_2$P); 28.6 (d, J = 25.4 Hz, 2 CH of $^{i}Pr_2$P); 29.4 (s, 3 CH_3 of N^{t}*Bu*); 61.7 (s, C_q of N^{t}*Bu*); 112.2 (d, J = 12.3 Hz, *C*H); 120.7 (s, *C*H); 126.2 (s, *C*H); 148.5 (s, C_q); 150.7 (d, J = 37.4 Hz, C_q); 165.3 (d, J = 11.2 Hz, C_q); 165.9 (s, *C*H=N^{t}Bu). $^{31}P\{^{1}H\}$-NMR (202.5 MHz; C_6D_6; δ, ppm): 193.2 (s, O$P^{i}Pr_2$). C,H,N analysis (%): calcd for $C_{17}H_{27}BrNNiOP$ (430.98): C 47.38, H 6.31, N 3.25; found: C 47.72, H 6.40, N 3.17.

($^{i\text{-Pr}}$POCN^{Ph})NiBr (1-Ph):[4]

^{1}H-NMR (500 MHz; C_6D_6; δ, ppm): 1.15 (m, 6H, 2 CH_3 of $^{i}Pr_2$P); 1.44 (m, 2 CH_3 of $^{i}Pr_2$P); 2.25 (m, 2H, 2CH of $^{i}Pr_2$P); 6.66 (m, 2H, *m*-C*H*, central ring); 6.79 (m, 1H, *p*-C*H*, central ring); 7.00-7.23 (m, 5H, N*Ph*); 7.34 (br s, 1H, C*H*=NPh). ^{13}C{^{1}H}-NMR (125.8 MHz; C_6D_6; δ, ppm): 16.8 (s, 2 CH_3 of $^{i}Pr_2$P); 18.2 (br s, 2 CH_3 of $^{i}Pr_2$P); 29.0 (d, J = 24.1 Hz, 2 CH of $^{i}Pr_2$P); 113.6 (d, J = 12.2 Hz, *C*H); 122.1 (s, *C*H); 124.6 (s, 2 *C*H); 126.7 (s, *C*H); 127.3 (s, *C*H); other aromatic ^{13}C resonances of CH resonances are obscured by the signal of C_6D_6; 148.3 (s, C_q); 148.9 (s, C_q); 154.4 (d, J = 35.2 Hz, C_q); 165.8 (d, J = 9.8 Hz, C_q); 172.2 (s, *C*H=N*Ph*). ^{31}P{^{1}H}-NMR (202.5 MHz; C_6D_6; δ, ppm): 201.3 (s, O$P^{i}Pr_2$). NMR data are consistent with the previously published data.[4]

($^{i\text{-Pr}}$POCN$^{Ar'}$)NiBr (1-Ar'): 80% yield

^{1}H-NMR (500 MHz; C_6D_6; δ, ppm): 1.14 (dd, J = 6.9 and 15.0 Hz, 6H, 2 CH_3 of $^{i}Pr_2$P); 1.40 (dd, J = 7.2 and 17.8 Hz, 6H, 2 CH_3 of $^{i}Pr_2$P); 2.18 (m, 2H, 2CH of $^{i}Pr_2$P); 2.33 (s, 6H, 2 CH_3 of N*Ar'*); 6.62 (d, $^{3}J_{H\text{-}H}$ = 7.4 Hz, 1H, aromatic C*H*); 6.68 (d, $^{3}J_{H\text{-}H}$ = 8.0 Hz, 1H, aromatic C*H*); 6.78 (t, $^{3}J_{H\text{-}H}$ = 7.6 Hz, 1H, aromatic C*H*); 6.98 (m, 4H, 3 aromatic CH and C*H*=NAr). ^{13}C{^{1}H}-NMR (125.8 MHz; C_6D_6; δ, ppm): 16.8 (s, 2 CH_3 of $^{i}Pr_2$P); 18.1 (d, J = 4.0 Hz, 2 CH_3 of $^{i}Pr_2$P); 19.3 (s, 2 CH_3 of N*Ar'*); 28.9 (d, J = 23.6 Hz, 2 CH of $^{i}Pr_2$P); 113.7 (d, J = 12.5 Hz, *C*H); 121.7 (s, *C*H); 126.4 (s, *C*H); 126.6 (s, *C*H); 130.6 (s, *C*H); 148.0 (d, J = 8.0 Hz, C_q); 155.2 (d, J = 34.4 Hz, C_q); 165.9 (br s, C_q); 174.3 (s, *C*H=N^{t}Bu); other aromatic ^{13}C resonances are obscured by the signal of C_6D_6. ^{31}P{^{1}H}-NMR (202.5 MHz; C_6D_6; δ, ppm): 203.0 (s, O$P^{i}Pr_2$). C,H,N analysis (%): calcd for $C_{21}H_{27}BrNNiOP$ (479.02): C 52.66, H 5.68, N 2.92; found: C 52.96 H 6.79, N 2.85.

($^{i\text{-Pr}}$POCN^{Ar})NiBr (1-Ar): 69% yield

^{1}H-NMR (500 MHz; C_6D_6; δ, ppm): 1.15 (m, 12H, 2 CH_3 of $^{i}Pr_2$P and 2 CH_3 of N*Ar*); 1.40 (dd, J = 7.2 and 17.9 Hz, 6H, 2 CH_3 of $^{i}Pr_2$P); 1.57 (d, J = 6.8 Hz, 6H, 2 CH_3 of N*Ar*); 2.19 (m, 2H, 2CH of $^{i}Pr_2$P); 3.60 (sept, J = 6.8 Hz, 2H, 2 CH of N*Ar*); 6.65 (m, 2H, aromatic C*H*); 6.76 (t, $^{3}J_{H\text{-}H}$ = 7.7 Hz, 1H, aromatic C*H*); 7.14

(m, 3H, aromatic C*H*); 7.48 (d, *J* = 4.0 Hz, 1H, C*H*=NAr). $^{13}C\{^1H\}$-NMR (125.8 MHz; C_6D_6; *δ*, ppm): 16.8 (s, 2 CH_3 of $^{i}Pr_2P$); 18.1 (d, *J* = 4.1 Hz, 2 CH_3 of $^{i}Pr_2P$); 23.4 (s, 2 CH_3 of N*Ar*); 24.4 (s, 2 CH_3 of N*Ar*); 28.8 (d, *J* = 23.6 Hz, 2 CH of $^{i}Pr_2P$); 29.3 (s, 2 CH, N*Ar*); 113.8 (d, *J* = 12.3 Hz, *C*H); 121.6 (s, *C*H); 123.2 (s, 2 *C*H); 126.7 (s, *C*H); 127.2 (s, *C*H); 141.2 (s, 2 C_q); 145.4 (s, C_q); 147.8 (s, C_q); 155.4 (d, *J* = 33.6 Hz, C_q); 166.0 (d, *J* = 10.3 Hz, C_q); 173.4 (d, *J* = 3.4 Hz, *C*H=N^{t}Bu). $^{31}P\{^1H\}$-NMR (202.5 MHz; C_6D_6; *δ*, ppm): 203.1 (s, O*P*^{i}Pr$_2$). C,H,N analysis (%): calcd for $C_{25}H_{35}BrNNiOP$ (535.13): C 56.11, H 6.59, N 2.62; found: C 56.34 H 6.66, N 2.53.

Preparation of ($^{i\text{-Pr}}$POCN$^{\text{Ar}}$)Ni(η^2-BH$_4$) (2-Ar)

A solution of $LiBH_4$ in THF (2.0 M, 96.3 μL, 0.1925 mmol) was added via syringe at room temperature to a solution of 1-Ar (98.1 mg, 0.1833 mmol) in 20 mL of toluene. An immediate colour change from orange-red to barberry red was observed, accompanied by the formation of white precipitate. The reaction mixture was left with stirring for 24 h, then all volatiles were pumped off and the product was extracted with hexanes (3 x 20 mL) and dried in vacuum to give the barberry red powder of **2-Ar** (75 mg, 93%). Single crystals of **2-Ar** suitable for X-ray diffraction analysis were obtained by crystallization from Et_2O solution at -30 °C. ^{1}H-NMR (500 MHz; C_6D_6; *δ*, ppm): -0.95 (br s, 2H, B*H*$_4$); -0.72 (br s, 2H, B*H*$_4$); 1.07 (dd, *J* = 6.9 and 14.8 Hz, 6H, 2 CH_3 of $^{i}Pr_2P$); 1.08 (d, *J* = 6.9 Hz, 6H, 2 CH_3 of N*Ar*); 1.24 (dd, *J* = 7.2 and 18 Hz, 6H, 2 CH_3 of $^{i}Pr_2P$); 1.50 (d, *J* = 6.9 Hz, 6H, 2 CH_3 of N*Ar*); 2.06 (m, 2H, 2 CH of $^{i}Pr_2P$); 3.56 (sept, *J* = 6.9 Hz, 2H, 2 CH of N*Ar*); 6.74 (m, 3H, aromatic protons of C_6H_3/N*Ar*); 7.12 (m, 2H, aromatic protons of C_6H_3/N*Ar*); 7.18 (m, 1H, aromatic proton of C_6H_3/N*Ar*); 7.57 (d, *J* = 3.5 Hz, 1H, C*H*=NAr). $^{31}P\{^1H\}$-NMR (202.5 MHz; C_6D_6; *δ*, ppm): 208.2 (s, O*P*^{i}Pr$_2$). $^{11}B\{^1H\}$-NMR (160.5 MHz; C_6D_6; *δ*, ppm): -30.8 (br s, *B*H$_4$). $^{13}C\{^1H\}$-NMR (125.8 MHz; C_6D_6; *δ*, ppm): 16.6 (d, *J* = 2.5 Hz, 2 CH_3 of $^{i}Pr_2P$); 16.9 (d, *J* = 4.2 Hz, 2 CH_3 of $^{i}Pr_2P$); 23.1 (s, 2 CH_3 of N*Ar*); 25.4 (s, 2 CH_3 of N*Ar*); 28.6 (d, *J* = 22.8 Hz, 2 CH of $^{i}Pr_2P$); 28.7 (s, 2 CH of N*Ar*); 112.8 (d, *J* = 13.1 Hz, CH of C_6H_3/N*Ar*); 121.5 (s, CH of C_6H_3/N*Ar*); 123.4 (s, 2 CH of C_6H_3/N*Ar*); 125.6 (s, CH of C_6H_3/N*Ar*); 127.3 (s, CH of C_6H_3/N*Ar*); 141.5 (s, Cq of C_6H_3/N*Ar*); 145.7

(s, Cq of *C*$_6$*H*$_3$/N*Ar*); 146.5 (s, Cq of *C*$_6$*H*$_3$/N*Ar*); 156.7 (s, Cq of *C*$_6$*H*$_3$/N*Ar*); 157.0 (s, Cq of *C*$_6$*H*$_3$/N*Ar*); 166.0 (d, J = 10.1 Hz, Cq of *C*$_6$*H*$_3$); 172.2 (d, J = 3.0 Hz, *CH*=NAr). C,H,N analysis (%): calcd for $C_{25}H_{39}BNNiOP$ (470.07): C 63.88, H 8.36, N 2.98; found: C 64.18, H 8.59, N 3.06. IR (nujol, selected bands): 1902 cm^{-1} (w, B-H), 1927 cm^{-1} (w, B-H), 1954 cm^{-1} (w, B-H), 2039 cm^{-1} (w, B-H), 2251 cm^{-1} (w, B-H), 2284 cm^{-1} (w, B-H).

Preparation of ($^{i\text{-Pr}}$POCN$^{\text{Ar}}$)Ni(BF$_4$) (3-Ar)

A solution of $AgBF_4$ (76.6 mg, 0.3934 mmol) in 10 mL of toluene was added at room temperature to a solution of **1-Ar** (200.5 mg, 0.3747 mmol) in 15mL of toluene. The colour immediately changed from orange-red to yellow and formation of white precipitate was observed. The reaction mixture was stirred at room temperature for 1 h, filtered and the residue was washed with a mixture of hexanes/toluene (5/1) until the filtrate became colourless. The solvent was removed in vacuum to give yellow powder of **3-Ar** which was additionally dried in vacuum for 5 h (120 mg, 59%). Single crystals of **3-Ar** suitable for X-ray diffraction analysis were obtained by slow room temperature vaporization of Et_2O solution into hexanes. ^{1}H-NMR (500 MHz; C_6D_6; δ, ppm): 1.05 (dd, J = 7.1 and 14.7 Hz, 6H, 2 CH_3 of ^{i}*Pr*$_2$P); 1.09 (d, J = 6.9 Hz, 6H, 2 CH_3 of N*Ar*); 1.41 (dd, J = 7.2 and 19.4 Hz, 6H, 2 CH_3 of ^{i}*Pr*$_2$P); 1.59 (d, J = 6.9 Hz, 6H, 2 CH_3 of N*Ar*); 2.26 (m, 2H, 2 CH of ^{i}*Pr*$_2$P); 3.59 (sept, J = 6.9 Hz, 2H, 2 CH of N*Ar*); 6.37 (d, J = 8.1 Hz, 1H, C$_6$*H*$_3$/N*Ar*); 6.43 (d, J = 7.4 Hz, 1H, C$_6$*H*$_3$/N*Ar*); 6.61 (t, J = 7.8 Hz, 1H, C$_6$*H*$_3$/N*Ar*); 7.10 (m, 2H, C$_6$*H*$_3$/N*Ar*); 7.19 (m, 1H, C$_6$*H*$_3$/N*Ar*); the resonance of C*H*=NAr is obscured by the residual resonance of C_6D_6 (found by ^{1}H-^{13}C HSQC NMR). ^{31}P{^{1}H}-NMR (202.5 MHz; C_6D_6; δ, ppm): 199.5 (s, O*P*^{i}Pr$_2$). ^{11}B{^{1}H}-NMR (160.5 MHz; C_6D_6; δ, ppm): -1.4 (br s, *B*F$_4$). ^{19}F{^{1}H}-NMR (470.6 MHz; C_6D_6; δ, ppm): -173.8 (br s, B*F*$_4$). ^{13}C{^{1}H}-NMR (125.8 MHz; C_6D_6; δ, ppm): 16.5 (d, J = 3.1 Hz, 2 CH_3 of ^{i}*Pr*$_2$P); 17.4 (d, J = 6 Hz, 2 CH_3 of ^{i}*Pr*$_2$P); 23.0 (s, 2 CH_3 of N*Ar*); 24.7 (s, 2 CH_3 of N*Ar*); 28.5 (d, J = 21.7 Hz, 2 CH of ^{i}*Pr*$_2$P); 29.5 (s, 2 CH of N*Ar*); 114.6 (d, J = 11.3 Hz, CH of C$_6$*H*$_3$/N*Ar*); 122.7 (s, CH of C$_6$*H*$_3$/N*Ar*); 123.9 (s, 2 CH of C$_6$*H*$_3$/N*Ar*); 128.6 (s, CH of C$_6$*H*$_3$/N*Ar*); 129.3 (s, Cq of C$_6$*H*$_3$/N*Ar*); 141.1 (s, 2 Cq of C$_6$*H*$_3$/N*Ar*); 142.8 (s, Cq of C$_6$*H*$_3$/N*Ar*); 147.2 (s, Cq

of *C*$_6$*H*$_3$/N*Ar*); 167.5 (d, *J* = 8.4 Hz, Cq of *C*$_6$*H*$_3$/N*Ar*); 172.9 (d, *J* = 3.3 Hz, *CH*=NAr); other resonance for aromatic carbons are obscured by the signal of C_6D_6. C,H,N analysis (%): calcd for $C_{25}H_{35}BF_4NNiOP$ (542.03): C 55.40, H 6.51, N 2.58; found: C 55.82, H 6.72, N 2.69.

Preparation of [($^{i\text{-Pr}}$POCN^{Ar})Ni(CH$_3$CN)][BPh$_4$] (4-Ar)

First, a solution of **1-Ar** (182.7 mg, 0.3414 mmol) in 30 mL of toluene and then CH_3CN (0.5 mL, 9.57 mmol) were added at room temperature to the solid $NaBPh_4$ (175.3 mg, 0.5121 mmol). The reaction mixture allowed to stir at room temperature for 24 h and during this time changed the colour from orange-red to yellow and formation of white precipitate was observed. The mixture was filtered and the precipitate was washed with toluene until the filtrate became colourless. Toluene was removed in vacuum to give yellow oil, which was dried in high vacuum for 10 h and triturated with hexanes and hexanes/Et_2O (1/1) mixture. All volatiles were pumped off to give yellow foamy material which was dried in vacuum for additional 5 h (230 mg, 83%). ^{1}H-NMR (400 MHz; C_6D_6; *δ*, ppm): -0.12 (s, 3H, *CH*$_3$CN); 0.95 (dd, *J* = 6.9 and 15.2 Hz, 6H, 2 CH$_3$ of ^{i}*Pr*$_2$P); 0.97 (d, *J* = 6.8 Hz, 6H, 2 CH$_3$ of N*Ar*); 1.03 (dd, *J* = 7.2 and 19.7 Hz, 6H, 2 CH$_3$ of ^{i}*Pr*$_2$P); 1.13 (d, *J* = 6.8 Hz, 6H, 2 CH$_3$ of N*Ar*); 1.81 (m, 2H, 2 CH of ^{i}*Pr*$_2$P); 2.98 (sept, *J* = 6.8 Hz, 2H, 2 CH of N*Ar*); 6.42 (d, *J* = 8.1 Hz, 1H, C$_6$*H*$_3$/N*Ar*); 6.47 (d, *J* = 7.4 Hz, 1H, C$_6$*H*$_3$/N*Ar*); 6.62 (t, *J* = 7.8 Hz, 1H, C$_6$*H*$_3$/N*Ar*); 6.81 (m, 2H, C$_6$*H*$_3$/N*Ar*); 6.91 (m, 1H, C$_6$*H*$_3$/N*Ar*); 7.08 (br t, *J* = 7.2 Hz, 4H, *p*-H of B*Ph*$_4$); 7.27 (t, *J* = 7.4 Hz, 8H, *m*-H of B*Ph*$_4$); 8.05 (br s, 9H, *CH*=NAr and *o*-H of B*Ph*$_4$). ^{31}P{^{1}H}-NMR (202.5 MHz; C_6D_6; *δ*, ppm): 205.5 (s, O*P*^{i}Pr$_2$). ^{11}B{^{1}H}-NMR (160.5 MHz; C_6D_6; *δ*, ppm): -5.8 (s, *B*Ph$_4$). ^{13}C{^{1}H}-NMR (125.8 MHz; C_6D_6; *δ*, ppm): -0.6 (s, *CH*$_3$CN); 16.8 (br s, 2 CH$_3$ of ^{i}*Pr*$_2$P); 17.5 (d, *J* = 5.1 Hz, 2 CH$_3$ of ^{i}*Pr*$_2$P); 22.8 (s, 2 CH$_3$ of N*Ar*); 23.7 (s, 2 CH$_3$ of N*Ar*); 28.9 (d, *J* = 23.5 Hz, 2 CH of ^{i}*Pr*$_2$P); 29.1 (s, 2 CH of N*Ar*); 115.9 (d, *J* = 10.7 Hz, CH of *C*$_6$*H*$_3$/N*Ar*); 122.2 (s, B*Ph*$_4$); 123.2 (s, CH of *C*$_6$*H*$_3$/N*Ar*); 123.4 (s, CH$_3$*C*N); 123.8 (s, 2 CH of *C*$_6$*H*$_3$/N*Ar*); 126.5 (s, B*Ph*$_4$); 128.3 (s, CH of *C*$_6$*H*$_3$/N*Ar*); 129.7 (s, CH of *C*$_6$*H*$_3$/N*Ar*); 137.0 (s, B*Ph*$_4$); 140.1 (s, 2 Cq of *C*$_6$*H*$_3$/N*Ar*); 141.2 (s, Cq of *C*$_6$*H*$_3$/N*Ar*); 142.9 (s, Cq of *C*$_6$*H*$_3$/N*Ar*); 147.5 (s, Cq of *C*$_6$*H*$_3$/N*Ar*); 166.2 (d, *J* = 7.9 Hz, Cq of *C*$_6$*H*$_3$/N*Ar*);

176.0 (br s, *CH*=NAr). C,H,N analysis (%): calcd for $C_{51}H_{58}BN_2NiOP$ (815.52): C 75.11, H 7.17, N 3.44; found: C 74.71, H 7.18, N 4.15.

Preparation of [($^{i\text{-Pr}}$POCN^{Ar})Ni(CH_3CN)][BAF] (5-Ar)

Method A. Generation of 6-Ar on NMR scale. A yellow solution of **3-Ar** (11.5 mg, 0.0212 mmol) and CH_3CN (1.3 μL, 0.0255 mmol) in CH_2Cl_2 (0.6 mL) was added at room temperature to the solid $LiB(C_6F_5)_4{\cdot}Et_2O$ (16.1 mg, 0.0212 mmol). No colour change and immediate formation of cloudy white precipitate was observed. The reaction mixture was transferred to an NMR tube, left at room temperature for 30 min and then checked with NMR spectroscopy, showing complete conversion of **3-Ar** to **5-Ar**. All volatiles were pumped off and the product with extracted with toluene (app. 2 mL) to give yellow oily material (22.4 mg, 90%), which dried in vacuum and dissolved in CD_2Cl_2 for NMR analysis (**5-Ar** is poorly soluble in C_6D_6).

Method B. A solution of CH_3CN (20 μL, 0.383 mmol) in CH_2Cl_2 (20 mL) was added to the mixture of solid **4-Ar** (117.5 mg, 0.1441 mmol) and $LiB(C_6F_5)_4{\cdot}Et_2O$ (109.6 mg, 0.1441 mmol). Formation of yellow solution and white precipitate was observed. The reaction mixture was left with stirring at room temperature overnight, then filtered and the residue was washed with CH_2Cl_2 (5 mL). The resulting solution was concentrated to app. 3 mL, layered with hexanes (app. 5 mL) and left at -30 °C for 24 h to give yellow oily precipitate. The filtrate was decanted, and the residue was washed with hexanes/toluene (30ml/5ml) and dried in vacuum to give yellow foamy material of **5-Ar** (148.3 mg, 88%). ^{1}H-NMR (400 MHz; C_6D_6; δ, ppm): 1.24 (d, J = 6.8 Hz, 6H, 2 CH_3 of N*Ar*); 1.37 (m, 18H, 2 CH_3 of N*Ar* and 4 CH_3 of ^{i}*Pr*$_2$P); 1.68 (s, 3H, *CH*$_3$CN); 2.34 (m, 2H, 2 CH of ^{i}*Pr*$_2$P); 3.33 (sept, J = 6.8 Hz, 2H, 2 CH of N*Ar*); 6.86 (m, 1H, C$_6$*H*$_3$/N*Ar*); 7.2 (m, 2H, C$_6$*H*$_3$/N*Ar*); 7.27 (m, 2H, C$_6$*H*$_3$/N*Ar*); 7.33 (m, 1H, C$_6$*H*$_3$/N*Ar*); 8.1 (d, J = 4.0, 1H *CH*=NAr). ^{31}P{^{1}H}-NMR (202.5 MHz; C_6D_6; δ, ppm): 203.9 (s, O*P*^{i}Pr$_2$). ^{19}F{^{1}H}-NMR (376.5 MHz; C_6D_6; δ, ppm): -133.1 (br s, 8F, *o*-F of B*(C$_6$F$_5$)$_4$*); -163.8 (t, $^3J_{F\text{-}F}$ = 20.3 Hz, 4F, *p*-F of B*(C$_6$F$_5$)$_4$*); -167.6 (br m, 8F, *m*-F of B*(C$_6$F$_5$)$_4$*). ^{11}B{^{1}H}-NMR (128.4 MHz; C_6D_6; δ, ppm): -16.7 (s, *B*$(C_6F_5)_4$). ^{13}C{^{1}H}-NMR (125.8 MHz; C_6D_6; δ, ppm): 2.18 (s, *CH*$_3$CN); 17.0 (br s, 2 CH_3 of ^{i}*Pr*$_2$P); 17.6 (d, J = 5.4

Hz, 2 CH_3 of $^{i}Pr_2P$); 23.0 (s, 2 CH_3 of N*Ar*); 24.0 (s, 2 CH_3 of N*Ar*); 29.2 (d, J = 24 Hz, 2 CH of $^{i}Pr_2P$); 29.4 (s, 2 CH of N*Ar*); 116.5 (d, J = 12.7 Hz, CH of C_6H_3/N*Ar*); 124.1 (s, CH of C_6H_3/N*Ar*); 124.2 (s, 2 CH of C_6H_3/N*Ar*); 126.6 (s, CH_3CN); 128.5 (s, CH of C_6H_3/N*Ar*); 130.0 (s, CH of C_6H_3/N*Ar*); 135.6 (br s, B$(C_6F_5)_4$); 137.6 (br s, B$(C_6F_5)_4$); 140.9 (s, 2 Cq of C_6H_3/N*Ar*); 143.0 (s, Cq of C_6H_3/N*Ar*); 146.9 (s, Cq of C_6H_3/N*Ar*); 147.5 (br s, B$(C_6F_5)_4$); 147.8 (s, Cq of C_6H_3/N*Ar*); 149.4 (br s, B$(C_6F_5)_4$); 166.3 (d, J = 8.2 Hz, Cq of C_6H_3/N*Ar*); 176.4 (d, J = 3.4 Hz, *CH*=NAr). C,H,N analysis (%): calcd for $C_{51}H_{38}BF_{20}N_2NiOP$ (1175.32): C 52.12, H 3.26, N 2.38; found: C 51.20, H 3.24, N 2.33.

