Supporting Information for

Mechanistic insight into cooperative catalysis with pentanuclear nickel clusters: catalytic alkene dimerization and silyl-silylene and silylyne clusters.

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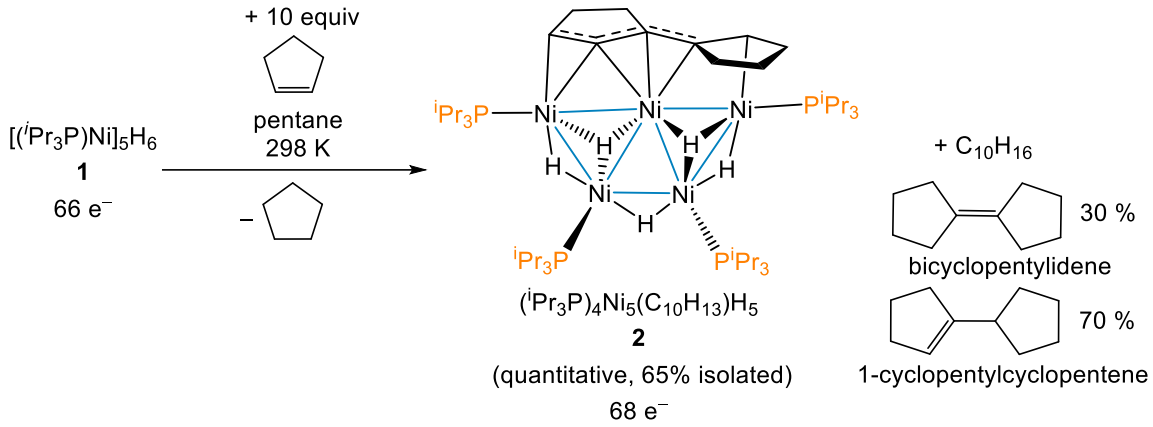
General experimental considerations. Unless otherwise stated, all reactions were carried out in an inert atmosphere under standard Schlenk or glovebox techniques. Benzene-d_6, and toluene-d_8 were degassed by three freeze-pump-thaw cycles, and subsequently dried by running through a column of activated alumina. Anhydrous solvents and reagents were purchased from Millipore Aldrich (Sigma Aldrich), or Oakwood Chemicals. Silane reagents were degassed by three freeze-pump-thaw cycles and dried by standing over 4Å molecular sieves for 24 hrs prior to use. ^{1}H, ^{13}C{^{1}H}, ^{29}Si{^{1}H} and ^{31}P{^{1}H} NMR spectra were recorded on a Bruker AMX Spectrometer operating at either 300 MHz or 500 MHz with respect to proton nuclei. The compound [Ni(^{i}Pr$_3$P)]$_5$H$_6$ (**1**) was synthesized according to reported procedures.[1]

Catalytic [2+2] cyclodimerization of norbornadiene (*exo-trans-exo* isomer). To a n-pentane solution (3 mL) of [(^{i}Pr$_3$P)Ni]$_5$H$_6$ (100 mg, 0.045 mmol) kept at 253 K was added dropwise a n-pentane solution (2 mL) of norbornadiene (85 mg, 0.45 mmol). The mixture was stirred at 253 K for 15 min before filtration through silica plug to remove the inorganics. A clear oil (72 mg, 86%) was obtained containing trace amounts of norbornene dimer due to hydrogenation of norbornadiene to norbornene. The crude mixture containing primarily [2+2] cyclodimerized norbornadiene was then sublimed under vacuum at 323 K and identified as exclusively the *exo-trans-exo* isomer, by comparison to the literature ^{1}H and ^{13}C{^{1}H} NMR spectra.[2] ^{1}H NMR (500

MHz, 298K, benzene-d_6): δ 1.31 (s, 4H), 1.34 (d of m, 2H, *J* = 8.8 Hz), 1.67 (d of m, 2H, *J* = 8.8 Hz), 2.55 (br t, 4H), 6.01 (br t, 4H). $^{13}C\{^1H\}$ NMR (125 MHz, 298K, benzene-d_6): δ 40.2 (4C), 42.6 (2C), 44.6 (4C), 136.4 (4C).

Synthesis of 2. To a stirring n-pentane solution of $[Ni(^iPr_3P)]_5H_6$ (**1**) (1 g, 0.91 mmol) was added dropwise a solution of excess cyclopentene (680 mg, 9.98 mmol) at 298 K, as shown in Scheme S1. The reaction mixture was stirred for an additional 30 min before the volatiles were removed under vacuum. To isolate **2**, which appeared to be formed nearly quantitatively from $^{31}P\{^1H\}$ NMR, the crude was dissolved in minimal amount of n-pentane and crystalized at 233 K to afford crystalline solid (65 %, 635 mg). The crystals were suitable for single-crystal X-ray diffraction studies. Multiple crystals provided the same unit cell and structure, despite the clear presence of two isomers in slow-exchange in the solution NMR spectra; there is no indication that a second isomer crystallizes from solution under these conditions. It should be noted that although the cocrystallized pentane observed in the X-ray structure can be removed under vacuum, trace amounts of the organic catalysis products, $C_{10}H_{16}$, are difficult to fully remove from the samples via a single recrystallization. ^1H NMR (298 K, Benzene-d_6, 500 MHz): δ –21.10 (br s, 1H), –17.96 (br s, 2H associated with isomer 2a), –16.17 (br s, 2H), –15.12 (br s, 1H), –10.80 (br s, 1H), 0.65 (m, 1H), 0.73 (m, 1H), 1.04 (dd, 9H, J=13, 6.7 Hz), 1.05 (dd, 9H, J=13, 6.7 Hz), 1.12 (dd, 9H, J=12, 7 Hz), 1.17 (dd, 9H, J=13, 6.7 Hz), 1.19(dd, 9H, J=13, 6.7 Hz), 1.25-1.39 (overlapping dd, 90 H), 1.52 (dd, 9H, J=13, 6.7 Hz), 1.57 (m, 1H), 1.72 (d of sept, 3H, J = 7.6, 7 Hz), 1.77 (d of sept, 3H, J = 7.6, 7 Hz), 1.82 (d of sept, 3H, J = 7.6, 7 Hz), 1.89 (m, 1H), 2.01 (d of sept, 3H, J = 7.6, 7 Hz), 2.31 (d of sept, 3H, J = 7.6, 7 Hz), 2.31 (d of sept, 3H, J = 7.6, 7 Hz), 2.38 (dt, 1H, J= 11.6, 7 Hz), 2.54 (m, 2H), 2.58 (d of sept, 3H, J = 7.6, 7 Hz), 2.82 (dd, 1H, J = 11.8, 7 Hz), 2.87 (dd, 1H, J = 7.6, 3 Hz), 2.96 (dt, 1H, J = 24, 4 Hz), 3.02 (dd, 1H, J = 14, 5 Hz), 3.54 (dt, 1H, J = 20, 5Hz), 3.98 (m, 1H). $^{31}P\{^1H\}$ NMR (298 K, Benzene-d_6, 121.5 MHz): δ 40.8 (m, P), 43.8 (m, 2P) 52.5 (m, 1P), 63.3 (br s, 1P), 67.6 (br s, 1P). 63.1 (m, 1P), 69.4 (m, 1P). $^{13}C\{^1H\}$ NMR (298 K, benzene-d_6, 125 MHz): δ 20.3 (d, J = 2.3 Hz), 20.3 (d, J = 3.5 Hz), 20.4 (d, J = 2.8 Hz), 20.6 (d, J = 2.9 Hz), 20.6 (d, J = 3.7 Hz), 20.7 (d, J = 2 Hz), 20.7 (d, J = 3.3 Hz), 20.8 (s), 20.9 (d, J = 4.6 Hz), 21.1 (d, J = 4.2 Hz), 21.1 (d, J = 4.2 Hz), 21.2 (d, J = 5 Hz), 21.3(d, J = 4 Hz), 21.3(d, J = 4.2 Hz), 21.5 (d, J = 4 Hz), 21.5 (d, J = 4.7 Hz), 23.6 (d, P*C*H, J = 13.5 Hz), 24.9(d, P*C*H, J = 13.4 Hz), 26.1 (d, P*C*H, J = 11 Hz), 26.2(d overlapped, P*C*H, J = 14 Hz), 26.2 (d overlapped, P*C*H, J = 12 Hz), 26.6 (d, P*C*H, J = 12.5 Hz), 26.8 (d, J = 14.2 Hz), 27.3 (s, CH_2), 27.4 (s, CH_2), 27.6(d, P*C*H, J = 13.6 Hz), 29.3 (s), 30.9 (d, J = 6 Hz), 31.4 (d, J = 6.5 Hz), 32.4 (s), 34.6 (s), 35.2 (s), 35.3 (s), 36.3 (s), 36.4 (s), 37.8 (s), 39.1 (d, J = 7 Hz), 50.9 (d, J = 4.6Hz), 59.1 (s), 62.2 (m), 71.8 (s), 83.6 (s), 83.8(s), 84.8(s). Anal Calc for $C_{46}H_{102}Ni_5P_4$ (1072.68 g·mol^{-1}): Calc: C, 51.51; H, 9.58 Found: C, 51.96; H, 9.72.



Scheme S1. Synthesis of **2** and catalytic dimerization of cyclopentene.

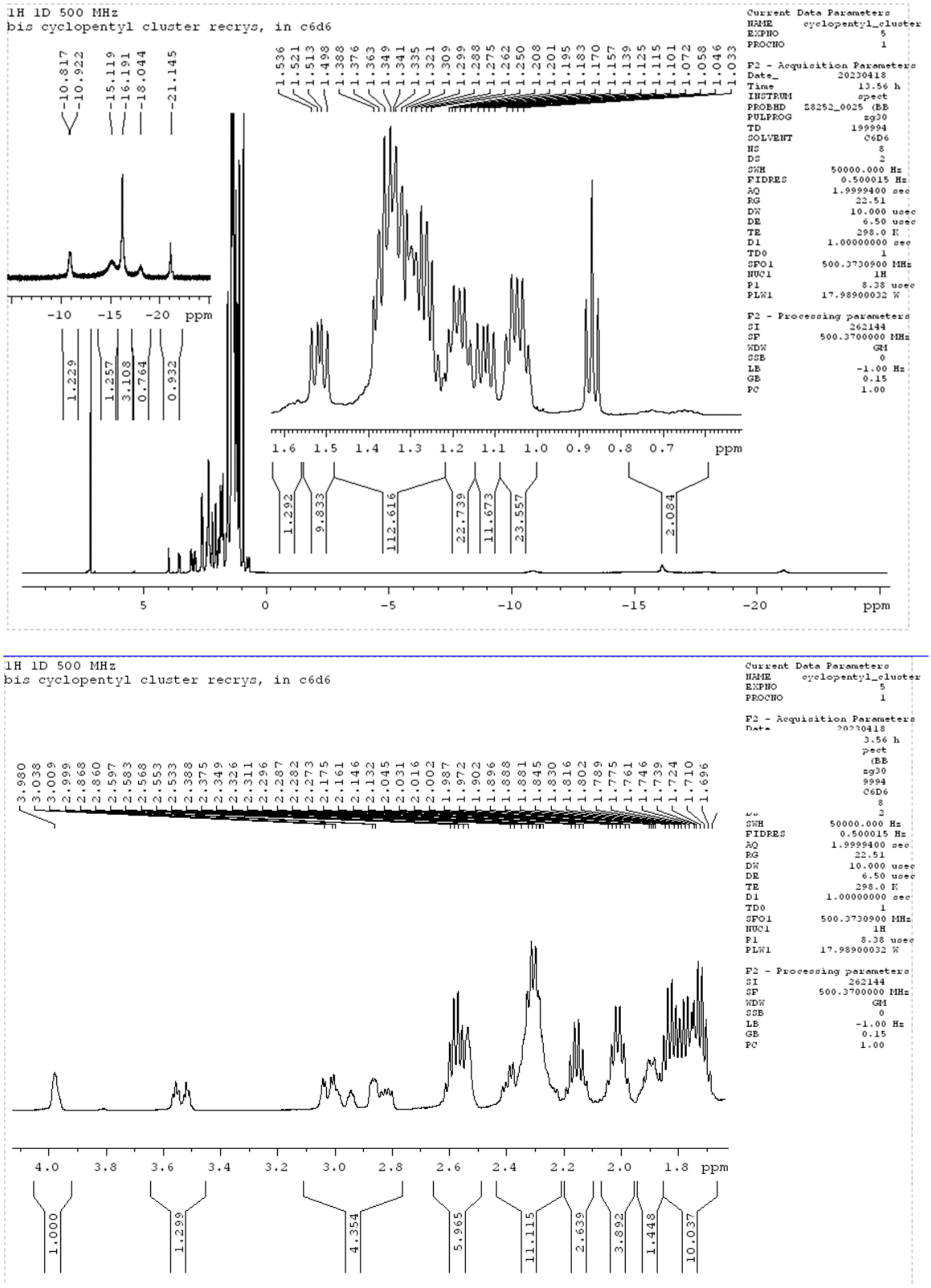


Figure S1. ^{1}H NMR of **2** (500.4 MHz, C_6D_6, 298 K) with expansions of hydride region from 0 to –25 ppm (top left), alkyl region 0.5 to 1.6 ppm (top right) and 1.6 to 4 ppm (bottom).

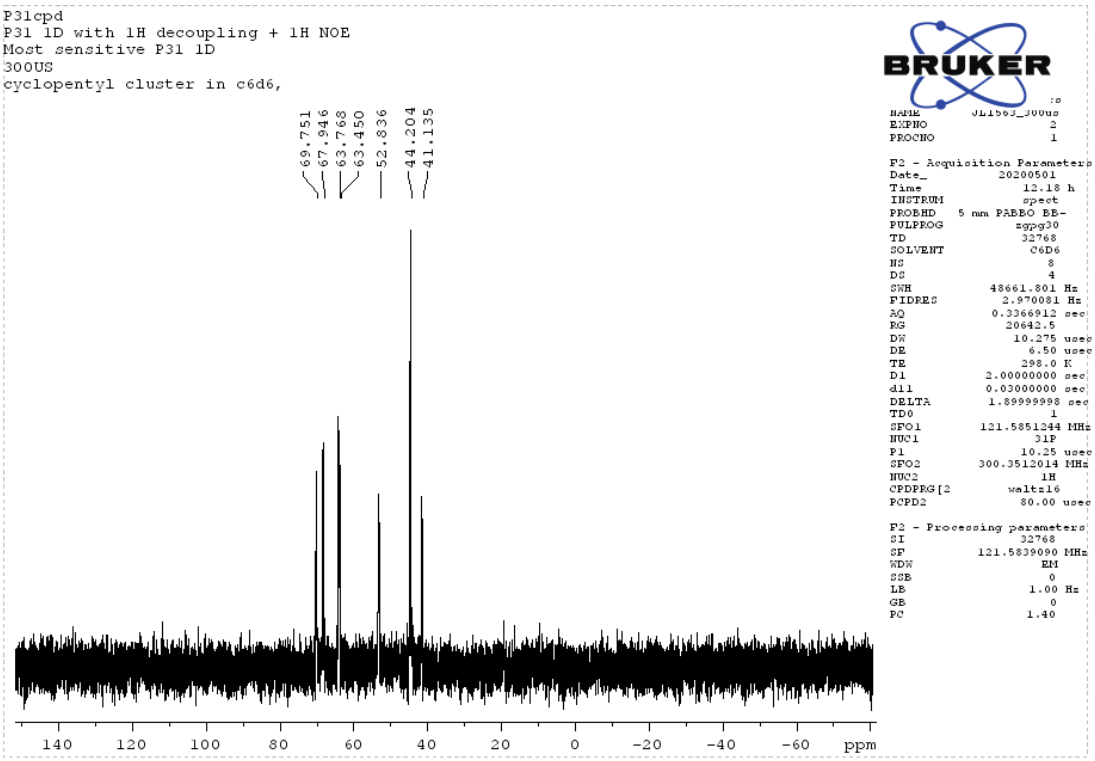
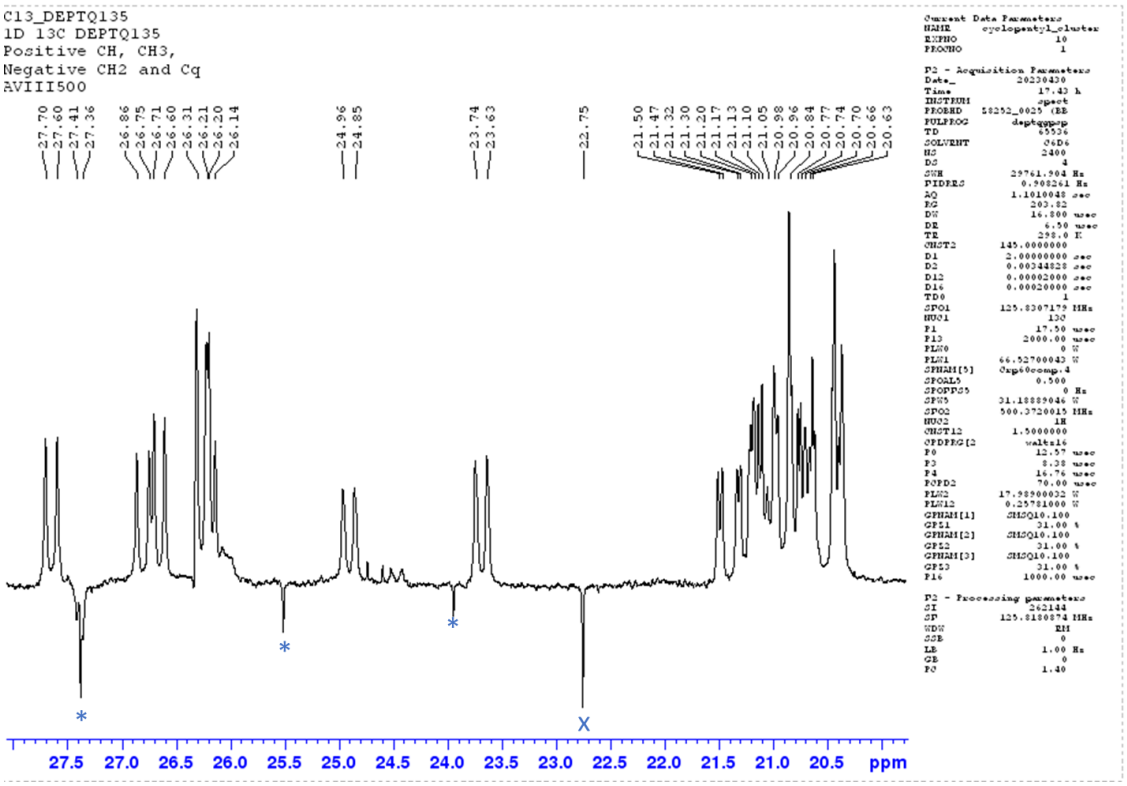


Figure S2. $^{31}P\{^{1}H\}$ NMR spectrum of **2** (121.6 MHz ,C_6D_6, 298 K).



