Complexes of iron and cobalt with new tripodal amido-polyphosphine hybrid ligands

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Supporting Information

Experimental Section

All manipulations were carried out using standard Schlenk or glove-box techniques under a dinitrogen atmosphere. Unless otherwise noted, solvents were deoxygenated and dried by thorough sparging with N_2 gas followed by passage through an activated alumina column. Non-halogenated solvents were typically tested with a standard purple solution of sodium benzophenone ketyl in tetrahydrofuran in order to confirm effective oxygen and moisture removal. Deuterated solvents were degassed and stored over activated 3-Å molecular sieves prior to use. THF-d_8 was dried by passage over activated alumina and stored over activated sieves prior to use. DippN(H)$SiMe_2(CH_2Cl)$[1] and Li[$NH(2,6\text{-}Me_2C_6H_3)$][2] were prepared according to literature procedures. Diphenylphosphine (Strem), tetrakis(triphenylphoshine) palladium (Strem), bis(chloromethyl)methylchlorosilane (Gelest), and *n*-butyllithium (Aldrich) were used as received without further purification. Phosphorus (III) chloride (Strem) and 2-iodobromobenzene (Alfa Aesar) were degassed via three freeze-pump-thaw cycles prior to use. Triethylamine (Aldrich) was degassed and distilled from CaH_2 prior to use. All reagents were purchased from commercial vendors and used without further purification unless explicitly stated. Elemental analyses were carried out at Desert Analytics, Tucson, Arizona. NMR spectra were recorded at ambient temperature on Varian Mercury 300 MHz, Joel 400 MHz, and an Inova 500 MHz spectrometers, unless otherwise noted. ^{1}H NMR chemical shifts were referenced to residual solvent. ^{31}P NMR chemical shifts are reported relative to an external standard of 85% H_3PO_4. UV-vis measurements were taken on a Hewlett Packard 8452A diode array spectrometer using a quartz crystal cell with a Teflon cap. Electrochemical analysis was performed on a CHI

[1] R. R. Schrock, S. W. Seidel, Y. Schrodi and W. M. Davis, *Organometallics*, 1999, **18**, 428.
[2] J. T. Patton, S. G. Feng and K. A. Abboud, *Organometallics*, 2001, **20**, 3399.

600B Potentiostat/Galvanostat. X-ray diffraction studies were carried out in the Beckman Institute Crystallographic Facility on a Bruker Smart 1000 CCD diffractometer.

X-ray Crystallography Procedures. X-ray quality crystals were grown as indicated in the experimental procedures for each complex. The crystals were mounted on a glass fiber with Paratone-N oil. Structures were determined using direct methods with standard Fourier techniques using the Bruker AXS software package. In some cases, Patterson maps were used in place of the direct methods procedure.

2-$Ph_2PC_6H_4Br$ (6). 2-$Ph_2PC_6H_4Br$ was prepared by modification of a literature procedure.[3] 2-iodobromobenzene (24.1337 g, 85.3070 mmol), diphenylphosphine (15.8848 g, 85.3150 mmol), triethylamine (10.0945 g, 99.7579 mmol), and a catalytic amount of $Pd(PPh_3)_4$ (513.0 mg, 0.4439 mmol) were dissolved in 15 mL of toluene to give a clear, bright yellow solution. The solution was heated at 80 °C with stirring for 16 hours in a sealed bomb, resulting in the precipitation of triethylammonium iodide. The resulting orange solution was dried in vacuo at 50 °C, extracted into diethyl ether (400 mL), and filtered through a 1" pad of silica gel to give a clear, pale yellow solution, from which the volatiles were removed in vacuo to yield the phosphine as a creamy white powder (24.9352 g, 86%). Characterization data matched those previously reported for the complex.

$(2\text{-}Ph_2PC_6H_4)_2PCl$ (7). To a colorless solution of **6** (1.170 g, 3.42 mmol) in 30 mL of diethyl ether stirring at -80 °C, ^{n}BuLi (1.60 M solution in hexanes, 2.15 mL, 3.44 mmol) was added

[3] D. Brauer, M. Hingst, M., K. Kottsieper, C. Liek, T. Nickel, M. Tepper, O. Stelzer and W. Sheldrick, *J. Organomet. Chem.*, 2002, **645**, 14.

dropwise by syringe, causing the solution to become deep orange and cloudy. The reaction was stirred at -80 °C for 15 min, followed by 35 min at room temperature. The orange suspension of Li[2-$Ph_2PC_6H_4$] was added slowly by pipette (over 20 min) to a stirring solution of PCl_3 (230 mg, 1.67 mmol) in 5 mL of diethyl ether at -80 °C. After the addition, the cloudy pale yellow suspension was allowed to stir at room temperature for 3 h and evaporated to dryness in vacuo. The resulting pale yellow powder was extracted into benzene (40 mL) and filtered through Celite to remove LiCl. The volatiles were removed in vacuo and the orange residue dissolved in 3 mL CH_2Cl_2 and layered with 2 mL of petroleum ether. A pale yellow microcrystalline solid was obtained by cooling the solution to -35 °C for 16 h (0.667 g, 66%). ^{1}H NMR (C_6D_6): δ 7.76 (d, 2H, Ar-*H*), 7.33 (m, 4H, Ar-*H*), 7.17 (m, 6H, Ar-*H*), 6.99 (m, 6H, Ar-*H*), 6.80 – 6.94 (m, 10H, Ar-*H*). ^{13}C NMR (CD_2Cl_2): δ 134.8 (d), 134.4 – 133.6 (m), 132.9, 130.6 (d), 129.4 – 128.4 (m). ^{31}P NMR (C_6D_6): δ 68.6 (t, $^3J_{PP}$ = 245.6 Hz, Ar_2*P*Cl), -15.7 (d, $^3J_{PP}$ = 245.6 Hz, Ph_2*P*-). Attempts to obtain combustion analysis data repeatedly yielded low results for carbon, likely due to the presence of small amounts of (2-$Ph_2PC_6H_4)_2$Br (evident by ^{31}P NMR spectroscopy).

(2-$Ph_2PC_6H_4)_2$PH (8). Pale yellow **7** (485.2 mg, 0.8238 mmol) was added in portions to a solution of $LiAlH_4$ (40.2 mg, 1.06 mmol) in 35 mL of diethyl ether at -35 °C. The reaction immediately became cloudy while remaining colorless and was allowed to proceed at room temperature with stirring for 2 h. The volatiles were removed and the reaction mixture was extracted into 40 mL of benzene and filtered through a 1" pad of silica to give a colorless solution that was dried to a white foam (369.4 mg, 81 %). ^{1}H NMR (C_6D_6): δ 7.30 (m, 9H, Ar-*H*), 7.15 (m, 3H, Ar-*H*), 6.80 (m, 5H, Ar-*H*), 5.68 (dt, $^1J_{HP}$ = 221.8 Hz, $^4J_{HP}$ = 8.0 Hz, P-*H*). ^{13}C NMR (C_6D_6): 138.0 (m), 136.2 (m), 135.0 – 134.2 (m), 129.5, 129.3 – 128.8 (m). ^{31}P NMR

(C_6D_6): δ -10.9 (d, $^3J_{PP}$ = 116.6 Hz, Ph_2P-), -53.8 (dt, $^1J_{HP}$ = 222.2 Hz, $^3J_{PP}$ = 116.0 Hz, Ar_2PH). *m/z* (ESI): 555.1 (M+1). Anal. Calcd. for $C_{36}H_{29}P_3$: C, 77.97; H, 5.27. Found: C, 77.75; H, 5.23.