Preparation of ($^{i\text{-Pr}}$POCN$^{\text{Ar}}$)NiMe (6-Ar)

A solution of MeLi in Et_2O (1.6 M, 0.2025 mmol) was added via syringe to a solution of **1-Ar** (103.2 mg, 0.1929 mmol) in 30 mL of toluene at -80 °C. The mixture allowed to warm up to room temperature slowly and then stirred for additional 1.5 h (in total took app. 12 h). During this time the colour of the reaction mixture turned to crimson red. All volatiles were pumped off, the residue was dried in vacuum and the product was extracted with hexanes (3 x 20 mL) to give dark-red solid (69 mg, 76%). Single crystals of **6-Ar** suitable for X-ray diffraction analysis were obtained by slow vaporization of Et_2O solution into hexanes at -28 °C. ^{1}H-NMR (500 MHz; C_6D_6; δ, ppm): -0.81 (d, J = 3.6 Hz, 3H, NiCH_3); 1.10 (d, J = 6.8 Hz, 6H, 2 CH_3 of N*Ar*); 1.15 (m, 6H, 2 CH_3 of $^{i}Pr_2P$); 1.19 (dd, J =3.2 and 7.1 Hz, 6H, 2 CH_3 of $^{i}Pr_2P$); 1.38 (d, J = 6.8 Hz, 6H, 2 CH_3 of N*Ar*); 2.05 (m, 2H, 2 CH of $^{i}Pr_2P$); 3.49 (sept, J = 6.8 Hz, 2H, 2 CH of N*Ar*); 6.84-6.90 (m, 3H, C_6H_3/N*Ar*); 7.13-7.16 (m, 3H, C_6H_3/N*Ar* overlapping with the residual resonance of C_6D_6); 7.73 (d, J = 4.2 Hz, 1H, *CH*=NAr). ^{31}P{^{1}H}-NMR (202.5 MHz; C_6D_6; δ, ppm): 199.2 (s, OP^{i}Pr$_2$). ^{13}C{^{1}H}-NMR (125.8 MHz; C_6D_6; δ, ppm): -8.4 (d, J = 22.3 Hz, Ni*Me*); 17.2 (s, 2 CH_3 of $^{i}Pr_2P$); 18.0 (d, J = 5.2 Hz, 2 CH_3 of $^{i}Pr_2P$); 23.0 (s, 2 CH_3 of N*Ar*); 24.5 (s, 2 CH_3 of N*Ar*); 28.3 (d, J = 23.6 Hz, 2 CH of $^{i}Pr_2P$); 28.8 (s, 2 CH of N*Ar*); 112.8 (d, J = 11.8 Hz, aromatic *C*H); 120.9 (s, aromatic *C*H); 123.3 (s, aromatic 2 *C*H); 125.7 (s, aromatic *C*H); 126.6 (s, aromatic *C*H); 141.1 (s, aromatic 2 C_q); 146.0 (s, aromatic 2 C_q); 147.3 (s, aromatic 2 C_q); 164.2 (br s, aromatic 2 C_q); 173.4 (br s, aromatic 2 C_q); 176.0 (s, *C*H=NAr). C,H,N

analysis (%): calcd for co-crystal of 0.81 **6-Ar** and 0.19 ($^{i\text{-Pr}}$POCN$^{\text{Ar}}$)NiCl: C 65.42, H 7.97, N 2.95; found: C 65.88, H 8.23, N 2.82.

Preparation of ($^{i\text{-Pr}}$POC(H)N$^{\text{Ar}}$)Ni(COD) (9-Ar)

A solution of 1-(^{i}Pr$_2$PO)-3-(CH=NAr)-C$_6$H$_4$ (124.2 mg, 0.31 mmol) in 10 mL of PhMe was added at room temperature to a solution of Ni(COD)$_2$ (85.9 mg, 0.31 mmol) in 10 mL of PhMe. The reaction mixture was clear and had bright red colour. The mixture was stirred 24 h at room temperature and the colour of the mixture became dark-brown. All volatiles were pumped of and the product was crystallized from pentane (app. 20 mL) at -20 °C overnight. After the crystallization was complete, pentane was carefully decanted while still cold to give an orange powder of **9-Ar**, which was dried in vacuum (120.0 mg, 69%). ^{1}H-NMR (500 MHz; C$_6$D$_6$; δ, ppm): 0.74 (dd, J = 7.1 and 17.6 Hz, 3H, CH$_3$ of $^{i}Pr_2$P); 0.87 (m, 3H, CH$_3$ of $^{i}Pr_2$P); 1.00 (dd, J = 7.2 and 16.8 Hz, 3H, CH$_3$ of $^{i}Pr_2$P); 1.06 (dd, J = 6.9 and 12.9 Hz, 3H, CH$_3$ of $^{i}Pr_2$P); 1.18 (d, J = 6.9 Hz, 12H, 4 CH$_3$ of N*Ar*); 1.27 (m, 1H, CH_2 of COD); 1.37-1.63 (m, 4H, CH_2 of COD); 1.80 (m, 1H, CH_2 of COD); 1.89 (m, 2H, 2 CH of $^{i}Pr_2$P); 1.97 (m, 2H, CH_2 of COD); 2.47 (m, 1H, =C*H* of COD); 3.27 (sept, 6.9 Hz, 2H, 2 CH of N*Ar*); 3.75 (m, 1H, =C*H* of COD); 4.59 (m, 1H, =C*H* of COD); 4.81 (m, 1H, =C*H* of COD); 7.13-7.20 (m, 4H, aromatic C*H*, overlapping with the residual resonance of C$_6$D$_6$); 7.54 (d, J = 7.3 Hz, aromatic C*H*); 8.06 (s, aromatic C*H*); 8.20 (s, C*H*=NAr); 8.26 (d, J = 7.4 Hz, aromatic C*H*). ^{13}C{^{1}H}-NMR (125.8 MHz; C$_6$D$_6$; δ, ppm): 16.6 (s, *C*H$_3$ of $^{i}Pr_2$P); 17.2 (d, J = 8.4 Hz, *C*H$_3$ of $^{i}Pr_2$P); 17.7 (s, *C*H$_3$ of $^{i}Pr_2$P); 18.0 (d, J = 5.6 Hz, *C*H$_3$ of $^{i}Pr_2$P); 23.7 (s, 2 *C*H$_3$ of N*Ar*); 23.8 (s, 2 *C*H$_3$ of N*Ar*); 28.4 (s, 2 *C*H of N*Ar*); 28.57 (s, COD); 28.62 (d, J = 23.7 Hz, 2 *C*H of $^{i}Pr_2$P); 29.2 (d, J = 4.0 Hz, COD); 30.2 (s, COD); 31.8 (d, J = 3.0 Hz, COD); 32.1 (s, COD); 62.4 (s, COD); 82.1 (d, J = 24.2 Hz, COD); 109.3 (d, J = 11.7 Hz, aromatic *C*H$_{\text{bridgehead}}$); 111.7 (s, COD); 123.3 (s, aromatic 2 *C*H); 123.5 (s, aromatic *C*H); 124.2 (s, aromatic *C*H); 135.3 (s, aromatic C_q); 138.1 (s, aromatic 2 C_q); 144.5 (s, aromatic *C*H); 150.9 (s, aromatic C_q); 153.2 (d, J = 16.3 Hz, aromatic C_q); 163.0 (s, *C*H=NAr); 170.0 (d, J = 14.3 Hz, aromatic C_q). ^{31}P{^{1}H}-NMR (202.5 MHz; C$_6$D$_6$; δ, ppm): 197.2 (s,

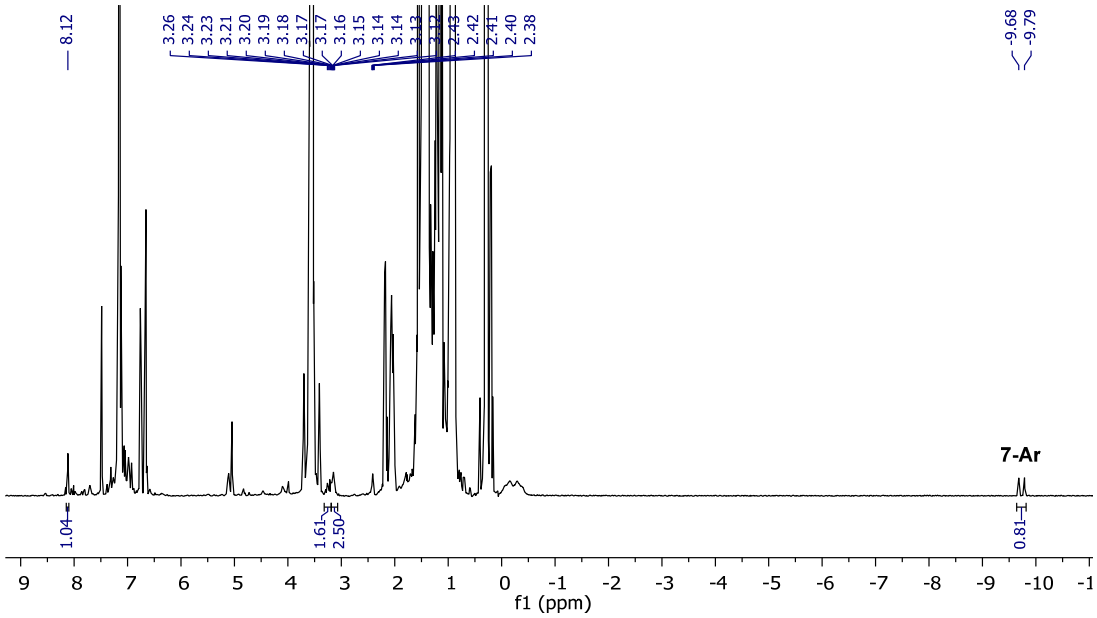
O*P*^{i}Pr$_2$). C,H,N analysis (%): calcd for $C_{33}H_{48}NNiOP$ (564.42): C 70.22, H 8.57, N 2.48; found: C 70.58, H 8.69, N 2.36.

NMR scale reaction of ($^{i\text{-Pr}}$POCN^{Ar})NiBr (1-Ar) with L-Selectride

A solution of L-Selectride in THF (20.2 μL, 0.0202 mmol, 1.0 M solution) was added *via* syringe to a frozen in liq. N_2 solution of **1-Ar** (10.8 mg, 0.0202 mmol) in 0.6 mL of C_6D_6 in an NMR tube. The mixture was allowed to warm up slowly to room temperature, left at room temperature for 10 min and then was monitored by NMR at room temperature, showing after 10 min selective formation of **7-Ar** (16% conversion of **1-Ar** by $^{31}P\{^1H\}$-NMR). Monitoring the reaction mixture by NMR during the next 24 h at room temperature revealed decomposition of **7-Ar** to a mixture of unidentified products together with the release of POC(H)N ligand and H_2 and formation of black precipitate of metallic nickel.

7-Ar; selected NMR resonances: ^{1}H-NMR (500 MHz; C_6D_6; δ, ppm): -9.72 (d, $^2J_{H\text{-}P}$ = 54 Hz, 1H, Ni*H*; coupled in the ^{1}H-^{31}P HSQC NMR spectrum to the ^{31}P resonance at 205.1 ppm); 1.16 (m, 6H, 2 CH_3 of P^i*Pr$_2$*; found by ^{1}H-^{31}P HSQC NMR); 2.15 (m, 2H, 2 CH of P^i*Pr$_2$*); 3.03 (sept, $^2J_{H\text{-}H}$ = 6.8 Hz, 2H, 2 CH of N*Ar*); 7.94 (s, 1H, C*H*=NAr; coupled in the ^{1}H-^{13}C HSQC NMR spectrum to the ^{13}C resonance at 161.1 ppm); other resonances are overlapped with the resonances of **1-Ar**. $^{31}P\{^1H\}$-NMR (202.5 MHz; C_6D_6; δ, ppm): 205.1 (s, O*P*^{i}Pr$_2$).

(A)



(B)

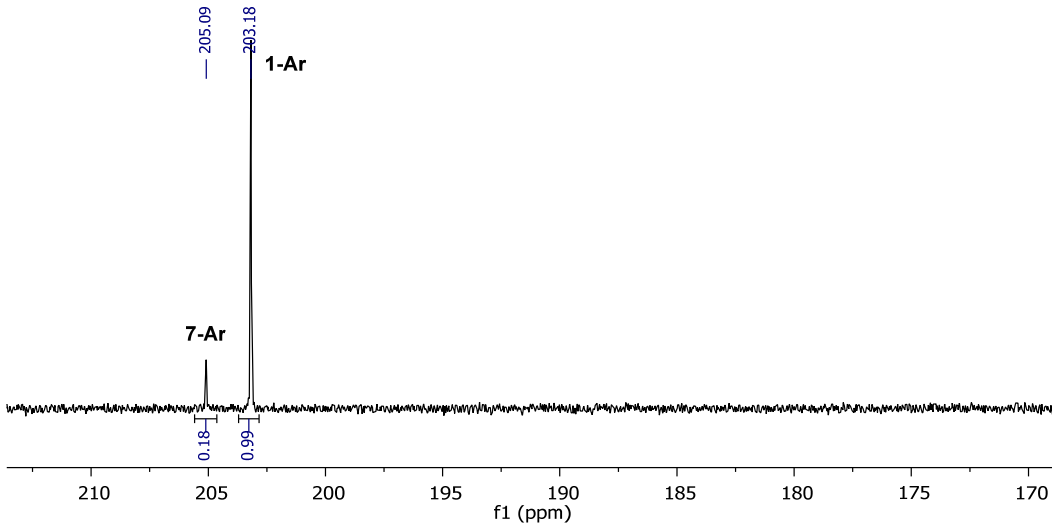


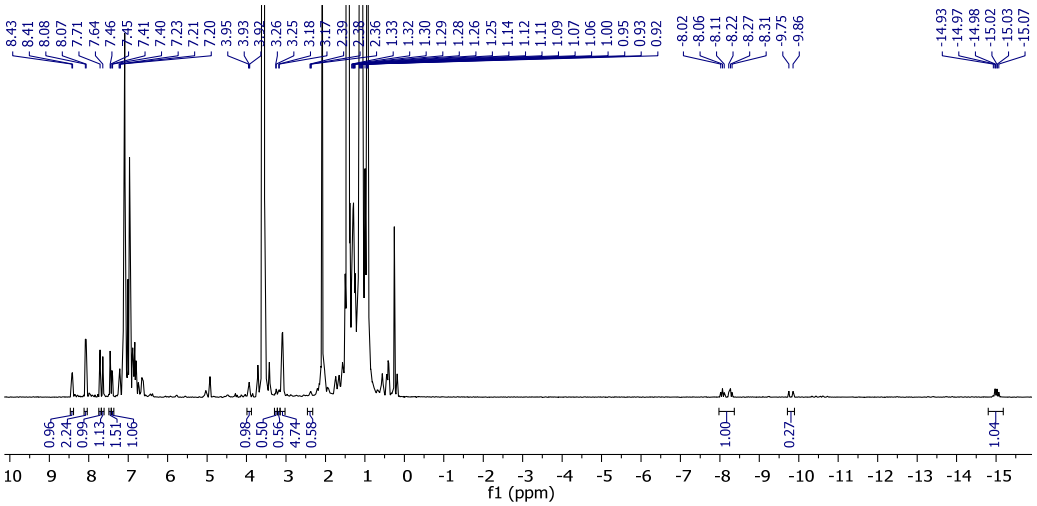
Figure S1. ^{1}H- (**A**) and ^{31}P{^{1}H}-NMR (**B**) spectra from the reaction of **1-Ar** with L-Selectride in C_6D_6 taken after 10 min at room temperature, showing 16% conversion (by ^{31}P{^{1}H}-NMR) of **1-Ar** to **7-Ar**.

NMR scale reaction of ($^{i\text{-Pr}}$POCN^{Ar})NiBr (1-Ar) with $LiHBEt_3$

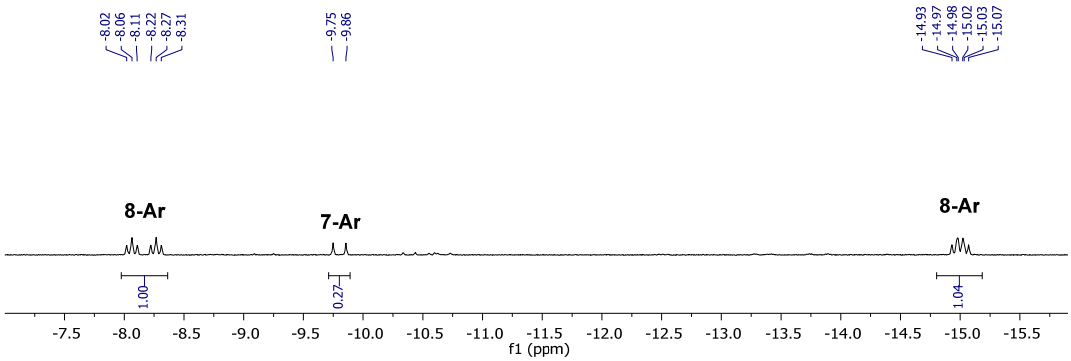
A solution of $LiHBEt_3$ in THF (20.0 μL, 0.02 mmol, 1.0 M solution) was added slowly *via* syringe to a cold (app. -30 °C) solution of **1-Ar** (10.8 mg, 0.02 mmol) in 0.6 mL of PhMe-d_8 in an NMR tube. The mixture was slowly warmed up to room temperature, left at room temperature for 10 minutes (during this time the colour change first to dark-red and then to green was observed) and then the reaction was monitored by NMR, showing formation of a mixture of **7-Ar** and **8-Ar** (app. 1:4 ratio by ^{1}H-NMR, respectively; app. 74% overall conversion of **1-Ar** by ^{31}P{^{1}H}-NMR). Further monitoring the reaction by NMR during 24 h at room temperature revealed decomposition of both **7-Ar** and **8-Ar** to a mixture of unidentified products together with the release of POC(H)N ligand and H_2 and formation of black precipitate of metallic nickel. An attempted variable temperature NMR analysis of the reaction mixture (-80 °C to room temperature) gave the result identical to the room temperature experiment.

8-Ar; selected NMR resonances: ^{1}H-NMR (500 MHz; PhMe-d_8; δ, ppm): -15.00 (dt, J = 22 Hz and 23.8 Hz, 1H, Ni*H*); -8.17 (dt, J = 22 Hz, 101.5 Hz, 1H, Ni*H*); the CH_3 resonances of P^i*Pr*$_2$ and N*Ar* of **8-Ar** (in the region of 0.93-1.51 ppm are overlapping with the corresponding resonances for **1-Ar**, **7-Ar** and the residual CH_3 resonance of PhMe-d_8; 2.10 (m, 4 CH of P^i*Pr*$_2$, overlapping with the CH resonances of **7-Ar** and with the residual resonance of PhMe-d_8); 3.10 (m, 4 CH of N*Ar*; overlapping with the CH resonances of **7-Ar**); 7.64 and 7.71 (both s, 1H, C*H*=NAr); other resonances are overlapped with the resonances of **1-Ar**, **7-Ar** and with the residual resonances of PhMe-d_8. ^{31}P{^{1}H}-NMR (202.5 MHz; PhMe-d_8; δ, ppm): 197.6 (br s, 1P, O*P*^{i}Pr$_2$); 208.5 (br s, 1P, O*P*^{i}Pr$_2$).

(A)



(B)



(C)

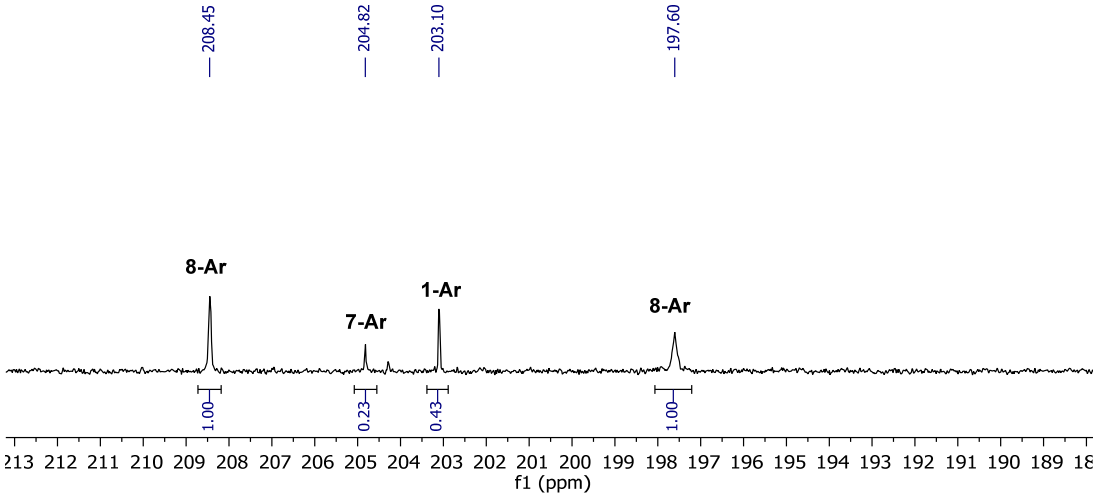


Figure S2. ^{1}H- (**A**), expanded hydride region (**B**) and ^{31}P{^{1}H}-NMR (**C**) spectra from the reaction of **1-Ar** with $LiBHEt_3$ in PhMe-d_8 taken after 10 min at room temperature, showing 74% conversion (by ^{31}P{^{1}H}-NMR) of **1-Ar** to a mixture of **7-Ar** and **8-Ar** (app. 1:4 ratio by ^{1}H-NMR, respectively).

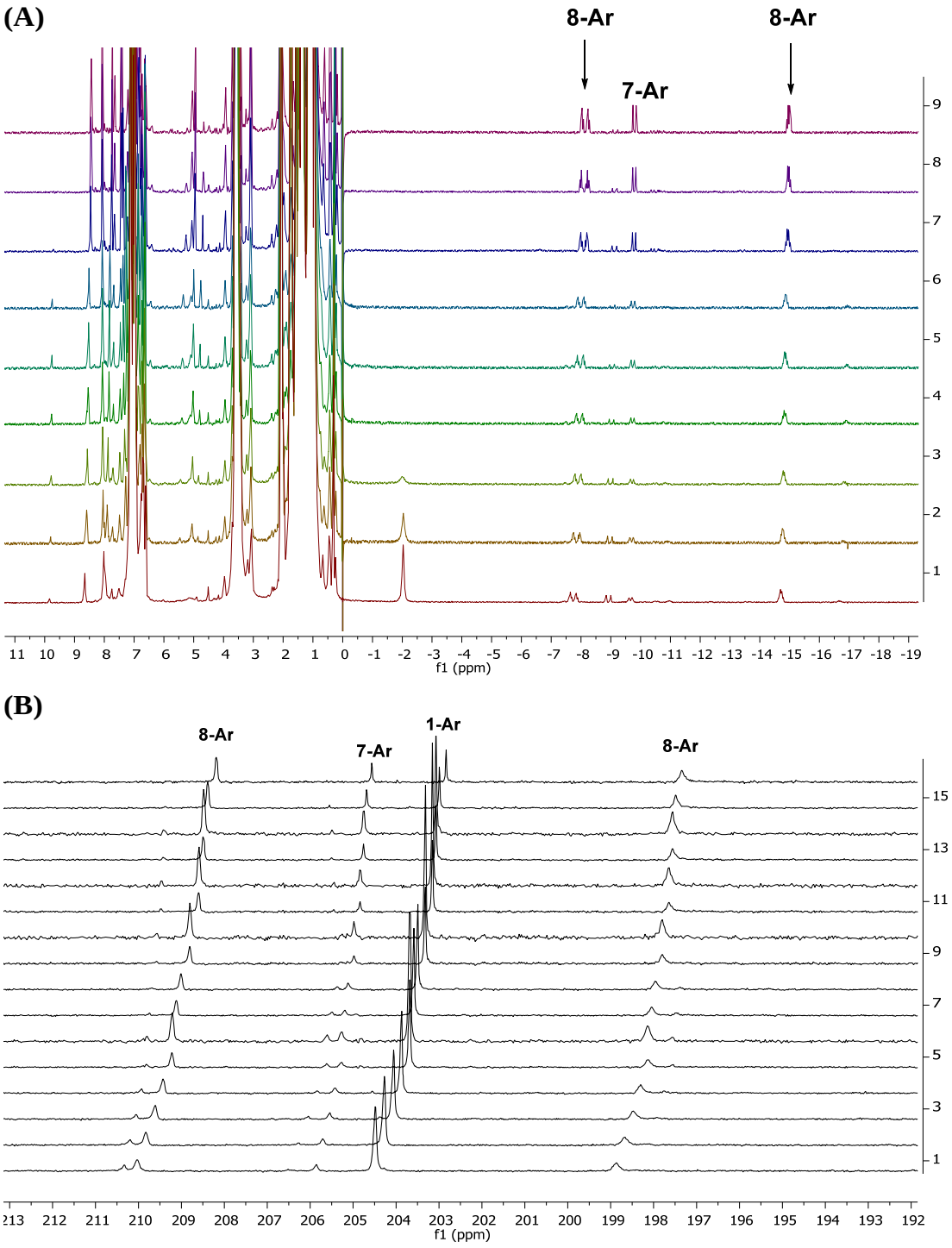


Figure S3. Variable temperature NMR analysis (-80 °C to room temperature) of the reaction of **1-Ar** with $LiBHEt_3$ in PhMe-d_8, showing formation of a mixture of **7-Ar** and **8-Ar**: ^{1}H-NMR spectra (**A**) and $^{31}P\{^{1}H\}$-NMR spectra (**B**).

NMR scale reaction of ($^{i\text{-Pr}}$POCN^{Ar})NiMe (6-Ar) with $PhSiH_3$

$PhSiH_3$ (5.0 μL, 0.0405 mmol, 2.7 equiv to Ni) was added in one portion at room temperature to a solution of **6-Ar** (7.1 mg; 0.015 mmol) in 0.6 mL of C_6D_6 in an NMR tube. The reaction was monitored by NMR spectroscopy overnight at room temperature, showing no consumption of both **6-Ar** and $PhSiH_3$. The mixture was heated at 65 °C for 12 h, showing by $^{31}P\{^1H\}$-NMR 72% conversion of **6-Ar**, complete consumption of $PhSiH_3$ and formation of $PhMeSiH_2$ in a mixture with the silane redistribution products, Ph_2SiH_2 and SiH_4 ($PhMeSiH_2$:Ph_2SiH_2 = 1:2.4 by ^1H-NMR),[3] and unidentified Ni decomposition species.