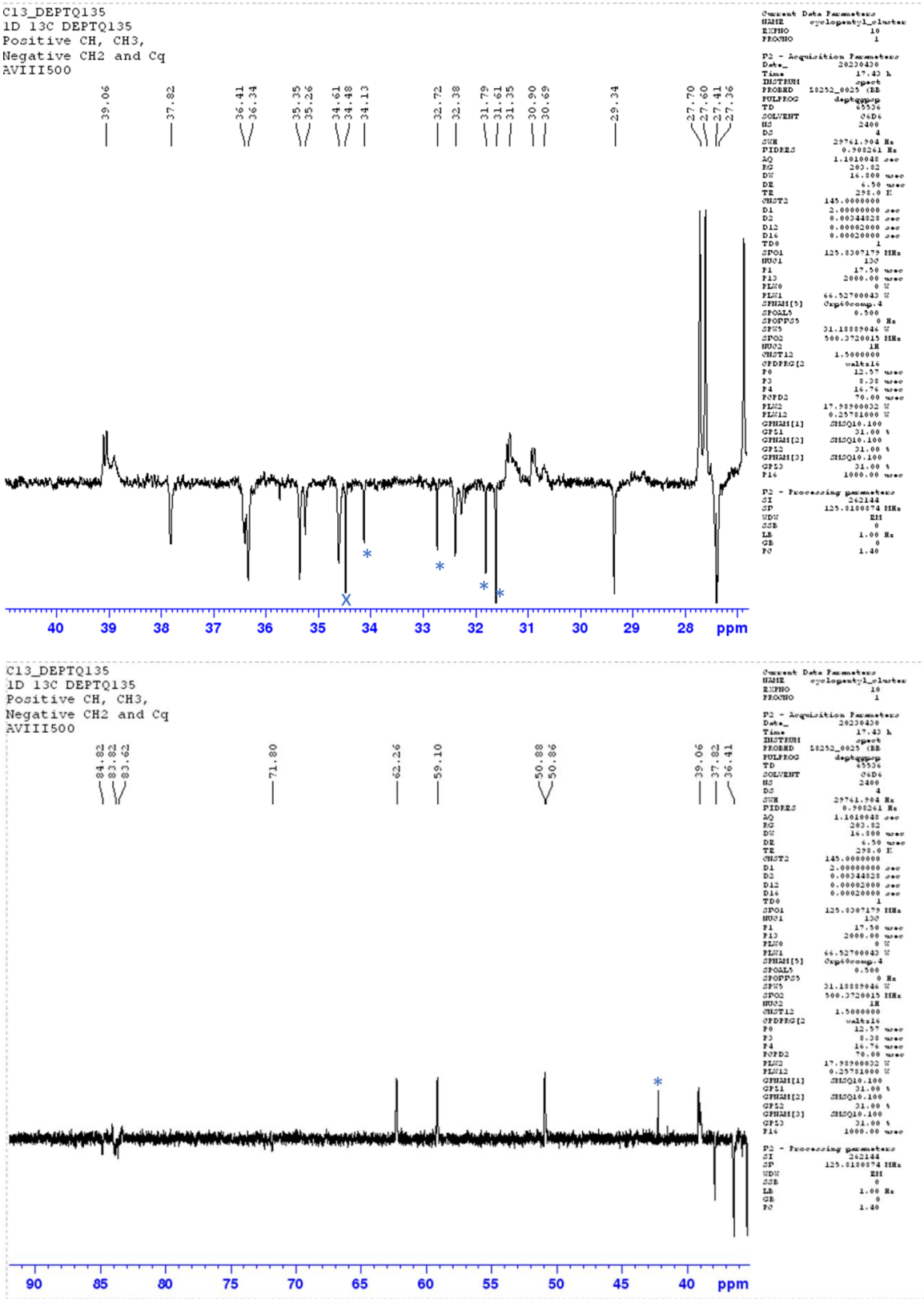


Figure S3. $^{13}C\{^{1}H\}$ DEPT NMR spectrum of NMR of **2** (125.8 MHz , C_6D_6, 298 K), shown as three

expansions, with positively phased CH and CH_3 and negatively phased CH_2. X = n-pentane. * = $C_{10}H_{16}$ (dimerized cyclopentene isomers).

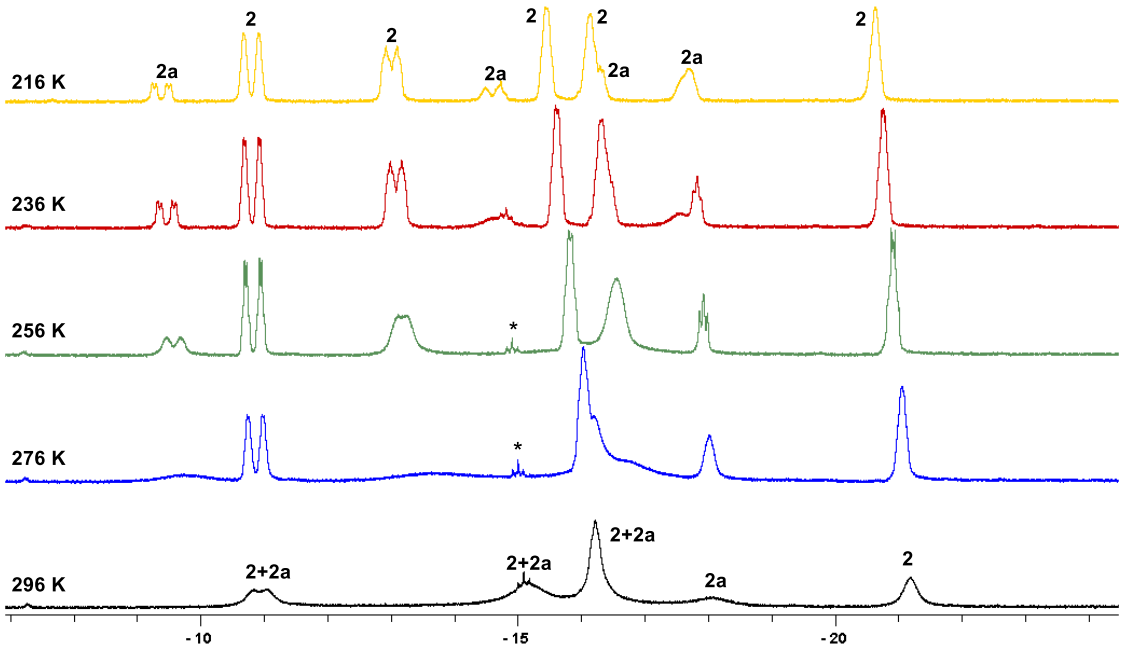


Figure S4. Hydride region of the variable-temperature ^{1}H NMR of **2** (500.4 MHz, d_8-toluene). The sharp 2nd order multiplet near δ –15 marked with * is assigned as the trace impurity [(^{i}Pr$_3$P)Ni]$_4$(μ_4-O)H$_4$ from adventitious oxygen.[3]

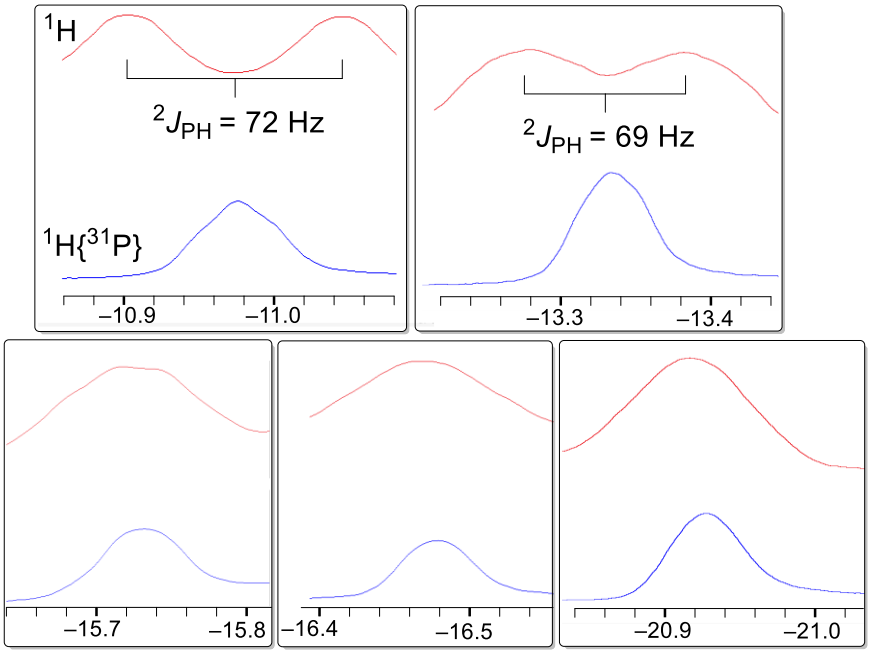


Figure S5. Expansions of the hydride signals for major isomer **2** in the ^{1}H (top, red) and ^{1}H{^{31}P} (bottom, blue) NMR spectra (500.4 MHz, THF, 223 K). Although some of the multiplets show peak shapes suggestive of proton-proton coupling, none were sufficiently resolved to determine coupling constants at this temperature.

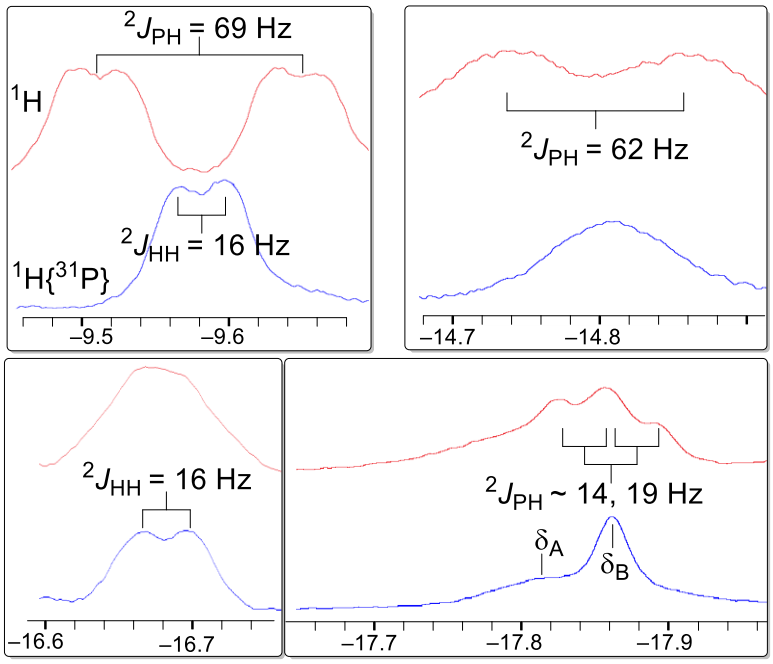


Figure S6. Expansions of the hydride signals for minor isomer **2a** of the ^{1}H (top, red) and ^{1}H{^{31}P} (bottom, blue) NMR spectra (500.4 MHz, THF, 223 K). The only proton-proton coupling resolved is the $^2J_{HH}$ = 16 Hz between the hydride peaks at δ –9.58 and –16.68.

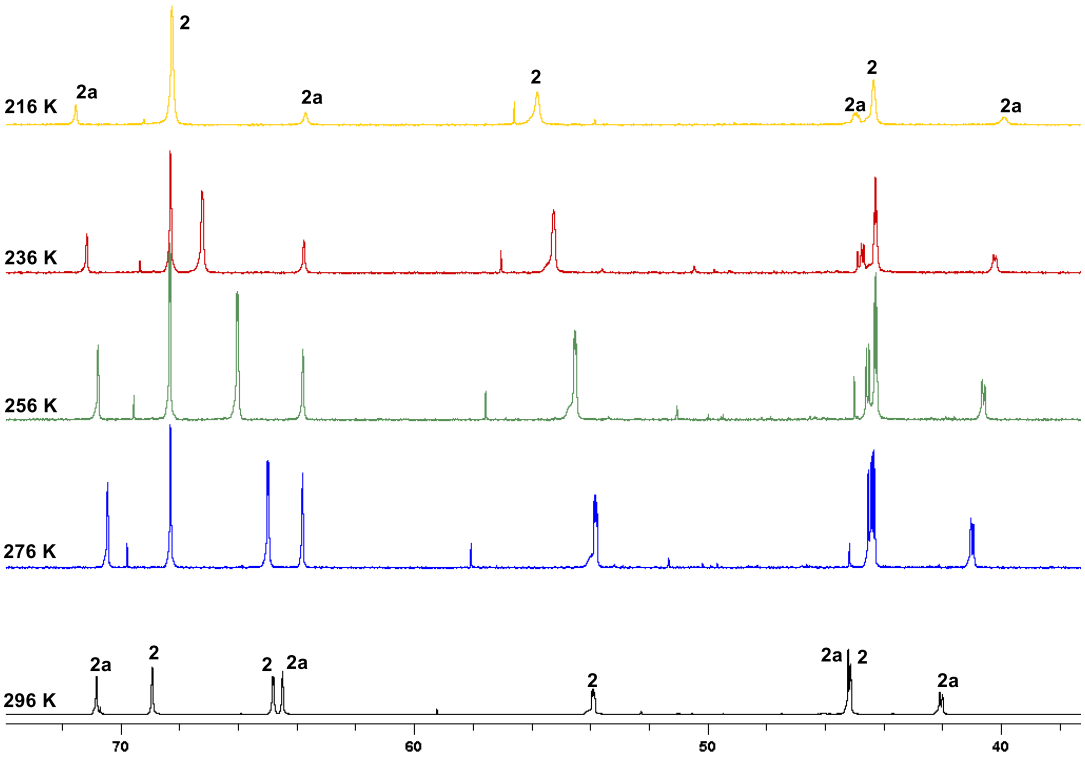


Figure S7. Variable low-temperature $^{31}P\{^{1}H\}$ NMR of **2** (121.6 MHz, d_8-toluene)

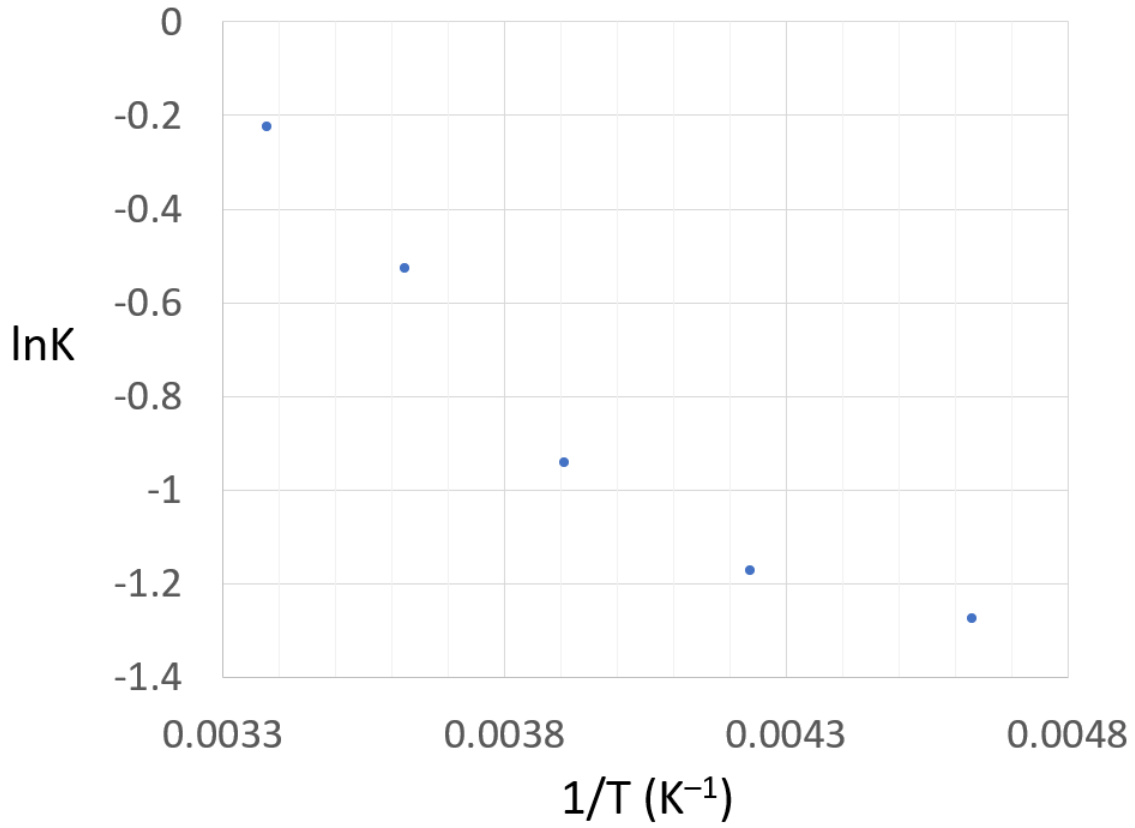


Figure S8. Van't Hoff Plot for complex **2**. Equilibrium constant determined from the relative integrals of **2** and **2a** in the variable-temperature $^{31}P\{^{1}H\}$ NMR of **2**. A slope of –1107 K and an intercept of 3.56 were determined. The lowest temperature data point at 216 K was excluded. This curvature at low temperature is possibly because the interconversion of **2** and **2a** is too slow to reach equilibrium at this temperature under the experimental time constraints.

Organic products from the synthesis of 2. The synthesis of 2 catalytically generated a mixture of cyclopentylidenecyclopentane and 1-cyclopentylcyclopentene. The mother liquor obtained from recrystallization of **2** in the above step was filtered through silica plug under air to remove inorganics and washed with n-hexane to give a clear liquid. N-hexane was removed using rotary evaporation to obtain a clear oil, which contained a mixture of cyclopentylidenecyclopentane (30%) and 1-cyclopentylcyclopentene (70%) as characterized by comparison of the ^{1}H and $^{13}C\{^{1}H\}$ spectra of the products in $CDCl_3$ with those in the literature.[4,5] **Cyclopentylidenecyclopentane.** ^{1}H NMR (298 K, Chloroform-d, 500 MHz): δ 1.66 (m, 8H), 2.12 (m, 8H). $^{13}C\{^{1}H\}$ NMR (298 K, Chloroform-d, 125 MHz): δ 26.9, 31.3, 132.4. **1-cyclopentylcyclopentene.** ^{1}H NMR (298 K, Chloroform-d, 500 MHz): δ 1.38-1.42 (m, 2H), 1.56-1.58 (m, 2H), 1.66 (m overlap with cyclopentylidenecyclopentane, 2H), 1.76-1.79 (m, 2H), 1.85 (p, J = 7.6 Hz, 2H), 2.26-2.97 (m, 4H), 2.49 (p, J = 8 Hz, 1H), 5.32-5.34 (m, 1H). $^{13}C\{^{1}H\}$ NMR (298 K, Chloroform-d, 125 MHz): δ 23.5, 25.2, 31.4, 32.3, 33.8, 41.8, 121.4, 148.5.