[(2-$Ph_2PC_6H_4$)$_2$P$CH_2Si(CH_3)_2$N(Dipp)]Li·$(Et_2O)_{1.5}$ (Li[^{Si}NP$_3$], 9). To a stirring solution of **8** (1.6029 g, 2.8905 mmol) in 30 mL of THF at -35 °C was added dropwise a solution of ^{n}BuLi (1.60 M in hexanes, 1.890 mL, 3.024 mmol). The mixture immediately adopted a deep orange hue. After 1 hr, this phosphide solution was added dropwise to a stirring solution of DippN(H)$SiMe_2(CH_2Cl)$ (820.7 mg, 2.891 mmol) in 20 mL THF. The deep orange color of the solution quickly faded, and after 3 hours volatiles were removed from the pale yellow solution to give a yellow foam. The foam was dissolved in 30 mL Et_2O, filtered through a pad of Celite to remove LiCl, and chilled to -35 °C. ^{n}BuLi (1.60 M in hexanes, 1.890 mL, 3.024 mmol) was added dropwise with stirring, and after 2 hours stirring at room temperature the solution was diluted with 50 mL of petroleum ether and chilled to -35 °C for 12 hours to yield a crop of white crystals which were isolated on a frit and washed with petroleum ether (3 x 10 mL) (2.0968 mg, 79 %). ^{1}H NMR (C_6D_6): δ 7.50 (m, 2H, Ar-*H*), 7.20 – 7.40 (m, 8H, Ar-*H*), 7.05 (t, 4H, Ar-*H*), 6.80 – 7.05 (m, 17H, Ar-*H*), 4.25 (septet, J = 6.9 Hz, 2H, -C*H*$(CH_3)_2$), 3.11 (q, 6H, Et_2O) 1.60 (d, $^2J_{HP}$ = 5.4 Hz, 2H, -C*H*$_2$), 1.38 (d, J = 6.0 Hz, 12H, -CH(C*H*$_3)_2$), 0.82 (t, 9H, Et_2O), 0.20 (s, 6H, Si(C*H*$_3)_2$). ^{13}C NMR (THF-d^8): δ 143.8, 135.5 – 134.5 (m), 134.0 – 133.0 (m), 129.5, 129.0 – 128.8 (m), 128.7, 122.7, 115.4, 66.5 (Et_2O), 27.4 (-*C*H$(CH_3)_2$), 25.7 (-CH(*C*H$_3)_2$), 20.2 – 19.0 (d, -*C*H$_2$P), 15.9 (Et_2O), 4.4 (-Si(*C*H$_3)_2$). ^{31}P NMR (C_6D_6): δ -15.9 (d, $^3J_{PP}$ = 165 Hz, *P*Ph$_2$), -29.0 (br t, $^3J_{PP}$ = 165 Hz, Ar_2PCH_2). Anal. Calcd. for $C_{57}H_{68}LiNO_{1.5}P_3Si$: C, 74.49; H, 7.46; N, 1.52. Found: C,73.23; H, 7.17; N, 1.60.

[^{Si}NP$_3$]FeCl (1). A yellow solution of **9** (171.9 mg, 0.1870 mmol) in 2 mL of THF was added to a suspension of $FeCl_2$ (23.9 mg, 0.1886 mmol) in THF (5 mL). The mixture immediately gained a dark brown hue and was allowed to stir for 12 h. The volatiles were removed and the resulting dark brown oily residue was extracted into benzene (10 mL), filtered through a pad of Celite, dried in vacuo, triturated with petroleum ether (3 x 5 mL), isolated on a frit and washed with petroleum ether (3 x 10 mL) to give a brown powder (106.9 mg, 64 %). Yellow-green crystals suitable for X-ray diffraction were obtained by vapor diffusion of petroleum ether into a concentrated benzene solution of **1**. ^{1}H NMR (C_6D_6): δ 50.8, 25, 16.1, 15.0, 13.1, 10.8, 8.0, 3.1, -4.0, -4.7, -6.5, -8.5, -49.1. UV-vis (C_6H_6) λ_{max}, nm (ε, M^{-1} cm^{-1}): 387 (3640). Evans Method (C_6D_6): 4.57 μ_B. *m/z* (ESI): 856.2 ([^{Si}NP$_3$]Fe$^+$, 100%), 857.2 (64%), 858.3 (18%). Anal. Calcd. for $C_{51}H_{53}ClFeNP_3Si$: C, 68.65; H, 5.99; N, 1.57. Found: C, 68.30; H, 5.90; N, 1.69.

[^{Si}NP$_3$]CoCl (2). A yellow solution of **9** (560.8 mg, 0.6102 mmol) in 8 mL of THF was added to a light blue suspension of $CoCl_2$ (79.2 mg, 0.610 mmol) in 8 mL THF. The mixture immediately gained a dark maroon hue and was allowed to stir for 12 h. The volatiles were removed and the resulting dark red oil was extracted into benzene (100 mL), filtered through a pad of Celite to remove salts, dried in vacuo, triturated with petroleum ether (2 x 10 mL), isolated on a frit and washed with 9:1 petroleum ether / CH_2Cl_2 (3 x 10 mL) to give a maroon powder (120.0 mg, 22 %). ^{1}H NMR (CD_2Cl_2): δ 10.8, 9.2, 8.3, 7.6, 7.4, 7.2, 7.0, 3.7, 1.3, 1.0, 0.5, 0.1, -3.0. UV-vis (C_6H_6) λ_{max}, nm (ε, M^{-1} cm^{-1}): 820 (480), 490 (3300), 422 (4500), 335 (8125). Anal. Calcd. for $C_{51}H_{53}ClCoNP_3Si$: C, 68.41; H, 5.97; N, 1.56. Found: C, 68.24; H, 5.90; N, 1.37.

[^{Si}NP$_3$]CoI (3). This compound was generated in the same manner as described for **2**. Although analytically pure samples were not be obtained, dark red plates suitable for XRD analysis were obtained by vapor diffusion of petroleum ether into a concentrated benzene solution of **3**.

HN(Dipp)SiMe(CH$_2$Cl)$_2$ (10). Li[NH(2,6-Me$_2$C$_6$H$_3$)] (623.0 mg, 3.400 mmol) was added in portions to a stirring solution of (ClCH$_2$)$_2$SiMeCl (603.9 mg, 3.401 mmol) in Et$_2$O (10 mL) at -35 °C. A white solid formed, and the reaction was stirred overnight at room temperature. The volatiles were removed in vacuo and the residues extracted into 15 mL of petroleum ether, filtered through a pad of Celite, and solvent was removed in vacuo to give a clear, slightly yellow oil (1.0397, 96%). ^{1}H NMR (C$_6$D$_6$): δ 6.95 – 7.05 (m, 3H, Ar-*H*), 3.20 – 3.40 (septet, J = 6.9 Hz, 2H, –C*H*(CH$_3$)$_2$), 2.74 (s, 4H, -Si(C*H*$_2$)$_2$), 2.37 (s, 1H, -N*H*), 1.09 (d, J = 6.0 Hz, 12H, -CH(C*H*$_3$)$_2$), -0.02 (s, 3H, SiC*H*$_3$). ^{13}C NMR (C$_6$D$_6$): δ 145.9, 125.9, 123.9, 28.8, 28.6, 24.2 (-CH(*C*H$_3$)$_2$), -6.6 (-Si*C*H$_3$). *m/z* (CI): 317 (M$^+$, 100%), 318 (26%), 319 (67%).

LiN(Dipp)SiMe(CH$_2$PPh$_2$)$_2$ (11, Li[^{Si}NP$_2$]). Diphenylphosphine (1.2786 g, 6.8672 mmol) was dissolved in 10 mL of THF and chilled to -80 °C. ^{n}BuLi (1.60 M in hexanes, 4.30 mL, 6.88 mmol) was added dropwise to the stirring solution, causing a color change to orange and then to red. After 10 minutes, the solution was warmed to room temperature and stirred for 40 minutes. The red phosphide solution was cooled to -35 °C and added dropwise to a cold (-35 °C) solution of **10** (1.0927 mg, 3.4316 mmol), and the color rapidly dissipated with each drop. The reaction was allowed to proceed for 5 hours, and volatiles were removed in vacuo to leave a yellow oil. The residues were extracted into petroleum ether (60 mL), filtered through a pad of Celite, and chilled to -35 °C. ^{n}BuLi (1.60 M in hexanes, 2.00 mL, 3.20 mmol) was added dropwise to the

stirring solution, causing a white solid to precipitate. After 2 hours, the solid was isolated on a frit and washed with petroleum ether (3 x 10 mL) to yield the pure lithium amide (1.3700 g, 64%). ^{1}H NMR (C_6D_6): δ 7.36 – 7.52 (m, 8H, Ar-*H*), 6.88 – 7.10 (m, 14H, Ar-*H*), 3.72 (br s, 2H, -C*H*$(CH_3)_2$), 1.40 – 1.80 (dd, 4H, -Si(CH_2)$_2$), 1.10 – 1.20 (d, J = 5.7 Hz, 6H, -CH(CH_3)$_2$), 1.00 (br s, 6H, -CH(CH_3)$_2$), -0.20 (s, 3H, -SiCH_3). ^{13}C NMR (THF-d^8): δ 155.1, 144.0 – 143.0 (m), 134.0 (d), 133.0 (d), 129.2 – 128.6 (m), 128.5, 122.9, 116.0, 27.2 (-*C*H$(CH_3)_2$), 25.6 (-CH(CH_3)$_2$), 17.8 (dd, $^{1}J_{CP}$ = 28.0 Hz, $^{3}J_{CP}$ = 2.6 Hz). ^{31}P NMR (C_6D_6): δ -23.4 (s). Anal. Calcd. for $C_{39}H_{44}LiNP_2Si$: C, 75.10; H, 7.11; N, 2.25. Found: C, 75.06; H, 7.22; N, 2.33.