NMR scale reaction of ($^{i\text{-Pr}}$POCN^{Ar})NiMe (6-Ar) with HBPin

HBPin (3.2 μL, 0.022 mmol) was added at room temperature to a solution of **6-Ar** (12.2 mg, 0.022 mmol) in 0.6 mL of C_6D_6 in an NMR tube. The mixture was left at room temperature for 10 min and then the reaction was monitored by ^1H and $^{31}P\{^1H\}$-NMR at room temperature, showing after 24 h decomposition of **6-Ar** (42% consumption of **6-Ar** by $^{31}P\{^1H\}$-NMR relative to **1-Ar**, which is known to be unreactive towards HBPin and was used as an internal standard) and formation of small amounts of **8-Ar** (7% by $^{31}P\{^1H\}$-NMR). Further monitoring of the reaction by NMR showed only decomposition, along with H_2 release, to metallic Ni and unidentified products. The reaction at low temperature showed an identical result.

NMR scale reaction of ($^{i\text{-Pr}}$POCN^{Ar})Ni(BF_4) (3-Ar) with PhC(O)H

PhC(O)H (5.3 μL, 0.0523 mmol) was added at room temperature to a solution of **3-Ar** (28.4 mg, 0.0523 mmol) in 0.6 mL of C_6D_6 in an NMR tube. The mixture was left at room temperature for 10 min and then checked with NMR, which chowed complete conversion of **3-Ar** to a weak adduct [($^{i\text{-Pr}}$POCN^{Ar})Ni(η^1-O=CHPh)][BF_4]. In an attempt to isolate the product, all volatiles were pumped off in vacuum and this resulted in the formation of a difficult to separate mixture of **3-Ar** and [($^{i\text{-Pr}}$POCN^{Ar})Ni(η^1-O=CHPh)][BF_4]. ^1H-NMR (500 MHz; C_6D_6; δ, ppm): 1.04 (d, J = 6.8 Hz, 6H, 2 CH_3 of N*Ar*); 1.14 (dd, J = 7.0 and 14.9 Hz, 6H, 2 CH_3 of $^iPr_2$P); 1.41 (m, 12H, 2 CH_3 of N*Ar* and 2 CH_3 of $^iPr_2$P); 2.45 (m, 2H, 2 CH of

$^{i}Pr_2$P); 3.49 (sept, J = 6.8 Hz, 2H, 2 CH of N*Ar*); 6.43 (m, 1H); 6.69 (m, 2H); 6.97 (m, 3H); 7.05 (m, 3H); 7.34 (br s, 1H, C*H*=NAr); 7.56 (br d, $^{3}J_{H\text{-}H}$ = 7.5 Hz, 1H, *o*-H of η^1-O=CH*Ph*); 9.72 (br s, 1H, η^1-O=C*H*Ph). $^{31}P\{^{1}H\}$-NMR (202.5 MHz; C_6D_6; δ, ppm): 200.3 (br s, O$P^{i}Pr_2$). $^{13}C\{^{1}H\}$-NMR (125.8 MHz; C_6D_6; δ, ppm): 16.6 (br s, 2 *C*H$_3$ of $^{i}Pr_2$P); 17.6 (br s, 2 *C*H$_3$ of $^{i}Pr_2$P); 22.8 (br s, 2 *C*H$_3$ of N*Ar*); 24.5 (br s, 2 *C*H$_3$ of N*Ar*); 28.5 (br d, J = 22.1 Hz, 2 *C*H of $^{i}Pr_2$P); 29.4 (br s, 2 *C*H of N*Ar*); 114.9 (br d, J = 11.7 Hz); 123.2 (br s); 124.0 (s); 124.6 (s); 129.0 (s); 130.3 (s); 134.7 (s); 136.6 (s); 141.1 (s); 147.2 (s); 167.3 (d, J = 8.3 Hz); 174.1 (br s, *C*H=NAr); 194.7 (br s, η^1-O=*C*HPh). $^{19}F\{^{1}H\}$-NMR (470.6 MHz; C_6D_6; δ, ppm): -164.6 (br s, B*F*$_4$). $^{11}B\{^{1}H\}$-NMR (160.5 MHz; C_6D_6; δ, ppm): -1.2 (br s, *B*F$_4$).

NMR scale reaction of ($^{i\text{-}Pr}$POCN^{Ar})Ni(BF$_4$) (3-Ar) with PhSiH$_3$

PhSiH$_3$ (1.7 μL, 0.018 mmol) was added *via* syringe to a frozen in liq. N_2 solution of **3-Ar** (7.0 mg, 0.013 mmol) in 0.6 mL of PhMe-d$_8$ in an NMR tube. The tube was placed into the pre-cooled to -80 °C NMR machine and the reaction was monitored by ^{1}H, $^{31}P\{^{1}H\}$, $^{19}F\{^{1}H\}$ and $^{11}B\{^{1}H\}$ NMR upon gradual increasing the temperature up to 25 °C. NMR analysis showed to reaction between **3-Ar** and PhSiH$_3$ below 0 °C, but above this temperature formation of BF_3 and PhSiH$_2$F,[5] followed by conversion of the latter compound to PhSiHF$_2$[5] was observed (see Figure S4). Also, formation of a complex mixture of unidentified Ni decomposition species along with large amount of H_2 was observed by NMR.

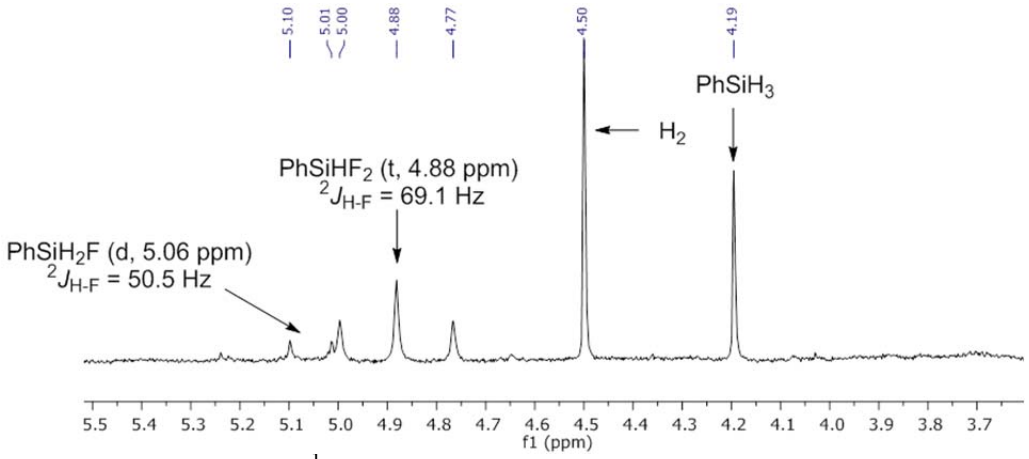


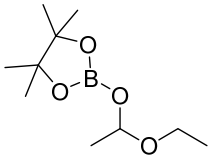
Figure S4. A fragment of ^{1}H-NMR spectrum of the reaction of **3-Ar** with PhSiH$_3$ in PhMe-d$_8$ at 0 °C, showing formation of PhSiH$_2$F, PhSiHF$_2$ and H_2.

General procedure for catalytic hydrosilylation and hydroboration reactions

A substrate of interest or a mixture of substrates, as in competitive hydroboration of benzaldehyde (Table 4), each 0.162 mmol, was mixed with an appropriate amount of either $PhSiH_3$ (see Tables 1 and 2) or HBPin (see Tables 3 and 4) in 0.6 mL of C_6D_6 (unless another solvent is specified, see Tables 1-4) at room temperature. The mixture was transferred to an NMR tube equipped with a Teflon valve, left at room temperature for 15 min and checked with ^{1}H-NMR, confirming no reaction in the absence of the catalyst. This solution was then added to the solid pre-catalyst, the mixture was transferred back to the NMR tube and the reaction was monitored with ^{1}H- and ^{31}P{^{1}H}-NMR either at room temperature or at elevated temperatures (see Tables 1-4). Conversion of substrates and the yields of the hydrosilylation and hydroboration products were determined by ^{1}H-NMR spectroscopy using $Si(SiMe_3)_4$ as an internal standard. All hydrosilylation and hydroboration products were characterized without isolation. NMR signals for new hydrosilylation and hydroboration products are given below. Concerning hydrosilylation of styrene and 1-octene with the bromide pre-catalysts, the activity of **1-Ar'**/$LiBHEt_3$ system was found to be very similar to **1-Ph**/$LiBHEt_3$, whereas under analogous reaction conditions (20 h at 60 °C) **1-^{t}Bu**/$LiBHEt_3$ showed low activity in hydrosilylation of styrene (18% conversion to $PhCH(Me)SiH_2Ph$) and 1-octene (only trace amounts of (^{n}Oct)SiH_2Ph and no octane isomerization products were detected).

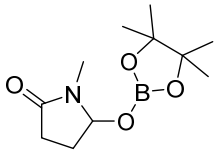
NMR data for hydrosilylation and hydroboration products

The hydrosilylation products $PhCH(SiH_2Ph)CH_3$,[6] $Ph(CH_2)_2SiH_2Ph$,[6] (*n*-Hex)SiH_2Ph, (*n*-Oct)SiH_2Ph,[7] $Ph(CH_2)_3SiH_2Ph$,[8] $PhH_2Si(OBn)$,[9] $PhHSi(OBn)_2$,[9,10,11] $PhH_2Si(OCy)$,[10,12,13] $PhHSi(OCy)_2$,[10,12,13] PhMeHSi(OBn), [14] $Et_3Si(OBn)$ [15] and hydroboration products BnOBPin, [16] ^{i}PrOBPin,[16a] CyOBPin, [17] PhMeC(H)OBPin,[16c,d, 18] $Ph_2C(H)OBPin$,[18, 19] EtOBPin,[20] $EtN(Bpin)_2$[21] have been previously described, and NMR spectra for these compounds have been listed for a variety of solvents including C_6D_6.

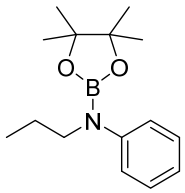


A compound was not obtained in pure form and was observed in a mixture with EtOAC during the catalytic hydroboration of EtOAc with HBPin mediated by **6-Ar**. Characteristic NMR signals: ^{1}H-NMR (500 MHz; C_6D_6; δ, ppm): 1.15 (br s, 12 H, 4 CH_3 of B*Pin*); 1.29 (m, 3H, OCH_2CH_3);

1.53 (br d, $^{3}J_{H\text{-}H}$ = 5.2 Hz, 3H, *CH₃*CH(O)-); 3.49 (m, 1H, O*CH₂*CH₃); 3.88 (m, 1H, O*CH₂*CH₃); 5.52 (q, $^{3}J_{H\text{-}H}$ = 5.2 Hz, 3H, CH₃C*H*(O)-). ^{1}H-^{13}C HSQC NMR (f1: 500 MHz; f2: 128.5 MHz; C_6D_6; δ, ppm): 17.3 (OCH₂*CH₃*); 23.0 (OCH*CH₃*); 24.4 (CH₃ of B*Pin*); 62.6 (O*CH₂*CH₃); 96.2 (O*CH*CH₃).



^{1}H-NMR (500 MHz; C_6D_6; δ, ppm): 1.05 (br s, 12 H, 4 CH₃ of B*Pin*); 1.57 (m, 2H, *CH₂*); 1.84 (m, 1H, *CH₂*); 2.24 (m, 1H, *CH₂*); 2.69 (s, 3H, N*CH₃*); 5.21 (m, 1H, *CH*). ^{1}H-^{13}C HSQC NMR (f1: 500 MHz; f2: 128.5 MHz; C_6D_6; δ, ppm): 24.5 (CH₃ of B*Pin*); 26.6 (N*CH₃*); 27.5 (*CH₂*); 27.8 (*CH₂*); 86.2 (*CH*). ^{11}B{^{1}H}-NMR (160.5 MHz; C_6D_6; δ, ppm): 21.2 (br s, *B*Pin).



^{1}H-NMR (500 MHz; C_6D_6; δ, ppm): 0.79 (t, $^{3}J_{H\text{-}H}$ = 7.5 Hz, 3H, *CH₃*CH₂CH₂N); 1.08 (br s, 12H, B*Pin*); 1.49 (m, 2H, CH₃*CH₂*CH₂N); 3.51 (t, $^{3}J_{H\text{-}H}$ = 7.2 Hz, 2H, CH₃CH₂*CH₂*N); 6.85 (t, $^{3}J_{H\text{-}H}$ = 7.2 Hz, 1H, *p*-H of N*Ph*); 7.16 (t, $^{3}J_{H\text{-}H}$ = 7.9 Hz, 2H, *m*-H of N*Ph*); 7.37 (d, $^{3}J_{H\text{-}H}$ = 8.0 Hz, 1H, *o*-H of N*Ph*). ^{13}C{^{1}H}- NMR (128.5 MHz; C_6D_6; δ, ppm): 11.3 (s, CH₃ of N*Pr*); 22.6 (s, CH₂ of N*Pr*); 25.0 (s, 4 CH₃ of B*Pin*); 48.7 (s, CH₂ of N*Pr*); 83.2 (s, 2 C_q of B*Pin*); 121.78 (s, CH of N*Ph*); 121.83 (s, CH of N*Ph*); 128.9 (s, CH of N*Ph*); 146.4 (s, C_q of N*Ph*). ^{11}B{^{1}H}-NMR (160.5 MHz; C_6D_6; δ, ppm): 23.7 (br s, *B*Pin).

MeC(O)NH(BPin): was obtained in a mixture with $MeC(O)NH_2$ and $EtN(BPin)_2$ (see Table 3, entry 13 and Figure S5). ^{1}H-NMR (500 MHz; C_6D_6; δ, ppm): 0.96 (br s, 12H, B*Pin*); 2.10 (br s, 3H, *CH₃*); 6.36 (br s, 1H, N*H*).

EtC(O)N(BPin)Ph: was obtained in a mixture with EtC(O)NHPh and ^{n}PrN(BPin)Ph (see Table 3, entry 15 and Figure S6). ^{1}H-NMR (500 MHz; C_6D_6; δ, ppm): 0.94 (br s, 12H, B*Pin*); 1.23 (t, $^{3}J_{H\text{-}H}$ = 7.2 Hz, 3H, *CH₃*); 2.78 (q, $^{3}J_{H\text{-}H}$ = 7.2 Hz, 3H, *CH₃*); 6.99 (t, $^{3}J_{H\text{-}H}$ = 7.0 Hz, 1H, *p*-H of N*Ph*); 7.13 (m, 4H, *m*-H and *o*-H of N*Ph*).

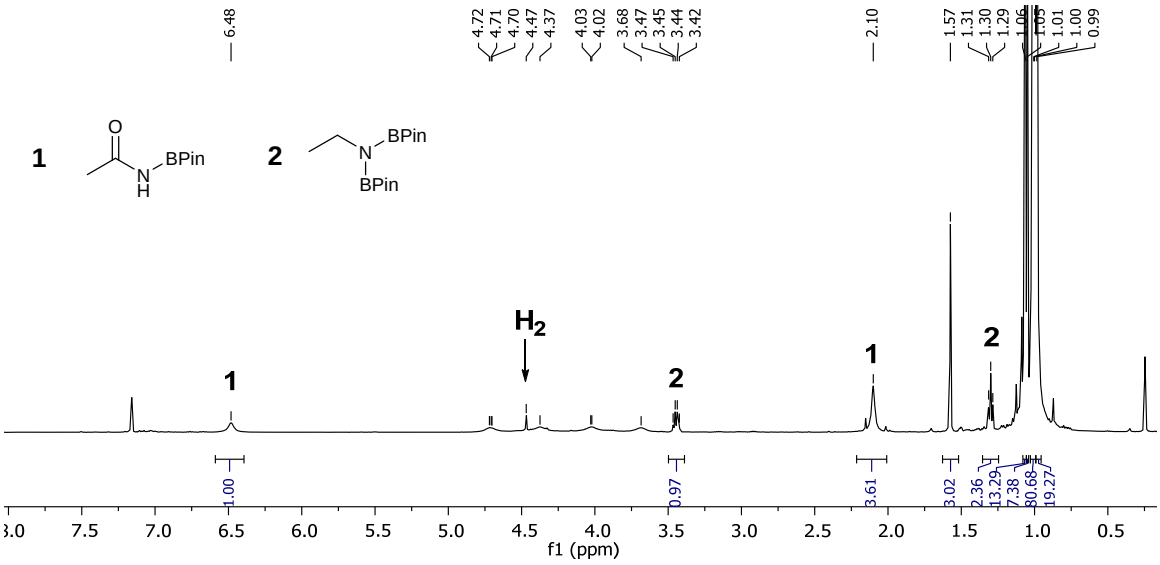


Figure S5. ^{1}H-NMR spectrum for hydroboration of acetamide with HBPin at 60 °C in the presence of 5 mol% of **6-Ar**, taken after 5 h and showing formation of a mixture of MeC(O)NH(BPin) and EtN(BPin)$_2$.

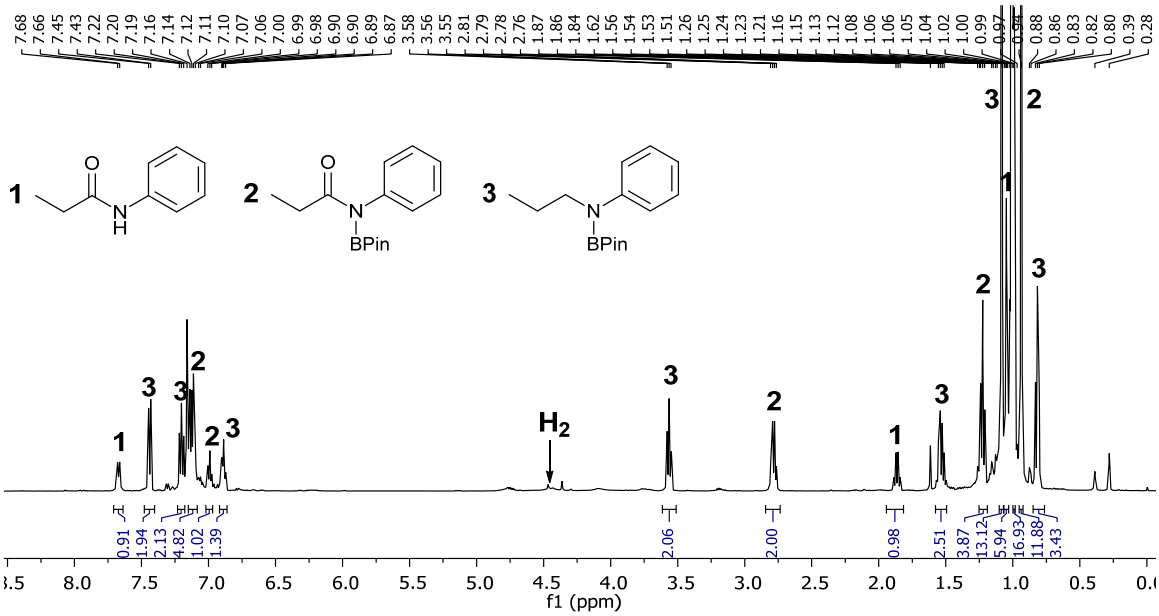


Figure S6. ^{1}H-NMR spectrum for hydroboration of *N*-phenylpropanamide with HBPin at room temperature in the presence of 5 mol% of **6-Ar**, taken after 5 days at room temperature and showing formation of a mixture of EtC(O)NHPh (19%), EtC(O)N(BPin)Ph (40%) and ^{n}PrN(BPin)Ph (41%).

X-Ray diffraction analysis

The single crystals of **1-Ar** and **2-Ar** suitable for X-Ray diffraction analysis were obtained by crystallization from there solutions in hexanes at -30 °C, whereas the single crystals of **3-Ar** and **6-Ar** were obtained by slow ambient pressure vaporization of their Et_2O solutions into hexanes at room temperature and at -28 ºC, respectively. The later crystallization technique consists of a two vials system: the small vial with Et_2O solution of a complex was placed in a larger vial with hexanes, the system was closed with a screw cap and left either at room temperature or at -28 ºC, showing slow transfer of the lower boiling point Et_2O from the inner vial solution into higher boiling point hexanes in the outer vial.

X-ray diffraction data for **1-Ar**, **2-Ar, 3-Ar** and **6-Ar** were collected on a SMART APEX II area-detector diffractometer (graphite monochromator, ω-scan technique), using $Mo_{K\alpha}$-radiation (0.71073 Å). The intensity data were integrated by the SAINT program[22] and were corrected for absorption and decay using SADABS.[23] All structures were solved by direct methods using SHELXS,[24] and were refined on F^2 using SHELXL-2014/2017.[25] All non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms were placed in ideal calculated positions and refined as riding atoms with relative isotropic displacement parameters taken as $U_{iso}(H)=1.5U_{eq}(C)$ for methyl groups and $U_{iso}(H)=1.2U_{eq}(C)$ for rest ones. The hydrogen atoms of BH4 group were located from the Fourier density synthesis and refined in the isotropic approximation. In the crystal of **3-Ar** the fluorine atoms of CF_3 group are disordered by three positions with the occupancies equal to 0.31054, 0.37834 and 0.31088. In crystal of **6-Ar** in both independent molecules the superposition of Cl and Me-group was observed with slightly different ratio of occupancies (0.23, 0.77 and 0.15, 0.85). The positional and anisotropic displacement parameters of the fluorine atoms in **3-Ar** and **Cl** and **Me** groups in two independent molecules in **6-A**r were refined with the constraints DFIX and EADP. Crystal data, data collection and structure refinement details are summarized in Table S1. The general view of **1-Ar**, **2-Ar, 3-Ar** and **6-Ar** are shown on the Figures S7-S10.

Table S1. X-ray crystallographic data and refinement details for complexes **1-Ar**, **2-Ar**, **3-Ar** and **6-Ar**.

	1-Ar	**2-Ar**	**3-Ar**	**6-Ar**
Empirical formula	$C_{25}H_{35}BrNNiOP$	$C_{25}H_{39}BNNiOP$	$C_{25}H_{35}BF_4NNiOP$	$C_{25\cdot81}H_{37\cdot43}Cl_{0\cdot19}NNiOP$
Formula weight	535.13	470.06	542.03	474.18
Temperature (K)	120	120	120	120
Crystal system	Monoclinic	Monoclinic	Monoclinic	Orthorhombic
Space group	$P2_1/c$	$P2_1/c$	$P2_1/n$	$Pca2_1$
Z(Z')	4(1)	4(1)	4(1)	8(2)
Unit cell dimensions				
a, Å	15.4795(10)	15.5364(18)	12.0222(5)	28.3028(16)
b, Å	10.0302(6)	10.1575(12)	13.5884(5)	12.4428(7)
c, Å	16.4542(11)	16.462(2)	16.3723(6)	14.4107(8)
α, °	90	90	90	90
β, °	93.9154(17)	94.059(3)	90.8780(10)	90
γ, °	90	90	90	90
V, $Å^3$	2548.8(3)	2591.4(6)	2674.31(18)	5075.0(5)
d_{calc}, $g\cdot cm^{-3}$	1.395	1.205	1.346	1.241
μ, cm^{-1}	24.08	8.26	8.31	8.64
F(000)	1112	1008	1136	2028
$2\theta_{max}$, °	58	58	58	58
Completeness	1.0	0.99	1.00	1.00
Refl. collected	22748	24001	31862	59956
Refl. unique (R_{int})	6780 (0.0687)	6879 (0.0416)	7117 (0.0423)	13472 (0.0422)
Refl. with I > 2σ(I)	4746	5622	5660	11538
Variables	279	295	325	570
Final R_1 with I>2σ(I)	0.0417	0.0332	0.0459	0.0337
wR_2 (all data)	0.0970	0.0843	0.1204	0.0836
GOF	0.949	1.006	1.022	1.037
Largest difference in peak / hole ($e/Å^3$)	0.527/-0.464	0.539/-0.286	1.243/-1.183	0.370/-0.302
CCDC number	1883579	1883581	1883582	1883580

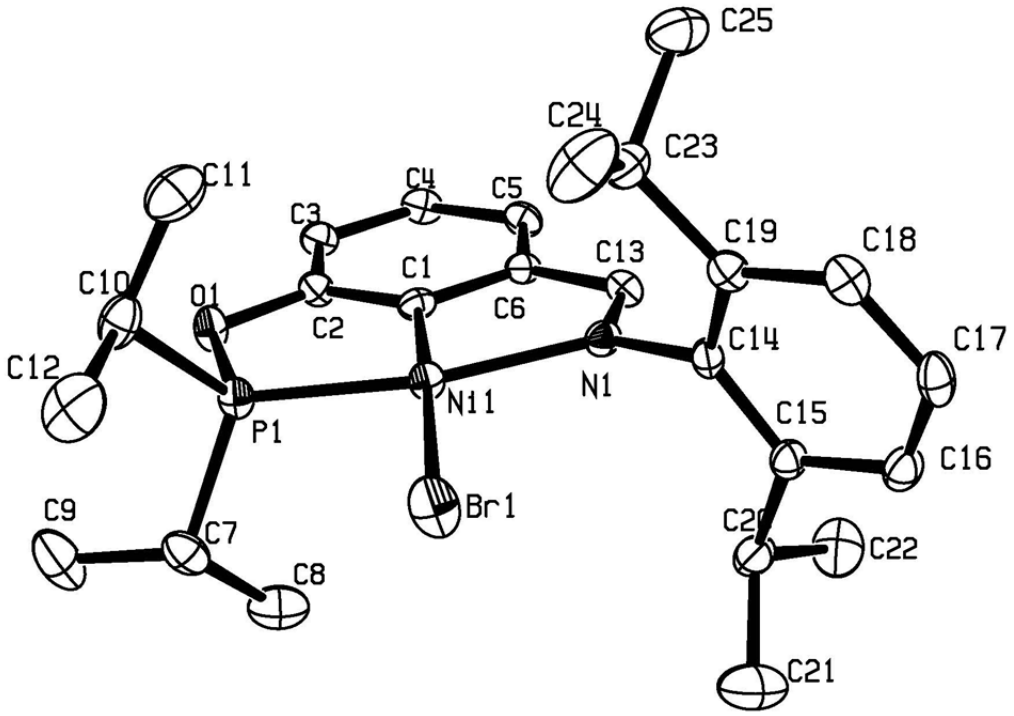


Figure S7. Molecular structure of **1-Ar** (hydrogen atoms are omitted for clarity). Thermal ellipsoids are drawn to 50% probability level

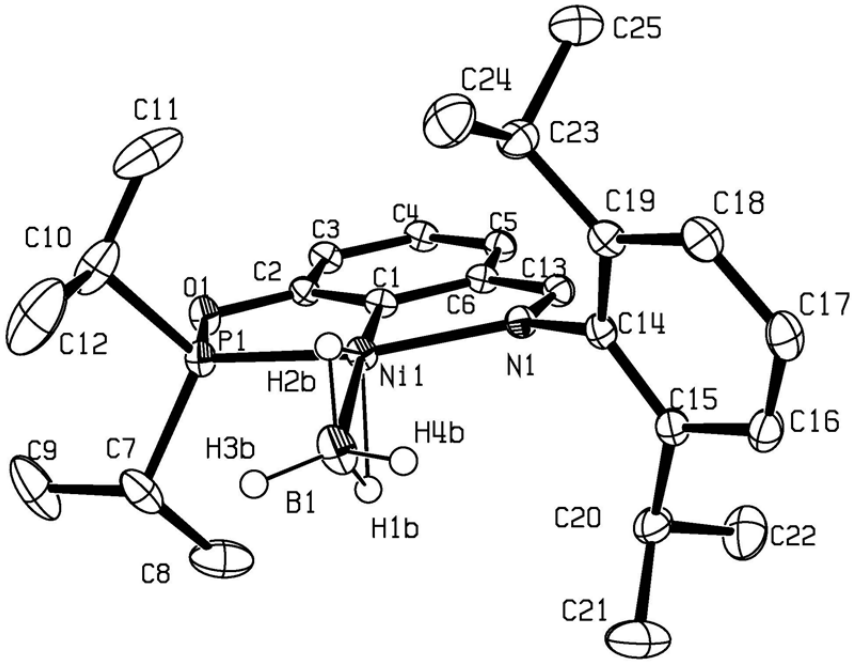


Figure S8. Molecular structure of **2-Ar** (hydrogen atoms except for BH_4 unit are omitted for clarity). Thermal ellipsoids are drawn to 50% probability level.