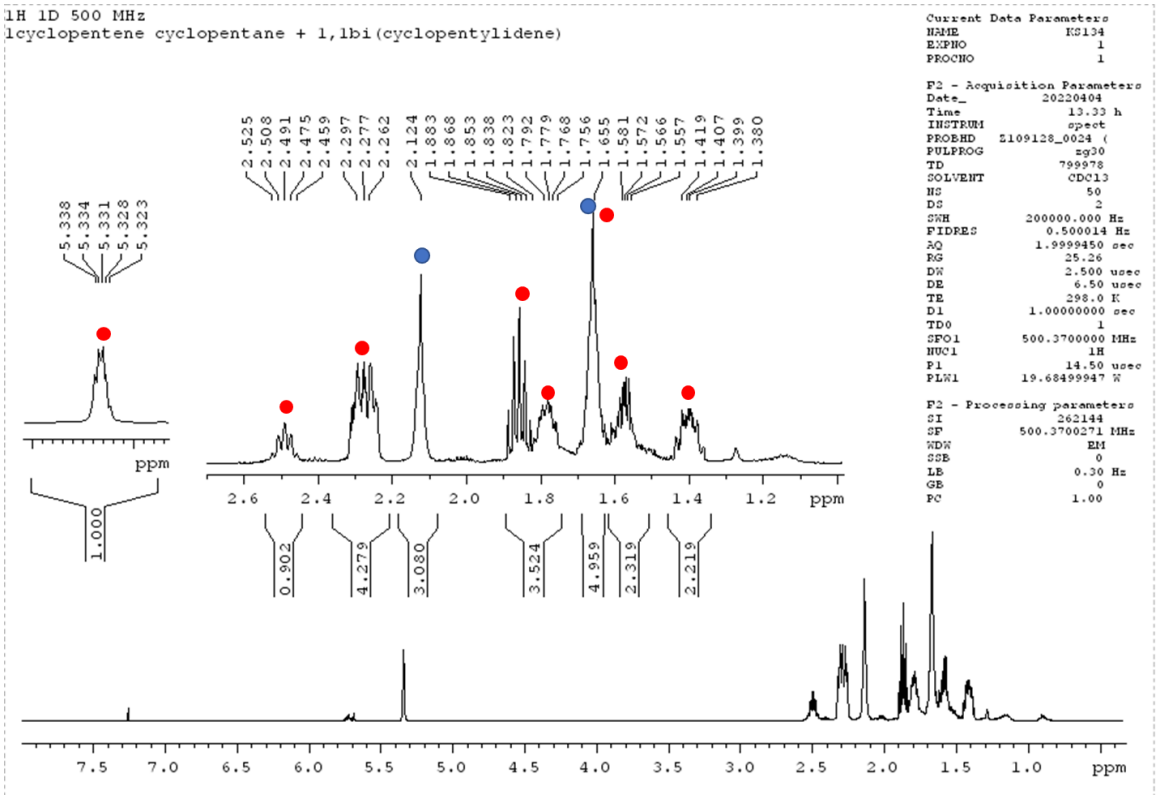


Figure S9. ^{1}H NMR of the catalytic cyclopentene dimerization products from synthesis of **2**. **blue**: cyclopentylidenecyclopentane, **red**: 1-cyclopentyl-cyclopentene

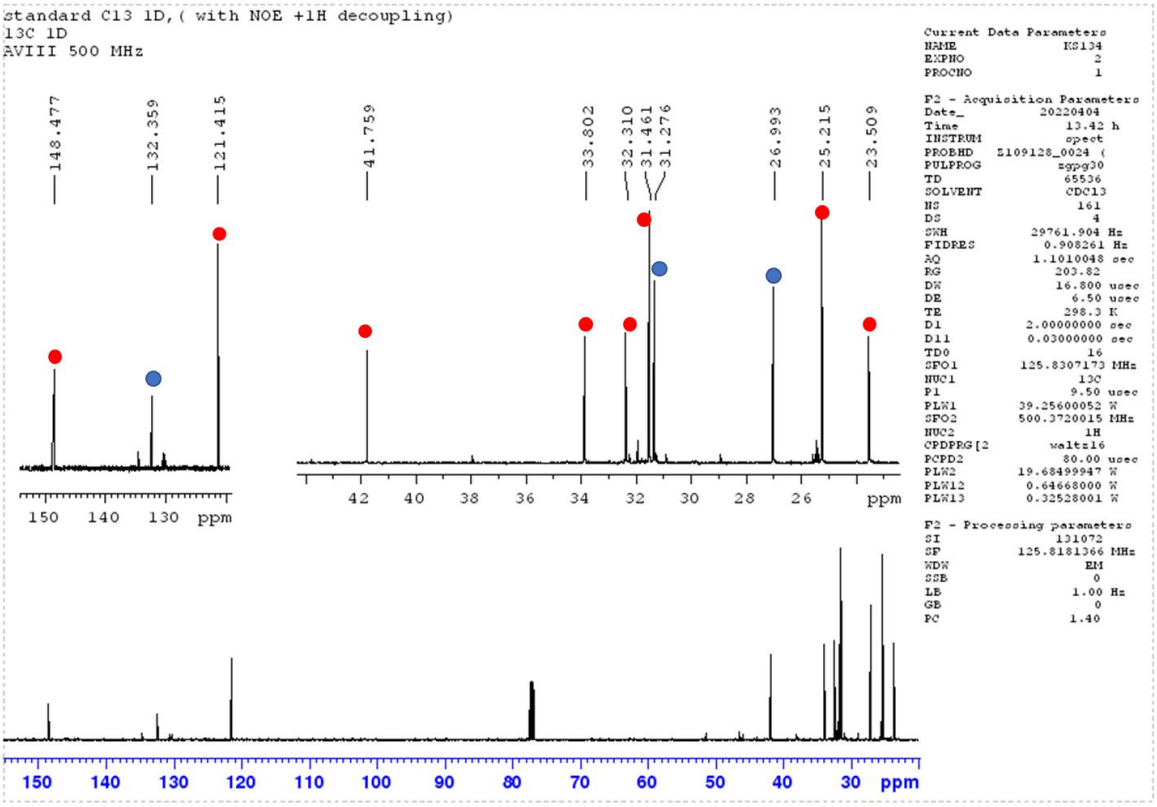


Figure S10. ^{13}C NMR of the catalytic cyclopentene dimerization products from synthesis of **2**. **blue**: cyclopentylidenecyclopentane, **red**: 1-cyclopentyl-cyclopentene

Reaction of 2 with hydrogen gas. In a J. Young NMR tube, **2** (20 mg, 0.019 mmol) and one drop of $^{i}Pr_3P$ was dissolved in 500 mg of n-pentane and the sample was frozen under liquid nitrogen, placed under vacuum and then refilled 1 atm of hydrogen gas. The tube was sealed and warmed to room temperature. ^{1}H and ^{31}P{^{1}H} NMR show clean conversion to **2** and liberation of a mixture of cyclopentylidenecyclopentane and 1-cyclopentylcyclopentene.

Synthesis of 3. To an n-pentane solution (3 mL) of **2** (100 mg, 0.09 mmol) was added an n-pentane solution (2 mL) of Ph_2SiH_2 (34 mg, 0.18 mmol) and stirred for 1 h at 298 K before it was pumped dry under vacuum. The solid crude was then redissolved in minimal amount of n-pentane to crystalize at 233 K yielding 88 mg of **3** (73 %).

Alternative synthesis of **3** from **1**: To a stirring n-pentane (7 mL) solution of $[Ni(^{i}Pr_3P)]_5H_6$ (**1**) (500 mg, 0.45 mmol) was added dropwise an n-pentane solution (3 mL) of Ph_2SiH_2 (166 mg, 0.9 mmol), a precipitate immediately formed, along with noticeable gas liberation from the solution. The mixture was stirred for another 5 min prior to filtration and the solid was dried under vacuum to obtain essentially pure **3** (399 mg, 0.31 mmol, 68%). Crystals of **3** suitable for single-crystal X-ray diffraction studies were grown from a concentrated toluene solution of **3**. ^{1}H NMR (298 K, Benzene-d_6, 500 MHz): δ –22.65 (br s, $W_{1/2}$ = 63 Hz, 1H), –15.06 (br s, $W_{1/2}$ = 57 Hz, 1H), −9.40 (br

s, $W_{1/2}$ = 860 Hz, 1H), −4.12 (br s, $W_{1/2}$ = 59 Hz, 1H), 0.96-1.53 (overlapping br s, 72 H), 1.88-1.99 (overlapping br s, 12 H). $^{13}C\{^1H\}$ NMR (298 K, Benzene-d_6, 125 MHz): δ 20.8 (overlapping br s, 24 C), 23.5 (br s, 3C), 25.1 (br s, 3C), 26.2 (br s, 3C), 27.2 (br s, 3C), 126.6 (br s), 127.3 (s), 136.8 (br s), 137.3 (s). $^{31}P\{^1H\}$ NMR (298 K, Benzene-d_6, 202 MHz): δ 48.2 (br s, $W_{1/2}$ = 57 Hz, 1P), 58.8 (br s, $W_{1/2}$ = 39 Hz, 1P), 68.4 (br s, $W_{1/2}$ = 54 Hz, 1P), 74.4 (br s, $W_{1/2}$ = 40 Hz, 1P). Anal Calc for $C_{60}H_{110}Ni_5P_4Si_2$ (1305.07 g·mol^{-1}): Calc: C, 55.22; H, 8.50 Found: C, 54.91; H, 8.39.

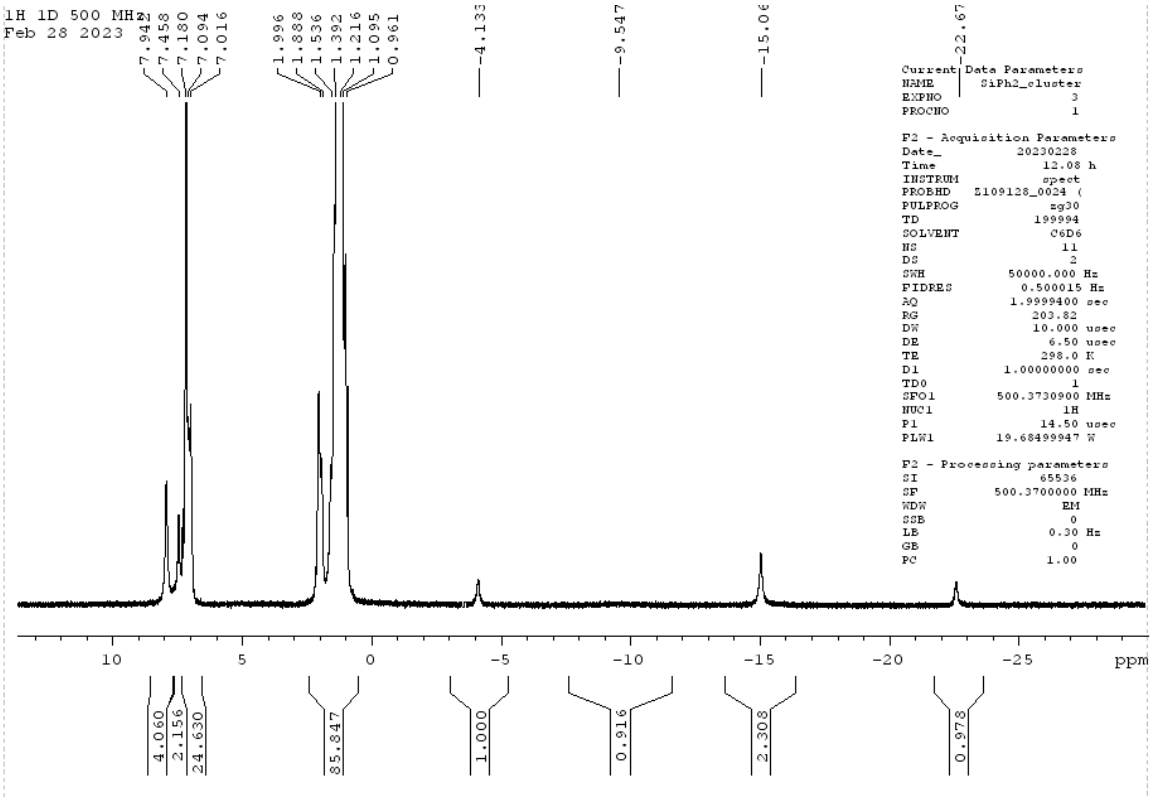


Figure S11. ^1H NMR of **3** (500 MHz, C_6D_6, 298 K).

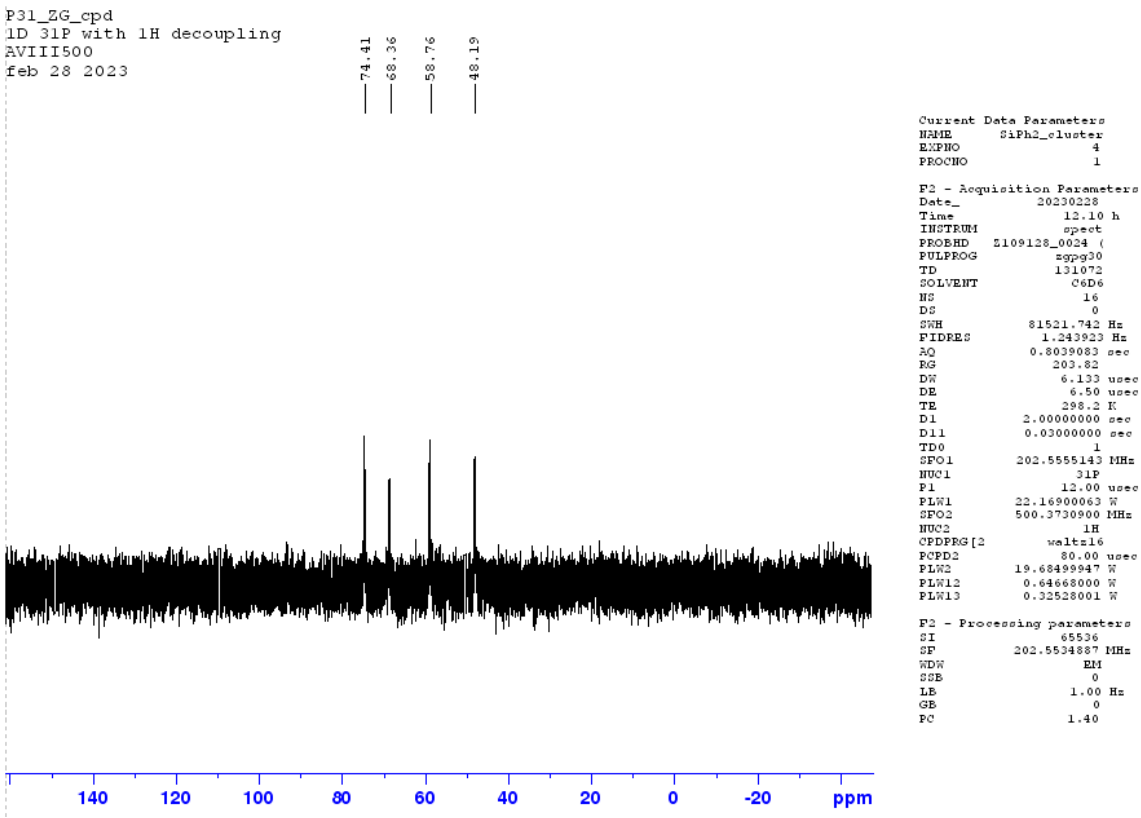


Figure S12. $^{31}P\{^{1}H\}$ NMR of **3** in (202.56 MHz, C_6D_6, 298 K).

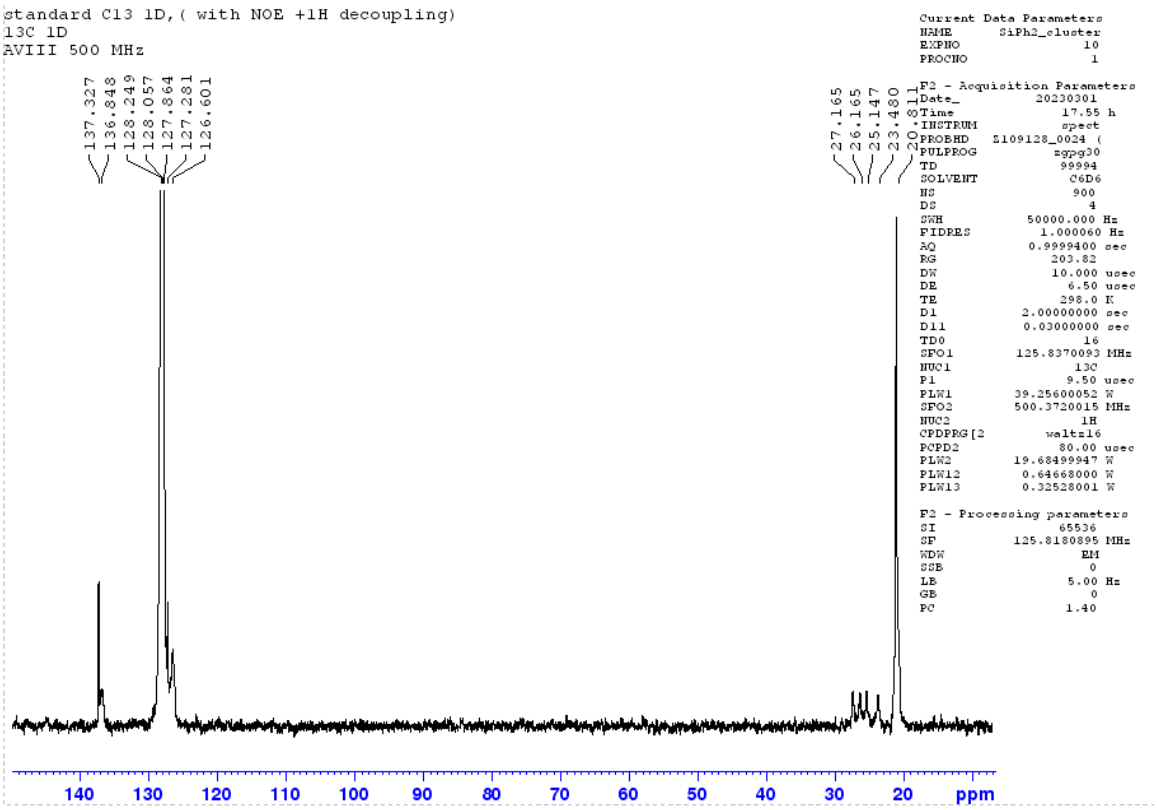


Figure S13. $^{13}C\{^{1}H\}$ NMR of **3** (125.84 MHz, C_6D_6, 298 K).