[^{Si}NP$_2$]FeCl (4). A yellow solution of **11** (232.8 mg, 0.3732 mmol) in 5 mL of THF was added to a slurry of $FeCl_2$ (47.4 mg, 0.374 mmol) in 5 mL of THF, causing an immediate color change to dark brown. After 3 hours, the solution had lightened to a golden hue, and volatiles were removed in vacuo, leaving a dark yellow oil. The residues were extracted into benzene (10 mL), filtered through a pad of Celite, lyophilized to a golden powder, then washed with petroleum ether to give a canary yellow powder (219.0 mg, 83%). Crystals suitable for X-ray diffraction were grown by diffusion of petroleum ether into a concentrated benzene solution of the product. ^{1}H NMR (C_6D_6): δ 64.0, 55.0, 21.0, 18.1, 13.4, 10.4, 1.9, 0.9, -7.9, -45.1, -56.0. UV-vis (Et_2O) λ_{max}, nm (ε, M^{-1} cm^{-1}): 370 (2300). Evans Method (C_6D_6): 4.80 μ_B. Anal. Calcd. for $C_{39}H_{44}ClFeNP_2Si$: C, 66.15; H, 6.26; N, 1.98. Found: C, 66.53; H, 6.26; N, 1.69.

[^{Si}NP$_2$]CoCl (5a). A yellow solution of **11** (360.0 mg, 0.5771 mmol) in 8 mL of Et_2O was added to a slurry of $CoCl_2$ (74.9 mg, 0.5769 mmol) in 5 mL of Et_2O, causing an immediate change in color from light blue to dark green. After 5 hours, the solution was filtered to remove LiCl, dried

in vacuo, extracted into benzene (10 mL), filtered through a pad of Celite, and dried to a green oil. The oil was dissolved in 1 mL of Et_2O, and 15 mL of petroleum ether was added, causing a green solid to precipitate. The solid was isolated on a frit and washed with petroleum ether (3 x 10 mL) to give **5a** as a green powder (231.1 mg, 58%). ^{1}H NMR (THF-d^8): 44.6, 35.0, 26.5, 22.1, 12.3, 11.4, 9.2, 7.3, -1.0, -20.0, -58.4. UV-vis (Et_2O) λ_{max}, nm (ε, M^{-1} cm^{-1}): 735 (510), 600 (660), 490 (980), 360 (2900). Evans Method (C_6D_6): 3.74 μ_B. Anal. Calcd. for $C_{39}H_{44}ClCoNP_2Si$: C, 65.86; H, 6.24; N, 1.97. Found: C, 64.15; H, 5.98; N, 1.88.

[^{Si}NP$_2$]CoI (5b). A yellow solution of **11** (209.4 mg, 0.3357 mmol) in 5 mL of Et_2O was added to a dark blue solution of CoI_2 (0.3357) in 5 mL of Et_2O, causing an immediate change in color to dark brown. The reaction was allowed to proceed 5 hours, filtered through a pad of Celite, and dried in vacuo to a brown oil. The oil was triturated with petroleum ether to give a brown powder, which was isolated on a frit and washed with 5:1 pet. ether / Et_2O (2 x 5 mL) to afford **11** as a light brown powder (125.0 mg, 46 %). Dark brown blocks of crystalline **11** suitable for XRD analysis were obtained by slow evaporation of Et_2O from a concentrated solution. ^{1}H NMR (C_6D_6): 77.1, 26.5, 20.7, 20.2, 11.4, 5.7, 3.5, 1.3, -4.3, -7.4, -8.7, -13.5, -59.0, -79.4. UV-vis (Et_2O) λ_{max}, nm (ε, M^{-1} cm^{-1}): 790 (320), 620 (1000), 500 (1900), 320 (6700). Evans method (C_6D_6): 4.04 μ_B. Anal. Calcd. for $C_{39}H_{44}CoINP_2Si$: C, 58.36; H, 5.53; N, 1.75. Found: C, 57.53; H, 5.20; N, 1.73. *N.b.:* Attempts to obtain elemental analyses of compounds **4a** and **4b** repeatedly yielded low results in carbon, even with recrystallized samples.

Figure 1. Cyclic voltammogram of [$^{Si}NP_3$]FeCl (**1**) in 0.35 M [TBA][PF_6]/THF, scan rate = 250 mV/s, V vs Fc/Fc^+.

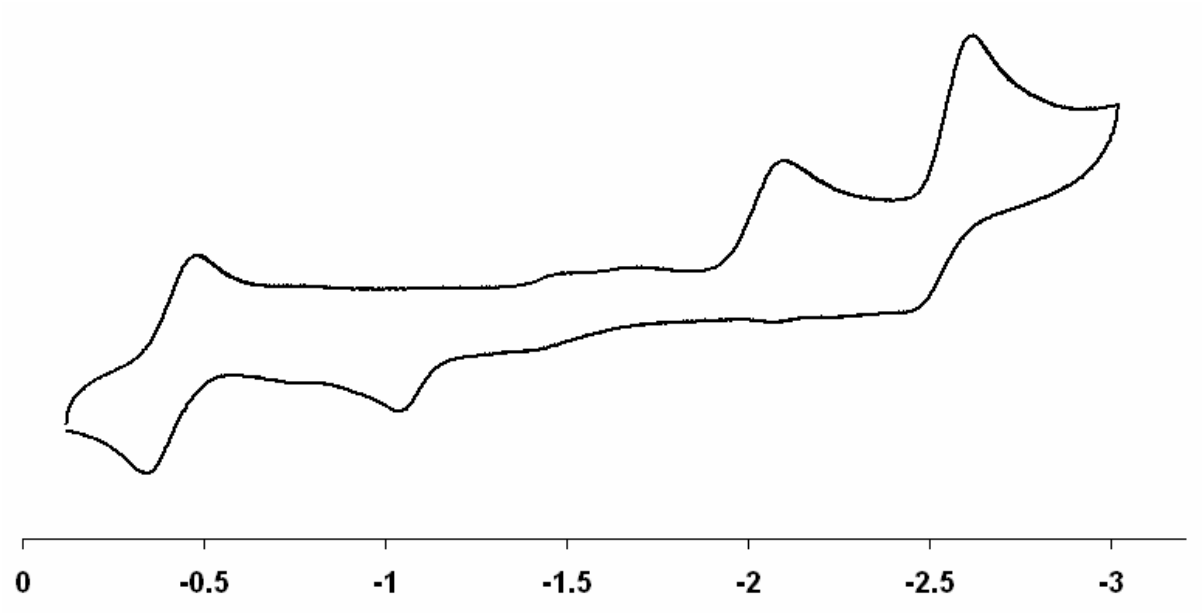

Figure 2. Cyclic voltammogram of [$^{Si}NP_3$]CoCl (**2a**) in 0.35 M [TBA][PF_6]/THF, scan rate = 400 mV/s, V vs. Fc/Fc^+.