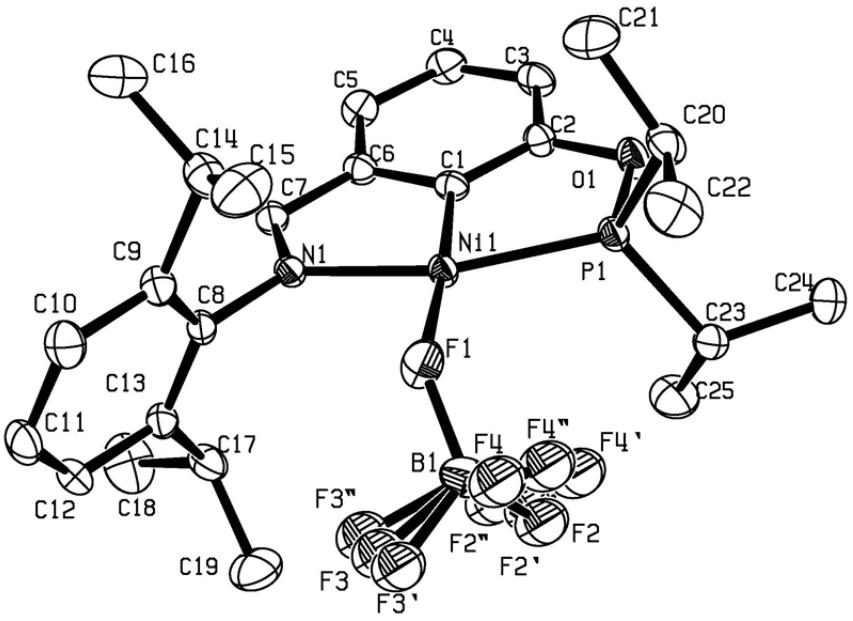


Figure S9. Molecular structure of **3-Ar** (hydrogen atoms are omitted for clarity). Thermal ellipsoids are drawn to 50% probability level.

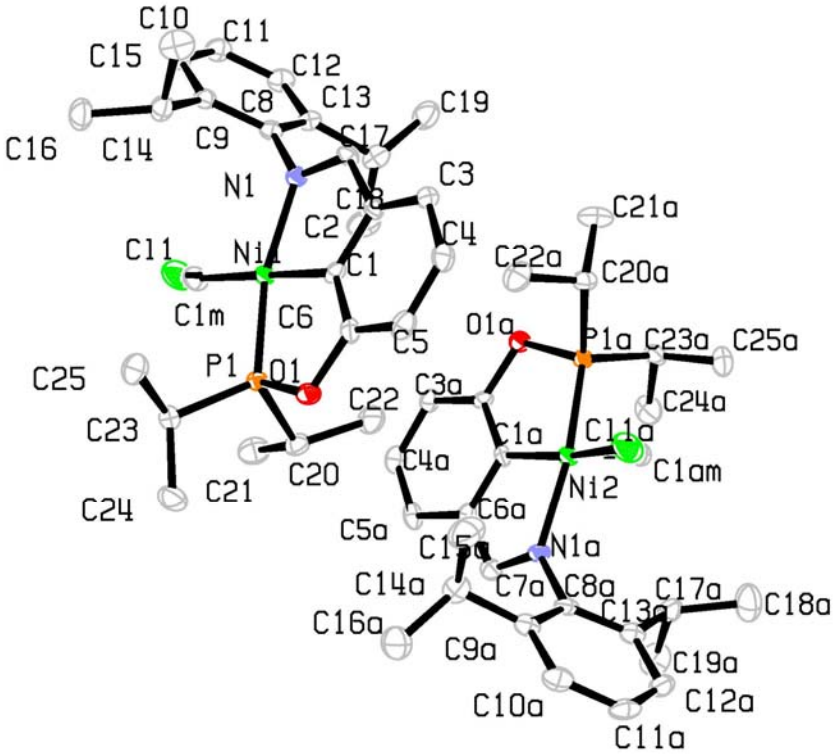


Figure S10. The general view of one of the independent molecules of co-crystal of 0.81 **6-Ar** and 0.19 ($^{i\text{-Pr}}$POCN^{Ar})NiCl illustrating the superposition of Cl(1) and Me-groups. Atoms are shown by thermal ellipsoids (50% probability level). Hydrogen atoms are omitted for clarity.

Computational Details

Gibbs free energies at 60 °C and a reference pressure of 1 bar were obtained within the rigid-rotator and harmonic oscillator approximations at the PBE0-D3/def2-TZVPP//PBE-D3/dhf-SV(P) level of theory with TURBOMOLE, using the RI-approximation.[26,27]

Figure S11 shows the free energy diagram for the direct addition of $PhSiH_3$. Figure S12 shows the transition states for Markovnikov and *anti*-Markovnikov olefin insertion. Figure S13 shows the transition state energies for various conformers. Figure S14 shows the reaction pathways also including dissociation of the N-arm, while Figure S15 shows the corresponding free energy diagram.

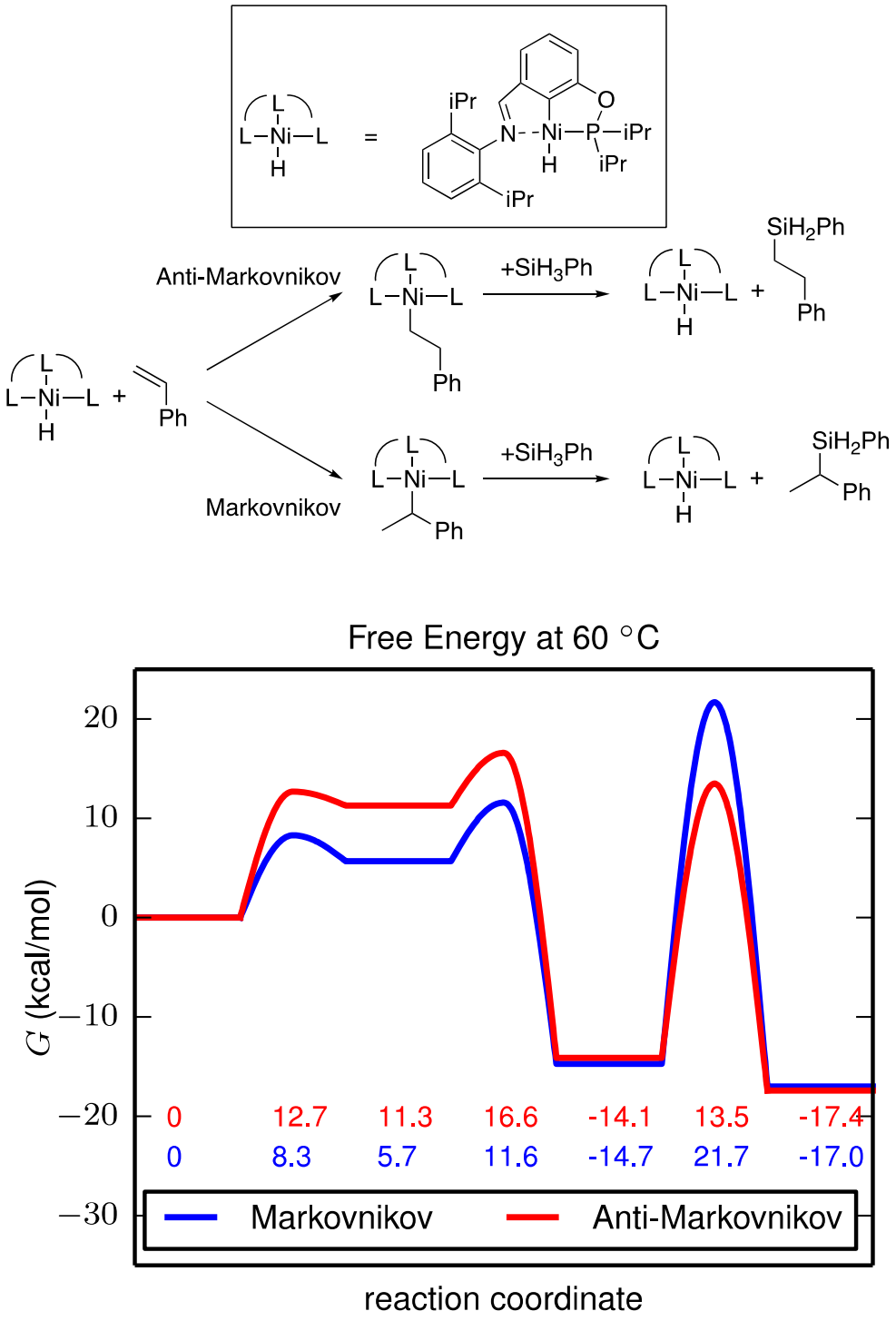


Figure S11. Computed mechanism for direct addition of $PhSiH_3$ to the alkylnickel species

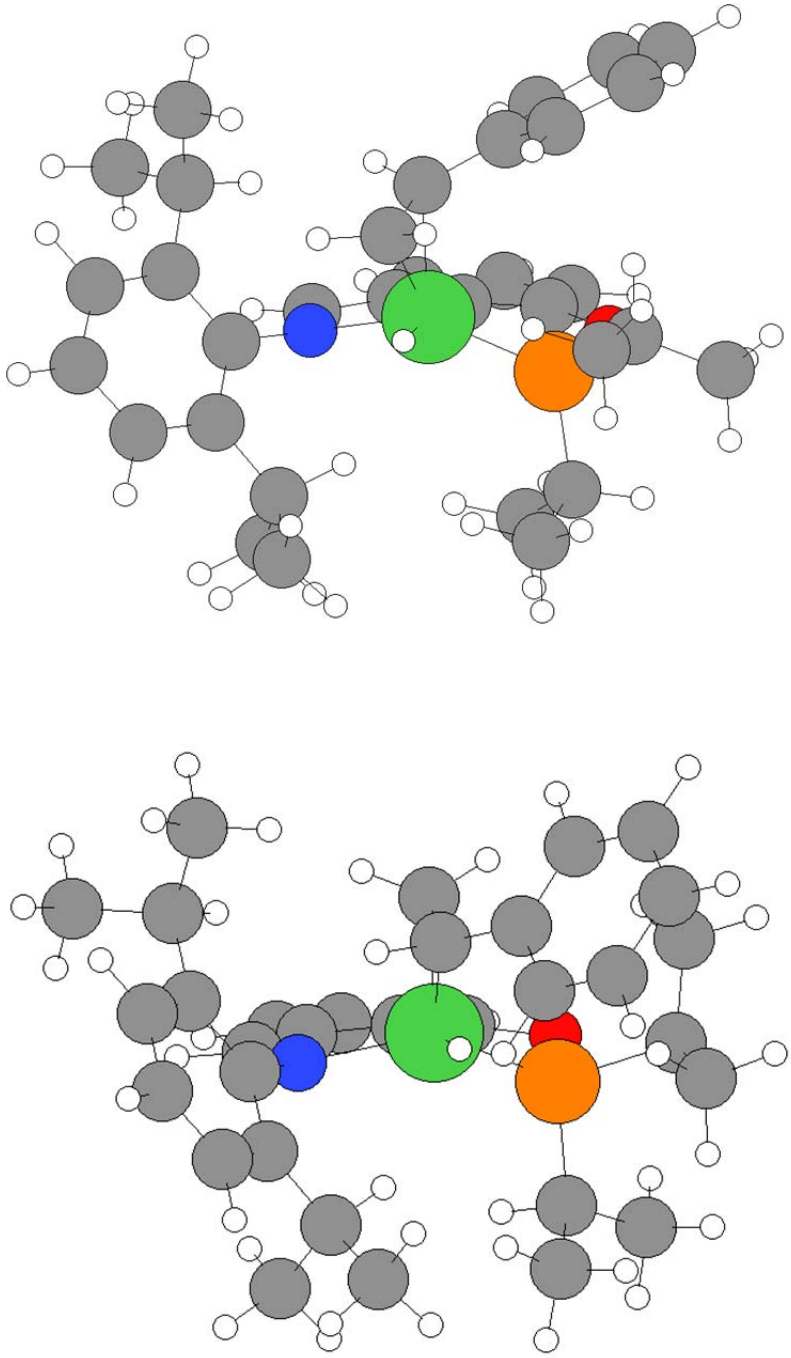


Figure S12. Computed structures of the transition state for styrene insertion, towards intermediates **C** (top) and **E** (bottom), showing more favorable interaction of the alkyl ligand in the intermediate **C** with P-arm of the POCN ligand (Ph-group is unhindered)

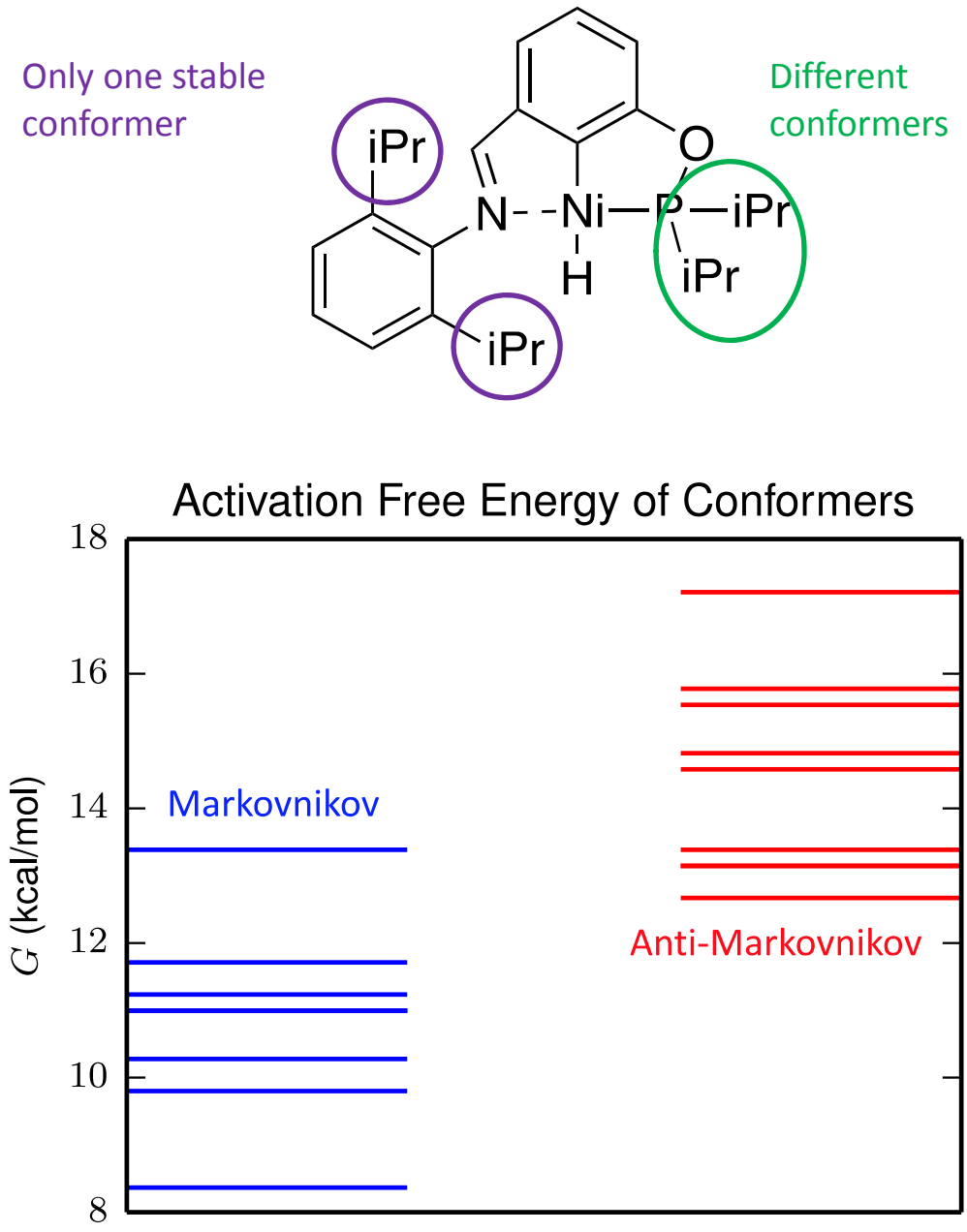


Figure S13. Analysis of the conformers of insertion of styrene into the Ni-H bond of **7-Ar** (transition states free energies are shown at the bottom). In principle, there are 3^4=81 conformers; 9 conformers for different orientations of ^{i}Pr groups on phosphine. For Markovnikov insertion product some converged to same conformer The ^{i}Pr groups of the Ar substituent have only one stable orientation.

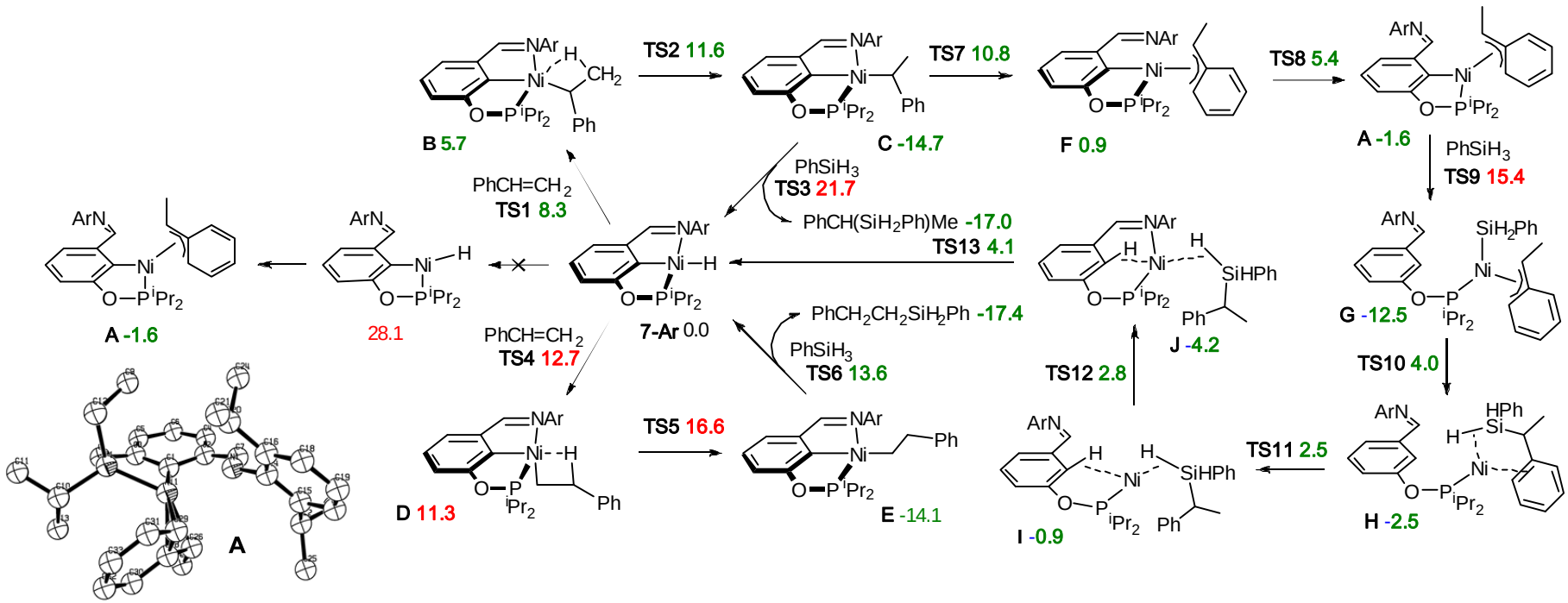


Figure S14. DFT-calculated mechanism for **7-Ar**-catalyzed hydrosilylation of styrene with $PhSiH_3$ at 60 °C (free energies are in kcal·mol^{-1}).

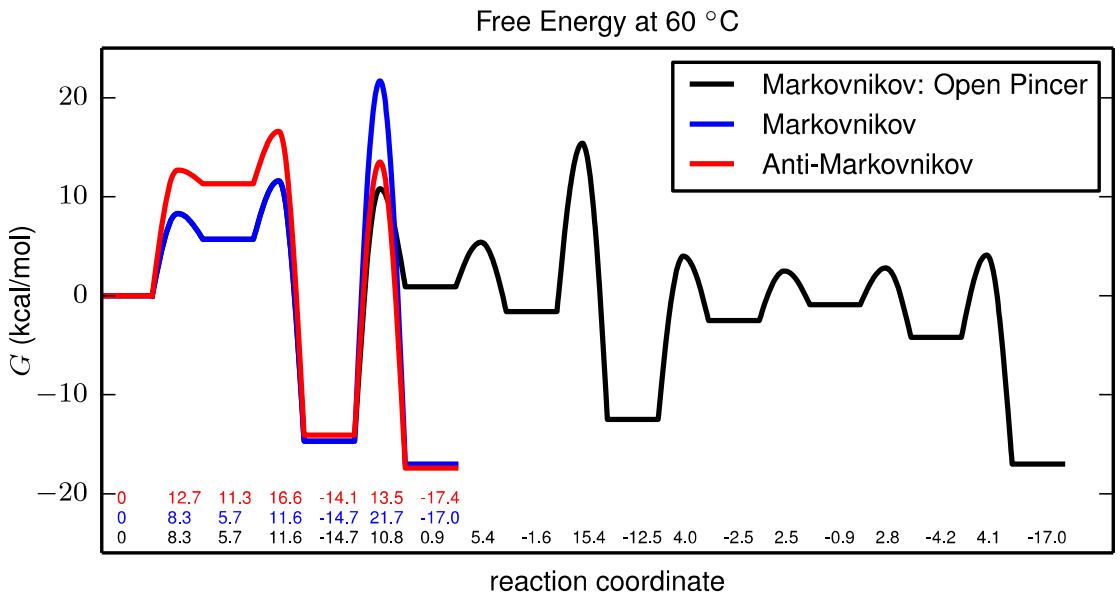


Figure S15. DFT-calculated reaction coordinate for **7-Ar**-catalyzed hydrosilylation of styrene with $PhSiH_3$ at 60 °C.