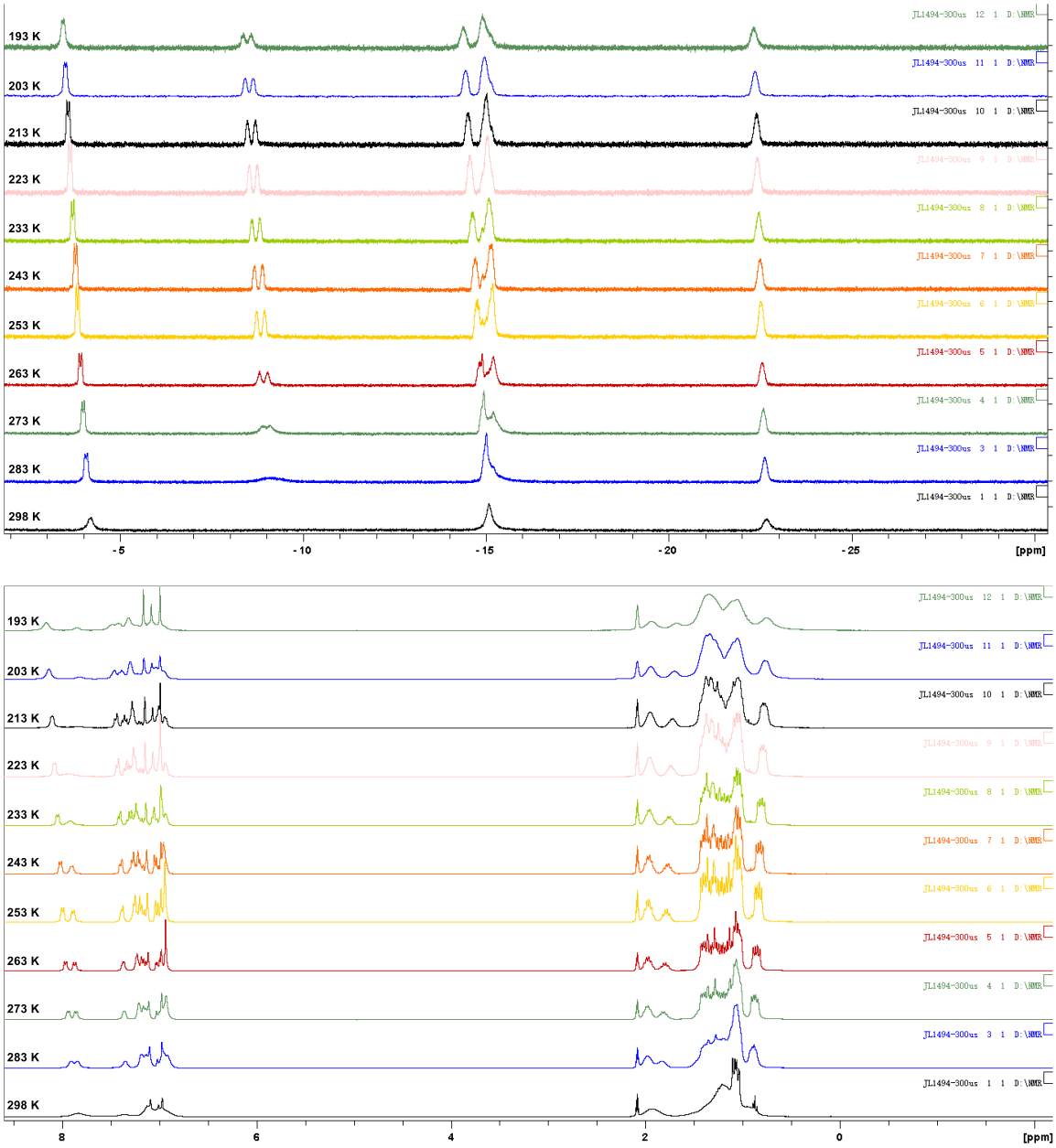


Figure S14. Variable-temperature ^{1}H NMR of **3** (300 MHz ,d_8-toluene). Hydride region (top), alkyl and aromatic region (bottom).

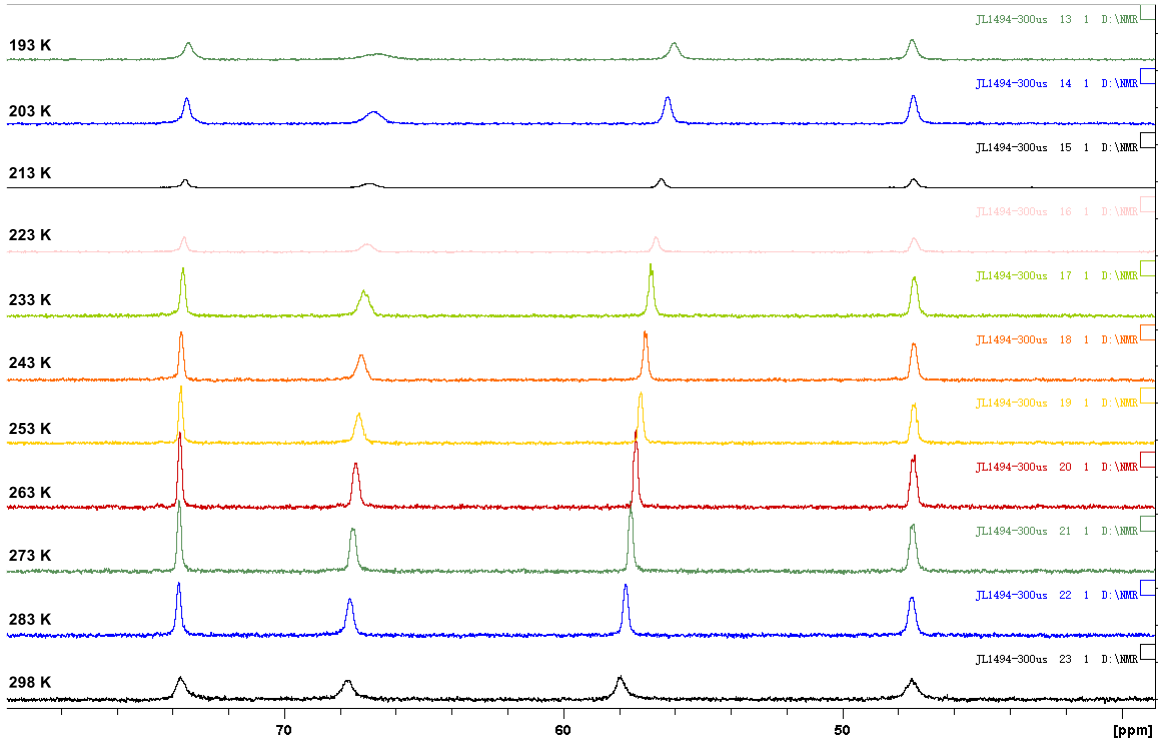


Figure S15. Variable-temperature $^{31}P\{^{1}H\}$ NMR of **3** in (202.56 MHz, d_8-toluene).

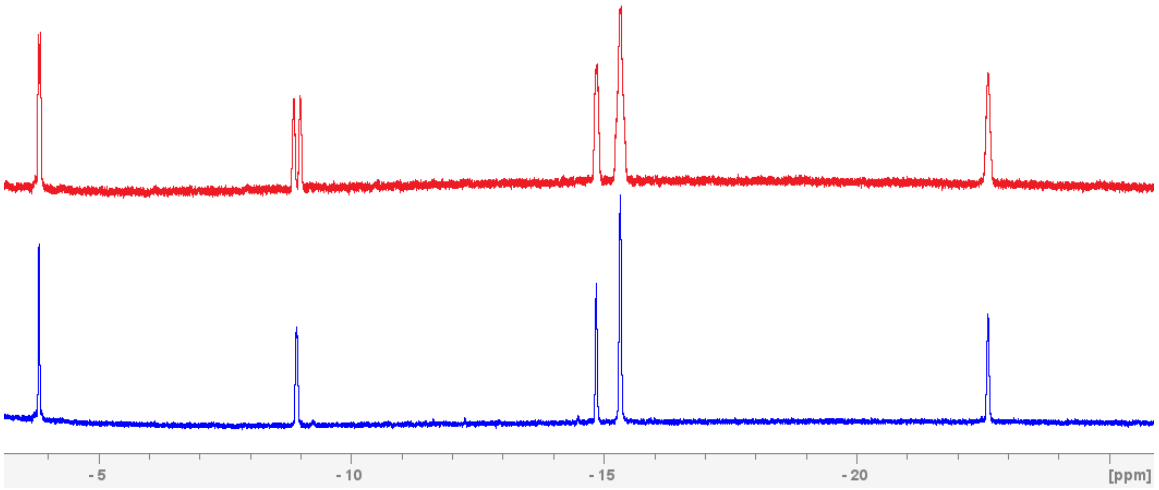


Figure S16. ^{1}H (top) and $^{1}H\{^{31}P\}$ (bottom) NMR spectra of the hydride region of **3** at 213 K (500.37 MHz, THF). No proton-proton couplings were resolved.

Synthesis of 4. To a stirring n-pentane (7 mL) solution of $[Ni(^{i}Pr_3P)]_5H_6$ (**1**) (500 mg, 0.45 mmol) was added dropwise an n-pentane solution (3 mL) of Et_3SiH over the course of 15 min. The reaction mixture was stirred for 3 hours at 298 K and the reaction progress was monitored by NMR spectroscopy using aliquots from the reaction mixture. The solvent and excess Et_3SiH was removed under vacuum and crude **4** was redissolved in minimal n-pentane and cooled in a –40 °C freezer inside the glovebox to afford crystals of **4** suitable for single crystal X-ray diffraction studies. The mother liquor was reduced to afford a second crop with a total yield of 189 mg, 0.16 mmol, 36%). ^{1}H NMR (298 K, Benzene-d_6, 500 MHz): δ –18.83 (br s, $W_{1/2}$ = 146 Hz, 2H), −11.82 (br s, $W_{1/2}$ = 176 Hz, 5H), 1.37 (dd, J = 12.2 Hz, 7.1 Hz, 90 H), 1.58 (t, J = 7.7 Hz, 3H), 2.07 (q, J = 7.7 Hz, 2H), 2.09 (sept, J = 7.1 Hz, 15H). $^{13}C\{^{1}H\}$ NMR (298 K, Benzene-d_6, 125 MHz): δ 13.9 (s, $SiCH_2CH_3$ 1C), 20.9 (d, $PCH(CH_3)$ $^{3}J_{CP}$= 2.4 Hz, 30C), 24.9 (d, $PCH(CH_3)$ $^{3}J_{CP}$= 9.1 Hz, 15C), 28.4 (s, $SiCH_2CH_3$ 1C). $^{31}P\{^{1}H\}$ NMR (298 K, Benzene-d_6, 202 MHz): δ 49.9 (br s, $W_{1/2}$ = 107 Hz, 5P). Anal Calc for $C_{47}H_{117}Ni_5P_4$ (1158.87 g·mol^{-1}): Calc: C, 48.71; H, 10.18 Found: C, 48.34; H, 9.99.

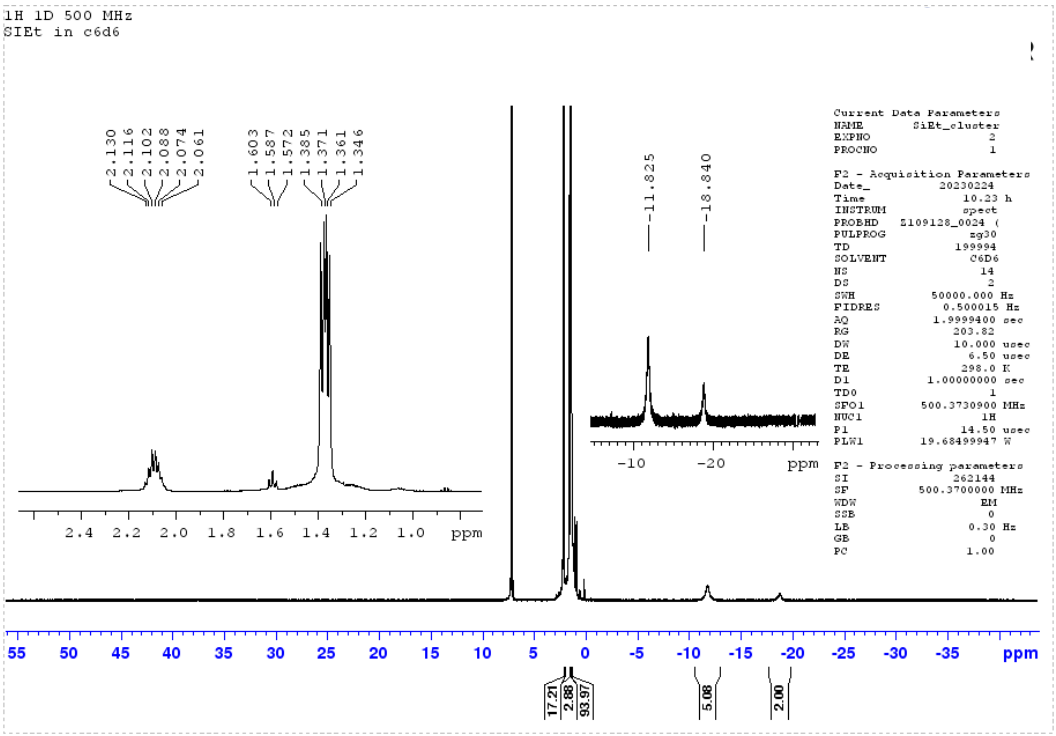


Figure S17. ^{1}H NMR of **4** (500 MHz, C_6D_6, 298 K).

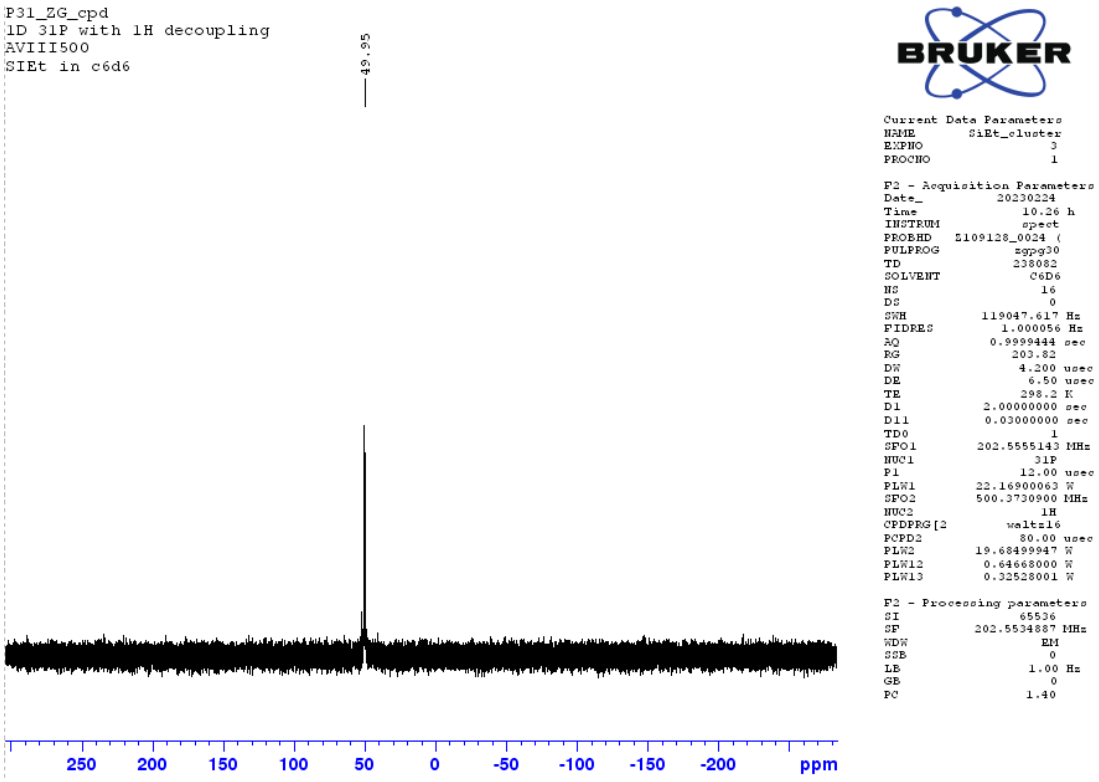


Figure S18. $^{31}P\{^{1}H\}$ NMR of **4** (202.56 MHz, C_6D_6, 298 K).

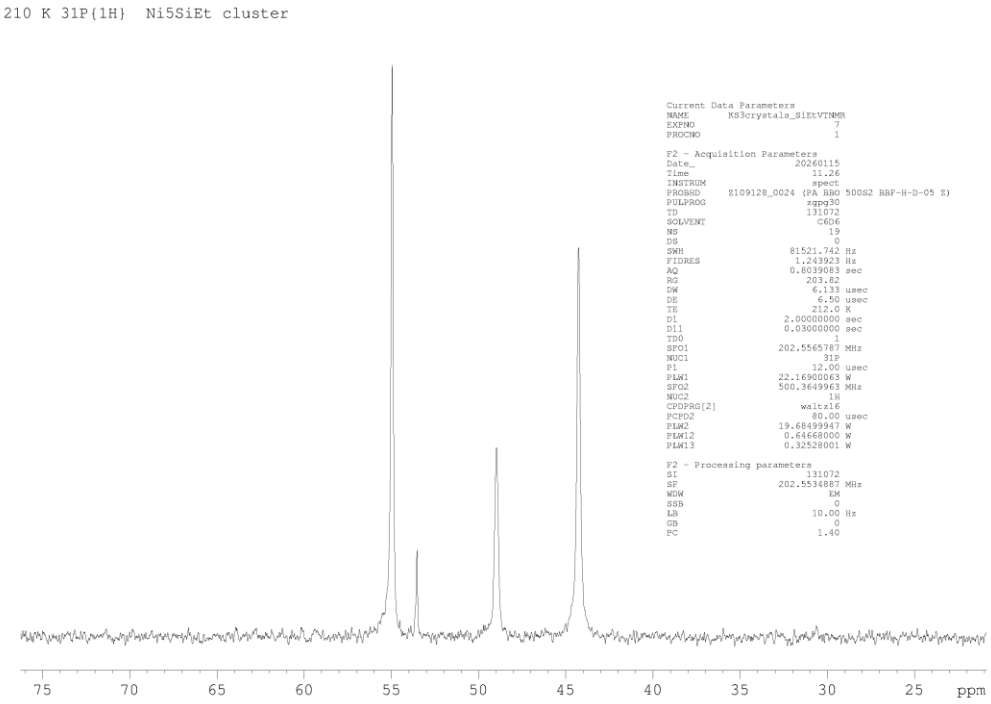


Figure S19. $^{31}P\{^{1}H\}$ NMR of **4** at 210 K (202.56 MHz, THF). The small peak at 53.5 is an impurity.

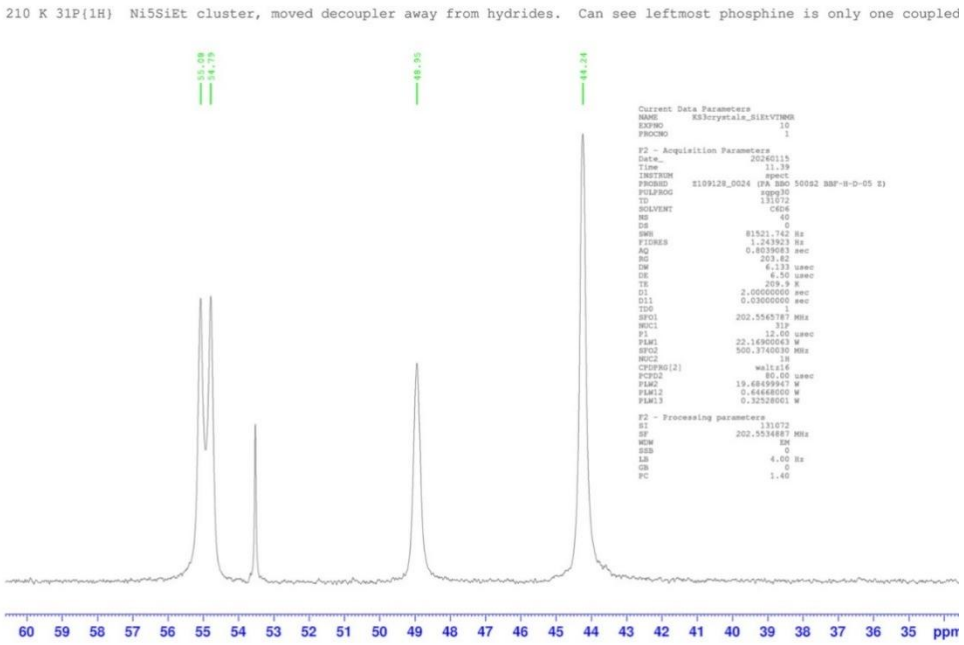


Figure S20. $^{31}P\{^{1}H\}$ NMR of **4** at 210 K with the decoupler offset moved away from the hydride region to show the large $^{2}J_{PH}$ coupling to the ^{31}P environment at δ 54.9 (202.56 MHz, THF, 210 K). The small peak at 53.5 is an impurity.