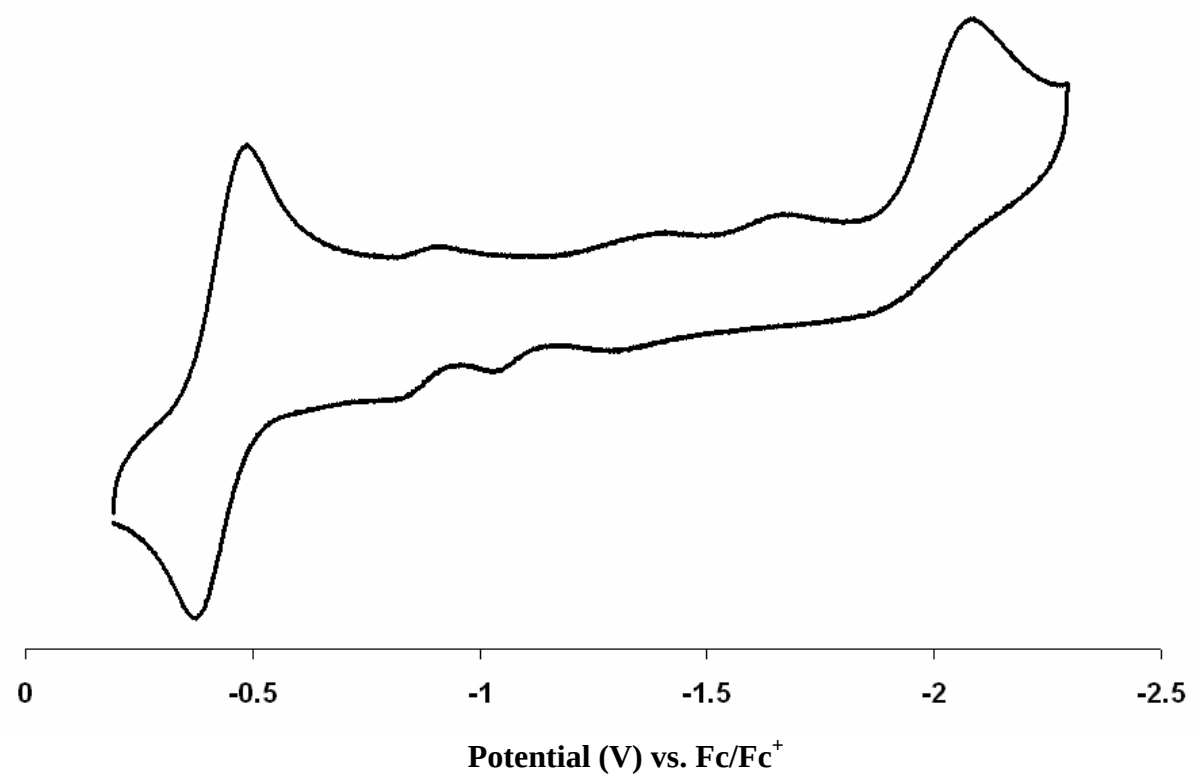

Figure 3. Cyclic voltammogram of [$^{Si}NP_2$]FeCl (**3**) in 0.35 M [TBA][PF_6]/THF, scan rate = 250 mV/s, V vs. Fc/Fc^+.

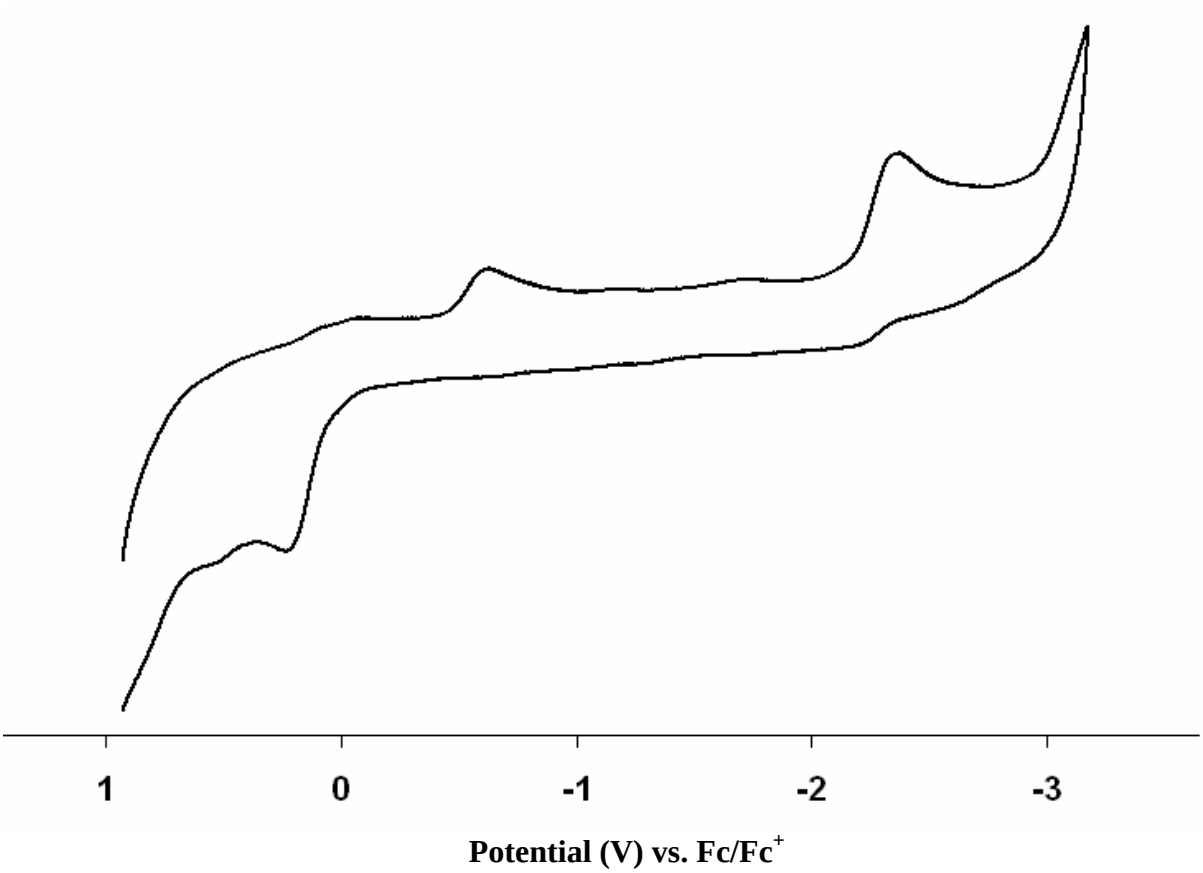

Figure 4. Cyclic voltammogram of [$^{Si}NP_2$]CoCl (**4a**) in 0.35 M [TBA][PF_6]/THF, scan rate = 500 mV/s, V vs. Fc/Fc^+.

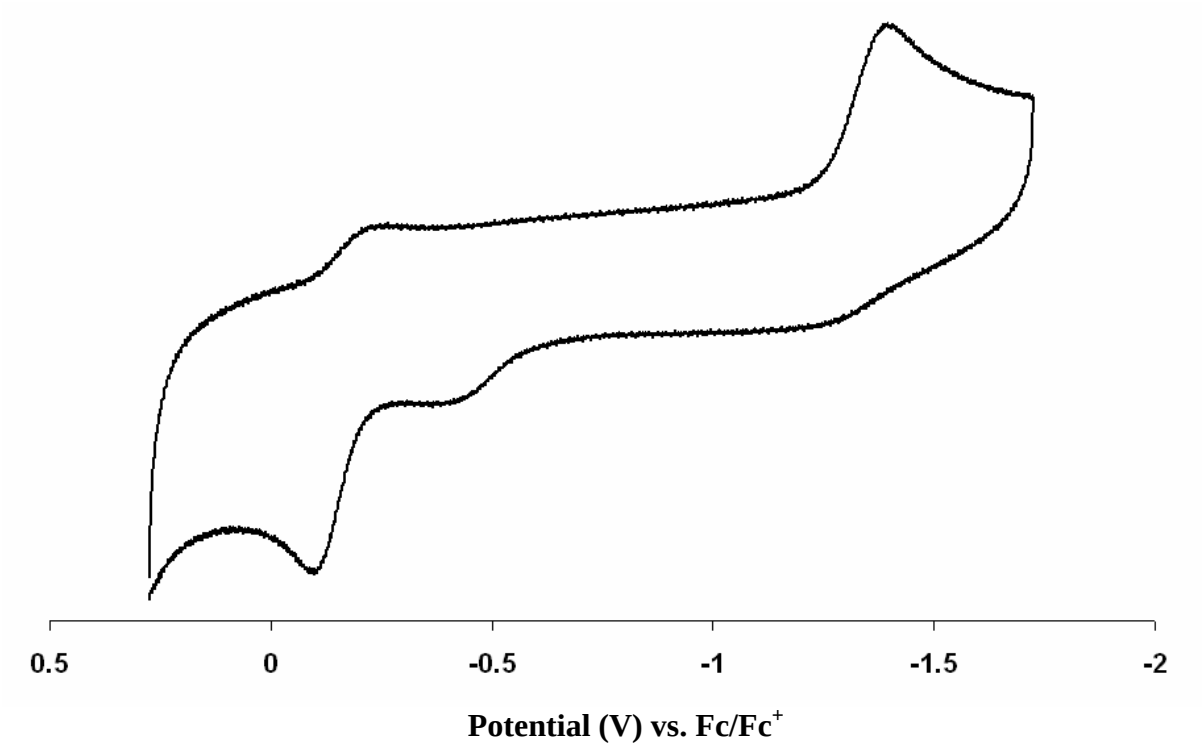

Figure 5. UV-vis spectrum of Fe($^{Si}NP_3$)Cl (**1**) at various temperatures (**blue** = -80 °C; **red** = 25 °C; gray and green lines traces are intermediate spectra obtained during warming of the sample).