Table S2. Total energy and free energy contribution (including zero-point correction) for all structures in kcal/mol.

structure	E PBE0-D3/def2-TZVPP	ΔG (vib-rot-trans)
styrene	-194139.15800	58.85037
SiH_3Ph	-327951.82790	48.45362
$PhCH(SiH_2Ph)Me$	-522123.56349	122.88955
$PhCH_2CH_2SiH_2Ph$	-522123.20147	122.14147
7-Ar	-1852926.66005	290.14095
TS1	-2047075.47715	366.97172
TS2	-2047074.68155	369.46933
B	-2047079.91331	368.75709
TS4	-2047071.23596	367.12229
TS5	-2047069.24920	369.02956
D	-2047074.21007	368.68539
C	-2047101.43584	369.90671
E	-2047098.56533	367.62659
TS3	-2375035.81125	437.33260
TS6	-2375042.63602	435.94159
TS7	-2047077.23230	371.15671
F	-2047086.46511	370.52334
TS8	-2047079.60252	368.21933
A	-2047085.31370	366.88568
TS9	-2375037.41291	432.58117
G	-2375065.55817	432.82018
TS10	-2375051.59631	435.43968
H	-2375058.15611	435.45163
TS11	-2375050.42029	432.74608
I	-2375053.76454	432.63375
TS12	-2375050.31317	432.89905
J	-2375057.65120	433.22888
TS13	-2375048.72407	432.64092

Table S3. Cartesian coordinates in xyz-format.

styrene

16

Energy =

C -2.8989348 -4.4486348 -4.9060087

H -3.8450549 -3.9445270 -4.6304896

C -2.5237216 -5.5251278 -4.1795529

H -3.1448924 -5.8837697 -3.3411340

H -1.5956845 -6.0883267 -4.3843712

C -2.1948243 -3.8407459 -6.0483850

C -2.7598218 -2.7065168 -6.6793532

C -0.9680739 -4.3357314 -6.5558835

C -2.1307616 -2.0893919 -7.7706535

H -3.7151254 -2.3043089 -6.3001499

C -0.3383648 -3.7216012 -7.6448274

H -0.4982237 -5.2171882 -6.0900199

C -0.9155282 -2.5946467 -8.2591653

H -2.5937178 -1.2069394 -8.2429105

H 0.6161459 -4.1258144 -8.0214460

H -0.4168603 -2.1133257 -9.1166912

SiH_3Ph

15

Energy =

H 0.4869892 1.7826316 11.2028233

Si 0.7231362 1.4505087 12.6560245

H 0.0923196 0.1178738 12.9780426

H 2.2142867 1.3240108 12.8669209

C -0.0155922 2.7952091 13.7560095

C -0.0622185 4.1415896 13.3255485

C -0.5099448 2.4894974 15.0452184

C -0.5808210 5.1489202 14.1552908

H 0.3081421 4.4128346 12.3212492

C -1.0293764 3.4941279 15.8779611

H -0.4954987 1.4468372 15.4083777

C -1.0649401 4.8264418 15.4341010

H -0.6104580 6.1925921 13.7997638

H -1.4122324 3.2343849 16.8792032

H -1.4748578 5.6160750 16.0858788

PhCH(SiH_2Ph)Me

31

Energy =

C -4.2652232 -9.5284275 -3.5376605

H -4.0911326 -8.7744071 -4.3400871

C -3.0804306 -9.4788706 -2.5558482

H -2.9020290 -8.4384060 -2.2059395

H -3.2531536 -10.1008060 -1.6489580

H -2.1462096 -9.8467495 -3.0382118

C -4.5083731 -10.8707891 -4.1987729

C -4.9509817 -10.9348528 -5.5401134

C -4.3468326 -12.0891005 -3.5007989

C -5.2185989 -12.1631260 -6.1619666

H -5.0846291 -9.9967305 -6.1068229

C -4.6128125 -13.3204330 -4.1208553

H -4.0065377 -12.0798039 -2.4524558

C -5.0500620 -13.3650963 -5.4542818

H -5.5573693 -12.1814167 -7.2114904

H -4.4748842 -14.2559694 -3.5530302

H -5.2569607 -14.3324367 -5.9411888

Si -5.8972056 -8.9717141 -2.6803185

H -7.0046104 -8.9531617 -3.7062485

H -6.2161651 -9.9718981 -1.5932559

C -5.7134793 -7.2522159 -1.9202298

C -5.2262180 -7.0841985 -0.6024392

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C -5.0252873 -5.8040062 -0.0609149

H -5.0029121 -7.9703602 0.0176770

C -5.7962494 -4.8084740 -2.1403715

H -6.3835554 -6.1869747 -3.7069135

C -5.3099326 -4.6632864 -0.8302051

H -4.6475953 -5.6953907 0.9697170

H -6.0258503 -3.9160620 -2.7466571

H -5.1553916 -3.6571008 -0.4057786

$PhCH_2CH_2SiH_2Ph$

31

Energy =

C -5.5448923 -11.5209401 -3.8997430

H -6.5108208 -11.4690640 -4.4522865

C -5.1082237 -10.0951188 -3.4910366

H -4.1391945 -10.1372057 -2.9406667

H -4.9103366 -9.4815198 -4.4007985

H -5.7388593 -12.1261622 -2.9847940

C -4.5100196 -12.2211448 -4.7576374

C -4.5239301 -12.0876704 -6.1617058

C -3.4754536 -12.9783088 -4.1695506

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H -5.3285063 -11.5021069 -6.6403026

C -2.4844217 -13.5840606 -4.9581204

H -3.4505948 -13.0973987 -3.0720555

C -2.5107293 -13.4416751 -6.3554927

H -3.5683915 -12.5779206 -8.0521026

H -1.6872545 -14.1759572 -4.4777323

H -1.7350290 -13.9189448 -6.9771179

Si -6.3666830 -9.1640820 -2.4070824

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H -6.6102858 -9.9598131 -1.1435519

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H -4.5757702 -8.1135903 -0.2306106

C -5.5743670 -5.0382238 -2.4276639

H -6.7744807 -6.4223004 -3.5870710

C -4.7029353 -4.8726303 -1.3383757

H -3.6666457 -5.8577839 0.3047453

H -5.8603232 -4.1691539 -3.0438032

H -4.3019868 -3.8738524 -1.0972551

7-Ar

65

Energy =

Ni 1.9458392 -0.1425017 6.2968761

C 1.0351659 -0.1615326 4.6597884

C 1.8270495 -0.0726713 3.4882736

C -0.3628770 -0.2046626 4.5417264

C 1.2255258 -0.0470124 2.2072651

C -0.9843430 -0.1832907 3.2818360

C -0.1751551 -0.1064178 2.1226833

H 1.8376924 0.0222286 1.2923010

H -2.0826523 -0.2211941 3.2019877

H -0.6630083 -0.0892167 1.1341536

N 3.5257963 -0.0048454 5.1092759

C 3.2348340 0.0141367 3.8273284

H 4.0404476 0.1135880 3.0708575

P 0.0268989 -0.2818638 7.0633358

O -1.0781916 -0.2620366 5.7226770

C -0.5991607 1.1661587 8.0526915

C -2.1119011 1.1541041 8.3070800

H -0.0503282 1.0567710 9.0179914

H -2.4115915 2.0778758 8.8523260

H -2.6731256 1.1237554 7.3479057

H -2.4288289 0.2864175 8.9249762

C -0.4652309 -1.8500584 7.9651322

C -1.8538709 -2.3754128 7.5722391

H -0.4680773 -1.5490974 9.0398365

H -2.0932244 -3.2791161 8.1775040

H	-2.6595810	-1.6295097	7.7334831
H	-1.8772950	-2.6623058	6.4993794
C	-0.1238875	2.4561380	7.3639876
H	-0.5917086	2.5677613	6.3606912
H	-0.4017385	3.3447554	7.9745701
H	0.9805229	2.4508639	7.2281621
C	0.6306609	-2.9082923	7.7522394
H	0.6915660	-3.2055642	6.6813442
H	1.6285439	-2.5198667	8.0486138
H	0.4073904	-3.8213496	8.3498800
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C	5.7263315	-1.0672179	5.4308607
C	5.2898813	1.2509496	6.2196304
C	7.0414261	-0.9472884	5.9193775
C	6.6129576	1.3165490	6.6915535
C	7.4875189	0.2331708	6.5313850
H	7.7343982	-1.7978986	5.8290476
H	6.9664486	2.2298770	7.1959304
H	8.5243205	0.3020142	6.9003301
C	4.3016600	2.3990090	6.3816792
C	4.5138632	3.2241809	7.6578519
H	3.2974347	1.9148698	6.4728178
H	3.6711040	3.9385748	7.7924101
H	4.5553731	2.5692826	8.5554534
H	5.4500031	3.8262425	7.6215559
C	5.1845751	-2.3861884	4.8772754
C	6.2688769	-3.3822885	4.4433480
H	4.5813023	-2.1556538	3.9706212
H	5.8002281	-4.2627741	3.9512988
H	6.9846861	-2.9277229	3.7232346
H	6.8511879	-3.7652491	5.3112976
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H	4.0368139	2.7118973	4.2132423
H	3.4924188	4.0877343	5.2330011

H 5.2529266 3.7950940 4.9750816

C 4.2251803 -3.0274209 5.9024917

H 3.7679767 -3.9555097 5.4915342

H 4.7693155 -3.2870619 6.8380177

H 3.4028992 -2.3274134 6.1748970

H 2.5995089 -0.0937909 7.7310180

TS1

81

Energy =

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Ni -0.0734601 -0.2306944 0.2066498

C -0.6736212 1.5152505 -0.1332250

C 0.3050004 2.4654482 -0.5236445

C -1.9880715 1.9441935 0.1253888

C -0.0829576 3.7982880 -0.8296731

C -2.3910545 3.2496858 -0.1863630

C -1.4271635 4.1619633 -0.6886264

H 0.6668628 4.5388477 -1.1548722

H -3.4307102 3.5644356 -0.0030501

H -1.7430116 5.1906626 -0.9286801

N 1.7410929 0.6723335 -0.0412954

C 1.6344523 1.9138450 -0.4841915

H 2.5347721 2.4928025 -0.7734634

P -1.8322960 -0.2347601 1.4144723

O -2.8079245 1.0457999 0.7721067

C -1.7560835 0.2942457 3.2118791

C -0.9910758 1.6211514 3.3284761

H -0.9258349 1.9257103 4.3979908

H 0.0439022 1.5220567 2.9322112

H -1.4883689 2.4402336 2.7672896

C -3.1111029 -1.5856287 1.2755410

C -4.4093152 -1.2835836 2.0354355

H -5.1965572 -2.0131817 1.7374339

H	-4.2757746	-1.3725327	3.1370531
H	-4.7852732	-0.2641980	1.8043793
C	-1.1074962	-0.8128202	4.0567487
H	-0.1202315	-1.1089012	3.6353925
H	-0.9364099	-0.4493236	5.0953433
H	-1.7391485	-1.7243149	4.1228927
H	-3.3212684	-1.5278587	0.1824709
C	2.9956258	0.0097226	-0.0298446
C	3.7121257	-0.2456325	-1.2365980
C	3.4852372	-0.4597164	1.2278405
C	4.9243766	-0.9618240	-1.1487685
C	4.6984603	-1.1662758	1.2544358
C	5.4191834	-1.4174523	0.0769770
H	5.4938992	-1.1678703	-2.0705399
H	5.0949880	-1.5276772	2.2162783
H	6.3702819	-1.9737066	0.1179726
C	2.7193382	-0.1366924	2.5043252
C	2.9015514	-1.1682790	3.6253618
H	2.2115619	-0.9398343	4.4677563
H	2.6779341	-2.1982555	3.2694002
H	3.9337664	-1.1644328	4.0432597
C	3.2269419	0.2147700	-2.6113862
C	4.1422684	1.3125244	-3.1891210
H	3.7525316	1.6758824	-4.1665440
H	4.2180951	2.1837481	-2.5016328
H	5.1746323	0.9303637	-3.3557233
C	3.0541184	1.2855737	2.9978474
H	2.8450205	2.0451046	2.2137315
H	2.4438261	1.5448883	3.8924279
H	4.1291003	1.3664641	3.2777598
C	3.0749340	-0.9547388	-3.6029813
H	2.6580762	-0.5905886	-4.5684895
H	4.0510080	-1.4419085	-3.8231925
H	2.3861882	-1.7329907	-3.2087488

C -0.3493312 -0.9452761 -1.7343290

H 0.2775951 -0.2505874 -2.3200578

H -0.2051502 -2.8799703 -0.7266159

H 1.4092554 -2.0558018 -1.0723921

C -1.7517039 -1.0289568 -2.1857812

C -2.3642921 0.1094852 -2.7707565

C -2.5335318 -2.2067580 -2.0806634

C -3.6959114 0.0813405 -3.2001158

H -1.7791464 1.0402841 -2.8558200

C -3.8691260 -2.2354822 -2.5106370

H -2.0878213 -3.1242731 -1.6626124

C -4.4630061 -1.0907293 -3.0678935

H -4.1452517 0.9893457 -3.6363246

H -4.4495668 -3.1690828 -2.4162742

H -5.5127337 -1.1130889 -3.4039479

C -2.5512629 -2.9838183 1.5709215

H -1.5703402 -3.1475910 1.0761754

H -2.4138138 -3.1591019 2.6600991

H -3.2583268 -3.7577868 1.1957629

H -2.8095174 0.4523764 3.5353299

H 2.2186830 0.6631873 -2.4887258

H 1.6423100 -0.1377145 2.2170855

TS2

81

Energy =

H -0.8093417 -1.2666949 -0.2153718

C 0.2525120 -1.8288482 -0.3097927

Ni -0.1870388 0.3285221 -0.1935984

C -0.2356953 2.1768209 -0.0617318

C 0.0134632 2.7235678 1.2365939

C -0.6202106 3.0590083 -1.0955108

C 0.0240477 4.1337612 1.4265561

C -0.6243874 4.4440811 -0.9151371

C -0.2719414 4.9750658 0.3539086

H	0.2452054	4.5504064	2.4233787
H	-0.9236988	5.0991433	-1.7482135
H	-0.2692886	6.0683572	0.4943316
N	-0.0231210	0.4620778	1.7756616
C	0.1513176	1.7055931	2.2216046
H	0.3530982	1.8988646	3.2912935
P	-1.1023579	0.7937473	-2.0908501
O	-1.0489858	2.4849034	-2.2745744
C	-2.9353168	0.4567465	-2.2435215
C	-3.6870317	1.1704256	-1.1119893
H	-4.7812545	0.9867528	-1.2068643
H	-3.3535916	0.7977068	-0.1177182
H	-3.5165701	2.2678402	-1.1357499
C	-0.3089896	0.3040754	-3.7086633
C	-1.2067721	0.4940326	-4.9400786
H	-0.6233283	0.2547252	-5.8579157
H	-2.1003630	-0.1667532	-4.9346104
H	-1.5490635	1.5489669	-5.0293650
C	-3.1858572	-1.0584300	-2.2442216
H	-2.8613649	-1.5143406	-1.2812077
H	-4.2729574	-1.2669628	-2.3608464
H	-2.6533410	-1.5823939	-3.0692152
C	0.0982987	-0.6417774	2.6612902
C	1.3501782	-0.9818649	3.2552483
C	-1.0672542	-1.4296873	2.9022929
C	1.3971753	-2.1150267	4.0930391
C	-0.9620690	-2.5481094	3.7464695
C	0.2608041	-2.8937296	4.3393651
H	2.3533633	-2.3940874	4.5657518
H	-1.8563374	-3.1586511	3.9529343
H	0.3269552	-3.7747902	4.9989588
C	-2.4105662	-1.0201657	2.3080376
C	-3.2299771	-0.2081765	3.3295522
H	-4.1815268	0.1504258	2.8752321

H	-3.4831013	-0.8242824	4.2223827
H	-2.6611425	0.6811678	3.6788828
C	2.6210070	-0.1598272	3.0389010
C	2.9768837	0.6516542	4.3017227
H	3.8758087	1.2830508	4.1218734
H	2.1438676	1.3196981	4.6115964
H	3.1993256	-0.0228591	5.1592288
H	-2.1826267	-0.3369739	1.4600694
C	3.8203583	-1.0225102	2.5984797
H	4.6867613	-0.3720730	2.3445586
H	4.1515940	-1.7160949	3.4032578
H	3.5791037	-1.6325943	1.7011531
C	1.4676735	-0.9714908	-0.4276109
H	1.9850301	-0.7835519	0.5254523
H	0.0532322	-2.4624497	-1.1989136
H	0.2194425	-2.4441859	0.6161377
C	2.3886235	-1.0382960	-1.5571133
C	3.5712785	-0.2408413	-1.5296913
C	2.2139424	-1.8683874	-2.7000557
C	4.4930222	-0.2488103	-2.5798735
H	3.7386026	0.4153894	-0.6577343
C	3.1382982	-1.8739527	-3.7545604
H	1.3452779	-2.5459888	-2.7592711
C	4.2837412	-1.0607331	-3.7125725
H	5.3897200	0.3915019	-2.5196449
H	2.9643540	-2.5356733	-4.6207436
H	5.0083665	-1.0660092	-4.5430166
H	-0.0671003	-0.7753163	-3.5817662
H	2.4208501	0.5662198	2.2216655
C	-3.2158583	-2.1992662	1.7404686
H	-3.5702497	-2.8946750	2.5343301
H	-4.1170810	-1.8258691	1.2045474
H	-2.6095158	-2.7910224	1.0186276
H	-3.2461138	0.8923102	-3.2195458

C 1.0096317 1.0854939 -3.8392982

H 0.8072732 2.1527228 -4.0717139

H 1.6126675 1.0375422 -2.9083783

H 1.6259673 0.6470374 -4.6540079

B

81

Energy =

H 0.4003029 -1.8216161 0.2733397

C 0.2676806 -2.0340833 -0.9217303

Ni -0.1059370 -0.2101452 0.1546244

C -0.6608751 1.5143094 -0.2182184

C 0.3431771 2.4392281 -0.6055415

C -1.9620479 1.9681319 0.0641867

C -0.0198478 3.7808126 -0.9087807

C -2.3371754 3.2800525 -0.2564820

C -1.3561518 4.1702843 -0.7668229

H 0.7457674 4.5075236 -1.2283843

H -3.3692934 3.6170665 -0.0694721

H -1.6519215 5.2046422 -1.0083159

N 1.7394303 0.6241581 -0.0883878

C 1.6598500 1.8608354 -0.5585108

H 2.5704643 2.4140105 -0.8635783

P -1.8298455 -0.1639180 1.4570175

O -2.7872384 1.1018115 0.7432534

C -1.7640354 0.4851501 3.2187480

C -0.9376099 1.7794010 3.2562926

H -0.8557690 2.1467669 4.3048894

H 0.0917492 1.6083841 2.8687254

H -1.3958539 2.5851658 2.6447259

C -3.1431908 -1.4896320 1.4027358

C -4.4127763 -1.1463945 2.1912572

H -5.2194881 -1.8734968 1.9427351

H -4.2472456 -1.1990047 3.2908078

H -4.7818575 -0.1298786 1.9368749

C	-1.1755786	-0.5900631	4.1448505
H	-0.1945830	-0.9542047	3.7622439
H	-1.0037568	-0.1685065	5.1612864
H	-1.8462486	-1.4688490	4.2586106
H	-3.3852086	-1.4602619	0.3147487
C	2.9636672	-0.0883356	-0.1009386
C	3.6630912	-0.3515184	-1.3177177
C	3.4344824	-0.6164709	1.1423807
C	4.8449327	-1.1186897	-1.2515097
C	4.6173843	-1.3731428	1.1466899
C	5.3256939	-1.6220720	-0.0388063
H	5.4017217	-1.3278166	-2.1803767
H	4.9997659	-1.7775291	2.0969847
H	6.2539954	-2.2164947	-0.0147772
C	2.6791776	-0.3082676	2.4292685
C	3.0346454	1.0988510	2.9505972
H	2.4346549	1.3460123	3.8553681
H	4.1127203	1.1596503	3.2235606
H	2.8283648	1.8766625	2.1842032
C	3.1863133	0.1475599	-2.6821993
C	4.1317513	1.2260379	-3.2474937
H	3.7487179	1.6166229	-4.2170260
H	4.2378322	2.0835677	-2.5471150
H	5.1510814	0.8148644	-3.4252040
H	1.5988056	-0.2841565	2.1481075
C	2.9956991	-0.9994102	-3.6934763
H	2.5794389	-0.6071433	-4.6481080
H	3.9562127	-1.5081328	-3.9323977
H	2.2910995	-1.7680666	-3.3079653
C	-0.4130197	-0.9568940	-1.6879748
H	0.2341052	-0.3663609	-2.3614667
H	-0.2851911	-2.9949549	-0.8635221
H	1.3198263	-2.2127105	-1.2272591
C	-1.8074738	-1.0484021	-2.1517481

C -2.3689728 0.0510074 -2.8564982

C -2.6453127 -2.1731698 -1.9379992

C -3.6950484 0.0362084 -3.2987043

H -1.7434956 0.9437082 -3.0252767

C -3.9762216 -2.1890918 -2.3842508

H -2.2517195 -3.0624466 -1.4183672

C -4.5148712 -1.0840472 -3.0627033

H -4.1000809 0.9142661 -3.8295529

H -4.5974171 -3.0827893 -2.2024743

H -5.5611309 -1.0956341 -3.4096246

C -2.5904512 -2.8857617 1.7215799

H -1.6458307 -3.0893361 1.1721734

H -2.3848170 -3.0197463 2.8060774

H -3.3310159 -3.6625293 1.4243281

H -2.8118447 0.7124102 3.5174630

H 2.1919047 0.6227108 -2.5469866

C 2.8514447 -1.3637642 3.5294451

H 3.8831739 -1.3758826 3.9483059

H 2.1625759 -1.1460744 4.3756581

H 2.6209381 -2.3857734 3.1549956

TS4

81

Energy =

Ni -0.2253042 0.2904407 -0.2366768

C -0.0832504 -1.6366142 -1.0739806

H -0.2294586 -1.1124207 0.3959124

C -0.2078601 2.0988371 -0.7144102

C 1.0687901 2.7243065 -0.7644221

C -1.3604096 2.9092513 -0.7446859

C 1.1728121 4.1101321 -1.0667759

C -1.2760928 4.2737169 -1.0469801

C 0.0037126 4.8575053 -1.2377815

H 2.1619705 4.5941248 -1.1298718

H -2.1918679 4.8846022 -1.0915386

H	0.0693243	5.9327001	-1.4728005
N	1.7512115	0.6444795	0.0829341
C	2.1240171	1.8350604	-0.3608477
H	3.1936396	2.1268169	-0.3705784
P	-2.2082545	0.8009848	0.3942374
O	-2.5481862	2.3118885	-0.3690537
C	-2.5154701	1.2286424	2.1895376
H	-3.5403416	1.6561440	2.2545763
C	-3.7232244	-0.1501175	-0.1684471
C	-5.0342162	0.2847351	0.5039570
H	-5.8834994	-0.2807754	0.0571750
H	-5.0478626	0.0879888	1.5970292
H	-5.2295823	1.3676382	0.3393366
C	-1.5022104	2.2853710	2.6506280
H	-1.6099087	3.2337243	2.0822850
H	-1.6512847	2.5105584	3.7312906
H	-0.4586106	1.9262774	2.5111372
C	-3.8351245	-0.0517936	-1.6986198
H	-4.0946657	0.9835427	-2.0073671
H	-2.8873596	-0.3316866	-2.1993206
H	-4.6265853	-0.7440796	-2.0624222
C	2.7136476	-0.3338539	0.4450725
C	3.6449305	-0.8534461	-0.5026489
C	2.6753248	-0.8377477	1.7824559
C	4.5336798	-1.8630769	-0.0770726
C	3.5833191	-1.8440411	2.1496751
C	4.5114086	-2.3563336	1.2307763
H	5.2618055	-2.2746420	-0.7960124
H	3.5719367	-2.2357334	3.1790078
H	5.2176941	-3.1453877	1.5377623
C	1.7039383	-0.2368358	2.7896641
C	1.2457818	-1.2136550	3.8806425
H	0.8055579	0.0567393	2.2001684
H	0.4424109	-0.7493980	4.4942790

H	0.8415719	-2.1528364	3.4408074
H	2.0682629	-1.4887193	4.5791085
C	3.7169136	-0.3777178	-1.9531589
C	5.0260663	0.3870541	-2.2310118
H	2.8818715	0.3336707	-2.1233287
H	5.0452396	0.7668076	-3.2773057
H	5.1432015	1.2558355	-1.5462864
H	5.9147578	-0.2688961	-2.0910716
C	2.2831681	1.0538108	3.4032849
H	2.5408181	1.7937366	2.6147908
H	1.5447374	1.5299617	4.0873977
H	3.2064208	0.8372446	3.9874732
C	3.5308932	-1.5357903	-2.9528661
H	3.5010452	-1.1464413	-3.9951496
H	4.3643266	-2.2710712	-2.8952203
H	2.5816724	-2.0835605	-2.7654635
H	0.9051164	-2.0934281	-0.8457267
C	-0.0546545	-0.5961288	-2.0669609
H	0.9052180	-0.3158298	-2.5289131
H	-0.9400849	-0.4081993	-2.6973741
C	-1.2208364	-2.6236715	-0.9918794
C	-1.5684424	-3.2328449	0.2352810
C	-1.9470559	-2.9929754	-2.1427160
C	-2.6156335	-4.1611682	0.3151678
H	-1.0138157	-2.9520063	1.1481974
C	-3.0043618	-3.9152760	-2.0664865
H	-1.6734292	-2.5518647	-3.1145644
C	-3.3467364	-4.5004038	-0.8374221
H	-2.8690153	-4.6185818	1.2862721
H	-3.5622374	-4.1810051	-2.9800205
H	-4.1766538	-5.2238794	-0.7768696
C	-2.4266960	-0.0625133	3.0173193
H	-2.5584343	0.1629141	4.0997833
H	-3.1998938	-0.8098094	2.7313358