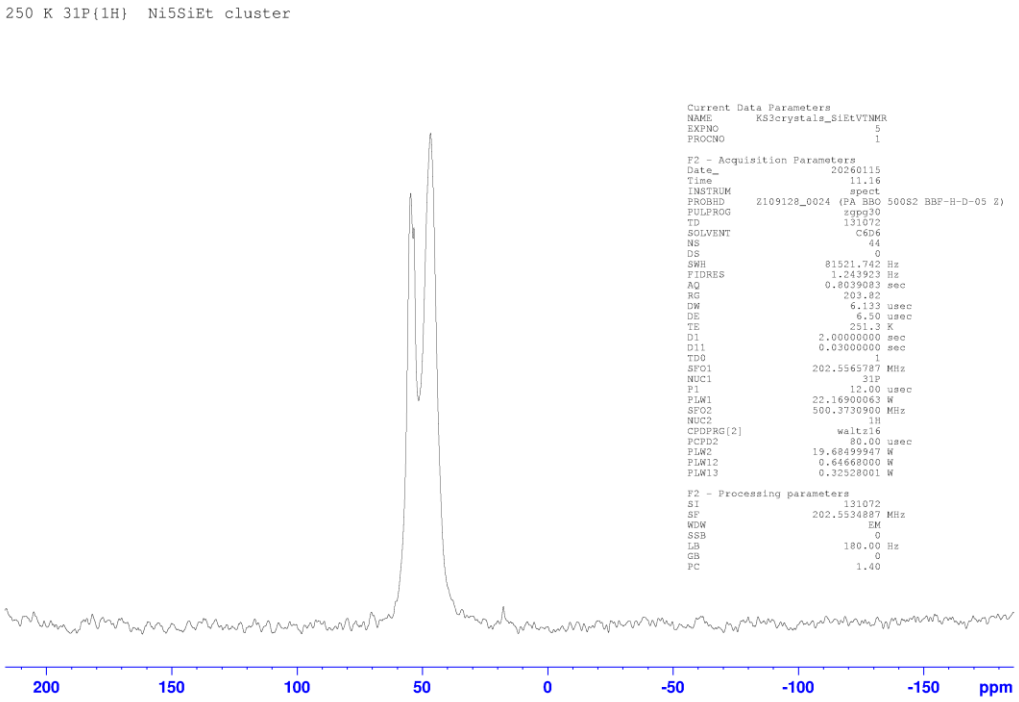


Figure S21. $^{31}P\{^{1}H\}$ NMR of **4** at 253 K (202.56 MHz, THF).

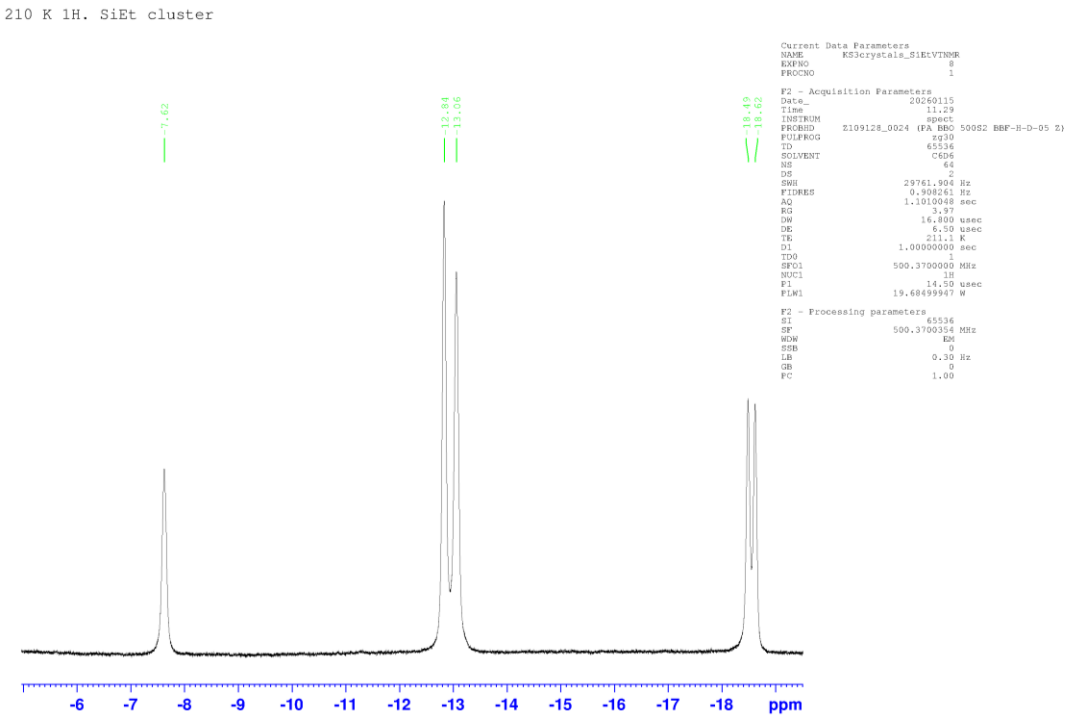


Figure S22. ^{1}H NMR of **4**, hydride region at low temperature (500.4 MHz, THF, 210 K). There are four hydride environments, at –7.62 (s, 1H), –12.84 (s, 2H), –13.06 (s, 2H) and –18.55 (d, 2H, $^{2}J_{PH}$ = 66.2 Hz).

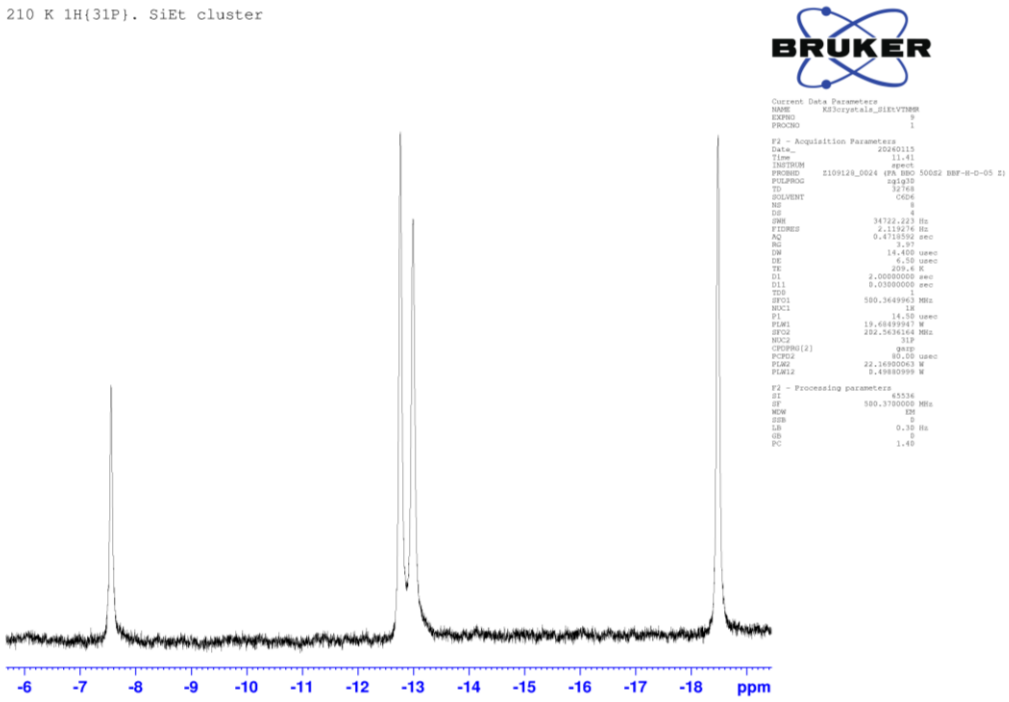


Figure S23. ^{1}H{^{31}P} NMR of **4**, hydride region at low temperature (500.4 MHz, THF, 210 K). No proton-proton couplings were resolved.

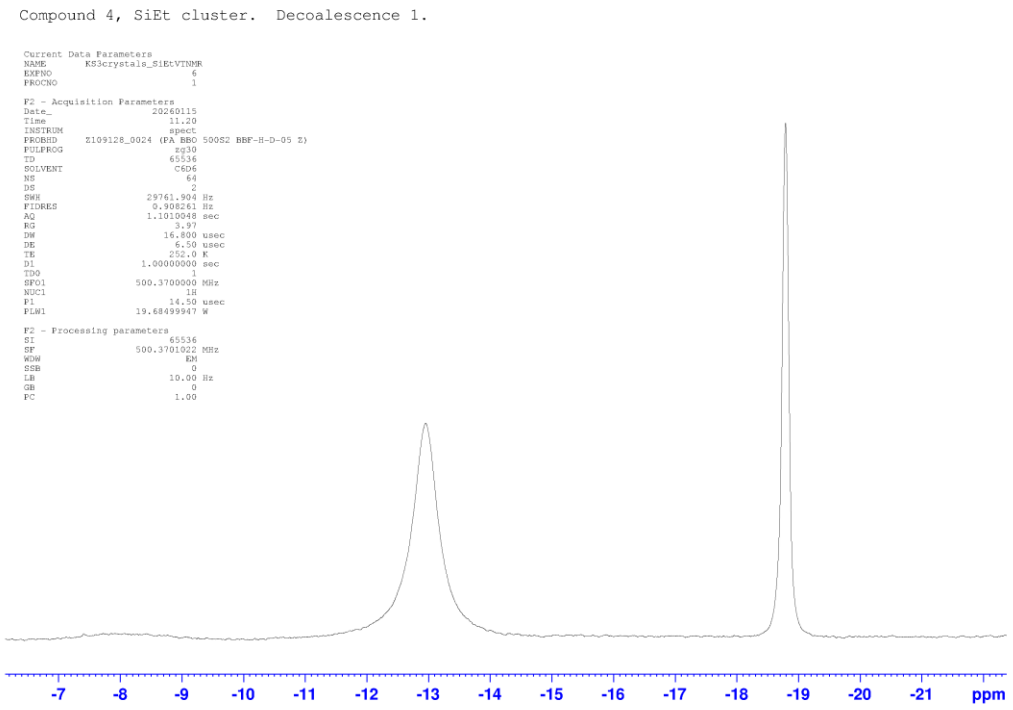


Figure S24. ^{1}H NMR of **4**, hydride region at 253 K, the temperature where decoalescence of the peak near –8 ppm was observed (500.4 MHz, THF).

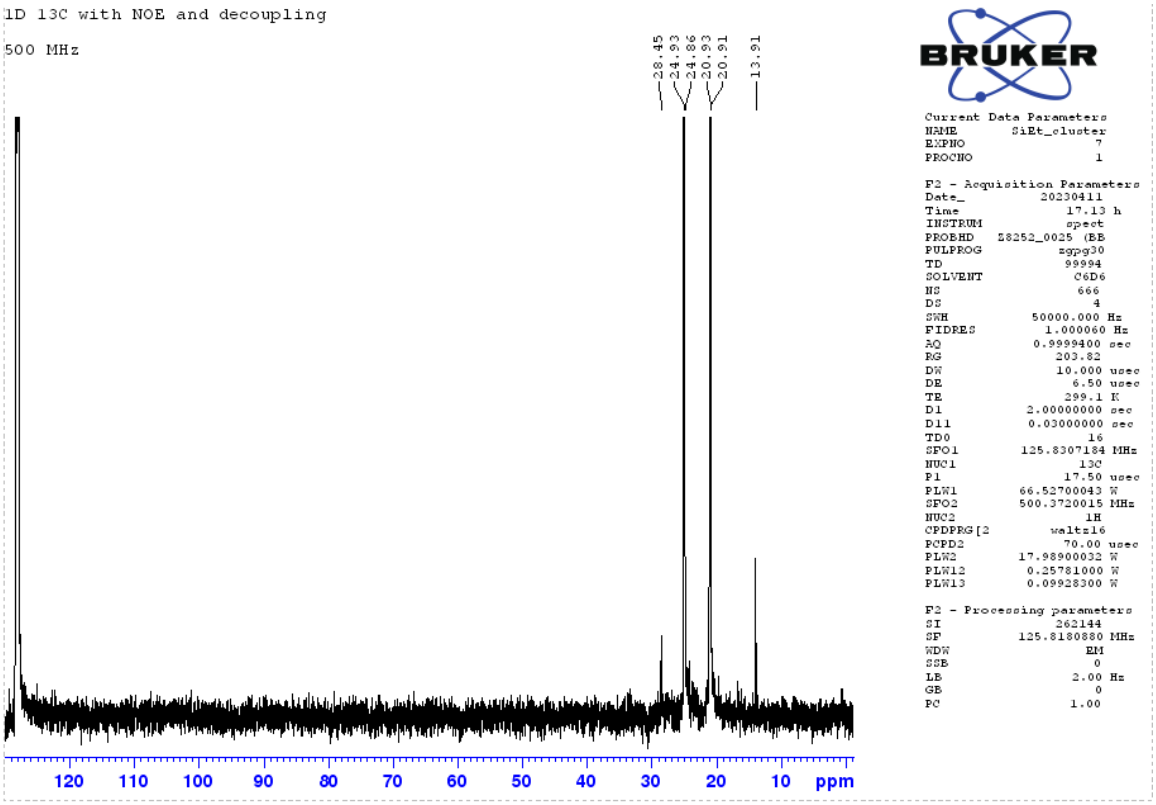


Figure S25. $^{13}C\{^{1}H\}$ NMR of **4** (125.84 MHz, C_6D_6, 298 K).

X-ray crystallography. X-ray structure collection and solution parameters for complexes **2**, **3** and **4** are provided in Tables 1-3. Unless otherwise stated, the hydrogen moieties associated with carbons that are not bound to Ni were placed in idealized positions and treated as riding on the carbon atom and methyl group hydrogens were modelled with the SHELX AFIX 137 command. Nickel hydride locations were assigned from electron-density difference maps and their locations were refined, as were their isotropic thermal parameters.

For the structure of **2**, the hydrogen atoms on carbons bound to nickel (H2A, H3A and H7A) were located in electron density difference maps, and their locations were refined. The thermal parameters were treated as riding on the attached atom. The hydride ligands H1-H5 were located in an electron density difference map and their locations and isotropic thermal parameters were refined. The structure contains a cocrystallized pentane molecule, treated as two-fold disordered. The SHELX SAME command was used to restrain the disordered pentane moieties to have similar bond distances as well as symmetry in both directions along the pentane chain. The nearly overlapped C51A and C51B atoms were forced to have identical anisotropic thermal parameters using the EADP command, as were the proximal C50A and C50B atoms. The thermal parameters of C47A-C51A and C47B-C51B were also restrained using the SHELX DELU command.

For the structure of **3**, the Si-H(1) and hydride ligands H2-H6 were located in the electron density difference map, and their locations and isotropic thermal parameters were refined. The isopropyl substituents C34-C36 and C49-51 were treated as twofold disordered, with refined occupancies of 0.8254 and 0.73508 for the higher occupancy sites, respectively. The proximal disordered atoms were constrained to have equal anisotropic thermal parameters using the SHELX EADP command (C34A and C34B, C36A and C36B, C49A and c49B, C50A and c50B). The asymmetric unit contains a cocrystallized toluene two-fold disordered around the inversion centre of the unit cell (C61-C67). The thermal parameters for this moiety were constrained to be equal using the EADP command, and the AFIX 66 command was unit to constrain the geometry of the aromatic ring. The hydrogens of the toluene methyl group were treated as idealized 2-fold disordered.

For the structure of **4**, hydride ligands H1-H7 were located in the electron density difference map, and their locations and isotropic thermal parameters were refined.

Table S1. Crystal data and structure refinement for **2**.

Identification code	CCDC 2371930
Empirical formula	$C_{51}H_{114}Ni_5P_4$
Formula weight	1144.85
Temperature/K	170(2)
Crystal system	triclinic
Space group	P-1
a/Å	12.6719(8)
b/Å	13.4829(9)
c/Å	18.3772(10)
α/°	91.850(3)
β/°	101.576(2)
γ/°	103.972(3)
Volume/Å^3	2974.2(3)
Z	2
ρ_{calc}g/cm^3	1.278
μ/mm^{-1}	1.691
F(000)	1240.0
Crystal size/mm^3	0.22 × 0.05 × 0.04
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.468 to 49.998
Index ranges	-15 ≤ h ≤ 15, -16 ≤ k ≤ 16, -21 ≤ l ≤ 21
Reflections collected	111006
Independent reflections	10456 [R_{int} = 0.0893, R_{sigma} = 0.0394]
Data/restraints/parameters	10456/44/640
Goodness-of-fit on F^2	1.047
Final R indexes [I>=2σ (I)]	R_1 = 0.0309, wR_2 = 0.0669
Final R indexes [all data]	R_1 = 0.0507, wR_2 = 0.0756
Largest diff. peak/hole / e Å^{-3}	0.47/-0.40

Table S2. Crystal data and structure refinement for **3**.

Identification code	CCDC 2371929
Empirical formula	$C_{127}Ni_{10}P_8Si_4H_{228}$
Formula weight	2702.30
Temperature/K	170(2)
Crystal system	triclinic
Space group	P-1
a/Å	12.835(3)
b/Å	14.971(3)
c/Å	19.994(4)
α/°	86.749(7)
β/°	73.097(7)
γ/°	69.214(7)
Volume/Å^3	3432.0(12)
Z	1
ρ_{calc}g/cm^3	1.307
μ/mm^{-1}	1.510
F(000)	1446.0
Crystal size/mm^3	0.18 × 0.18 × 0.15
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.284 to 55
Index ranges	-16 ≤ h ≤ 16, -19 ≤ k ≤ 19, -25 ≤ l ≤ 25
Reflections collected	193944
Independent reflections	15780 [R_{int} = 0.0936, R_{sigma} = 0.0461]
Data/restraints/parameters	15780/8/738
Goodness-of-fit on F^2	1.038
Final R indexes [I>=2σ (I)]	R_1 = 0.0493, wR_2 = 0.1129
Final R indexes [all data]	R_1 = 0.0691, wR_2 = 0.1206
Largest diff. peak/hole / e Å^{-3}	0.87/-0.70

Table S3. Crystal data and structure refinement for **4**.