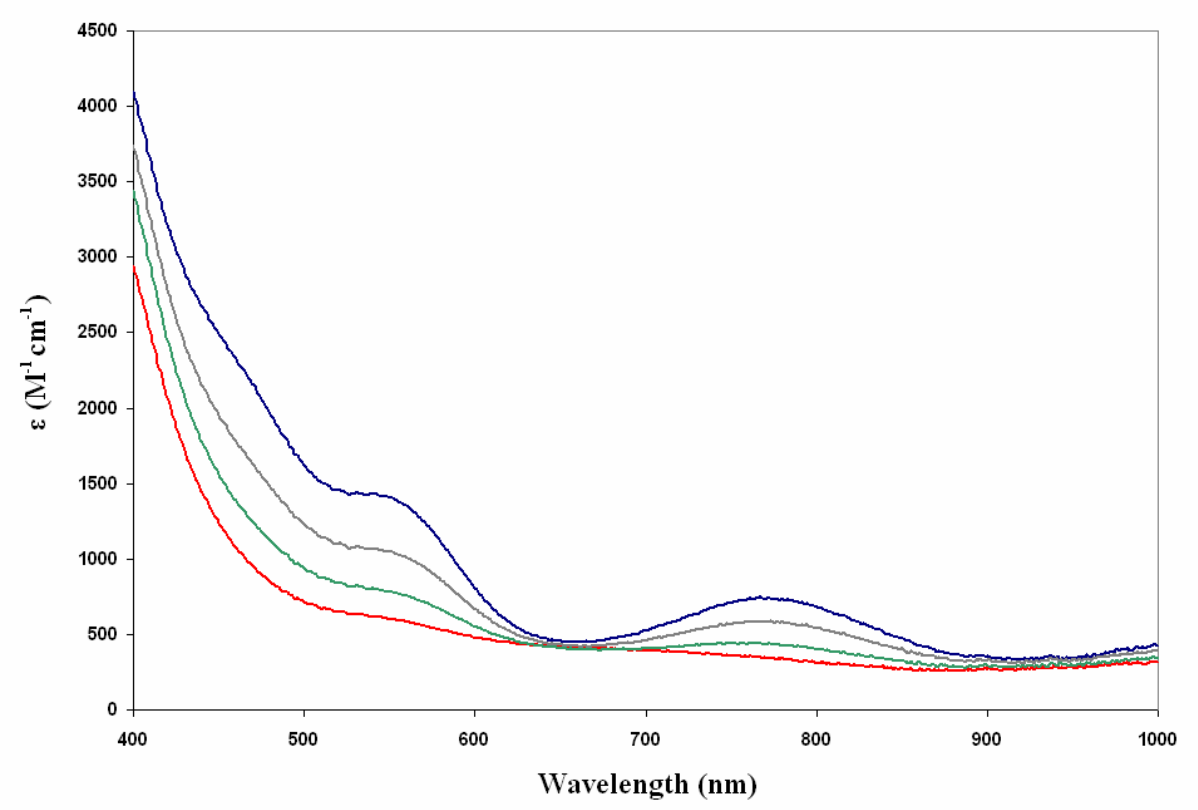

Figure 6. Fully labeled drawing of [$^{Si}NP_3$]FeCl (**1**)

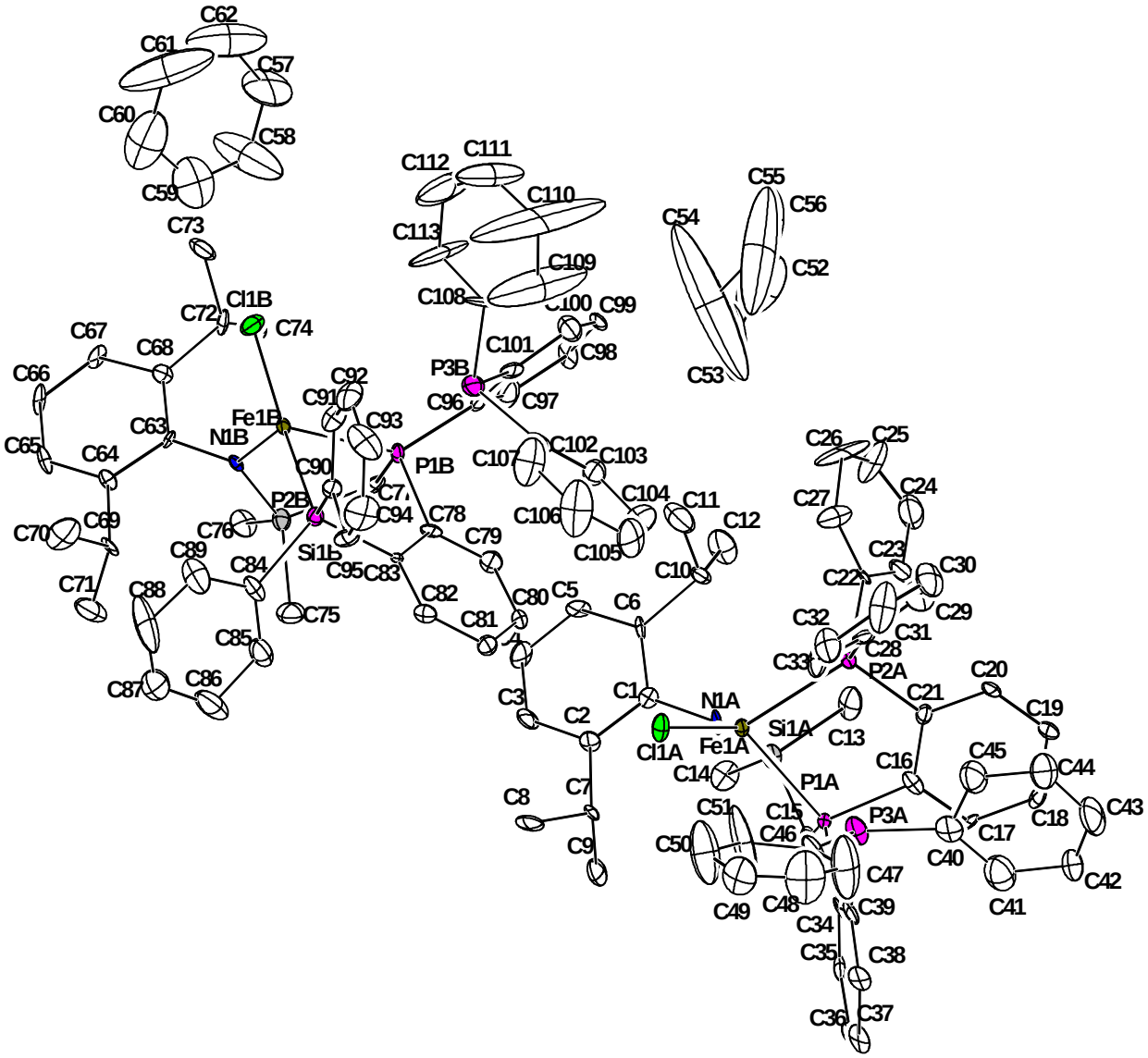

Table 1. Crystal data and structure refinement for [$^{Si}NP_3$]FeCl (**1**).