H -1.4306482 -0.5419310 2.8877492

H -3.4918804 -1.2060281 0.1033759

TS5

81

Energy =

H -0.5629383 -1.3778887 -0.1241371

C 0.5351253 -1.8214740 -0.3241859

Ni -0.0845776 0.3353616 -0.1635623

C -0.2785468 2.1648635 -0.0285813

C -0.1205937 2.7114958 1.2850013

C -0.5089659 3.0414582 -1.1130090

C -0.1181326 4.1248254 1.4616236

C -0.5302594 4.4248011 -0.9391721

C -0.3117079 4.9588283 0.3612023

H 0.0325604 4.5501303 2.4679360

H -0.7354959 5.0792212 -1.8008440

H -0.3186787 6.0528699 0.4959766

N -0.0573272 0.4452980 1.7776928

C -0.0110239 1.6878830 2.2659961

H 0.0792906 1.8643539 3.3535575

P -0.9250443 0.7719852 -2.0937803

O -0.7685801 2.4500052 -2.3356168

C -2.7700772 0.5361866 -2.3019331

C -3.5282429 1.4005146 -1.2850514

H -4.6249916 1.2561143 -1.4139975

H -3.2584710 1.1183414 -0.2430252

H -3.3045094 2.4808593 -1.4113284

C -0.1111158 0.1308104 -3.6496544

C 1.2251998 0.8714366 -3.8375019

H 1.8448225 0.3431781 -4.5963898

H 1.0490775 1.9108443 -4.1877420

H 1.8029435 0.9302929 -2.8907950

C -3.1241595 -0.9507291 -2.1670073

H -2.8904233 -1.3125550 -1.1409946

H	-4.2140251	-1.1013647	-2.3370776
H	-2.5743566	-1.6005977	-2.8828095
H	0.0990313	-0.9367195	-3.4042602
C	-0.0738668	-0.6766642	2.6518279
C	1.1246061	-1.1394904	3.2625248
C	-1.3154661	-1.3492962	2.8546158
C	1.0497122	-2.2762677	4.0931034
C	-1.3327319	-2.4826166	3.6862132
C	-0.1615249	-2.9453327	4.3045018
H	1.9651842	-2.6485330	4.5820564
H	-2.2818740	-3.0147523	3.8603769
H	-0.1947970	-3.8356042	4.9542431
C	-2.5917336	-0.8064841	2.2206242
C	-3.2782893	0.2099341	3.1549154
H	-4.1684313	0.6594225	2.6589102
H	-3.6159485	-0.2794102	4.0968401
H	-2.5867925	1.0368179	3.4257686
C	2.4567090	-0.4252642	3.0543057
C	2.8408075	0.4016980	4.2978337
H	3.7939404	0.9507878	4.1261245
H	2.0559369	1.1480573	4.5488839
H	2.9783050	-0.2541118	5.1875055
H	-2.2693804	-0.2474820	1.3127925
C	3.5926927	-1.3915708	2.6696116
H	4.5102228	-0.8201321	2.4054328
H	3.8595434	-2.0765012	3.5057011
H	3.3153658	-2.0170495	1.7930793
C	1.5732661	-0.7625028	-0.5711037
H	2.3797920	-0.7053600	0.1788681
H	1.9670063	-0.6993908	-1.6001778
H	0.6962528	-2.3134571	0.6636223
C	0.2620264	-2.8770876	-1.3861797
C	1.1889153	-3.1677325	-2.4070639
C	-0.9367686	-3.6219041	-1.3464277

C 0.9185580 -4.1579261 -3.3679693

H 2.1416783 -2.6152721 -2.4405395

C -1.2102239 -4.6135825 -2.2985044

H -1.6688377 -3.4154949 -0.5459622

C -0.2833470 -4.8808275 -3.3220260

H 1.6588805 -4.3664466 -4.1585971

H -2.1540738 -5.1814924 -2.2434008

H -0.4967746 -5.6554893 -4.0771741

C -0.9748047 0.1970519 -4.9175617

H -1.8815841 -0.4413716 -4.8546917

H -1.2914344 1.2406537 -5.1389384

H -0.3793508 -0.1622655 -5.7874603

H -3.0063394 0.8938482 -3.3291756

H 2.3203487 0.2816992 2.2084893

C -3.5746202 -1.8966368 1.7693711

H -4.0414074 -2.4294563 2.6283176

H -4.4006460 -1.4451672 1.1762317

H -3.0720756 -2.6580893 1.1319480

D

81

Energy =

Ni -0.2395968 0.3103116 -0.2239103

C -0.0751113 -1.6952888 -0.9706586

H -0.1068070 -1.2939721 0.1959192

C -0.2377364 2.0516239 -0.8461413

C 1.0320807 2.6856106 -0.9361417

C -1.4059268 2.8344092 -0.9271158

C 1.1119522 4.0478132 -1.3402958

C -1.3405231 4.1713566 -1.3389102

C -0.0689359 4.7586167 -1.5729042

H 2.0929000 4.5435863 -1.4326971

H -2.2659931 4.7620073 -1.4318622

H -0.0199966 5.8134440 -1.8901412

N 1.7393785 0.6843010 0.0660171

C	2.0994986	1.8404122	-0.4758207
H	3.1664155	2.1351889	-0.5311362
P	-2.2003240	0.8821672	0.5097387
O	-2.5766116	2.2561765	-0.4816938
C	-2.4116901	1.6388218	2.2146758
H	-3.3943333	2.1594422	2.2309512
C	-3.7825279	-0.0801606	0.2135240
C	-5.0456442	0.6572834	0.6850760
H	-5.9485586	0.0698074	0.4016146
H	-5.0775312	0.7993668	1.7864863
H	-5.1250689	1.6553594	0.2010393
C	-1.2980214	2.6653735	2.4654663
H	-1.3539219	3.5177979	1.7554182
H	-1.3793594	3.0714527	3.4997353
H	-0.2925627	2.2024094	2.3527021
C	-3.8800726	-0.4607276	-1.2719361
H	-3.9238867	0.4483252	-1.9101706
H	-3.0171527	-1.0764805	-1.5946909
H	-4.8020108	-1.0591918	-1.4481353
C	2.7043206	-0.2861390	0.4335031
C	3.6119210	-0.8384547	-0.5208981
C	2.6790061	-0.7694323	1.7797071
C	4.5046409	-1.8407519	-0.0871749
C	3.5904451	-1.7698359	2.1541039
C	4.5051337	-2.3018836	1.2327944
H	5.2169453	-2.2739344	-0.8093472
H	3.5909792	-2.1435241	3.1901199
H	5.2153332	-3.0848602	1.5461950
C	1.7088621	-0.1605288	2.7838787
C	1.2800339	-1.1175886	3.9039154
H	0.7972826	0.1052314	2.1979058
H	0.4731295	-0.6529468	4.5129169
H	0.8912996	-2.0763653	3.4936212
H	2.1138435	-1.3568061	4.6021184

C	3.6470931	-0.4091924	-1.9877937
C	4.9436004	0.3547564	-2.3215155
H	2.8009336	0.2879835	-2.1618731
H	4.9355406	0.7009208	-3.3795415
H	5.0715507	1.2455960	-1.6680004
H	5.8395912	-0.2913002	-2.1815192
C	2.2709033	1.1552914	3.3583088
H	2.5015814	1.8805861	2.5483577
H	1.5343212	1.6330146	4.0430939
H	3.2071566	0.9695601	3.9323363
C	3.4487548	-1.5982909	-2.9480340
H	3.3952043	-1.2400581	-4.0004293
H	4.2866799	-2.3281039	-2.8864561
H	2.5065158	-2.1458461	-2.7268043
H	0.9483377	-2.1390241	-0.9509459
C	-0.1839248	-0.6019677	-1.9754569
H	0.7183585	-0.3726612	-2.5698166
H	-1.1193589	-0.5374521	-2.5603205
C	-1.1408430	-2.7736308	-0.9507651
C	-1.7624573	-3.1728741	0.2496627
C	-1.5182818	-3.4144235	-2.1488744
C	-2.7429276	-4.1772316	0.2556904
H	-1.4798302	-2.6721058	1.1930689
C	-2.4977696	-4.4197359	-2.1472571
H	-1.0395892	-3.1076912	-3.0939496
C	-3.1169328	-4.8025144	-0.9454251
H	-3.2221046	-4.4698609	1.2050042
H	-2.7840398	-4.9054925	-3.0950720
H	-3.8912236	-5.5875284	-0.9450667
C	-2.3965009	0.5055444	3.2520522
H	-2.4187726	0.9239068	4.2839227
H	-3.2674754	-0.1792434	3.1493671
H	-1.4689215	-0.1045853	3.1575104
H	-3.6498557	-1.0158789	0.8056443

C

81

Energy =

Ni	1.9553503	-0.2182705	6.6594782
C	1.0561591	-0.1405474	4.9822040
C	1.8388545	0.1572724	3.8396290
C	-0.3283428	-0.2992857	4.8137757
C	1.2544380	0.3032330	2.5584388
C	-0.9365223	-0.1713142	3.5524981
C	-0.1326105	0.1355378	2.4308836
H	1.8744610	0.5408641	1.6776677
H	-2.0245478	-0.3111762	3.4487040
H	-0.6098343	0.2403672	1.4426576
N	3.5629971	0.0550734	5.4350037
C	3.2408387	0.2416572	4.1750185
H	4.0302324	0.4266208	3.4184980
P	-0.0090617	-0.6430181	7.3311814
O	-1.0534108	-0.5911001	5.9427782
C	-0.9642916	0.5445530	8.4011825
C	-0.9160306	1.9239971	7.7218498
H	-1.3149274	2.6981599	8.4142262
H	0.1234524	2.2105739	7.4544516
H	-1.5272590	1.9297881	6.7927748
C	-0.4313393	-2.3859043	7.8548988
H	-1.5318558	-2.4407537	7.6908664
H	-0.3854378	0.5928824	9.3509562
C	0.2636097	-3.3680015	6.8980539
H	0.0084174	-3.1587327	5.8369792
H	1.3706753	-3.3042455	6.9998697
H	-0.0468248	-4.4123672	7.1291433
C	4.9417942	0.0075088	5.7974871
C	5.6187348	-1.2414166	5.7369394
C	5.5748836	1.1853545	6.2731780
C	6.9717902	-1.2726411	6.1226446

C	6.9285880	1.0988840	6.6500892
C	7.6244348	-0.1149047	6.5697996
H	7.5266583	-2.2236519	6.0813786
H	7.4491472	1.9979758	7.0170738
H	8.6844480	-0.1622540	6.8693397
C	4.8041388	2.5011431	6.3267300
C	5.1361480	3.3508757	7.5641459
H	3.7234094	2.2336606	6.3834749
H	4.4495979	4.2242016	7.6248842
H	5.0248719	2.7635487	8.5016129
H	6.1736591	3.7526120	7.5289266
C	4.8893316	-2.4954572	5.2555190
C	5.0621774	-2.6951015	3.7357197
H	3.8043793	-2.3274529	5.4500163
H	4.5071716	-3.5968469	3.3921098
H	4.6851709	-1.8253048	3.1564531
H	6.1368055	-2.8308672	3.4777498
C	5.0054722	3.3102543	5.0295514
H	4.6923319	2.7318269	4.1330605
H	4.4095921	4.2503227	5.0543907
H	6.0768206	3.5830460	4.8969530
C	5.3011101	-3.7727646	6.0079247
H	4.6330539	-4.6148556	5.7209634
H	6.3414698	-4.0839904	5.7634778
H	5.2336733	-3.6413672	7.1096014
C	2.9988705	-0.0938907	8.4119707
H	3.8054541	0.5774868	8.0424676
C	3.6191984	-1.4457021	8.7552928
H	4.2441446	-1.8110353	7.9145184
H	4.2845566	-1.3866807	9.6532031
H	2.8642735	-2.2359449	8.9641744
C	2.3070576	0.6151425	9.5238770
C	2.0635556	2.0125950	9.4346441
C	1.8617251	-0.0298512	10.7067044

C 1.3781673 2.7125477 10.4347321

H 2.4170270 2.5519037 8.5384326

C 1.1678885 0.6670216 11.7103896

H 2.0625109 -1.1029591 10.8483096

C 0.9099495 2.0415726 11.5805217

H 1.2043498 3.7961600 10.3197635

H 0.8313888 0.1261352 12.6117284

H 0.3655605 2.5881066 12.3680862

C -0.1178437 -2.6868972 9.3252736

H 0.9768783 -2.6931658 9.5080143

H -0.5689264 -1.9506230 10.0243596

H -0.5088332 -3.6952125 9.5903653

C -2.4062793 0.0994569 8.6822792

H -2.9696006 -0.0470402 7.7346496

H -2.4589472 -0.8413950 9.2711192

H -2.9285681 0.8872012 9.2713187

E

81

Energy =

Ni 0.1575323 -0.3490622 6.7897042

C 0.2113599 -0.2132153 4.9017016

C -1.0271876 -0.2287893 4.2122132

C 1.3958774 -0.0577427 4.1622053

C -1.0800673 -0.0742963 2.8050365

C 1.3724284 0.0893675 2.7658719

C 0.1228526 0.0856514 2.1003484

H -2.0445495 -0.0796157 2.2696491

H 2.3126002 0.2004300 2.2020653

H 0.1025705 0.2062668 1.0046781

N -1.8543182 -0.5617145 6.3958569

C -2.1344884 -0.4669885 5.1154016

H -3.1735578 -0.6193007 4.7572334

P 2.2149460 -0.3444689 6.5584611

O 2.5744511 -0.0704916 4.8842560

C	3.0816550	-1.9771775	6.8081351
C	2.3639590	-3.0611786	5.9893461
H	4.1058778	-1.8317699	6.3947274
H	2.9029399	-4.0306757	6.0869353
H	1.3216361	-3.2031812	6.3531090
H	2.3146148	-2.7987970	4.9110945
C	3.2704795	0.9885513	7.3163803
C	4.7597454	0.8803559	6.9634764
H	3.1257489	0.8457476	8.4131105
H	5.3155250	1.7443828	7.3935711
H	5.2255418	-0.0460906	7.3641433
H	4.9047893	0.8963723	5.8609410
C	3.1620546	-2.3390476	8.2981183
H	2.1450234	-2.4677900	8.7299501
H	3.7117176	-3.2991442	8.4244239
H	3.6926325	-1.5677696	8.8988730
C	2.6689665	2.3461962	6.9154451
H	2.7897807	2.5233242	5.8243538
H	1.5825791	2.3885058	7.1487404
H	3.1791855	3.1715154	7.4607215
C	-2.8557936	-0.9122767	7.3422355
C	-3.8805689	0.0022102	7.7099028
C	-2.7465571	-2.1950530	7.9547292
C	-4.8233882	-0.4205288	8.6694398
C	-3.7037727	-2.5589333	8.9167726
C	-4.7439407	-1.6846811	9.2661440
H	-5.6318783	0.2666060	8.9678416
H	-3.6397217	-3.5465007	9.4005411
H	-5.4908086	-1.9874515	10.0184058
C	-1.6394931	-3.1447972	7.5129608
C	-1.1080261	-4.0521887	8.6305550
H	-0.7906035	-2.4936876	7.1871228
H	-0.2024577	-4.5956502	8.2793070
H	-0.8262001	-3.4616732	9.5298829

H	-1.8512977	-4.8212712	8.9401349
C	-3.9720195	1.4048496	7.1118719
C	-5.0999543	1.4956457	6.0637561
H	-3.0105083	1.6091662	6.5920823
H	-5.1369885	2.5118631	5.6107402
H	-4.9635888	0.7581543	5.2427975
H	-6.0902834	1.2930373	6.5306646
C	-2.0699332	-3.9611238	6.2791488
H	-2.3815438	-3.2992743	5.4417270
H	-1.2289109	-4.5938751	5.9152669
H	-2.9269180	-4.6286610	6.5237292
C	-4.1465511	2.4950256	8.1874661
H	-4.0704444	3.5044306	7.7255216
H	-5.1417556	2.4339235	8.6817006
H	-3.3714354	2.4176015	8.9804605
C	0.0974184	-0.2502179	8.7787671
C	-0.5243797	1.1092430	9.1562749
H	1.0459866	-0.3778175	9.3503498
H	-0.5809077	-1.0685480	9.1211503
H	0.1756902	1.9370523	8.9002769
H	-1.4434474	1.2798308	8.5519539
C	-0.8807446	1.1976053	10.6267663
C	-0.0493040	1.8655645	11.5489558
C	-2.0387857	0.5542417	11.1175636
C	-0.3617607	1.8956055	12.9184093
H	0.8596969	2.3746280	11.1820304
C	-2.3570260	0.5844037	12.4835097
H	-2.6989251	0.0204108	10.4123800
C	-1.5187871	1.2550105	13.3915864
H	0.3020867	2.4273055	13.6212927
H	-3.2703422	0.0796922	12.8420880
H	-1.7680816	1.2798547	14.4656801

TS3

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Energy =

Ni	-0.0483490	-0.1542956	-0.1643087
Si	-0.3125252	1.1237319	1.8712253
C	0.1165234	-1.2453253	1.9689236
C	-0.2340968	-1.7321141	-1.2125112
C	0.9677503	-2.4058959	-1.5431163
C	-1.4405232	-2.2001269	-1.7639971
C	0.9332727	-3.6204515	-2.2777789
C	-1.5001071	-3.4021534	-2.4830376
C	-0.3007177	-4.1188086	-2.7124243
H	1.8683097	-4.1565780	-2.5105579
H	-2.4628017	-3.7543941	-2.8855786
H	-0.3420132	-5.0644642	-3.2772031
N	1.9775117	-0.5318030	-0.5208035
C	2.1444368	-1.6888350	-1.1288782
H	3.1580944	-2.0605832	-1.3672281
P	-1.9351779	0.1708767	-1.1388967
O	-2.5300535	-1.3761244	-1.6099760
C	-1.8748091	1.0204709	-2.8092443
H	-2.8825765	0.8417503	-3.2463693
C	-3.4652774	0.8158461	-0.2965237
H	-3.1835566	1.8463522	0.0164020
C	-0.8211905	0.3804494	-3.7234814
H	-1.0420658	-0.6861737	-3.9376628
H	-0.7902251	0.9263916	-4.6939009
H	0.1901014	0.4296332	-3.2649740
C	-4.6837483	0.8759421	-1.2324831
H	-4.5596405	1.6108513	-2.0563751
H	-4.9037991	-0.1205462	-1.6741219
H	-5.5748883	1.1903222	-0.6439130
C	3.1174693	0.2040508	-0.0778968
C	4.0876200	-0.3587832	0.8141324
C	3.2633895	1.5455684	-0.5518138
C	5.1325275	0.4752765	1.2634113

C	4.3266086	2.3248097	-0.0665586
C	5.2501094	1.8040799	0.8482052
H	5.8799220	0.0652874	1.9609278
H	4.4460577	3.3600341	-0.4206703
H	6.0741594	2.4320496	1.2249072
C	2.3577964	2.0777318	-1.6554503
C	2.2483458	3.6082233	-1.7025498
H	1.3420339	1.6662541	-1.4574848
H	1.4349754	3.9102343	-2.3987851
H	2.0213866	4.0371663	-0.7024832
H	3.1841632	4.0842272	-2.0731350
C	4.0993094	-1.8214855	1.2695298
C	5.0927536	-2.6514261	0.4236094
H	3.0802533	-2.2416330	1.1212415
H	5.0621425	-3.7232476	0.7229677
H	4.8885237	-2.5929125	-0.6671287
H	6.1313498	-2.2820335	0.5777160
C	2.8087835	1.5260143	-3.0247289
H	2.7980386	0.4148195	-3.0404421
H	2.1338405	1.8838509	-3.8343057
H	3.8427759	1.8634854	-3.2630612
C	4.4609959	-2.0067540	2.7590130
H	4.2356608	-3.0489313	3.0755106
H	5.5456966	-1.8396445	2.9422670
H	3.8950163	-1.3191726	3.4195581
H	0.6167252	-1.8603409	1.1976839
C	1.1336532	-1.0114564	3.0886970
H	2.0550500	-0.5373881	2.6972121
H	0.7573975	-0.3599909	3.9086256
H	1.4088436	-1.9884990	3.5543574
C	-1.1273752	-1.9583161	2.3989802
C	-1.7212022	-2.9371651	1.5628239
C	-1.7443292	-1.7324064	3.6557862
C	-2.8891287	-3.6151499	1.9308461

H	-1.2442060	-3.1715481	0.5990411
C	-2.9236880	-2.4020276	4.0238789
H	-1.2937697	-1.0272431	4.3702109
C	-3.5126112	-3.3391471	3.1616000
H	-3.3161356	-4.3694944	1.2482322
H	-3.3797347	-2.1928823	5.0066030
H	-4.4373410	-3.8648414	3.4525365
H	0.1672427	1.3233418	0.1633898
H	-1.1144359	0.7215485	3.1032312
H	1.0481165	1.5945219	2.3326101
C	-1.3198044	2.7472264	1.5582300
C	-0.9437160	3.7168264	0.6030773
C	-2.4698944	3.0142877	2.3349558
C	-1.6793014	4.8991803	0.4207083
H	-0.0485427	3.5449271	-0.0195804
C	-3.2255037	4.1858866	2.1518942
H	-2.7884189	2.2784838	3.0952278
C	-2.8327278	5.1321086	1.1903479
H	-1.3546644	5.6408666	-0.3293249
H	-4.1268552	4.3618552	2.7636680
H	-3.4222549	6.0528028	1.0431182
C	-3.7553849	-0.0143217	0.9614466
H	-4.6020901	0.4435030	1.5192810
H	-4.0254951	-1.0608565	0.7050633
H	-2.8862990	-0.0599484	1.6510922
C	-1.6431384	2.5275793	-2.6384141
H	-1.6575163	3.0254064	-3.6341947
H	-2.4089667	3.0182526	-1.9998334
H	-0.6516535	2.7215681	-2.1763030

TS6

0

Energy =

TS7

81

Energy =

Ni	0.3953987	-0.3938249	0.3946077
C	2.2461313	-0.4504609	0.3480040
C	2.9204067	0.8006690	0.1972520
C	3.0205899	-1.6224096	0.5037832
C	4.3357533	0.8614564	0.3211178
C	4.4138346	-1.5704683	0.6011317
C	5.0633770	-0.3108817	0.5323197
H	4.8482556	1.8349450	0.2443922
H	4.9845909	-2.5070302	0.7007955
H	6.1612728	-0.2686954	0.6200889
N	0.7453234	1.5470586	-0.1994185
C	2.0270221	1.8752778	-0.0908896
H	2.3617359	2.9193923	-0.2400113
P	0.7191726	-2.4900961	0.0389034
O	2.3370351	-2.8181923	0.4839257
C	0.7225200	-3.0038119	-1.7629841
C	1.7092767	-2.1512630	-2.5717831
H	1.0845581	-4.0563786	-1.7552974
H	1.7045111	-2.4841826	-3.6347473
H	1.4308476	-1.0753711	-2.5415676
H	2.7479678	-2.2399017	-2.1889368
C	-0.1169495	-3.8633835	0.9727947
C	0.2020113	-5.2708770	0.4467048
H	-1.2022451	-3.6497659	0.8441355
H	-0.2595340	-6.0266876	1.1221297
H	-0.2038276	-5.4502665	-0.5718671
H	1.2980926	-5.4608465	0.4306082
C	-0.6996067	-2.9456319	-2.3370467
H	-1.0884466	-1.9043766	-2.3201471
H	-0.6955527	-3.2951705	-3.3942001
H	-1.4216430	-3.5729645	-1.7697674
C	0.2432931	-3.7115129	2.4586053
H	1.3016401	-3.9985258	2.6387123

H	0.1109387	-2.6636772	2.8011023
H	-0.4117927	-4.3638617	3.0777857
C	-0.2199181	2.5380523	-0.5164833
C	-0.5319615	3.5927385	0.3905299
C	-0.8990762	2.4157470	-1.7669821
C	-1.5202559	4.5222963	0.0066488
C	-1.8779146	3.3682659	-2.0956353
C	-2.1881454	4.4178340	-1.2180549
H	-1.7745265	5.3492752	0.6900748
H	-2.4086367	3.2942273	-3.0578908
H	-2.9591836	5.1568784	-1.4917018
C	-0.5145874	1.2961556	-2.7285416
C	-1.6530147	0.8398626	-3.6514095
H	-0.2275347	0.4283856	-2.0893814
H	-1.3541155	-0.0830195	-4.1959600
H	-2.5801011	0.6151260	-3.0796088
H	-1.9033754	1.6054405	-4.4200769
C	0.1716543	3.7556464	1.7375708
C	1.1626130	4.9375601	1.7082761
H	0.7563390	2.8299502	1.9274916
H	1.7023278	5.0216754	2.6782852
H	1.9201164	4.8231666	0.9024684
H	0.6300363	5.8989389	1.5293866
C	0.7357003	1.6793822	-3.5459798
H	1.5937734	1.9234566	-2.8835782
H	1.0450799	0.8387427	-4.2073741
H	0.5303026	2.5660933	-4.1873734
C	-0.8177164	3.9157836	2.9086698
H	-0.2689851	3.9081361	3.8766207
H	-1.3763246	4.8767382	2.8522034
H	-1.5607854	3.0898329	2.9305384
C	-0.9049227	0.2728028	2.0573921
H	-1.0037935	1.3175877	1.7152785
C	-0.5033260	0.1454452	3.5065142

H 0.3425663 0.8294830 3.7372872

H -1.3368626 0.4013008 4.2111671

H -0.1621746 -0.8800172 3.7713079

C -1.8942587 -0.5978214 1.4585320

C -2.3194925 -0.3760282 0.0964147

C -2.4841815 -1.7238196 2.1294048

C -3.2075310 -1.2534573 -0.5463674

H -2.0228038 0.5582439 -0.4105504

C -3.3812362 -2.5712752 1.4795448

H -2.2447367 -1.8982783 3.1898185

C -3.7366336 -2.3677617 0.1250983

H -3.5143030 -1.0408477 -1.5847776

H -3.8292117 -3.4112300 2.0390819

H -4.4458742 -3.0447522 -0.3774528

F

81

Energy =

Ni -0.5064754 -0.1895149 0.0699576

C -0.3351926 -1.6970104 -1.0489551

C 0.9324863 -2.3264016 -1.1745329

C -1.3345378 -2.0696109 -1.9731150

C 1.1004464 -3.4662428 -2.0070369

C -1.1968333 -3.1996499 -2.7919826

C 0.0221247 -3.9191317 -2.7733359

H 2.0846923 -3.9605756 -2.0731301

H -2.0167429 -3.4832302 -3.4713807

H 0.1350374 -4.8056963 -3.4187999

N 1.7796614 -0.4478656 -0.0077169

C 2.0170808 -1.6279831 -0.5273031

H 3.0415689 -2.0585996 -0.5287548

P -2.0383002 0.2995449 -1.3690764

O -2.4068199 -1.2157158 -2.1163428

C -1.6690370 1.3475059 -2.8763580

C -0.4437679 0.7794264 -3.6058236

H	-2.5513926	1.2935475	-3.5514122
H	-0.1593208	1.4447196	-4.4529019
H	0.4283317	0.6991915	-2.9200868
H	-0.6427977	-0.2342713	-4.0139743
C	-3.7793481	0.7446284	-0.8406045
C	-4.6968031	1.2410451	-1.9678321
H	-3.6268652	1.5598830	-0.0963454
H	-5.7186172	1.4198713	-1.5613874
H	-4.3520937	2.1949582	-2.4207077
H	-4.7883340	0.4820612	-2.7762388
C	-1.4482909	2.7945340	-2.4086581
H	-0.6172743	2.8449853	-1.6708197
H	-1.1794775	3.4446485	-3.2720138
H	-2.3497714	3.2310576	-1.9242333
C	-4.3989738	-0.4684815	-0.1266010
H	-4.6780188	-1.2520187	-0.8626340
H	-3.6946986	-0.9220700	0.6017223
H	-5.3126122	-0.1576726	0.4283889
C	2.7664726	0.2457531	0.7203071
C	3.4584287	-0.3327683	1.8322517
C	2.9855954	1.6170306	0.3662800
C	4.3749757	0.4752776	2.5359838
C	3.9104762	2.3717575	1.1051752
C	4.6092852	1.8076327	2.1822231
H	4.9214883	0.0437884	3.3911510
H	4.0958290	3.4227434	0.8337867
H	5.3349225	2.4125189	2.7505992
C	2.2624348	2.2014451	-0.8394475
C	2.0707679	3.7230969	-0.7809170
H	1.2530995	1.7243995	-0.8530833
H	1.4135778	4.0572707	-1.6135872
H	1.6007692	4.0415548	0.1760812
H	3.0327389	4.2732943	-0.8883049
C	3.2504013	-1.7714634	2.3090070