Identification code	CCDC 2371931
Empirical formula	$C_{47}H_{117}SiP_5Ni_5$
Formula weight	1158.89
Temperature/K	170(2)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	15.7736(12)
b/Å	20.5782(14)
c/Å	18.9188(13)
α/°	90
β/°	102.478(3)
γ/°	90
Volume/Å^3	5995.8(7)
Z	4
ρ_{calc}g/cm^3	1.284
μ/mm^{-1}	1.723
F(000)	2512.0
Crystal size/mm^3	0.22 × 0.19 × 0.09
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.032 to 66.476
Index ranges	-24 ≤ h ≤ 24, -31 ≤ k ≤ 31, -28 ≤ l ≤ 29
Reflections collected	305888
Independent reflections	22941 [R_{int} = 0.0816, R_{sigma} = 0.0364]
Data/restraints/parameters	22941/0/582
Goodness-of-fit on F^2	1.083
Final R indexes [I>=2σ (I)]	R_1 = 0.0371, wR_2 = 0.0823
Final R indexes [all data]	R_1 = 0.0538, wR_2 = 0.0881
Largest diff. peak/hole / e Å^{-3}	0.66/-0.86

Computational details. All calculations were performed using Gaussian 16 C01.[6] Geometry optimizations, vibrational frequency and single point energy calculations were performed using the BP86 functional with the Def2SVP basis set. The energies of the species are summarized in Table 4. The nature of all stationary points was confirmed by the number of imaginary frequencies; all minima were assessed to have zero imaginary frequencies. Optimized XYZ coordinates are included below.

Table S4. Calculated energies for the species examined by DFT.

	Energy (ΔG°) Ha	Energy (ΔG°) Ha
	P^iPr_3 analogues	PMe_3 analogues
2	-10719.03648	-9776.957045
2a	-10719.02586	-9776.951611
2b	-10719.02114	-9776.946003
2c	-10719.0254	-9776.949393
3	-11835.73871	
4	-11396.74703	

XYZ coordinates of DFT optimized complexes.

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Ni	2.37514	-1.30970	0.10287
Ni	1.35881	0.93644	-0.47311
Ni	-0.96152	0.88177	0.50334
Ni	-2.47175	-0.93300	-0.57020
Ni	-0.02876	-1.05383	-0.64081
P	4.36270	-1.50556	0.99486
P	1.82314	2.35064	-2.05898
P	-1.23501	1.92214	2.40238
P	-4.63880	-0.83323	-0.28556
C	-0.07582	-2.98272	-0.83643
C	1.36532	-2.84520	-0.97048
C	2.03593	-3.29982	0.22444
C	0.95784	-3.76751	1.22558
H	0.87259	-3.08006	2.09540
H	1.19762	-4.76822	1.64670
C	-0.37976	-3.78080	0.42683
H	-0.66152	-4.82093	0.13538
H	-1.23368	-3.36820	1.00376
C	-1.00887	-2.49357	-1.80786
C	-2.46355	-2.58884	-1.71418
C	-2.99599	-2.55944	-3.15549

H	-3.04678	-3.60202	-3.55546
H	-4.01038	-2.12857	-3.27860
C	-1.92692	-1.76194	-3.92663
H	-2.08442	-0.67472	-3.75733
H	-1.94611	-1.93740	-5.02236
C	-0.60926	-2.19779	-3.26240
H	-0.24358	-3.15006	-3.71595
H	0.21009	-1.45674	-3.37200
C	5.51947	0.00356	1.10441
H	6.46646	-0.37193	1.55349
C	4.93747	1.08638	2.02524
H	5.56212	2.00469	1.97997
H	4.89823	0.76826	3.08604
H	3.90959	1.35644	1.70568
C	5.81917	0.57715	-0.28855
H	4.87322	0.82902	-0.81148
H	6.38857	-0.12660	-0.92713
H	6.42242	1.50660	-0.19918
C	4.41466	-2.09640	2.81942
H	5.35503	-1.67150	3.24044
C	3.21590	-1.50823	3.58583
H	2.26727	-1.93412	3.20013
H	3.13947	-0.40919	3.48585
H	3.28994	-1.75182	4.66841
C	4.45138	-3.62280	3.00561
H	4.42447	-3.86411	4.09067
H	5.36523	-4.09328	2.59186
H	3.56891	-4.11063	2.54290
C	5.46158	-2.79620	0.11410
H	4.99838	-3.74931	0.45027
C	6.93787	-2.81551	0.54302
H	7.44901	-3.70677	0.11703
H	7.06702	-2.85810	1.64440
H	7.48740	-1.92408	0.17481
C	5.31319	-2.75146	-1.41751
H	5.80534	-1.86202	-1.86036
H	4.24827	-2.72132	-1.72276
H	5.77961	-3.65073	-1.87563
C	3.11304	1.75764	-3.33587
H	4.06615	1.98970	-2.80623
C	3.03544	0.22741	-3.49507
H	2.20627	-0.06487	-4.17389
H	2.84728	-0.24985	-2.50985
H	3.97629	-0.17565	-3.92811
C	3.13519	2.45909	-4.70510
H	3.99139	2.08373	-5.30796
H	3.23891	3.55892	-4.63397
H	2.21577	2.24288	-5.28849

C	0.34501	2.92356	-3.10501
H	0.75369	3.60177	-3.88753
C	-0.33455	1.72558	-3.78613
H	-0.72976	1.02644	-3.01923
H	0.35249	1.15630	-4.44391
H	-1.18722	2.07015	-4.41071
C	-0.67379	3.69288	-2.24950
H	-1.57885	3.92973	-2.84945
H	-0.27637	4.65106	-1.85657
H	-0.98327	3.06496	-1.38541
C	2.49537	4.01160	-1.41138
H	1.63434	4.35326	-0.79415
C	3.66978	3.77804	-0.45066
H	4.57727	3.42559	-0.98606
H	3.41009	3.01408	0.30882
H	3.94215	4.71988	0.07352
C	2.81544	5.11152	-2.43567
H	3.02091	6.07103	-1.91156
H	1.98460	5.29861	-3.14639
H	3.72371	4.86944	-3.02630
C	-1.61038	0.67556	3.80135
H	-2.71639	0.57436	3.71706
C	-0.99683	-0.69036	3.44243
H	0.10874	-0.67870	3.53695
H	-1.22747	-0.94718	2.38643
H	-1.38728	-1.48801	4.11158
C	-1.27226	1.08147	5.24567
H	-1.64513	0.30673	5.95121
H	-1.72439	2.04649	5.54859
H	-0.17694	1.15835	5.40624
C	0.19994	2.95666	3.09223
H	-0.09108	3.27646	4.11744
C	0.47482	4.20440	2.23807
H	1.40671	4.70369	2.58160
H	-0.34007	4.95267	2.29244
H	0.61638	3.91912	1.17376
C	1.45935	2.08148	3.16860
H	1.67648	1.64940	2.16551
H	1.35187	1.23626	3.87729
H	2.33477	2.68463	3.49286
C	-2.75011	3.07705	2.46387
H	-3.57013	2.32772	2.36747
C	-2.81861	3.97873	1.21805
H	-3.83887	4.40417	1.10218
H	-2.57182	3.40869	0.30032
H	-2.11367	4.83167	1.28346
C	-2.97889	3.88074	3.75371
H	-2.15050	4.59367	3.95124

H	-3.09237	3.23493	4.64690
H	-3.90937	4.48441	3.66771
C	-5.13680	-0.37856	1.49468
H	-4.57425	0.57667	1.60021
C	-4.54255	-1.35264	2.52682
H	-4.58951	-0.90753	3.54472
H	-3.48176	-1.58128	2.30060
H	-5.09995	-2.30914	2.56723
C	-6.62232	-0.10159	1.77460
H	-7.22422	-1.03379	1.76436
H	-7.07766	0.60523	1.05124
H	-6.74014	0.34429	2.78697
C	-5.69333	-2.33979	-0.79550
H	-5.22312	-2.60028	-1.76774
C	-5.47305	-3.54139	0.14307
H	-6.07618	-3.45078	1.07024
H	-4.41080	-3.65542	0.44010
H	-5.78731	-4.48212	-0.35842
C	-7.19389	-2.11804	-1.05676
H	-7.64514	-3.05619	-1.44905
H	-7.39092	-1.32789	-1.80849
H	-7.74888	-1.85336	-0.13442
C	-5.42706	0.57634	-1.28972
H	-6.51851	0.55960	-1.07310
C	-5.22131	0.36321	-2.79845
H	-5.68972	1.19498	-3.36804
H	-5.66882	-0.58188	-3.16779
H	-4.13978	0.34798	-3.04845
C	-4.85233	1.93400	-0.86001
H	-3.74404	1.92043	-0.92292
H	-5.12592	2.20228	0.18009
H	-5.23321	2.74208	-1.52127
H	-2.86588	-3.39577	-1.06952
H	1.85177	-2.78187	-1.96015
H	2.94708	-3.91473	0.13457
H	0.19964	1.88014	0.05865
H	-1.11625	0.13515	-0.93836
H	-2.41221	0.20651	0.63580
H	2.77128	0.20780	-0.39231
H	0.88570	-0.23755	0.52662

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Ni	2.54820	-1.20097	0.02880
Ni	1.24168	0.90272	-0.53959
Ni	-1.18261	0.91492	0.31644
Ni	-2.42082	-1.24841	-0.21802
Ni	-0.00025	-1.14042	-0.41832

P	4.19473	-0.94541	1.45631
P	1.66820	2.20819	-2.22470
P	-1.85183	2.20200	1.95236
P	-4.56565	-1.28982	-0.57253
C	1.64038	-2.85699	-1.00391
C	1.90060	-2.78264	-2.52306
C	3.14224	-3.68342	-2.69809
C	3.94871	-3.49522	-1.38888
H	4.68962	-2.67826	-1.51794
H	4.53115	-4.40348	-1.11993
C	2.87563	-3.16389	-0.33361
H	2.85661	-3.77138	0.58848
C	0.31290	-3.05685	-0.45879
C	-0.01617	-3.76584	0.85168
C	-1.57413	-3.74507	0.94505
H	-1.98493	-4.76270	1.12941
H	-1.90499	-3.12444	1.80754
C	-2.07840	-3.18359	-0.40553
H	-2.87469	-3.75819	-0.91150
C	-0.90925	-2.83052	-1.19548
H	-0.95417	-2.73942	-2.29361
C	4.99898	0.77070	1.76211
H	6.00277	0.53886	2.18437
C	4.26473	1.67213	2.76416
H	4.79651	2.64519	2.84762
H	4.21376	1.23880	3.78279
H	3.23245	1.88979	2.42207
C	5.18210	1.52213	0.43276
H	4.19190	1.75247	-0.01134
H	5.75433	0.94601	-0.31881
H	5.71993	2.47972	0.60737
C	3.60020	-1.49491	3.18798
H	4.37015	-1.13025	3.90639
C	2.23938	-0.86966	3.54312
H	1.46509	-1.17631	2.80940
H	2.25524	0.23445	3.54505
H	1.91855	-1.20889	4.55241
C	3.48800	-3.02556	3.31489
H	3.21027	-3.29366	4.35730
H	4.42194	-3.56878	3.07156
H	2.68802	-3.41322	2.65223
C	5.78836	-1.98935	1.25860
H	5.38216	-3.00125	1.04198
C	6.69788	-2.07925	2.49757
H	7.56802	-2.73674	2.27909
H	6.19033	-2.49584	3.38937
H	7.11285	-1.08747	2.77849
C	6.62072	-1.54774	0.03942

H	7.20521	-0.62989	0.25963
H	5.99489	-1.34423	-0.85233
H	7.35125	-2.33977	-0.23304
C	3.31579	2.03518	-3.18525
H	4.00054	2.65787	-2.56409
C	3.84795	0.59316	-3.15177
H	3.31356	-0.05029	-3.88274
H	3.70703	0.14217	-2.14799
H	4.92705	0.56482	-3.41684
C	3.33700	2.58129	-4.62480
H	4.37301	2.54134	-5.02762
H	2.99185	3.62958	-4.70449
H	2.70849	1.96461	-5.30106
C	0.33234	2.12343	-3.57064
H	0.67170	2.78007	-4.40251
C	0.19707	0.68371	-4.09632
H	-0.12066	0.00134	-3.27841
H	1.14650	0.29054	-4.51356
H	-0.56761	0.63852	-4.90213
C	-1.01349	2.64026	-3.04043
H	-1.81965	2.44767	-3.78037
H	-1.00395	3.73027	-2.83564
H	-1.27498	2.11386	-2.09512
C	1.63820	4.04384	-1.72253
H	0.61074	4.11721	-1.30115
C	2.62112	4.28762	-0.56690
H	3.67854	4.20179	-0.89761
H	2.45926	3.55160	0.24677
H	2.48982	5.30879	-0.14796
C	1.78455	5.10673	-2.82210
H	1.55959	6.11435	-2.40762
H	1.09598	4.94362	-3.67659
H	2.82029	5.14977	-3.21926
C	-2.42496	1.15881	3.44968
H	-3.48709	0.95714	3.18377
C	-1.68956	-0.19322	3.45869
H	-0.63020	-0.08052	3.76867
H	-1.68799	-0.63685	2.43937
H	-2.17419	-0.90123	4.16629
C	-2.39183	1.81778	4.83887
H	-2.85910	1.14013	5.58678
H	-2.93689	2.78143	4.88332
H	-1.35245	2.00230	5.18190
C	-0.65986	3.46086	2.72099
H	-1.14878	3.86503	3.63466
C	-0.35323	4.62569	1.76780
H	0.46858	5.25078	2.17950
H	-1.22621	5.28955	1.61102

H	-0.02423	4.24662	0.77774
C	0.63152	2.72879	3.11585
H	1.04322	2.19179	2.23282
H	0.46690	1.97609	3.91304
H	1.39386	3.44848	3.48505
C	-3.42438	3.19011	1.52647
H	-4.15156	2.35369	1.40831
C	-3.30646	3.87433	0.15217
H	-4.31043	4.17864	-0.21569
H	-2.85294	3.19247	-0.59463
H	-2.68185	4.78925	0.19483
C	-3.96516	4.15329	2.59491
H	-3.24637	4.96861	2.82292
H	-4.21187	3.64167	3.54629
H	-4.89893	4.63863	2.23421
C	-5.62764	-0.36045	0.70125
H	-5.12658	0.63354	0.66055
C	-5.40794	-0.90555	2.12342
H	-5.78024	-0.17933	2.87869
H	-4.33153	-1.08884	2.31772
H	-5.95049	-1.85733	2.29269
C	-7.11922	-0.16059	0.39130
H	-7.69250	-1.10413	0.50280
H	-7.29990	0.22790	-0.63185
H	-7.56255	0.56999	1.10364
C	-5.41382	-2.96170	-0.92394
H	-4.65910	-3.43281	-1.59400
C	-5.49625	-3.83650	0.34009
H	-6.33828	-3.52731	0.99381
H	-4.56510	-3.79237	0.94048
H	-5.67295	-4.89847	0.06356
C	-6.75131	-2.95715	-1.68424
H	-7.05211	-4.00341	-1.91345
H	-6.69693	-2.41904	-2.65171
H	-7.57264	-2.50671	-1.09174
C	-4.90591	-0.34011	-2.18369
H	-5.99672	-0.41895	-2.39070
C	-4.13122	-0.99223	-3.34376
H	-4.35974	-0.47255	-4.29958
H	-4.38005	-2.06474	-3.48136
H	-3.03708	-0.92075	-3.16788
C	-4.52990	1.14246	-2.04543
H	-3.48272	1.24119	-1.69063
H	-5.18368	1.68247	-1.33085
H	-4.61933	1.65640	-3.02689
H	0.37183	-4.81118	0.80701
H	1.02934	-3.13821	-3.11051
H	2.81079	-4.74248	-2.77519

H	0.03972	1.85792	-0.06191
H	-1.18709	-0.12764	-0.91359
H	-2.61689	0.23461	0.48704
H	2.68868	0.35449	-0.44873
H	1.06259	-0.26943	0.55866
H	0.47047	-3.29068	1.72995
H	3.72867	-3.45380	-3.61369
H	2.10647	-1.74252	-2.85114

2b

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Ni	-2.49972	-1.11479	-0.26603
Ni	-1.20913	0.88562	0.64211
Ni	1.15784	0.90128	-0.36515
Ni	2.43037	-1.29795	-0.09389
Ni	-0.06251	-1.18147	0.21166
P	-4.35970	-0.74691	-1.33981
P	-1.52310	1.98585	2.50251
P	1.67601	2.32442	-1.94483
P	4.57396	-1.20400	0.35096
C	-1.38612	-2.91036	0.44165
C	-2.25016	-3.36896	1.63151
C	-3.06475	-4.53320	1.02627
C	-3.26378	-4.15585	-0.47197
H	-4.31551	-3.87060	-0.67439
H	-3.06200	-5.03254	-1.12802
C	-2.23658	-3.03834	-0.75071
H	-1.71293	-3.11795	-1.72393
C	0.04967	-3.09015	0.50122
C	0.98503	-2.91526	-0.59959
C	2.32027	-3.28315	-0.18224
H	3.02163	-3.67949	-0.93785
C	2.19417	-4.05297	1.13712
H	3.02006	-3.88037	1.85852
H	2.19264	-5.14869	0.92264
C	0.81950	-3.62859	1.71336
H	0.28964	-4.48057	2.19174
H	0.92828	-2.84868	2.50016
C	-5.09329	1.01164	-1.29630
H	-5.98994	0.97737	-1.95476
C	-4.10322	2.03534	-1.86083
H	-4.49419	3.06753	-1.72958
H	-3.90642	1.89137	-2.94165
H	-3.13579	1.96052	-1.32026
C	-5.52761	1.40720	0.12313
H	-4.67455	1.31175	0.82687
H	-6.36248	0.78806	0.50573
H	-5.86649	2.46576	0.13756

C	-4.19763	-1.00230	-3.23181
H	-4.91354	-0.28340	-3.69313
C	-2.76966	-0.64119	-3.68303
H	-2.04000	-1.37720	-3.28905
H	-2.44277	0.35252	-3.32215
H	-2.70348	-0.64675	-4.79326
C	-4.55244	-2.41868	-3.71509
H	-4.35042	-2.50184	-4.80527
H	-5.61866	-2.67937	-3.56223
H	-3.93217	-3.18727	-3.20902
C	-5.88998	-1.80137	-0.90444
H	-5.62517	-2.77852	-1.36160
C	-7.21762	-1.34471	-1.53240
H	-8.00029	-2.11852	-1.37189
H	-7.14103	-1.17775	-2.62684
H	-7.59514	-0.40688	-1.07452
C	-6.02469	-2.04178	0.61001
H	-6.37997	-1.13968	1.14752
H	-5.05510	-2.33125	1.06166
H	-6.75583	-2.85530	0.80847
C	-2.97667	1.42980	3.61024
H	-3.83601	1.94102	3.11744
C	-3.21190	-0.08630	3.49017
H	-2.48396	-0.65926	4.10231
H	-3.09116	-0.41650	2.43814
H	-4.22990	-0.35692	3.84462
C	-2.93694	1.85954	5.08774
H	-3.88508	1.56678	5.59029
H	-2.81220	2.95029	5.22772
H	-2.11640	1.35106	5.63630
C	-0.02444	1.98591	3.66402
H	-0.33848	2.51734	4.59032
C	0.37512	0.54438	4.02297
H	0.63499	-0.02022	3.10159
H	-0.43524	-0.00784	4.53991
H	1.26179	0.54560	4.69348
C	1.15828	2.73268	3.03089
H	2.05610	2.65273	3.68014
H	0.95606	3.81181	2.87439
H	1.39825	2.27945	2.04370
C	-1.81409	3.84559	2.21884
H	-0.88645	4.10848	1.66302
C	-2.98929	4.05818	1.25361
H	-3.96357	3.81513	1.72971
H	-2.88232	3.41641	0.35690
H	-3.04033	5.11867	0.92412
C	-1.91551	4.76770	3.44396
H	-1.87733	5.83159	3.12112