Identification code	mtw06	
Empirical formula	C56.50 H61 Cl Fe N P3 Si	
Formula weight	966.36	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.8604(17) Å	α= 72.318(3)°.
	b = 20.831(3) Å	β= 83.313(3)°.
	c = 23.586(4) Å	γ = 89.880(3)°.
Volume	5046.3(14) Å^3	
Z	4	
Density (calculated)	1.272 Mg/m^3	
Absorption coefficient	0.509 mm^{-1}	
F(000)	2036	
Crystal size	0.33 x 0.29 x 0.096 mm^3	
Theta range for data collection	1.03 to 25.08°.	
Index ranges	-12<=h<=12, -23<=k<=20, -26<=l<=26	
Reflections collected	19505	
Independent reflections	14316 [R(int) = 0.0801]	
Completeness to theta = 25.08°	79.9 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	14316 / 88 / 1156	
Goodness-of-fit on F^2	1.006	
Final R indices [I>2sigma(I)]	R1 = 0.1253, wR2 = 0.2861	
R indices (all data)	R1 = 0.1841, wR2 = 0.3269	
Largest diff. peak and hole	4.787 and -0.954 e.Å^{-3}	

Special Refinement Details.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full convariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles, and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes. The solvent molecules suffer from disorder in the atomic positions. Due to the low quality of the structure, the following atoms were restrained so that their U_{ij} components approximated isotropic behavior: C8, C17, C24, C25, C67, C72, C85, C86, C87, C88, C89, C101.

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for [$^{Si}NP_3$]FeCl (**1**). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Fe(1A)	8652(1)	1340(1)	2910(1)	10(1)
Fe(1B)	7376(1)	6328(1)	2918(1)	10(1)
Cl(1A)	9818(3)	2244(1)	2344(1)	20(1)
Cl(1B)	6453(3)	7214(1)	2356(1)	21(1)
N(1A)	8025(8)	1235(5)	3736(4)	12(2)
N(1B)	7636(8)	6242(5)	3737(4)	11(2)
P(1A)	9287(3)	183(1)	3175(1)	11(1)
P(2A)	7164(3)	949(1)	2354(1)	12(1)
P(3A)	10397(3)	424(2)	1823(2)	23(1)
P(1B)	6636(3)	5163(1)	3200(1)	12(1)
P(2B)	9124(3)	5943(1)	2343(1)	12(1)
P(3B)	6100(3)	5344(2)	1869(2)	22(1)
Si(1A)	7697(3)	440(2)	4230(1)	15(1)
Si(1B)	7772(3)	5447(2)	4221(1)	15(1)
C(1)	7967(10)	1802(5)	3969(5)	11(2)
C(2)	9023(10)	2050(6)	4126(5)	15(3)
C(3)	8901(11)	2539(6)	4418(5)	20(3)
C(4)	7779(11)	2797(6)	4542(5)	22(3)
C(5)	6727(10)	2584(6)	4343(5)	17(3)
C(6)	6798(10)	2111(5)	4051(5)	12(2)
C(7)	10327(10)	1817(6)	3972(5)	16(3)
C(8)	11260(10)	2407(6)	3693(6)	22(3)
C(9)	10784(12)	1318(6)	4515(5)	24(3)
C(10)	5657(10)	1916(6)	3808(5)	18(3)
C(11)	5315(13)	2523(7)	3311(7)	38(4)
C(12)	4574(12)	1660(8)	4279(6)	35(4)
C(13)	6206(12)	13(7)	4202(6)	29(3)
C(14)	7681(12)	429(6)	5034(5)	24(3)
C(15)	8958(11)	-86(6)	3993(5)	18(3)
C(16)	8153(10)	-304(6)	2932(5)	14(3)
C(17)	8195(10)	-993(5)	3087(5)	9(2)
C(18)	7399(10)	-1382(6)	2908(6)	19(3)
C(19)	6525(10)	-1064(6)	2550(6)	19(3)
C(20)	6459(10)	-361(6)	2384(5)	15(3)
C(21)	7258(10)	25(5)	2563(5)	13(2)
C(22)	5512(9)	1089(5)	2507(5)	12(2)
C(23)	4715(11)	613(7)	2956(6)	32(3)
C(24)	3497(13)	705(6)	3124(6)	42(4)
C(25)	3256(14)	1343(6)	2821(6)	40(4)
C(26)	3803(16)	1833(7)	2325(6)	71(7)
C(27)	5025(13)	1694(7)	2207(6)	35(3)
C(28)	7396(10)	1250(6)	1526(5)	15(3)
C(29)	6572(13)	1091(7)	1182(6)	29(3)
C(30)	6766(14)	1319(7)	577(6)	36(4)
C(31)	7863(16)	1713(7)	288(6)	45(4)
C(32)	8637(14)	1882(7)	623(6)	32(3)
C(33)	8445(12)	1655(6)	1235(6)	26(3)
C(34)	10749(10)	-218(6)	3017(5)	16(3)
C(35)	11331(11)	-643(6)	3472(7)	26(3)
C(36)	12475(13)	-933(7)	3322(8)	38(4)
C(37)	12991(12)	-795(8)	2751(9)	46(5)

C(38)	12405(11)	-371(7)	2289(7)	34(4)
C(39)	11285(11)	-86(6)	2403(6)	23(3)
C(40)	9924(11)	-195(7)	1481(6)	26(3)
C(41)	10003(14)	-896(8)	1744(7)	44(4)
C(42)	9520(15)	-1359(8)	1479(8)	50(5)
C(43)	9014(15)	-1121(9)	962(9)	57(5)
C(44)	8897(15)	-434(8)	698(7)	47(4)
C(45)	9325(13)	17(8)	966(7)	38(4)
C(46)	11595(11)	956(7)	1227(5)	22(3)
C(47)	12072(19)	818(10)	732(8)	73(7)
C(48)	12948(18)	1282(10)	309(8)	65(6)
C(49)	13368(14)	1793(8)	404(7)	43(4)
C(50)	12840(20)	1980(11)	878(8)	77(7)
C(51)	11971(19)	1532(11)	1308(8)	86(8)
C(52)	2390(20)	3496(11)	1511(13)	103(10)
C(53)	3710(20)	3556(13)	1372(12)	121(12)
C(54)	3750(50)	4140(30)	793(13)	398(11)
C(55)	2720(60)	4041(14)	545(13)	310(40)
C(56)	1540(30)	3826(11)	1190(8)	78(7)
C(57)	3510(20)	8532(12)	1117(12)	103(10)
C(58)	4600(20)	8324(13)	1343(13)	142(15)
C(59)	5580(20)	8722(11)	1231(8)	68(6)
C(60)	5490(20)	9385(12)	972(11)	90(8)
C(61)	4350(40)	9577(17)	764(13)	157(19)
C(62)	3310(30)	9165(18)	841(10)	113(12)
C(63)	7591(10)	6802(5)	3957(5)	9(2)
C(64)	8683(10)	7116(6)	4039(5)	11(2)
C(65)	8605(11)	7597(6)	4333(5)	16(3)
C(66)	7462(11)	7798(6)	4535(5)	19(3)
C(67)	6400(11)	7538(6)	4413(5)	17(3)
C(68)	6413(10)	7047(6)	4121(5)	13(2)
C(69)	9979(9)	6928(6)	3811(5)	15(3)
C(70)	10582(13)	7561(7)	3328(7)	39(4)
C(71)	10769(12)	6643(8)	4285(6)	33(3)
C(72)	5198(10)	6812(6)	3971(5)	17(3)
C(73)	4393(11)	7376(7)	3707(6)	27(3)
C(74)	4499(11)	6299(6)	4530(6)	24(3)
C(75)	9299(12)	5022(6)	4164(6)	26(3)
C(76)	7425(12)	5424(7)	5022(5)	23(3)
C(77)	6627(10)	4902(6)	4014(5)	14(2)
C(78)	7883(10)	4684(6)	2941(5)	12(2)
C(79)	7766(11)	3997(6)	3106(6)	22(3)
C(80)	8667(10)	3613(6)	2911(6)	18(3)
C(81)	9699(10)	3931(6)	2535(5)	17(3)
C(82)	9834(10)	4640(6)	2360(5)	14(2)
C(83)	8955(9)	5016(5)	2559(5)	10(2)
C(84)	10706(10)	6107(6)	2476(5)	19(3)
C(85)	11356(11)	5638(7)	2871(6)	30(3)
C(86)	12508(12)	5787(6)	3006(6)	41(4)
C(87)	12872(13)	6442(6)	2736(6)	36(3)
C(88)	12336(16)	6936(8)	2302(7)	70(5)
C(89)	11224(13)	6755(7)	2190(6)	34(3)
C(90)	9263(10)	6248(6)	1521(5)	15(3)
C(91)	8325(12)	6621(6)	1247(6)	25(3)
C(92)	8398(14)	6834(6)	621(6)	30(3)
C(93)	9334(13)	6661(8)	288(6)	36(4)