C 4.4891398 -2.6440478 2.0235210

H 2.4043836 -2.2109860 1.7388397

H 4.3087301 -3.6976786 2.3344502

H 4.7513856 -2.6422789 0.9425286

H 5.3786677 -2.2722166 2.5802326

C 2.9708237 1.7890908 -2.1464074

H 3.0321051 0.6835329 -2.2400930

H 2.4205027 2.1764897 -3.0329885

H 4.0067114 2.1965216 -2.1771241

C 2.8614037 -1.8421855 3.7991141

H 2.6182001 -2.8901999 4.0843778

H 3.6870598 -1.4999428 4.4618764

H 1.9709297 -1.2121688 4.0147205

C -0.4262965 -1.1312012 1.9092159

H 0.6526057 -1.1024300 2.1336642

C -1.0847238 -2.4603863 2.1703529

H -0.5059987 -3.2763051 1.6849375

H -1.1438031 -2.6980718 3.2619205

H -2.1150366 -2.5056758 1.7546346

C -1.1118418 0.1250606 2.0658180

C -0.4400300 1.3273372 1.5958257

C -2.4710006 0.2695366 2.5269846

C -1.1330176 2.5748364 1.5961418

H 0.6632640 1.3613208 1.5564476

C -3.1026877 1.5011501 2.5324021

H -2.9852219 -0.6137744 2.9379832

C -2.4458838 2.6681476 2.0375742

H -0.5900763 3.4793318 1.2723846

H -4.1284617 1.5838120 2.9304689

H -2.9676492 3.6391154 2.0445711

TS8

81

Energy =

Ni -1.3860897 -0.3660647 0.3327640

C	-0.5444110	-0.7048550	-1.3663970
C	0.7909442	-1.0882583	-1.6316002
C	-1.3696909	-0.5217279	-2.5074644
C	1.2115783	-1.4425859	-2.9348181
C	-0.9824824	-0.8761720	-3.8073861
C	0.3136160	-1.3782920	-4.0101343
H	2.2576791	-1.7492639	-3.1036978
H	-1.6840018	-0.7238345	-4.6429827
H	0.6397290	-1.6681284	-5.0226745
N	2.4825905	0.1108234	-0.4228751
C	1.8480468	-0.9901952	-0.5784272
H	2.1149575	-1.9017254	0.0162687
P	-2.5992362	0.9405624	-0.8425490
O	-2.5900764	0.1263106	-2.3433190
C	-1.9137135	2.6575247	-1.2130291
C	-1.7551366	2.9196258	-2.7178413
H	-2.6726781	3.3615630	-0.7955398
H	-1.3857972	3.9579365	-2.8794293
H	-1.0146733	2.2219739	-3.1664375
H	-2.7093559	2.8010068	-3.2727403
C	-4.4401001	1.1179469	-0.6473177
C	-5.1089756	1.9572990	-1.7458191
H	-4.5447379	1.6324379	0.3383217
H	-6.2070461	2.0077826	-1.5657020
H	-4.7297096	3.0015070	-1.7794911
H	-4.9495949	1.4962882	-2.7449005
C	-0.5927422	2.8497561	-0.4474126
H	0.1912885	2.1411022	-0.7974271
H	-0.2115741	3.8869202	-0.5901513
H	-0.7241180	2.6857233	0.6447741
C	-5.0557625	-0.2853364	-0.5381646
H	-4.9642451	-0.8264835	-1.5048007
H	-4.5482346	-0.8884369	0.2443653
H	-6.1355204	-0.2129625	-0.2765807

C	3.5771865	0.2505809	0.4534168
C	3.3890124	0.6393343	1.8079386
C	4.8876698	0.1211646	-0.0966023
C	4.5304219	0.8541171	2.6050444
C	5.9921056	0.3385651	0.7446424
C	5.8230980	0.6984668	2.0900174
H	4.4013511	1.1549929	3.6584486
H	7.0108745	0.2306249	0.3384503
H	6.7017128	0.8665979	2.7342840
C	5.0529450	-0.2607396	-1.5647023
C	6.2595440	0.4065145	-2.2446827
H	4.1361381	0.0989550	-2.0856446
H	6.2412923	0.2080145	-3.3394546
H	6.2525908	1.5081869	-2.0938083
H	7.2279635	0.0147223	-1.8595173
C	1.9951058	0.8751304	2.3810200
C	1.7591897	0.0853961	3.6816503
H	1.2601782	0.5149713	1.6281125
H	0.7092422	0.1981142	4.0337421
H	1.9563061	-0.9995266	3.5365359
H	2.4214469	0.4393181	4.5030306
C	5.1082584	-1.7926082	-1.7378205
H	4.2109730	-2.2875452	-1.3060617
H	5.1682992	-2.0697318	-2.8151606
H	6.0005242	-2.2147322	-1.2223029
C	1.7274631	2.3799564	2.5786244
H	0.6892802	2.5541767	2.9455570
H	2.4286588	2.8192394	3.3236539
H	1.8524080	2.9344407	1.6233168
C	-0.5819994	-1.8843245	1.3633775
H	0.3708804	-1.5018279	1.7797657
C	-0.5044345	-3.2857035	0.8059853
H	0.3548128	-3.3880320	0.1096619
H	-0.3727953	-4.0501356	1.6105706

H -1.4137144 -3.5513391 0.2249218

C -1.7736926 -1.4165799 2.0489036

C -1.8481766 -0.0027363 2.3628241

C -2.9785649 -2.1854295 2.2176702

C -3.0455388 0.5543703 2.9013735

H -0.9159012 0.5835324 2.4720140

C -4.1309868 -1.6126174 2.7368961

H -2.9617071 -3.2589832 1.9721501

C -4.1758753 -0.2317861 3.0805356

H -3.0535432 1.6185396 3.1926425

H -5.0269323 -2.2378188 2.8887394

H -5.0998625 0.2022350 3.4961862

A

81

Energy =

Ni 1.6636713 -0.8000179 7.2355616

C 1.2920008 -0.9647524 5.3378187

C 2.1945406 -0.9925503 4.2342508

C -0.0854748 -1.0519509 4.9963267

C 1.7419196 -1.2591552 2.9154372

C -0.5493174 -1.3261594 3.7027645

C 0.3855463 -1.4629720 2.6586521

H 2.4900618 -1.2732977 2.1065955

H -1.6340194 -1.4003750 3.5242475

H 0.0366787 -1.6824918 1.6359030

N 4.4625189 -0.4839561 3.4901652

C 3.5988580 -0.6209429 4.4394423

H 3.8712964 -0.4090168 5.4951875

P -0.3322488 -0.0288526 7.3146520

O -1.0441083 -0.7901770 5.9710454

C -0.5857190 1.8153166 7.0126245

C -1.5473898 2.0963827 5.8488520

H -1.0286809 2.2024385 7.9609248

H -1.6859720 3.1955624 5.7338107

H	-1.1393836	1.7020638	4.8926619
H	-2.5457734	1.6363766	6.0016376
C	-1.5716772	-0.5423282	8.6045476
C	-2.9807813	0.0308977	8.3925396
H	-1.1391789	-0.1403208	9.5520760
H	-3.6576403	-0.3310360	9.1996965
H	-3.0029988	1.1417618	8.4157728
H	-3.4031067	-0.3072602	7.4211107
C	0.7835680	2.4841605	6.8033311
H	1.2867760	2.0886909	5.8928925
H	0.6642739	3.5853445	6.6832211
H	1.4648990	2.3057624	7.6639299
C	-1.5877832	-2.0768829	8.6837363
H	-2.0194687	-2.5101669	7.7557924
H	-0.5637227	-2.4865709	8.8133225
H	-2.2055116	-2.4091480	9.5482699
C	5.7411252	0.0170308	3.7578236
C	5.9525616	1.2729460	4.4109137
C	6.8530203	-0.7441642	3.2757882
C	7.2808379	1.7012483	4.6101220
C	8.1536039	-0.2717494	3.5090724
C	8.3744529	0.9400125	4.1822912
H	7.4628327	2.6663181	5.1133206
H	9.0168434	-0.8595681	3.1577781
H	9.4023392	1.2969870	4.3605061
C	6.5865555	-2.0717817	2.5773851
C	7.6404657	-2.4469637	1.5248543
H	5.6063685	-1.9519983	2.0616200
H	7.3080361	-3.3406725	0.9512644
H	7.8103611	-1.6182267	0.8027104
H	8.6208794	-2.7047624	1.9861336
C	4.8089914	2.1956811	4.8390979
C	4.7192150	2.3286405	6.3721124
H	3.8523344	1.7507215	4.4925967

H 3.8672954 2.9843400 6.6631984

H 4.5703299 1.3371794 6.8558603

H 5.6498368 2.7696351 6.7952887

C 6.4135242 -3.2065792 3.6085560

H 5.6024035 -2.9742232 4.3320610

H 6.1565566 -4.1658980 3.1043083

H 7.3528922 -3.3607524 4.1867229

C 4.9104317 3.5811709 4.1707003

H 4.0221610 4.2024128 4.4262362

H 5.8147071 4.1386762 4.5029889

H 4.9593082 3.4867984 3.0640097

C 3.3363294 -1.9083068 7.4023185

H 4.1994279 -1.2281262 7.2459256

C 3.4704426 -3.2427037 6.7130334

H 3.7067934 -3.0980250 5.6369170

H 4.2923629 -3.8603521 7.1501925

H 2.5294769 -3.8320541 6.7596014

C 2.7129216 -1.7675851 8.7037300

C 2.4782211 -0.4127842 9.1611553

C 2.1075528 -2.8311427 9.4585681

C 1.7581495 -0.1773786 10.3694932

H 3.1041694 0.4092691 8.7603246

C 1.4013379 -2.5691720 10.6247071

H 2.2531432 -3.8700679 9.1223725

C 1.2173383 -1.2358104 11.0884203

H 1.6517612 0.8579371 10.7357925

H 0.9790063 -3.4070948 11.2043349

H 0.6607943 -1.0507671 12.0217610

TS9

96

Energy =

Ni -1.1287812 0.6994319 0.5746243

C -0.5744942 -0.1227562 -1.1941774

C 0.7074165 -0.5074794 -1.6885799

C	-1.6773937	-0.3636605	-2.0589382
C	0.8661219	-1.1029631	-2.9622716
C	-1.5230051	-0.9527286	-3.3252144
C	-0.2472752	-1.3353598	-3.7718078
H	1.8833568	-1.3827177	-3.2785820
H	-2.4190804	-1.0902867	-3.9508377
H	-0.1315505	-1.8033019	-4.7633306
N	3.0303260	-0.8582896	-1.0453882
C	1.8799419	-0.3184041	-0.8286061
H	1.7128972	0.3348285	0.0539069
P	-3.0905150	1.1000837	-0.3951922
O	-2.9484488	0.0257536	-1.7259057
C	-3.5609542	2.6448394	-1.3654582
C	-2.4284365	3.0112579	-2.3372506
H	-4.4533843	2.3593373	-1.9653609
H	-2.6966737	3.9336654	-2.9012757
H	-1.4694292	3.1994115	-1.8066714
H	-2.2450888	2.2018498	-3.0749807
C	-4.7100278	0.3674936	0.2146799
C	-5.1773274	0.9060050	1.5717869
H	-4.3836211	-0.6884265	0.3570231
H	-6.0557991	0.3177609	1.9214059
H	-4.3864532	0.8179656	2.3436253
H	-5.4957303	1.9705126	1.5191937
C	-3.9363052	3.8104198	-0.4380074
H	-3.0845658	4.1185297	0.2090925
H	-4.2242732	4.6998108	-1.0431018
H	-4.7935466	3.5687411	0.2264435
C	-5.8286068	0.3755662	-0.8357579
H	-6.2616198	1.3918857	-0.9732027
H	-5.4699156	0.0041016	-1.8189155
H	-6.6568086	-0.2904304	-0.5021893
C	4.0678802	-0.6526567	-0.1196500
C	5.2492392	-0.0112583	-0.5914609

C	3.9716254	-1.1297345	1.2263379
C	6.2990672	0.2204626	0.3154706
C	5.0583851	-0.8819303	2.0860163
C	6.2033896	-0.1976460	1.6493822
H	7.2126354	0.7318067	-0.0277909
H	5.0163899	-1.2330956	3.1283409
H	7.0328464	-0.0085071	2.3507523
C	2.7646183	-1.9569662	1.6829005
C	2.7327878	-3.3174062	0.9554801
H	1.8390355	-1.4129013	1.3905843
H	1.8175863	-3.8878021	1.2326729
H	2.7374773	-3.1829000	-0.1481034
H	3.6220738	-3.9281404	1.2301863
C	5.3182375	0.4313346	-2.0490040
C	4.6370636	1.7999751	-2.2523019
H	4.7165702	-0.3136450	-2.6192915
H	4.6448000	2.0905248	-3.3275435
H	3.5799794	1.7808655	-1.9107268
H	5.1691420	2.5929746	-1.6779873
C	2.6725518	-2.1559062	3.2016414
H	2.6854398	-1.1868837	3.7489652
H	1.7219776	-2.6733641	3.4555449
H	3.5067289	-2.7815236	3.5916017
C	6.7408696	0.4387846	-2.6285089
H	6.7066335	0.6144069	-3.7267331
H	7.3668834	1.2488778	-2.1901473
H	7.2605289	-0.5283413	-2.4506931
C	-0.9545002	1.4261747	2.4668589
H	-0.5551400	0.7765912	3.2746827
C	-2.0853136	2.2873886	3.0058348
H	-2.8718572	1.6554380	3.4693520
H	-1.7030054	2.9721397	3.8006148
H	-2.5702345	2.9112082	2.2263137
C	0.1554364	2.0587959	1.7311049

C -0.1081903 2.9904670 0.6801294

C 1.5223806 1.7403040 2.0080124

C 0.9535306 3.5525360 -0.0635170

H -1.1272253 3.3731550 0.5298490

C 2.5620563 2.3299186 1.2931728

H 1.7447075 1.0145814 2.8083164

C 2.2791581 3.2359771 0.2428075

H 0.7277056 4.2716394 -0.8684199

H 3.6061423 2.0662301 1.5295860

H 3.1052718 3.6935369 -0.3240544

Si -1.5611793 -1.0504196 1.9457036

H -0.3284680 -0.5305868 0.3306131

H -2.6647146 -0.8016845 2.9594444

C -2.1856497 -2.5302599 0.9260724

C -1.3644438 -3.1686720 -0.0330767

C -3.4989253 -3.0244125 1.1053640

C -1.8379772 -4.2513947 -0.7897267

H -0.3321146 -2.8164682 -0.2033884

C -3.9804998 -4.1054374 0.3471437

H -4.1578101 -2.5625645 1.8624081

C -3.1510802 -4.7181275 -0.6064310

H -1.1777417 -4.7276543 -1.5336562

H -5.0088364 -4.4729440 0.5041015

H -3.5276833 -5.5632093 -1.2068841

H -0.3649870 -1.5231957 2.7476528

G

96

Energy =

Ni -1.5667594 0.8689539 1.2345985

C -0.2132339 -0.1555744 -1.5411072

C 0.9940098 -0.8019310 -1.8755591

C -1.4135611 -0.5100401 -2.1751053

C 1.0116924 -1.7804443 -2.8925785

C -1.3924422 -1.4698027 -3.2073870

C	-0.1814287	-2.0895107	-3.5616257
H	1.9616372	-2.2797750	-3.1386182
H	-2.3413790	-1.7373799	-3.6971505
H	-0.1810914	-2.8453423	-4.3646097
N	3.3185429	-1.0064571	-1.1560880
C	2.1691233	-0.4341462	-1.0785849
H	1.9874412	0.3857244	-0.3444443
P	-2.8960715	1.0235835	-0.4685033
O	-2.6279085	0.0198014	-1.8360576
C	-3.0909609	2.6301651	-1.4211392
C	-1.7499445	3.0085620	-2.0680471
H	-3.8207714	2.3970520	-2.2282426
H	-1.8407731	3.9870458	-2.5927743
H	-0.9462429	3.1012651	-1.3059319
H	-1.4277327	2.2533072	-2.8160207
C	-4.6276539	0.4198012	-0.1113789
C	-5.0932329	0.8612303	1.2839225
H	-4.4431005	-0.6776368	-0.0715212
H	-6.0409975	0.3403721	1.5490135
H	-4.3341560	0.6046926	2.0580138
H	-5.2846490	1.9556689	1.3424993
C	-3.6628782	3.7465972	-0.5366909
H	-3.0343030	3.9206536	0.3627073
H	-3.7006447	4.7015727	-1.1083332
H	-4.6960794	3.5250279	-0.1927930
C	-5.6546204	0.6847966	-1.2169307
H	-5.9347939	1.7596522	-1.2868943
H	-5.2765932	0.3519783	-2.2075481
H	-6.5870677	0.1140951	-1.0044869
C	4.3160048	-0.6315719	-0.2322424
C	5.4323623	0.1109507	-0.7054043
C	4.2233930	-1.0482684	1.1318591
C	6.4527752	0.4442364	0.2037534
C	5.2760467	-0.6925534	1.9963601

C	6.3790818	0.0483016	1.5459035
H	7.3217832	1.0263338	-0.1431523
H	5.2361916	-1.0017221	3.0524062
H	7.1862903	0.3161412	2.2474917
C	3.0513317	-1.9126550	1.6011655
C	3.1632671	-3.3376632	1.0212848
H	2.1150954	-1.4752723	1.1875774
H	2.2732210	-3.9448042	1.3014676
H	3.2307413	-3.3112912	-0.0881505
H	4.0732664	-3.8477149	1.4101107
C	5.4445579	0.5756406	-2.1567728
C	4.6933848	1.9168213	-2.2996258
H	4.8678499	-0.1863989	-2.7304318
H	4.6442972	2.2356289	-3.3656791
H	3.6513587	1.8446822	-1.9169176
H	5.2102879	2.7176358	-1.7231757
C	2.8633343	-1.9562733	3.1239763
H	2.8080561	-0.9361091	3.5661521
H	1.9151606	-2.4835741	3.3689675
H	3.6891355	-2.5028942	3.6325798
C	6.8490387	0.6664822	-2.7722269
H	6.7788177	0.8729062	-3.8633680
H	7.4493548	1.4901416	-2.3237671
H	7.4148438	-0.2812261	-2.6364956
C	-0.7364123	0.8171350	3.0351125
H	-0.0486599	0.0095103	3.3588123
C	-1.7601476	1.1703389	4.1029123
H	-2.3111088	0.2628278	4.4297715
H	-1.2552309	1.6053520	4.9992147
H	-2.5177501	1.9084585	3.7613953
C	-0.0596524	1.8601725	2.2657657
C	-0.8094414	2.9768655	1.7542867
C	1.3097654	1.7353194	1.8471651
C	-0.1681725	3.9507122	0.9406531

H	-1.7854644	3.2373898	2.1990331
C	1.9055693	2.6881134	1.0310554
H	1.8959353	0.8762944	2.2129199
C	1.1666126	3.8105518	0.5703630
H	-0.7390429	4.8364376	0.6153437
H	2.9672909	2.5753487	0.7524621
H	1.6543069	4.5715072	-0.0601936
Si	-1.6154987	-1.3250550	1.7449576
H	-0.2135862	0.6169760	-0.7510481
H	-2.0496472	-1.6604720	3.1634915
C	-2.6647026	-2.5264091	0.7023843
C	-2.1266482	-3.1794626	-0.4294645
C	-4.0118462	-2.8004368	1.0423142
C	-2.9060597	-4.0547078	-1.2042930
H	-1.0743771	-3.0049028	-0.7122836
C	-4.7976421	-3.6722948	0.2711552
H	-4.4559083	-2.3255134	1.9362139
C	-4.2462335	-4.2981158	-0.8610232
H	-2.4603260	-4.5490039	-2.0842890
H	-5.8442517	-3.8718488	0.5582929
H	-4.8597541	-4.9841787	-1.4689861
H	-0.1940391	-1.8436944	1.5874676

TS10

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Energy =

Ni	1.1146594	0.1860867	1.0324924
C	-2.0637209	0.1162860	0.5083189
C	-2.8395244	-0.3731867	-0.5629665
C	-2.3467424	-0.2562855	1.8318036
C	-3.9458536	-1.2086808	-0.3037482
C	-3.4589207	-1.0947400	2.0857398
C	-4.2508725	-1.5559420	1.0237862
H	-4.5584605	-1.5885897	-1.1382156
H	-3.6736812	-1.3794463	3.1279884

H	-5.1132100	-2.2089640	1.2370193
N	-1.3648854	0.6140829	-2.1913217
C	-2.4603531	-0.0097386	-1.9376685
H	-3.1646590	-0.3139713	-2.7515029
P	0.0277993	0.7400471	2.7508891
O	-1.6041482	0.1403905	2.9013587
C	-0.3519158	2.5749197	2.9819613
C	-0.8681492	3.1735784	1.6658919
H	-1.1630040	2.6166078	3.7430350
H	-1.0090557	4.2736060	1.7697094
H	-0.1381794	2.9962308	0.8444543
H	-1.8434074	2.7380613	1.3615461
C	0.6119732	0.2264323	4.4603981
C	-0.3750617	0.5490968	5.5903448
H	1.5302444	0.8487942	4.5819920
H	0.0527720	0.2308378	6.5682707
H	-0.6049180	1.6339886	5.6645832
H	-1.3323581	0.0054027	5.4404691
C	0.8839175	3.3303153	3.4924791
H	1.7536825	3.1664674	2.8189544
H	0.6771066	4.4246389	3.5113043
H	1.1742942	3.0306036	4.5224892
C	1.0410690	-1.2444520	4.4707013
H	0.1765281	-1.9245002	4.3104843
H	1.7751158	-1.4522290	3.6637037
H	1.5074431	-1.5034555	5.4482073
C	-0.9940688	1.0291372	-3.4807303
C	0.0231153	0.3031247	-4.1625192
C	-1.5402096	2.2305490	-4.0262220
C	0.4553510	0.7729553	-5.4158510
C	-1.0662425	2.6572940	-5.2804753
C	-0.0844581	1.9373623	-5.9775997
H	1.2332552	0.2166671	-5.9635830
H	-1.4719327	3.5781654	-5.7275579

H	0.2649363	2.2917662	-6.9612881
C	-2.5406129	3.0529700	-3.2136295
C	-1.8226998	3.7500739	-2.0379944
H	-3.2765057	2.3451789	-2.7692081
H	-2.5481607	4.2980561	-1.3951542
H	-1.2876847	3.0130184	-1.4014568
H	-1.0753014	4.4823466	-2.4193632
C	0.5800193	-0.9704705	-3.5376699
C	-0.2294191	-2.2071499	-3.9767235
H	0.4313969	-0.8719863	-2.4385569
H	0.1397296	-3.1230539	-3.4619917
H	-1.3091557	-2.0906261	-3.7362069
H	-0.1444321	-2.3662188	-5.0756453
C	-3.3446324	4.0660819	-4.0402069
H	-3.8484309	3.5849513	-4.9073955
H	-4.1277224	4.5381140	-3.4067575
H	-2.7014782	4.8870966	-4.4295999
C	2.0830963	-1.1763353	-3.7832124
H	2.4526673	-2.0349758	-3.1791946
H	2.3088717	-1.4034562	-4.8494711
H	2.6680151	-0.2743780	-3.4960556
C	3.0531932	-0.5511661	0.2832680
H	3.2231667	-0.8587690	-0.7716950
C	4.1632257	-1.1006401	1.1776035
H	4.2815084	-2.1989686	1.0394695
H	5.1448285	-0.6257627	0.9418978
H	3.9472126	-0.9248588	2.2538010
C	2.8844854	0.9545429	0.2635502
C	3.5976754	1.8427830	1.1248664
C	2.0555758	1.5455952	-0.7517027
C	3.5116175	3.2297595	0.9601806
H	4.2381384	1.4291270	1.9192825
C	1.9588334	2.9448578	-0.8847091
H	1.5609601	0.9066084	-1.5032342