H	-1.09211	4.61663	4.17174
H	-2.87705	4.63255	3.98165
C	2.03580	1.41949	-3.59334
H	3.12407	1.20692	-3.49488
C	1.30461	0.06523	-3.61335
H	0.20805	0.19192	-3.72719
H	1.47051	-0.47289	-2.65552
H	1.66456	-0.56481	-4.45621
C	1.82122	2.19706	-4.90278
H	2.17458	1.58695	-5.76291
H	2.36960	3.15952	-4.93714
H	0.74840	2.41419	-5.08487
C	0.43955	3.67896	-2.42097
H	0.84487	4.20352	-3.31426
C	0.25260	4.69412	-1.28196
H	-0.58843	5.38251	-1.51531
H	1.15235	5.31760	-1.10972
H	0.00853	4.16893	-0.33374
C	-0.89960	3.01845	-2.77183
H	-1.23143	2.38318	-1.92326
H	-0.83672	2.36967	-3.66861
H	-1.67976	3.78623	-2.96457
C	3.31518	3.25132	-1.64712
H	4.04130	2.41754	-1.77957
C	3.43621	3.72492	-0.18807
H	4.48576	4.01136	0.04235
H	3.12715	2.92547	0.51468
H	2.80164	4.61085	0.01678
C	3.68123	4.36701	-2.63879
H	2.96317	5.21293	-2.59735
H	3.72552	4.01037	-3.68703
H	4.68315	4.78335	-2.39297
C	5.55611	0.05405	-0.68421
H	4.99086	0.97841	-0.42910
C	5.36770	-0.17442	-2.19431
H	5.67589	0.73051	-2.76268
H	4.30659	-0.38985	-2.43493
H	5.98084	-1.01701	-2.57053
C	7.03372	0.27707	-0.32525
H	7.66480	-0.58603	-0.62234
H	7.19363	0.45908	0.75714
H	7.42739	1.16443	-0.86854
C	5.56486	-2.83754	0.33607
H	4.82862	-3.53141	0.79602
C	5.82623	-3.34131	-1.09588
H	6.67776	-2.80730	-1.56662
H	4.94406	-3.21969	-1.75666
H	6.08946	-4.42104	-1.07969

C	6.85061	-2.90964	1.17966
H	7.26308	-3.94199	1.13863
H	6.68030	-2.67457	2.24914
H	7.64193	-2.22973	0.80500
C	4.86612	-0.57774	2.12091
H	5.96304	-0.62050	2.30217
C	4.16099	-1.49326	3.13577
H	4.34717	-1.13434	4.17118
H	4.50924	-2.54518	3.08282
H	3.06386	-1.49030	2.96567
C	4.39241	0.87410	2.28067
H	3.33729	0.97788	1.95205
H	5.00358	1.58935	1.69453
H	4.45699	1.18278	3.34642
H	0.68019	-2.86756	-1.65890
H	-1.65825	-3.66194	2.52152
H	-2.46792	-5.46833	1.09773
H	0.02632	1.82304	0.31357
H	1.20408	-0.29071	0.73799
H	2.56718	0.25490	-0.65248
H	-2.68208	0.29232	0.56600
H	-1.01412	-0.05990	-0.63376
H	-4.01990	-4.72071	1.56127
H	-2.92389	-2.54878	1.96176

2c

157

Ni	1.79768	-1.63246	0.16572
Ni	1.58981	0.86229	-0.28822
Ni	-0.82299	1.18677	0.27263
Ni	-2.43900	-0.42611	-0.86281
Ni	-0.08993	-0.63544	-1.20198
P	3.22541	-2.28342	1.67640
P	2.76814	2.17431	-1.55905
P	-1.35699	2.61521	1.84196
P	-4.39907	-1.06683	-0.11988
C	0.15875	-2.40945	-2.08142
C	1.45999	-2.87408	-2.74644
C	2.07580	-3.87121	-1.72479
C	1.39468	-3.53420	-0.39061
H	1.40791	-4.29656	0.40490
C	0.17292	-2.84900	-0.68864
H	-0.72746	-2.88579	-0.05421
C	-0.90739	-1.73158	-2.74064
C	-2.33801	-1.75249	-2.34333
C	-3.12097	-1.33783	-3.61072
H	-3.39466	-2.24842	-4.19900
H	-4.06415	-0.79230	-3.41255

C	-2.11107	-0.50219	-4.42200
H	-2.03597	0.51723	-3.98340
H	-2.38032	-0.39750	-5.49364
C	-0.79215	-1.25785	-4.18910
H	-0.75838	-2.15782	-4.85176
H	0.11977	-0.66794	-4.40792
C	4.09072	-0.94229	2.71453
H	4.62975	-1.48333	3.52559
C	3.04528	-0.00766	3.34180
H	3.54512	0.83600	3.86507
H	2.40240	-0.52264	4.08367
H	2.38862	0.41384	2.54927
C	5.10561	-0.14107	1.88529
H	4.62839	0.25581	0.96503
H	5.98587	-0.74416	1.58815
H	5.48100	0.72394	2.47359
C	2.41345	-3.30467	3.09194
H	2.97376	-3.00390	4.00687
C	0.94161	-2.88479	3.26184
H	0.33095	-3.22076	2.39903
H	0.81516	-1.78798	3.33601
H	0.51375	-3.34351	4.18031
C	2.50816	-4.83629	2.96862
H	2.00629	-5.30680	3.84229
H	3.54847	-5.21470	2.94865
H	1.99121	-5.21471	2.06243
C	4.66362	-3.39759	1.11491
H	4.12468	-4.33815	0.86368
C	5.72380	-3.70984	2.18555
H	6.41921	-4.49679	1.81918
H	5.28953	-4.07198	3.13932
H	6.34215	-2.81815	2.41852
C	5.31824	-2.89189	-0.18489
H	6.02654	-2.06067	0.00496
H	4.56200	-2.51762	-0.90200
H	5.89155	-3.70908	-0.67366
C	4.32221	1.43895	-2.40229
H	5.07766	1.52989	-1.58769
C	4.13638	-0.05944	-2.69075
H	3.52035	-0.21928	-3.60096
H	3.61915	-0.55586	-1.84375
H	5.11596	-0.55529	-2.86377
C	4.85873	2.16723	-3.64779
H	5.82107	1.70956	-3.96705
H	5.04472	3.24565	-3.48374
H	4.16083	2.07082	-4.50593
C	1.79836	2.94976	-2.99548
H	2.52719	3.52797	-3.60616

C	1.18633	1.83414	-3.85613
H	0.52093	1.20184	-3.22719
H	1.95347	1.17325	-4.30798
H	0.58071	2.26348	-4.68348
C	0.69602	3.89835	-2.50081
H	0.11047	4.28278	-3.36401
H	1.09516	4.77756	-1.95504
H	-0.00017	3.35421	-1.82812
C	3.44203	3.69676	-0.63436
H	2.49596	4.14277	-0.25821
C	4.24544	3.25300	0.59728
H	5.21285	2.78480	0.31417
H	3.67278	2.51441	1.19314
H	4.48107	4.12322	1.24794
C	4.18949	4.77146	-1.43888
H	4.34225	5.67706	-0.81089
H	3.64098	5.09277	-2.34796
H	5.19750	4.42678	-1.75052
C	-1.88511	1.71878	3.43978
H	-2.85107	1.27092	3.11085
C	-0.92680	0.55351	3.74532
H	0.03517	0.91247	4.16359
H	-0.69473	-0.02209	2.82577
H	-1.37637	-0.13458	4.49344
C	-2.14233	2.57058	4.69250
H	-2.48353	1.92230	5.52965
H	-2.92337	3.34121	4.53953
H	-1.22083	3.08372	5.04044
C	-0.13000	3.94024	2.42509
H	-0.62755	4.50769	3.24293
C	0.20704	4.90824	1.28037
H	0.98069	5.63655	1.60778
H	-0.66843	5.48864	0.92904
H	0.60837	4.34760	0.41222
C	1.14884	3.28009	2.96160
H	1.52715	2.53965	2.22293
H	0.98620	2.75083	3.92143
H	1.94155	4.04071	3.13063
C	-2.91746	3.61178	1.37863
H	-3.71611	2.87820	1.62966
C	-2.96056	3.82355	-0.14671
H	-3.95541	4.20700	-0.46283
H	-2.75562	2.86617	-0.67167
H	-2.19999	4.55835	-0.48352
C	-3.21367	4.91436	2.14123
H	-2.47362	5.70942	1.91507
H	-3.23633	4.78179	3.24074
H	-4.20859	5.30886	1.83848

C	-4.38411	-1.19146	1.77750
H	-4.24026	-0.11810	2.03645
C	-3.13407	-1.92818	2.28774
H	-3.02137	-1.77886	3.38314
H	-2.22430	-1.53379	1.78881
H	-3.18619	-3.02026	2.10843
C	-5.66858	-1.68338	2.46266
H	-5.84013	-2.76599	2.28937
H	-6.57421	-1.13816	2.12581
H	-5.59096	-1.54286	3.56344
C	-5.08705	-2.72775	-0.78524
H	-4.82553	-2.64781	-1.86359
C	-4.31548	-3.93681	-0.22298
H	-4.62636	-4.17247	0.81610
H	-3.21811	-3.77853	-0.22023
H	-4.52138	-4.83963	-0.83784
C	-6.60455	-2.97397	-0.70162
H	-6.84553	-3.95108	-1.17584
H	-7.19861	-2.20572	-1.23500
H	-6.97110	-3.02287	0.34370
C	-5.88532	0.08927	-0.42172
H	-6.78290	-0.45417	-0.05352
C	-6.05678	0.36591	-1.92476
H	-6.95453	0.99769	-2.10045
H	-6.18068	-0.55957	-2.52328
H	-5.17488	0.91023	-2.32452
C	-5.76964	1.41077	0.34820
H	-4.83537	1.93836	0.07411
H	-5.78084	1.27220	1.44818
H	-6.62300	2.07604	0.09308
H	-2.64464	-2.72869	-1.91872
H	1.25189	-3.35296	-3.72809
H	1.80920	-4.91843	-2.00596
H	0.53609	2.01604	0.01868
H	-1.12328	0.62221	-1.29096
H	-2.36534	0.68910	0.36514
H	2.66451	-0.24818	0.02957
H	0.54540	-0.18696	0.36881
H	3.18362	-3.83010	-1.70493
H	2.14448	-2.02483	-2.95018

2•PMe_3

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Ni	-2.11286	-1.12785	-0.50270
Ni	-1.46820	0.78178	0.94053
Ni	0.68360	1.43406	-0.03133
Ni	2.51279	-0.32901	0.05393
Ni	0.20054	-0.89991	0.30321

P	-3.90394	-0.79256	-1.61785
P	-2.24280	1.23392	2.86793
P	0.34014	3.07616	-1.36048
P	4.46353	0.31786	-0.52243
C	0.49406	-2.72151	-0.30335
C	-0.93855	-2.83317	-0.03582
C	-1.68321	-2.91417	-1.27362
C	-0.68290	-2.90940	-2.44648
H	-0.79086	-2.00348	-3.08294
H	-0.84753	-3.77876	-3.12093
C	0.73279	-2.95482	-1.79305
H	1.20039	-3.95912	-1.92560
H	1.43617	-2.21886	-2.23522
C	1.49135	-2.46977	0.70024
C	2.91838	-2.24152	0.45379
C	3.65151	-2.51326	1.77525
H	3.97054	-3.58382	1.82611
H	4.56717	-1.90444	1.92732
C	2.57847	-2.23922	2.85031
H	2.50174	-1.14400	3.02675
H	2.79506	-2.72498	3.82479
C	1.27681	-2.74172	2.19753
H	1.17002	-3.84442	2.33845
H	0.36335	-2.27433	2.62537
H	3.35995	-2.69371	-0.45821
H	-1.33182	-3.19628	0.93016
H	-2.56935	-3.57063	-1.34813
H	-0.39242	1.94274	1.05700
H	1.16567	0.25773	0.98522
H	2.12849	1.13405	-0.63615
H	-2.75385	-0.03124	0.54952
H	-0.82374	0.25230	-0.43907
C	5.01283	1.89953	0.28404
H	5.15032	1.72158	1.37000
H	5.95949	2.29164	-0.14574
H	4.20304	2.64648	0.16478
C	5.99132	-0.72892	-0.33126
H	6.88527	-0.23023	-0.76154
H	6.17746	-0.93276	0.74214
H	5.83991	-1.70242	-0.84023
C	4.58633	0.74651	-2.32948
H	4.39888	-0.16516	-2.93257
H	3.79694	1.48384	-2.57566
H	5.58195	1.16138	-2.59526
C	-0.97858	1.68711	4.15206
H	-0.22546	0.87546	4.20707
H	-0.45276	2.60492	3.82073
H	-1.42365	1.85201	5.15685

C	-3.45099	2.64259	3.02572
H	-3.77864	2.80434	4.07521
H	-2.97536	3.56843	2.64366
H	-4.33771	2.43079	2.39447
C	-3.16570	-0.13533	3.72190
H	-3.49494	0.14206	4.74629
H	-4.04845	-0.40732	3.10914
H	-2.50809	-1.02627	3.77493
C	-4.04604	-1.40293	-3.36935
H	-5.03428	-1.16191	-3.81531
H	-3.24912	-0.93848	-3.98474
H	-3.89454	-2.50069	-3.39154
C	-4.42272	0.98038	-1.81872
H	-5.41030	1.08631	-2.31700
H	-4.45091	1.44967	-0.81513
H	-3.65526	1.51368	-2.41558
C	-1.04522	4.25673	-0.97496
H	-1.98120	3.67415	-0.86012
H	-0.83625	4.74845	-0.00321
H	-1.17735	5.03367	-1.75855
C	-0.11601	2.52480	-3.07759
H	-1.01185	1.87568	-3.00751
H	-0.32067	3.37711	-3.76078
H	0.71011	1.91016	-3.48811
C	1.71072	4.28454	-1.72611
H	2.58548	3.73320	-2.12581
H	1.40493	5.06381	-2.45737
H	2.02269	4.77776	-0.78290
C	-5.43091	-1.53624	-0.85603
H	-5.30363	-2.63530	-0.78147
H	-5.54908	-1.13764	0.17157
H	-6.34656	-1.31302	-1.44455

2a•PMe_3

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Ni	-2.13319	-0.72530	-0.47753
Ni	-1.14196	1.20992	0.72080
Ni	1.19305	1.29298	-0.01869
Ni	2.54425	-0.81915	0.29008
Ni	0.16086	-0.84580	0.47279
P	-3.53860	-0.09324	-1.96173
P	-1.94455	2.09951	2.47577
P	1.46299	2.82674	-1.48220
P	4.66311	-0.67669	0.18141
C	-1.37753	-2.57282	0.35318
C	-2.03109	-2.77897	1.73846
C	-3.27281	-3.63666	1.40582
C	-3.71213	-3.17149	-0.00665

H	-4.47504	-2.36315	0.07827
H	-4.19122	-3.99186	-0.58527
C	-2.40481	-2.68598	-0.66171
H	-2.14254	-3.07790	-1.66193
C	0.04295	-2.75249	0.11979
C	0.67503	-3.19959	-1.19984
C	2.17356	-3.44523	-0.85262
H	2.36629	-4.54090	-0.76464
H	2.85237	-3.07650	-1.65224
C	2.40196	-2.77523	0.51839
H	3.18693	-3.21922	1.15916
C	1.08301	-2.57757	1.11017
H	0.91443	-2.57958	2.20107
H	0.17670	-4.12241	-1.57514
H	-1.34197	-3.27938	2.45051
H	-2.96703	-4.70481	1.35628
H	0.14831	2.13157	0.86757
H	1.32833	0.13845	1.11552
H	2.60104	0.67729	-0.43473
H	-2.53483	0.69991	0.24841
H	-0.56168	0.34413	-0.50527
H	0.54636	-2.43312	-1.99565
H	-4.07841	-3.55936	2.16736
H	-2.32519	-1.81006	2.19920
C	1.51359	2.19583	-3.23160
H	1.67711	3.00720	-3.97306
H	2.32335	1.44395	-3.31697
H	0.55608	1.68244	-3.45219
C	3.03532	3.82343	-1.41443
H	3.90296	3.13712	-1.48414
H	3.09505	4.57517	-2.23097
H	3.09319	4.34503	-0.43738
C	0.20870	4.19304	-1.62724
H	-0.78540	3.74063	-1.81495
H	0.15372	4.73162	-0.65982
H	0.45061	4.91388	-2.43791
C	5.31565	0.74142	1.19068
H	4.76091	1.65580	0.90039
H	5.10659	0.54774	2.26230
H	6.40726	0.89729	1.05263
C	5.40758	-0.32039	-1.48765
H	6.50705	-0.17045	-1.43388
H	5.18913	-1.16346	-2.17431
H	4.93141	0.58953	-1.90433
C	5.76196	-2.06365	0.75625
H	5.57740	-2.96550	0.13799
H	6.83737	-1.79487	0.69077
H	5.51616	-2.31508	1.80799

C	-5.27456	0.28628	-1.40866
H	-5.23157	1.03803	-0.59515
H	-5.90227	0.67535	-2.23863
H	-5.74317	-0.63247	-1.00085
C	-3.07061	1.50598	-2.78227
H	-2.93700	2.26835	-1.98868
H	-2.09626	1.37669	-3.29485
H	-3.83054	1.84897	-3.51693
C	-3.86444	-1.17897	-3.43608
H	-4.30198	-2.13889	-3.09527
H	-4.55521	-0.70297	-4.16401
H	-2.90281	-1.40355	-3.94050
C	-3.65355	1.63948	3.04768
H	-4.38692	1.94477	2.27409
H	-3.71257	0.53711	3.15049
H	-3.92260	2.11441	4.01546
C	-0.93360	1.73649	3.99261
H	-0.90359	0.63941	4.14993
H	0.10538	2.07343	3.80525
H	-1.33518	2.23123	4.90313
C	-2.03880	3.95779	2.52980
H	-2.42485	4.33525	3.50102
H	-1.02434	4.36743	2.35104
H	-2.69855	4.31277	1.71204

2b•PMe_3

85

Ni	-2.10453	-0.78111	-0.39445
Ni	-1.09958	1.10746	0.89221
Ni	1.12083	1.27722	-0.17605
Ni	2.57922	-0.76779	-0.20295
Ni	0.16355	-0.88537	0.31118
P	-3.71881	-0.18084	-1.64066
P	-1.87461	2.05695	2.63925
P	1.04177	2.89556	-1.56754
P	4.64043	-0.27350	0.09154
C	-1.00948	-2.65547	0.20361
C	-1.87546	-3.24674	1.33631
C	-2.77680	-4.25135	0.58872
C	-3.04980	-3.58697	-0.78691
H	-4.03003	-3.05821	-0.76903
H	-3.12360	-4.34373	-1.59950
C	-1.85543	-2.63038	-1.00362
H	-1.34739	-2.69323	-1.98603
C	0.44107	-2.78570	0.24867
C	1.37284	-2.44650	-0.82061
C	2.73171	-2.73765	-0.42688
H	3.48427	-3.00814	-1.19074