C(94)	10299(14)	6299(8)	546(6)	37(4)
C(95)	10278(10)	6075(6)	1168(5)	17(3)
C(96)	5245(10)	4746(5)	3076(5)	16(3)
C(97)	4440(12)	4333(6)	3558(7)	30(3)
C(98)	3375(11)	4032(7)	3465(8)	36(4)
C(99)	3079(12)	4130(7)	2911(8)	38(4)
C(100)	3883(12)	4548(7)	2406(7)	37(4)
C(101)	4982(10)	4834(6)	2483(6)	20(3)
C(102)	6781(11)	4698(6)	1554(6)	22(3)
C(103)	6578(11)	4008(6)	1833(6)	28(3)
C(104)	7201(13)	3539(7)	1594(7)	37(4)
C(105)	8048(14)	3758(8)	1073(6)	40(4)
C(106)	8246(18)	4435(9)	805(8)	63(6)
C(107)	7635(17)	4908(8)	1056(7)	51(5)
C(108)	5139(13)	5813(8)	1295(6)	41(4)
C(109)	4830(40)	5620(20)	856(17)	310(40)
C(110)	4120(60)	6040(30)	430(20)	470(60)
C(111)	3749(19)	6616(13)	440(9)	84(8)
C(112)	3970(20)	6769(12)	873(11)	95(9)
C(113)	4680(20)	6372(12)	1321(10)	111(11)

Table 3. Bond lengths [Å] and angles [°] for [$^{Si}NP_3$]FeCl (**1**).

Fe(1A)-N(1A)	1.933(9)	C(9)-H(9B)	0.9800
Fe(1A)-Cl(1A)	2.242(3)	C(9)-H(9C)	0.9800
Fe(1A)-P(1A)	2.420(3)	C(10)-C(12)	1.498(17)
Fe(1A)-P(2A)	2.480(3)	C(10)-C(11)	1.520(18)
Fe(1B)-N(1B)	1.939(9)	C(10)-H(10)	1.0000
Fe(1B)-Cl(1B)	2.233(3)	C(11)-H(11A)	0.9800
Fe(1B)-P(1B)	2.427(3)	C(11)-H(11B)	0.9800
Fe(1B)-P(2B)	2.478(3)	C(11)-H(11C)	0.9800
N(1A)-C(1)	1.445(13)	C(12)-H(12A)	0.9800
N(1A)-Si(1A)	1.720(10)	C(12)-H(12B)	0.9800
N(1B)-C(63)	1.412(13)	C(12)-H(12C)	0.9800
N(1B)-Si(1B)	1.719(10)	C(13)-H(13A)	0.9800
P(1A)-C(15)	1.830(12)	C(13)-H(13B)	0.9800
P(1A)-C(16)	1.842(11)	C(13)-H(13C)	0.9800
P(1A)-C(34)	1.845(11)	C(14)-H(14A)	0.9800
P(2A)-C(22)	1.829(11)	C(14)-H(14B)	0.9800
P(2A)-C(21)	1.841(11)	C(14)-H(14C)	0.9800
P(2A)-C(28)	1.846(12)	C(15)-H(15A)	0.9900
P(3A)-C(40)	1.820(13)	C(15)-H(15B)	0.9900
P(3A)-C(39)	1.831(13)	C(16)-C(17)	1.372(15)
P(3A)-C(46)	1.880(12)	C(16)-C(21)	1.415(16)
P(1B)-C(77)	1.827(11)	C(17)-C(18)	1.372(16)
P(1B)-C(78)	1.837(11)	C(17)-H(17)	0.9500
P(1B)-C(96)	1.839(11)	C(18)-C(19)	1.376(17)
P(2B)-C(84)	1.834(12)	C(18)-H(18)	0.9500
P(2B)-C(90)	1.835(12)	C(19)-C(20)	1.400(16)
P(2B)-C(83)	1.846(10)	C(19)-H(19)	0.9500
P(3B)-C(101)	1.833(12)	C(20)-C(21)	1.370(16)
P(3B)-C(102)	1.839(12)	C(20)-H(20)	0.9500
P(3B)-C(108)	1.844(13)	C(22)-C(27)	1.383(17)
Si(1A)-C(13)	1.866(12)	C(22)-C(23)	1.416(18)
Si(1A)-C(14)	1.887(12)	C(23)-C(24)	1.366(19)
Si(1A)-C(15)	1.890(12)	C(23)-H(23)	0.9500
Si(1B)-C(76)	1.869(12)	C(24)-C(25)	1.346(9)
Si(1B)-C(77)	1.887(11)	C(24)-H(24)	0.9500
Si(1B)-C(75)	1.888(12)	C(25)-C(26)	1.371(10)
C(1)-C(2)	1.392(16)	C(25)-H(25)	0.9500
C(1)-C(6)	1.442(16)	C(26)-C(27)	1.37(2)
C(2)-C(3)	1.392(16)	C(26)-H(26)	0.9500
C(2)-C(7)	1.534(15)	C(27)-H(27)	0.9500
C(3)-C(4)	1.366(17)	C(28)-C(29)	1.379(18)
C(3)-H(3)	0.9500	C(28)-C(33)	1.397(17)
C(4)-C(5)	1.405(17)	C(29)-C(30)	1.351(18)
C(4)-H(4)	0.9500	C(29)-H(29)	0.9500
C(5)-C(6)	1.360(15)	C(30)-C(31)	1.43(2)
C(5)-H(5)	0.9500	C(30)-H(30)	0.9500
C(6)-C(10)	1.529(15)	C(31)-C(32)	1.33(2)
C(7)-C(9)	1.518(17)	C(31)-H(31)	0.9500
C(7)-C(8)	1.526(16)	C(32)-C(33)	1.365(18)
C(7)-H(7)	1.0000	C(32)-H(32)	0.9500
C(8)-H(8A)	0.9800	C(33)-H(33)	0.9500
C(8)-H(8B)	0.9800	C(34)-C(35)	1.384(17)
C(8)-H(8C)	0.9800	C(34)-C(39)	1.440(17)
C(9)-H(9A)	0.9800	C(35)-C(36)	1.436(19)