C 2.6882761 3.7913778 -0.0390804

H 4.0878616 3.8896484 1.6303120

H 1.3170879 3.3613141 -1.6785645

H 2.6234373 4.8855481 -0.1543415

Si 1.4007739 -1.9341639 0.3741456

H -1.2188993 0.7799617 0.2687884

H 2.0332626 -2.7851595 -0.7103700

C 0.8242556 -3.1955811 1.6605266

C -0.5547497 -3.3092918 1.9518707

C 1.7251188 -4.0363627 2.3526580

C -1.0177775 -4.2261805 2.9083380

H -1.2821782 -2.6677055 1.4279111

C 1.2666917 -4.9454074 3.3202262

H 2.8082266 -3.9807088 2.1421037

C -0.1069852 -5.0414313 3.6024443

H -2.0991683 -4.2980871 3.1154816

H 1.9864729 -5.5865632 3.8568239

H -0.4673788 -5.7555584 4.3617722

H 0.2040019 -1.2331829 -0.2918634

H

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Energy =

Ni 0.3493856 0.9443170 0.6042328

C -1.9364475 -0.9487247 -0.0875096

C -1.9088583 -2.1077592 -0.8918570

C -2.4751462 -0.9853312 1.2120680

C -2.4784557 -3.3073716 -0.4142382

C -3.0467528 -2.1913791 1.6812997

C -3.0538599 -3.3351435 0.8673227

H -2.4635325 -4.2131401 -1.0429839

H -3.4706394 -2.2076880 2.6979065

H -3.5029399 -4.2671266 1.2485324

N -0.5534473 -1.0308327 -2.5687541

C -1.2649013 -2.0421933 -2.2113501

H	-1.4101484	-2.9220476	-2.8861895
P	-1.3265863	1.4003183	1.8188269
O	-2.4701515	0.0826577	2.0514710
C	-2.5992072	2.6601883	1.2242104
C	-2.9231610	2.4255860	-0.2577595
H	-3.5127935	2.4569752	1.8268626
H	-3.6450343	3.1919507	-0.6219639
H	-2.0014789	2.5001690	-0.8778096
H	-3.3768397	1.4273206	-0.4360846
C	-1.1101952	1.8541555	3.6270056
C	-2.4151434	1.9169302	4.4312256
H	-0.6639374	2.8745686	3.5539820
H	-2.1968663	2.1912407	5.4885495
H	-3.1300722	2.6688687	4.0326803
H	-2.9222108	0.9280879	4.4300960
C	-2.1204230	4.0981397	1.4690877
H	-1.1315483	4.2736108	0.9917098
H	-2.8433993	4.8197469	1.0246563
H	-2.0320277	4.3417416	2.5497711
C	-0.0734197	0.9340441	4.2813523
H	-0.4379043	-0.1145717	4.3402895
H	0.8719757	0.9214702	3.6975306
H	0.1547663	1.2784412	5.3156116
C	0.0302874	-0.9296756	-3.8434816
C	1.4142304	-1.2264072	-3.9883040
C	-0.7369589	-0.4213635	-4.9343844
C	2.0070122	-1.0549430	-5.2525961
C	-0.0932067	-0.2662443	-6.1756740
C	1.2625040	-0.5864171	-6.3430168
H	3.0751580	-1.2907178	-5.3867361
H	-0.6625248	0.1170176	-7.0367885
H	1.7415444	-0.4602297	-7.3278827
C	-2.1846558	0.0122804	-4.7068094
C	-2.2185377	1.3140663	-3.8768051

H	-2.6791010	-0.7754406	-4.0938459
H	-3.2651865	1.6091410	-3.6372135
H	-1.6694237	1.1873833	-2.9188199
H	-1.7422714	2.1472353	-4.4415516
C	2.1972142	-1.7381745	-2.7850396
C	2.1341983	-3.2752506	-2.6834608
H	1.6769965	-1.3357636	-1.8855558
H	2.6549558	-3.6308723	-1.7656388
H	1.0839492	-3.6380732	-2.6426050
H	2.6199311	-3.7484960	-3.5667128
C	-3.0107365	0.1612251	-5.9915715
H	-2.9772536	-0.7604579	-6.6134700
H	-4.0744543	0.3660778	-5.7388482
H	-2.6545901	1.0102492	-6.6174395
C	3.6531930	-1.2473664	-2.7420040
H	4.1164325	-1.5136331	-1.7657031
H	4.2761060	-1.7136439	-3.5381670
H	3.7165420	-0.1434069	-2.8654412
C	3.1864676	0.6729652	1.1164665
H	3.9163446	0.4202133	0.3096564
C	3.9712910	0.9695585	2.3980170
H	4.6398298	0.1216455	2.6634388
H	4.6141599	1.8710498	2.2736362
H	3.2994119	1.1532551	3.2653077
C	2.3316385	1.8243711	0.5878413
C	2.2065715	3.0787067	1.2508436
C	1.7461285	1.6918903	-0.7245305
C	1.5679823	4.1711201	0.6377755
H	2.6600201	3.2118256	2.2454663
C	0.9707307	2.7619400	-1.2524000
H	2.0432097	0.8678125	-1.3966770
C	0.9242062	4.0099329	-0.6015810
H	1.5312249	5.1409427	1.1607910
H	0.4988148	2.6331460	-2.2410240

H 0.3759082 4.8482072 -1.0613535

Si 2.0603391 -0.9169513 1.1831703

H -1.5305078 -0.0187637 -0.5185045

H 2.8021804 -1.9693446 0.3775733

C 1.5733357 -1.7205549 2.8203275

C 0.3379893 -2.4108373 2.8383211

C 2.3467508 -1.7145246 4.0033252

C -0.1171343 -3.0575697 3.9973766

H -0.2950813 -2.4325183 1.9355218

C 1.8895710 -2.3526486 5.1686009

H 3.3213812 -1.2015761 4.0302682

C 0.6549999 -3.0232225 5.1707662

H -1.0876698 -3.5816588 3.9812864

H 2.5050284 -2.3264161 6.0836583

H 0.2963759 -3.5207955 6.0874122

H 0.7499525 -0.7689587 0.3311836

TS11

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Energy =

Ni 0.5313935 0.7583891 1.0941049

C -1.6200803 0.5195883 0.7632029

C -2.2526219 -0.5770766 0.0925951

C -2.1125833 0.8840932 2.0539439

C -3.1976793 -1.3750517 0.7783628

C -3.0629339 0.0946392 2.7120780

C -3.5908344 -1.0493772 2.0793392

H -3.6346106 -2.2484077 0.2662989

H -3.3688016 0.3827189 3.7301939

H -4.3216138 -1.6790051 2.6121465

N -1.1734348 -0.1578902 -2.0347114

C -2.0114941 -0.8357487 -1.3236092

H -2.6481287 -1.6342956 -1.7773541

P 0.0078789 2.3967570 2.4137984

O -1.6480904 1.9980246 2.7133340

C	-0.2439033	4.1943422	1.9425585
C	-0.8170334	4.2428387	0.5188988
H	-0.9999649	4.6003760	2.6516738
H	-0.9886106	5.2965595	0.2013902
H	-0.1186458	3.7727908	-0.2093914
H	-1.7886028	3.7067104	0.4493422
C	0.6063306	2.4680767	4.1944853
C	-0.2567698	3.3540779	5.1036048
H	1.6317631	2.9029124	4.1108990
H	0.1203191	3.3123902	6.1507821
H	-0.2516361	4.4210225	4.7925753
H	-1.3111732	3.0011859	5.1052388
C	1.0606011	4.9945824	2.0658001
H	1.8727951	4.5450807	1.4504040
H	0.9079959	6.0348168	1.6993940
H	1.4238965	5.0613106	3.1143214
C	0.7320934	1.0381383	4.7427289
H	-0.2597377	0.5328383	4.7645673
H	1.4095905	0.4183706	4.1164547
H	1.1309130	1.0553204	5.7820745
C	-0.9703291	-0.4070727	-3.3974652
C	-0.5990665	-1.6880406	-3.9135245
C	-1.0829160	0.7217557	-4.2723860
C	-0.3590429	-1.8007198	-5.2991582
C	-0.8474449	0.5452793	-5.6433671
C	-0.4854637	-0.7085175	-6.1625366
H	-0.0686354	-2.7815104	-5.7126845
H	-0.9508551	1.4015602	-6.3284254
H	-0.3033638	-0.8303226	-7.2431254
C	-1.4427135	2.0859815	-3.6867646
C	-0.1894601	2.7433077	-3.0756645
H	-2.1532806	1.9037372	-2.8501717
H	-0.4425317	3.7239840	-2.6118603
H	0.2588120	2.0905859	-2.2968478

H	0.5806508	2.9216181	-3.8599778
C	-0.4090964	-2.9254818	-3.0366144
C	-1.4807290	-3.9977065	-3.3111719
H	-0.5152494	-2.6189903	-1.9756685
H	-1.3578846	-4.8620147	-2.6193217
H	-2.5066953	-3.5900285	-3.1738473
H	-1.4133346	-4.3826165	-4.3539616
C	-2.1326384	3.0354050	-4.6774448
H	-3.0127223	2.5575486	-5.1618196
H	-2.4846424	3.9484983	-4.1478484
H	-1.4416423	3.3740580	-5.4823714
C	1.0100477	-3.5099017	-3.1696392
H	1.1483640	-4.3627458	-2.4664389
H	1.2133646	-3.8895324	-4.1958522
H	1.7757872	-2.7402622	-2.9303213
C	3.0371246	-1.4751991	0.5175194
H	3.3425510	-2.3395237	-0.1122519
C	3.7707347	-1.5244631	1.8634660
H	3.6050543	-2.5054178	2.3608303
H	4.8690702	-1.3806342	1.7396261
H	3.4077902	-0.7427404	2.5689601
C	3.1706619	-0.2025828	-0.2850825
C	2.9519859	1.0690778	0.3225413
C	3.2967089	-0.2407460	-1.6910585
C	2.9097348	2.2435142	-0.4601962
H	2.9540991	1.1628866	1.4211527
C	3.2320919	0.9265644	-2.4674027
H	3.4375766	-1.2163236	-2.1868623
C	3.0366295	2.1763640	-1.8548756
H	2.7863822	3.2196111	0.0371664
H	3.3258187	0.8573551	-3.5637957
H	2.9852212	3.0935497	-2.4633240
Si	1.0996821	-1.4423991	0.6620535
H	-1.1601169	1.2990426	0.0930005

H 0.7065711 -1.5051189 -0.7954690

C 0.2198800 -2.8743451 1.5294161

C -0.3580711 -2.7063399 2.8083501

C 0.0530907 -4.1225195 0.8842576

C -1.0764519 -3.7449319 3.4229104

H -0.2675242 -1.7330389 3.3218969

C -0.6617595 -5.1659542 1.4940970

H 0.4830989 -4.2811019 -0.1210727

C -1.2292560 -4.9776040 2.7665585

H -1.5277514 -3.5882178 4.4173147

H -0.7828776 -6.1303433 0.9720199

H -1.7962016 -5.7937696 3.2454669

H 1.1212479 -0.3510610 1.9858439

I

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Energy =

Ni -0.0672350 0.4898192 0.9981860

C -2.1273926 -0.2154192 0.8836799

C -2.5900395 -1.1526928 -0.0824218

C -2.5481033 -0.3400921 2.2362556

C -3.3783324 -2.2481121 0.3248229

C -3.3355241 -1.4339250 2.6296589

C -3.7401690 -2.3859466 1.6729352

H -3.7056228 -2.9910642 -0.4213113

H -3.6157212 -1.5294856 3.6904713

H -4.3488833 -3.2472793 1.9934481

N -1.4272948 -0.0004086 -1.8241706

C -2.2593961 -0.9267658 -1.4920045

H -2.7952729 -1.5606941 -2.2375473

P -0.6847219 1.4103686 2.8526905

O -2.1730950 0.5746853 3.1878542

C -1.2746106 3.1731813 3.0551364

C -2.3059944 3.4836045 1.9604013

H -1.7694127 3.2606710 4.0479673

H	-2.6695632	4.5316565	2.0581860
H	-1.8619973	3.3710786	0.9458183
H	-3.1861274	2.8083956	2.0280250
C	0.2155130	1.0071198	4.4471894
C	-0.5037939	1.4677453	5.7215487
H	1.1815496	1.5577143	4.3376574
H	0.0542050	1.1244489	6.6222116
H	-0.5889321	2.5738833	5.7886762
H	-1.5277221	1.0359302	5.7719152
C	-0.0560286	4.1087102	2.9921593
H	0.5182260	3.9576225	2.0483723
H	-0.3833811	5.1725429	3.0230032
H	0.6425527	3.9502384	3.8436159
C	0.5199315	-0.4994620	4.4713247
H	-0.4187560	-1.0920878	4.5484167
H	1.0487443	-0.8237474	3.5492085
H	1.1571439	-0.7517099	5.3484230
C	-1.0042922	0.3207997	-3.1098433
C	-0.5914068	-0.6442536	-4.0828611
C	-0.8823725	1.7239073	-3.3805756
C	-0.1601342	-0.1710425	-5.3389983
C	-0.4615890	2.1336925	-4.6530974
C	-0.1157628	1.1941244	-5.6385100
H	0.1540332	-0.8985682	-6.1057750
H	-0.3901777	3.2073246	-4.8866625
H	0.2102861	1.5322986	-6.6359989
C	-1.1630713	2.7305652	-2.2636592
C	0.0267838	2.7756398	-1.2830719
H	-2.0474164	2.3609777	-1.6970216
H	-0.1093784	3.5763182	-0.5228497
H	0.1422332	1.7993154	-0.7422863
H	0.9868430	2.9634615	-1.8093002
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C	-1.6697991	-2.9106953	-4.4991002

H	-0.6447317	-2.2917185	-2.7012464
H	-1.6378046	-3.9925930	-4.2374802
H	-2.6706227	-2.5156723	-4.2165259
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H	1.0198907	-2.7429102	-5.2637777
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C	3.2202869	-0.7813030	-0.0091675
H	3.6609653	-1.3834561	-0.8359545
C	3.7686509	-1.2894930	1.3306920
H	3.6338873	-2.3902317	1.4127177
H	4.8535767	-1.0605981	1.4465058
H	3.2397754	-0.8388426	2.2019472
C	3.4470559	0.6819912	-0.3079987
C	3.3464249	1.6755959	0.6961910
C	3.6629062	1.1183567	-1.6365317
C	3.4671378	3.0400174	0.3859246
H	3.1737949	1.3794733	1.7434253
C	3.7882701	2.4799297	-1.9491092
H	3.7272118	0.3662425	-2.4419307
C	3.6916420	3.4513376	-0.9378448
H	3.3867311	3.7893938	1.1920747
H	3.9589128	2.7848126	-2.9953406
H	3.7871174	4.5224695	-1.1814350
Si	1.2857019	-0.9936584	-0.1601260
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H	1.1045676	-0.7125686	-1.6383547
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C	-0.0178951	-3.1373631	1.2772617

C 1.2991365 -3.8535411 -0.6257060

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H 1.9586852 -3.6273633 -1.4819882

C 0.1028680 -5.4999652 0.7098631

H -1.0412949 -4.7033384 2.3855016

H 1.3224793 -5.9928203 -1.0274949

H -0.1795398 -6.5479086 0.9076226

H 1.2315139 -0.1483446 1.3905858

TS12

96

Energy =

Ni 0.1800520 -0.8057630 0.4383855

C 2.2998185 -0.6805479 0.5995258

C 2.8236789 0.6323682 0.4424291

C 2.6675618 -1.4754295 1.7179832

C 3.7214050 1.1409906 1.4049971

C 3.5547010 -0.9621209 2.6708909

C 4.0839847 0.3407737 2.4991222

H 4.1115397 2.1677681 1.3106853

H 3.8193639 -1.5747468 3.5472139

H 4.7733725 0.7404409 3.2608462

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C 2.3517562 1.3545038 -0.7371478

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P 0.4942188 -2.8247374 1.1848523

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C 1.6842950 -4.1637220 -0.9375611

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H	-0.4972726	-4.9095109	4.2782941
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H	0.7674555	-2.1569599	4.1586018
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C	0.6589026	1.5021554	-2.4477020
C	0.4046152	2.9025866	-2.6075884
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C	-0.2902250	3.3183511	-3.7602848
C	-0.5419480	1.0329049	-4.5246721
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H	1.0521060	3.4122082	-0.6219636
H	2.3645696	5.4571947	-1.2126908
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H	1.8439181	5.3196935	-2.9314061
C	1.8494701	-1.2850324	-3.5512246
H	2.5833226	-0.6936634	-2.9622578
H	2.0579820	-2.3638797	-3.3758046
H	2.0293492	-1.0752011	-4.6295807
C	-0.3475943	4.9081185	-1.2173621
H	-0.0637425	5.5449132	-0.3500958
H	-0.5982611	5.5889408	-2.0612368
H	-1.2661712	4.3441805	-0.9452837
C	-2.9367227	1.0220896	1.1735932
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C	-3.2898533	0.6369734	2.6144087
H	-3.0285081	1.4627000	3.3113127
H	-4.3763219	0.4141686	2.7297054
H	-2.7289552	-0.2603293	2.9622167
C	-3.3531265	0.0465309	0.0975694
C	-3.4544357	-1.3443749	0.3405200
C	-3.5457635	0.4919646	-1.2330045
C	-3.7499834	-2.2456156	-0.6957234
H	-3.3093599	-1.7318410	1.3618412
C	-3.8391952	-0.4053106	-2.2691005
H	-3.4529352	1.5683592	-1.4574776
C	-3.9460676	-1.7824868	-2.0063816
H	-3.8315475	-3.3230107	-0.4722145
H	-3.9806294	-0.0226907	-3.2938202
H	-4.1783565	-2.4900514	-2.8194551
Si	-1.0150169	1.1873884	0.8794487
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C	1.3486172	2.5402326	4.0808761
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H -1.3026980 4.0967191 1.6659253

C 1.0018931 3.8963137 4.1971371

H 2.1036035 2.0992871 4.7534894

H -0.2270141 5.5146985 3.4101690

H 1.4778088 4.5268664 4.9671483

H -0.8840005 -0.4284953 1.4406207

J

96

Energy =

Ni 1.2065216 -0.7016460 -0.0896853

C 2.6930543 -1.1411028 1.1158631

C 3.1157938 0.0679118 1.8083965

C 2.5405385 -2.3462954 1.8915438

C 3.6235334 -0.0364803 3.1336534

C 3.0035825 -2.4219645 3.1926149

C 3.5969839 -1.2641089 3.7941293

H 3.9607073 0.8719411 3.6611534

H 2.8826638 -3.3568104 3.7629441

H 3.9644598 -1.3358704 4.8308165

N 1.8247296 1.1519659 0.1698782

C 2.7945697 1.2545373 1.0922859

H 3.3208042 2.2103146 1.2625283

P 0.7062354 -2.7579642 0.1094049

O 1.8432372 -3.3659498 1.2789591

C 1.1065142 -3.8871310 -1.3251526

C 2.5048158 -3.5535753 -1.8616055

H 1.1138869 -4.9254742 -0.9248675

H 2.7642058 -4.2226350 -2.7132765

H 2.5486025 -2.5011624 -2.2214635

H 3.2817441 -3.6779059 -1.0768099

C -0.8637175 -3.4699921 0.8483956

C -0.8338106 -4.9899448 1.0534640

H -1.6450316 -3.2069938 0.0944340

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H	-0.7699726	-5.5508519	0.0959021
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C	0.0239447	-3.7494783	-2.4064098
H	-0.0870523	-2.6907620	-2.7347329
H	0.2939541	-4.3538900	-3.3019826
H	-0.9722205	-4.0994177	-2.0565557
C	-1.1720279	-2.7159859	2.1504803
H	-0.3960463	-2.9206215	2.9211108
H	-1.2071886	-1.6174744	1.9926708
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C	1.3666180	2.2266945	-0.6156197
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C	1.0819338	1.9548123	-1.9963515
C	0.5105944	4.4889612	-0.9224677
C	0.5276123	2.9656936	-2.7974195
C	0.2556480	4.2367213	-2.2752287
H	0.2654639	5.4811657	-0.5094258
H	0.3042875	2.7594276	-3.8551094
H	-0.1685707	5.0247808	-2.9186082
C	1.4275901	0.5999429	-2.5934485
C	0.6429196	0.2337138	-3.8585820
H	1.1252471	-0.2105253	-1.8411982
H	0.8457640	-0.8239418	-4.1373055
H	-0.4529770	0.3417770	-3.7095687
H	0.9412753	0.8612409	-4.7284310
C	1.1997164	3.8640561	1.4196443
C	2.4352512	4.7561716	1.6589336
H	1.3394590	2.9184496	1.9848615
H	2.5726630	4.9610168	2.7448585
H	3.3706908	4.2941319	1.2725342
H	2.3179780	5.7339597	1.1392010
C	2.9448195	0.4605011	-2.8184288
H	3.5172087	0.6648585	-1.8887714

H	3.2054502	-0.5635018	-3.1687277
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H	-0.2249118	5.5516898	1.6087927
H	-0.9656515	3.9220013	1.8152375
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H	-4.3962377	1.0524631	-0.7728152
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H	-4.9278988	-1.4341343	-0.2752586
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C	-3.0199113	-1.4277702	-2.6430667
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C	-2.7619784	-1.7408177	-3.9878165
H	-2.9356087	-2.2221544	-1.8841994
C	-3.2213182	0.5548230	-4.6092748
H	-3.7591135	1.8951471	-2.9890729
C	-2.8610866	-0.7524101	-4.9793336
H	-2.4803949	-2.7718904	-4.2607139
H	-3.3042161	1.3436598	-5.3756024
H	-2.6578162	-0.9976923	-6.0346739
Si	-1.9824316	1.0938147	-0.2134361
H	3.1122627	-1.2867248	0.0754994
H	-1.8452871	2.3960685	-0.9602396
C	-1.9264809	1.3619086	1.6571798
C	-0.7905955	0.9425898	2.3883402
C	-2.9743691	1.9992253	2.3623389
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H	-3.8758737	2.3436315	1.8239071
C	-1.7445417	1.7970851	4.4545244

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H -3.7126618 2.7150934 4.2799928

H -1.6753617 1.9703834 5.5417269

H -0.8359245 0.1439119 -0.5358481

TS13

96

Energy =

Ni -0.4492723 0.1586569 -0.4038976

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C -0.2590705 1.4215568 -2.9125002

C -2.5479566 1.3027804 -2.0623045

C -0.7273571 2.1070052 -4.0671884

C -3.0201421 1.9590134 -3.2022730

C -2.0891633 2.3981734 -4.1812696

H -0.0288471 2.3630027 -4.8811726

H -4.1041150 2.0873654 -3.3503061

H -2.4645570 2.9213563 -5.0759871

N 1.1277380 0.0190317 -1.6466346

C 1.0228268 0.8116690 -2.7039745

H 1.8659929 0.9322226 -3.4108555

P -2.5113577 -0.5079274 -0.2742120

O -3.3894748 0.6942172 -1.1519324

C -3.4263676 -0.3952831 1.3477521

C -4.9109312 -0.7859734 1.3068047

H -2.8668255 -1.1100051 1.9954097

H -5.3752023 -0.5805988 2.2984656

H -5.4612453 -0.1887274 0.5475859

H -5.0649942 -1.8625829 1.0866222

C -2.9834770 -2.1060165 -1.1409693

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H	-2.1878462	1.3546593	1.8798763
C	-4.3774065	-2.1730291	-1.7769022
H	-5.1844541	-2.2712971	-1.0216498
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C	2.3322345	-0.6744863	-1.3535885
C	2.2660599	-2.1024836	-1.3384093
C	3.5388865	0.0107205	-1.0246451
C	3.4158048	-2.8213305	-0.9723482
C	4.6599043	-0.7640698	-0.6614433
C	4.6052130	-2.1613849	-0.6283274
H	3.3859442	-3.9218742	-0.9562171
H	5.6020722	-0.2558507	-0.3988126
H	5.4964427	-2.7426032	-0.3388256
C	3.6705192	1.5317958	-1.0887006
C	4.3674931	2.1434925	0.1412868
H	2.6422159	1.9540855	-1.1259203
H	4.3209353	3.2541783	0.0929043
H	3.8788644	1.8230091	1.0856725
H	5.4428804	1.8618358	0.1928883
C	0.9824098	-2.8047077	-1.7685593
C	0.8322809	-2.7875301	-3.3045022
H	0.1514427	-2.1875514	-1.3530575
H	-0.1474410	-3.2248791	-3.6044706
H	0.8794157	-1.7557536	-3.7125663
H	1.6380361	-3.3868068	-3.7861006
C	4.4056469	1.9652791	-2.3751544
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H	4.4473608	3.0753674	-2.4503457
H	5.4513115	1.5828059	-2.3765145
C	0.8260270	-4.2324242	-1.2311447

H	-0.1769257	-4.6295579	-1.5020736
H	1.5776169	-4.9299400	-1.6658742
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H	-0.7023798	0.2633303	3.5959673
C	1.3529592	0.5248996	4.2502422
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H	2.3908896	0.2838506	3.9306286
C	0.3784464	-1.4982291	3.0631027
C	-0.7196361	-2.3180260	3.4047916
C	1.5343448	-2.1311334	2.5469688
C	-0.6759481	-3.7115203	3.2320639
H	-1.6253298	-1.8496784	3.8289230
C	1.5885063	-3.5233203	2.3874050
H	2.4054314	-1.5232376	2.2494459
C	0.4825563	-4.3224910	2.7255846
H	-1.5512756	-4.3247696	3.5054864
H	2.5036582	-3.9835410	1.9792585
H	0.5229925	-5.4162444	2.5921640
H	-0.6081246	1.6473352	-0.2353900
Si	0.5704449	0.9090580	1.5217520
H	0.0615331	-0.7195109	0.7332497
H	2.0491771	0.7779463	1.2489313
C	0.3038059	2.7760853	1.8793430
C	0.8890052	3.7272758	1.0092648
C	-0.4731288	3.2659927	2.9534365
C	0.7147773	5.1050389	1.2053456
H	1.4907250	3.3814087	0.1498764
C	-0.6597898	4.6456656	3.1518239
H	-0.9482927	2.5640497	3.6601956
C	-0.0650792	5.5702295	2.2793296
H	1.1877812	5.8225789	0.5136280
H	-1.2741942	4.9992785	3.9972385

H -0.2092023 6.6526938 2.4336886

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