C	2.68620	-3.57147	0.85849
H	3.45133	-3.28263	1.60980
H	2.88228	-4.64306	0.61585
C	1.23954	-3.40088	1.40687
H	0.80314	-4.37301	1.72725
H	1.21688	-2.74225	2.30371
H	1.05806	-2.30410	-1.86800
H	-1.27688	-3.71627	2.14333
H	-2.20941	-5.19520	0.43263
H	0.21640	1.97052	0.99342
H	1.44971	0.02847	0.83159
H	2.47044	0.79015	-0.80021
H	-2.51400	0.44218	0.64477
H	-0.59885	0.43054	-0.47440
H	-3.70286	-4.51350	1.14415
H	-2.48835	-2.45343	1.81847
C	5.81438	-1.49020	0.86761
H	5.45139	-1.75633	1.88101
H	5.84112	-2.41794	0.26124
H	6.84316	-1.07980	0.95033
C	4.91947	1.22190	1.15707
H	5.98938	1.51666	1.21575
H	4.31502	2.05377	0.74372
H	4.53988	1.00991	2.17720
C	5.58305	0.18212	-1.44801
H	5.05184	1.00823	-1.96182
H	6.62511	0.49642	-1.22523
H	5.60379	-0.68814	-2.13513
C	-4.00906	-1.00088	-3.28481
H	-4.86137	-0.54899	-3.83524
H	-3.09024	-0.91150	-3.89895
H	-4.20893	-2.07993	-3.12890
C	-3.63278	1.60778	-2.13657
H	-3.50533	2.20819	-1.21361
H	-2.73462	1.76471	-2.76707
H	-4.53401	1.94421	-2.69279
C	-5.42233	-0.25748	-0.89138
H	-6.19869	0.15815	-1.56904
H	-5.67572	-1.31061	-0.65303
H	-5.41701	0.31376	0.05868
C	-0.67589	2.91530	3.77040
H	0.11194	2.19066	4.05901
H	-0.18380	3.73658	3.21145
H	-1.15961	3.32391	4.68343
C	-3.16200	3.37984	2.39456
H	-4.01944	2.94569	1.84181
H	-3.52191	3.80483	3.35625
H	-2.73364	4.19283	1.77393

C	-2.74281	0.91543	3.82110
H	-3.57334	0.41494	3.28424
H	-2.03114	0.12983	4.14626
H	-3.13929	1.44505	4.71395
C	2.57222	3.92877	-1.81108
H	2.85115	4.40181	-0.84746
H	3.40711	3.26881	-2.12110
H	2.42876	4.72303	-2.57519
C	0.68550	2.36998	-3.31512
H	1.47934	1.67015	-3.64478
H	-0.27473	1.81628	-3.32790
H	0.63058	3.22966	-4.01706
C	-0.22807	4.22976	-1.31042
H	-0.19911	5.00929	-2.10208
H	-1.23144	3.76015	-1.28143
H	-0.05099	4.70126	-0.32265

2c•PMe$_3$

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Ni	1.79768	-1.63246	0.16572
Ni	1.58981	0.86229	-0.28822
Ni	-0.82299	1.18677	0.27263
Ni	-2.43900	-0.42611	-0.86281
Ni	-0.08993	-0.63544	-1.20198
P	3.22541	-2.28342	1.67640
P	2.76814	2.17431	-1.55905
P	-1.35699	2.61521	1.84196
P	-4.39907	-1.06683	-0.11988
C	0.15875	-2.40945	-2.08142
C	1.45999	-2.87408	-2.74644
C	2.07580	-3.87121	-1.72479
C	1.39468	-3.53420	-0.39061
H	1.40791	-4.29656	0.40490
C	0.17292	-2.84900	-0.68864
H	-0.72746	-2.88579	-0.05421
C	-0.90739	-1.73158	-2.74064
C	-2.33801	-1.75249	-2.34333
C	-3.12097	-1.33783	-3.61072
H	-3.39466	-2.24842	-4.19900
H	-4.06415	-0.79230	-3.41255
C	-2.11107	-0.50219	-4.42200
H	-2.03597	0.51723	-3.98340
H	-2.38032	-0.39750	-5.49364
C	-0.79215	-1.25785	-4.18910
H	-0.75838	-2.15782	-4.85176
H	0.11977	-0.66794	-4.40792
C	4.09072	-0.94229	2.71453
H	4.62975	-1.48333	3.52559

C	3.04528	-0.00766	3.34180
H	3.54512	0.83600	3.86507
H	2.40240	-0.52264	4.08367
H	2.38862	0.41384	2.54927
C	5.10561	-0.14107	1.88529
H	4.62839	0.25581	0.96503
H	5.98587	-0.74416	1.58815
H	5.48100	0.72394	2.47359
C	2.41345	-3.30467	3.09194
H	2.97376	-3.00390	4.00687
C	0.94161	-2.88479	3.26184
H	0.33095	-3.22076	2.39903
H	0.81516	-1.78798	3.33601
H	0.51375	-3.34351	4.18031
C	2.50816	-4.83629	2.96862
H	2.00629	-5.30680	3.84229
H	3.54847	-5.21470	2.94865
H	1.99121	-5.21471	2.06243
C	4.66362	-3.39759	1.11491
H	4.12468	-4.33815	0.86368
C	5.72380	-3.70984	2.18555
H	6.41921	-4.49679	1.81918
H	5.28953	-4.07198	3.13932
H	6.34215	-2.81815	2.41852
C	5.31824	-2.89189	-0.18489
H	6.02654	-2.06067	0.00496
H	4.56200	-2.51762	-0.90200
H	5.89155	-3.70908	-0.67366
C	4.32221	1.43895	-2.40229
H	5.07766	1.52989	-1.58769
C	4.13638	-0.05944	-2.69075
H	3.52035	-0.21928	-3.60096
H	3.61915	-0.55586	-1.84375
H	5.11596	-0.55529	-2.86377
C	4.85873	2.16723	-3.64779
H	5.82107	1.70956	-3.96705
H	5.04472	3.24565	-3.48374
H	4.16083	2.07082	-4.50593
C	1.79836	2.94976	-2.99548
H	2.52719	3.52797	-3.60616
C	1.18633	1.83414	-3.85613
H	0.52093	1.20184	-3.22719
H	1.95347	1.17325	-4.30798
H	0.58071	2.26348	-4.68348
C	0.69602	3.89835	-2.50081
H	0.11047	4.28278	-3.36401
H	1.09516	4.77756	-1.95504
H	-0.00017	3.35421	-1.82812

C	3.44203	3.69676	-0.63436
H	2.49596	4.14277	-0.25821
C	4.24544	3.25300	0.59728
H	5.21285	2.78480	0.31417
H	3.67278	2.51441	1.19314
H	4.48107	4.12322	1.24794
C	4.18949	4.77146	-1.43888
H	4.34225	5.67706	-0.81089
H	3.64098	5.09277	-2.34796
H	5.19750	4.42678	-1.75052
C	-1.88511	1.71878	3.43978
H	-2.85107	1.27092	3.11085
C	-0.92680	0.55351	3.74532
H	0.03517	0.91247	4.16359
H	-0.69473	-0.02209	2.82577
H	-1.37637	-0.13458	4.49344
C	-2.14233	2.57058	4.69250
H	-2.48353	1.92230	5.52965
H	-2.92337	3.34121	4.53953
H	-1.22083	3.08372	5.04044
C	-0.13000	3.94024	2.42509
H	-0.62755	4.50769	3.24293
C	0.20704	4.90824	1.28037
H	0.98069	5.63655	1.60778
H	-0.66843	5.48864	0.92904
H	0.60837	4.34760	0.41222
C	1.14884	3.28009	2.96160
H	1.52715	2.53965	2.22293
H	0.98620	2.75083	3.92143
H	1.94155	4.04071	3.13063
C	-2.91746	3.61178	1.37863
H	-3.71611	2.87820	1.62966
C	-2.96056	3.82355	-0.14671
H	-3.95541	4.20700	-0.46283
H	-2.75562	2.86617	-0.67167
H	-2.19999	4.55835	-0.48352
C	-3.21367	4.91436	2.14123
H	-2.47362	5.70942	1.91507
H	-3.23633	4.78179	3.24074
H	-4.20859	5.30886	1.83848
C	-4.38411	-1.19146	1.77750
H	-4.24026	-0.11810	2.03645
C	-3.13407	-1.92818	2.28774
H	-3.02137	-1.77886	3.38314
H	-2.22430	-1.53379	1.78881
H	-3.18619	-3.02026	2.10843
C	-5.66858	-1.68338	2.46266
H	-5.84013	-2.76599	2.28937

H	-6.57421	-1.13816	2.12581
H	-5.59096	-1.54286	3.56344
C	-5.08705	-2.72775	-0.78524
H	-4.82553	-2.64781	-1.86359
C	-4.31548	-3.93681	-0.22298
H	-4.62636	-4.17247	0.81610
H	-3.21811	-3.77853	-0.22023
H	-4.52138	-4.83963	-0.83784
C	-6.60455	-2.97397	-0.70162
H	-6.84553	-3.95108	-1.17584
H	-7.19861	-2.20572	-1.23500
H	-6.97110	-3.02287	0.34370
C	-5.88532	0.08927	-0.42172
H	-6.78290	-0.45417	-0.05352
C	-6.05678	0.36591	-1.92476
H	-6.95453	0.99769	-2.10045
H	-6.18068	-0.55957	-2.52328
H	-5.17488	0.91023	-2.32452
C	-5.76964	1.41077	0.34820
H	-4.83537	1.93836	0.07411
H	-5.78084	1.27220	1.44818
H	-6.62300	2.07604	0.09308
H	-2.64464	-2.72869	-1.91872
H	1.25189	-3.35296	-3.72809
H	1.80920	-4.91843	-2.00596
H	0.53609	2.01604	0.01868
H	-1.12328	0.62221	-1.29096
H	-2.36534	0.68910	0.36514
H	2.66451	-0.24818	0.02957
H	0.54540	-0.18696	0.36881
H	3.18362	-3.83010	-1.70493
H	2.14448	-2.02483	-2.95018

3

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Ni	-0.02094	0.36699	0.12148
Ni	2.32454	-0.33750	0.10080
Ni	-1.57708	-1.47750	0.76037
Ni	-2.54913	0.53800	-0.24909
Ni	0.49315	-1.93742	-0.44887
P	4.51438	-0.45796	0.02894
Si	-0.99889	2.27486	-0.51654
Si	1.67598	1.71843	0.67617
P	-2.04018	-2.22942	2.73394
P	-4.52213	0.41197	-1.20533
P	1.08054	-3.47688	-1.88047
C	-0.80296	2.83156	-2.34555
C	-0.14255	2.00865	-3.28879

H	0.32438	1.07267	-2.94171
C	1.63962	2.02239	2.57582
C	2.11687	1.01425	3.45026
H	2.51865	0.08555	3.01305
C	2.46794	3.27538	-0.10286
C	5.08436	-0.83145	-1.75141
H	4.54303	-1.78769	-1.93046
C	2.55064	3.38888	-1.51477
H	2.11004	2.60204	-2.14629
C	-1.19386	3.86751	0.53177
C	1.11687	3.20090	3.16910
H	0.71572	4.00666	2.53463
C	-0.06813	2.35745	-4.64901
H	0.45760	1.69582	-5.35751
C	-2.03134	3.83834	1.67522
H	-2.54773	2.89905	1.93748
C	-1.40277	4.02141	-2.82989
H	-1.93409	4.68913	-2.13106
C	3.06166	4.30991	0.66674
H	3.03747	4.25474	1.76665
C	2.09914	1.17531	4.84638
H	2.49004	0.37551	5.49732
C	0.50029	-2.25474	4.01706
H	1.31533	-2.85156	4.48052
H	0.23436	-1.44672	4.72577
H	0.90263	-1.78544	3.09470
C	-0.68698	-3.16830	3.68046
H	-1.15948	-3.51056	4.62856
C	5.77198	0.80493	0.68736
H	6.73961	0.25685	0.69430
C	1.85686	-2.77271	-3.47371
H	2.92248	-2.66252	-3.17462
C	4.50801	0.20050	-2.73847
H	3.43786	0.39577	-2.52583
H	4.59631	-0.17257	-3.78180
H	5.03796	1.17218	-2.68739
C	-4.33031	0.74460	-3.06945
H	-4.02095	1.81210	-3.05935
C	-1.33491	4.37730	-4.18932
H	-1.80824	5.31140	-4.53546
C	-3.53381	-3.40690	2.78381
H	-4.37245	-2.69478	2.62335
C	1.08827	3.36469	4.56623
H	0.67318	4.29138	4.99589
C	-5.61741	-1.14090	-1.13142
H	-6.46422	-0.95184	-1.82857
C	-2.20680	4.97042	2.48936
H	-2.86701	4.91680	3.37086

C	-0.52470	5.08391	0.24420
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C	-0.66316	3.54758	-5.10498
H	-0.60387	3.82773	-6.16961
C	5.93277	2.04885	-0.20150
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C	5.01265	-2.06551	0.96048
H	4.85960	-2.83073	0.16634
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H	1.56749	2.48862	6.50539
C	3.17542	4.48575	-2.13121
H	3.21258	4.54754	-3.23124
C	6.58268	-1.08405	-1.98244
H	7.20128	-0.19362	-1.74591
H	6.76223	-1.32759	-3.05287
H	6.96699	-1.93581	-1.38709
C	-3.54539	-4.37379	1.58759
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H	-4.53867	-4.86381	1.49434
H	-2.78769	-5.17682	1.69141
C	-3.76210	-4.13093	4.12043
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C	-0.21241	-4.38229	2.86952
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C	-1.69030	0.41040	3.66660
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H	2.96007	-2.25423	1.69803
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H	1.94037	-0.82655	-4.48472
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H	0.27379	-1.36446	-4.09660
C	-1.49993	-3.48673	-3.05805
H	-1.78518	-2.76725	-2.26138

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H	-1.15871	-2.90436	-3.93682
C	-1.53833	6.16903	2.18026
H	-1.67480	7.06083	2.81395
C	-5.50597	3.12639	-1.35164
H	-4.46114	3.47365	-1.20340
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H	-5.71157	3.10100	-2.43954
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H	-5.92969	-0.45274	-3.99894
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H	-2.23722	-1.24378	4.97929
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H	-0.04631	-5.07647	-3.37277
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H	-5.37626	-1.47987	1.01903
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H	-6.89128	-0.60364	0.60215
C	2.14533	-5.24257	0.06426
H	2.51744	-4.37701	0.65056
H	2.76064	-6.13150	0.32441
H	1.10854	-5.43641	0.39795
C	-0.69381	6.22037	1.05627
H	-0.15993	7.15287	0.80905
C	1.79441	-3.66424	-4.72339
H	0.75747	-3.76886	-5.10507
H	2.19046	-4.68513	-4.54238
H	2.39614	-3.21654	-5.54471
C	3.74784	5.50348	-1.34593
H	4.23882	6.36612	-1.82580
C	-5.67694	1.96534	0.87106
H	-5.81102	1.02169	1.43337
H	-6.46529	2.67496	1.20406
H	-4.69416	2.38890	1.16312
C	-3.16203	-0.03577	-3.69870
H	-3.40474	-1.10792	-3.84305
H	-2.24994	0.02698	-3.07169
H	-2.91969	0.39022	-4.69552
C	-1.01961	-5.37979	-1.46126
H	-1.30630	-4.79804	-0.56054
H	-0.32089	-6.18310	-1.15280
H	-1.93450	-5.87435	-1.85378
C	-4.82294	-2.36331	-1.61545
H	-4.56583	-2.30427	-2.69046

H	-5.40852	-3.29534	-1.46107
H	-3.87141	-2.45106	-1.04702
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H	4.46469	1.75239	2.17739
H	6.21600	1.87283	2.53871
H	5.34479	0.33193	2.81017
C	3.69473	-4.77687	-1.87183
H	3.82474	-4.71809	-2.97026
H	4.29617	-5.64015	-1.51303
H	4.14122	-3.86320	-1.42515
C	6.45730	-2.18470	1.47347
H	7.21896	-2.01356	0.68751
H	6.62631	-3.20687	1.87810
H	6.65985	-1.47474	2.30212
C	-4.00825	-0.50901	3.96434
H	-4.33056	-0.19167	2.94963
H	-4.19427	0.34747	4.64762
H	-4.65929	-1.34152	4.29740
H	-2.90732	-0.65226	0.80457
H	-0.75753	-2.74423	0.22413
H	-1.23347	-0.65729	-0.59863
H	0.93150	-0.90782	0.77306
H	-2.68715	2.03651	-0.60194

4

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Ni	0.22221	-1.15968	0.97807
Ni	2.19514	-0.65069	-0.30351
Ni	1.13491	1.57904	-0.36276
Ni	-1.47910	1.29195	-0.40825
Ni	-1.91771	-1.13207	-0.15320
Si	0.01794	-0.20648	-1.16226
P	0.22207	-1.63233	3.15950
P	3.79941	-1.76142	-1.35052
P	2.33428	3.38156	0.17204
P	-3.04523	2.87083	-0.18540
P	-3.29362	-2.59106	-1.10343
C	0.07164	-0.73815	-3.02797
H	1.07051	-1.18447	-3.21822
H	-0.66698	-1.55535	-3.17688
C	-0.18549	0.41820	-4.00529
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C	0.68197	-4.38388	2.45502
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H	0.64825	-3.97741	1.42394
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H	-0.42244	-5.03255	4.93673
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C	-1.22796	-0.85313	4.12962
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C	-2.55747	-1.51035	3.71848
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H	-2.62461	-1.54904	2.60882
C	-1.31288	0.66301	3.87622
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C	1.71470	-1.30001	4.29781
H	1.40730	-1.61449	5.32116
C	2.09701	0.18821	4.32281
H	3.06193	0.32402	4.85829
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C	2.93259	-2.12898	3.86012
H	3.18222	-1.91498	2.79989
H	2.77444	-3.22017	3.96023
H	3.81696	-1.86333	4.47904
C	3.17088	-3.06106	-2.58929
H	2.83429	-2.40998	-3.42794
C	1.92133	-3.77259	-2.04107
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H	2.18953	-4.58476	-1.33444
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H	5.00676	-4.28111	1.27625
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H	4.93277	-1.25085	1.39863
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C	4.96523	-0.64431	-2.36742
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C	2.90412	5.63338	1.96773
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C	1.79628	3.57585	2.96894
H	2.76837	3.18668	3.33741
H	1.13669	2.70731	2.76953
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C	-2.59869	4.45994	0.76972
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C	-6.00136	-3.68156	-0.68527
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H	-6.03187	-4.03973	-1.73178
H	-7.04373	-3.42806	-0.39126
C	-3.43791	-2.41989	-2.99642
H	-2.37968	-2.58309	-3.30199
C	-3.80113	-0.97754	-3.38379
H	-3.66336	-0.82168	-4.47515
H	-3.16444	-0.25492	-2.83474
H	-4.86326	-0.74621	-3.15074
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H	-5.38981	-3.26868	-3.57078
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H	-4.14508	-3.33772	-4.84403
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