C(35)-H(35)	0.9500	C(63)-C(64)	1.416(15)
C(36)-C(37)	1.34(2)	C(63)-C(68)	1.431(15)
C(36)-H(36)	0.9500	C(64)-C(65)	1.380(15)
C(37)-C(38)	1.40(2)	C(64)-C(69)	1.539(15)
C(37)-H(37)	0.9500	C(65)-C(66)	1.386(17)
C(38)-C(39)	1.385(17)	C(65)-H(65)	0.9500
C(38)-H(38)	0.9500	C(66)-C(67)	1.371(16)
C(40)-C(45)	1.40(2)	C(66)-H(66)	0.9500
C(40)-C(41)	1.41(2)	C(67)-C(68)	1.396(15)
C(41)-C(42)	1.43(2)	C(67)-H(67)	0.9500
C(41)-H(41)	0.9500	C(68)-C(72)	1.525(16)
C(42)-C(43)	1.35(2)	C(69)-C(71)	1.470(17)
C(42)-H(42)	0.9500	C(69)-C(70)	1.543(18)
C(43)-C(44)	1.39(2)	C(69)-H(69)	1.0000
C(43)-H(43)	0.9500	C(70)-H(70A)	0.9800
C(44)-C(45)	1.39(2)	C(70)-H(70B)	0.9800
C(44)-H(44)	0.9500	C(70)-H(70C)	0.9800
C(45)-H(45)	0.9500	C(71)-H(71A)	0.9800
C(46)-C(47)	1.333(19)	C(71)-H(71B)	0.9800
C(46)-C(51)	1.34(2)	C(71)-H(71C)	0.9800
C(47)-C(48)	1.43(2)	C(72)-C(73)	1.487(17)
C(47)-H(47)	0.9500	C(72)-C(74)	1.541(16)
C(48)-C(49)	1.25(2)	C(72)-H(72)	1.0000
C(48)-H(48)	0.9500	C(73)-H(73A)	0.9800
C(49)-C(50)	1.36(2)	C(73)-H(73B)	0.9800
C(49)-H(49)	0.9500	C(73)-H(73C)	0.9800
C(50)-C(51)	1.41(2)	C(74)-H(74A)	0.9800
C(50)-H(50)	0.9500	C(74)-H(74B)	0.9800
C(51)-H(51)	0.9500	C(74)-H(74C)	0.9800
C(52)-C(56)	1.32(3)	C(75)-H(75A)	0.9800
C(52)-C(53)	1.42(3)	C(75)-H(75B)	0.9800
C(52)-H(52A)	0.9900	C(75)-H(75C)	0.9800
C(52)-H(52B)	0.9900	C(76)-H(76A)	0.9800
C(53)-C(54)	1.53(5)	C(76)-H(76B)	0.9800
C(53)-H(53A)	0.9900	C(76)-H(76C)	0.9800
C(53)-H(53B)	0.9900	C(77)-H(77A)	0.9900
C(54)-C(55)	1.37(6)	C(77)-H(77B)	0.9900
C(54)-H(54A)	0.9900	C(78)-C(79)	1.366(16)
C(54)-H(54B)	0.9900	C(78)-C(83)	1.423(15)
C(55)-C(56)	1.81(6)	C(79)-C(80)	1.388(16)
C(55)-H(55A)	0.9900	C(79)-H(79)	0.9500
C(55)-H(55B)	0.9900	C(80)-C(81)	1.377(16)
C(56)-H(56A)	0.9900	C(80)-H(80)	0.9500
C(56)-H(56B)	0.9900	C(81)-C(82)	1.411(16)
C(57)-C(62)	1.31(3)	C(81)-H(81)	0.9500
C(57)-C(58)	1.36(3)	C(82)-C(83)	1.364(15)
C(57)-H(57)	0.9500	C(82)-H(82)	0.9500
C(58)-C(59)	1.31(3)	C(84)-C(85)	1.384(19)
C(58)-H(58)	0.9500	C(84)-C(89)	1.399(18)
C(59)-C(60)	1.34(3)	C(85)-C(86)	1.385(18)
C(59)-H(59)	0.9500	C(85)-H(85)	0.9500
C(60)-C(61)	1.40(4)	C(86)-C(87)	1.356(9)
C(60)-H(60)	0.9500	C(86)-H(86)	0.9500
C(61)-C(62)	1.38(5)	C(87)-C(88)	1.394(10)
C(61)-H(61)	0.9500	C(87)-H(87)	0.9500
C(62)-H(62)	0.9500	C(88)-C(89)	1.34(2)

C(88)-H(88)	0.9500
C(89)-H(89)	0.9500
C(90)-C(91)	1.380(17)
C(90)-C(95)	1.416(15)
C(91)-C(92)	1.400(18)
C(91)-H(91)	0.9500
C(92)-C(93)	1.33(2)
C(92)-H(92)	0.9500
C(93)-C(94)	1.38(2)
C(93)-H(93)	0.9500
C(94)-C(95)	1.396(18)
C(94)-H(94)	0.9500
C(95)-H(95)	0.9500
C(96)-C(97)	1.405(17)
C(96)-C(101)	1.417(17)
C(97)-C(98)	1.387(18)
C(97)-H(97)	0.9500
C(98)-C(99)	1.34(2)
C(98)-H(98)	0.9500
C(99)-C(100)	1.44(2)
C(99)-H(99)	0.9500
C(100)-C(101)	1.390(18)
C(100)-H(100)	0.9500
C(102)-C(107)	1.37(2)
C(102)-C(103)	1.393(18)
C(103)-C(104)	1.405(18)
C(103)-H(103)	0.9500
C(104)-C(105)	1.40(2)
C(104)-H(104)	0.9500
C(105)-C(106)	1.36(2)
C(105)-H(105)	0.9500
C(106)-C(107)	1.42(2)
C(106)-H(106)	0.9500
C(107)-H(107)	0.9500
C(108)-C(113)	1.28(2)
C(108)-C(109)	1.30(3)
C(109)-C(110)	1.41(4)
C(109)-H(109)	0.9500
C(110)-C(111)	1.27(4)
C(110)-H(110)	0.9500
C(111)-C(112)	1.21(3)
C(111)-H(111)	0.9500
C(112)-C(113)	1.43(3)
C(112)-H(112)	0.9500
C(113)-H(113)	0.9500

N(1A)-Fe(1A)-Cl(1A)	121.8(3)
N(1A)-Fe(1A)-P(1A)	91.0(3)
Cl(1A)-Fe(1A)-P(1A)	125.94(12)
N(1A)-Fe(1A)-P(2A)	113.8(3)
Cl(1A)-Fe(1A)-P(2A)	113.27(12)
P(1A)-Fe(1A)-P(2A)	84.06(10)
N(1B)-Fe(1B)-Cl(1B)	121.9(3)
N(1B)-Fe(1B)-P(1B)	91.5(3)
Cl(1B)-Fe(1B)-P(1B)	125.70(12)
N(1B)-Fe(1B)-P(2B)	114.0(3)
Cl(1B)-Fe(1B)-P(2B)	112.89(12)
P(1B)-Fe(1B)-P(2B)	84.05(10)
C(1)-N(1A)-Si(1A)	118.5(7)
C(1)-N(1A)-Fe(1A)	121.4(7)
Si(1A)-N(1A)-Fe(1A)	119.7(5)
C(63)-N(1B)-Si(1B)	119.6(7)
C(63)-N(1B)-Fe(1B)	121.9(7)
Si(1B)-N(1B)-Fe(1B)	118.3(5)
C(15)-P(1A)-C(16)	104.6(5)
C(15)-P(1A)-C(34)	105.0(5)
C(16)-P(1A)-C(34)	101.7(5)
C(15)-P(1A)-Fe(1A)	102.0(4)
C(16)-P(1A)-Fe(1A)	107.4(4)
C(34)-P(1A)-Fe(1A)	133.4(4)
C(22)-P(2A)-C(21)	104.2(5)
C(22)-P(2A)-C(28)	101.4(5)
C(21)-P(2A)-C(28)	105.8(5)
C(22)-P(2A)-Fe(1A)	118.8(3)
C(21)-P(2A)-Fe(1A)	106.5(4)
C(28)-P(2A)-Fe(1A)	118.8(4)
C(40)-P(3A)-C(39)	101.8(6)
C(40)-P(3A)-C(46)	102.3(5)
C(39)-P(3A)-C(46)	104.9(6)
C(77)-P(1B)-C(78)	104.2(5)
C(77)-P(1B)-C(96)	105.0(5)
C(78)-P(1B)-C(96)	101.8(5)
C(77)-P(1B)-Fe(1B)	101.7(4)
C(78)-P(1B)-Fe(1B)	107.4(4)
C(96)-P(1B)-Fe(1B)	133.7(4)
C(84)-P(2B)-C(90)	101.2(5)
C(84)-P(2B)-C(83)	104.7(5)
C(90)-P(2B)-C(83)	106.4(5)
C(84)-P(2B)-Fe(1B)	118.1(3)
C(90)-P(2B)-Fe(1B)	118.4(4)
C(83)-P(2B)-Fe(1B)	106.7(4)
C(101)-P(3B)-C(102)	101.4(6)
C(101)-P(3B)-C(108)	104.6(7)
C(102)-P(3B)-C(108)	103.1(6)
N(1A)-Si(1A)-C(13)	117.4(6)
N(1A)-Si(1A)-C(14)	111.9(5)
C(13)-Si(1A)-C(14)	105.6(6)
N(1A)-Si(1A)-C(15)	103.7(5)
C(13)-Si(1A)-C(15)	105.4(6)
C(14)-Si(1A)-C(15)	112.8(5)
N(1B)-Si(1B)-C(76)	111.9(5)
N(1B)-Si(1B)-C(77)	104.7(5)
C(76)-Si(1B)-C(77)	111.5(5)
N(1B)-Si(1B)-C(75)	118.2(5)
C(76)-Si(1B)-C(75)	105.9(6)
C(77)-Si(1B)-C(75)	104.5(5)
C(2)-C(1)-C(6)	119.1(10)
C(2)-C(1)-N(1A)	120.9(9)
C(6)-C(1)-N(1A)	119.9(9)
C(3)-C(2)-C(1)	119.0(10)
C(3)-C(2)-C(7)	118.6(10)
C(1)-C(2)-C(7)	122.3(10)

C(4)-C(3)-C(2)	122.0(11)
C(4)-C(3)-H(3)	119.0
C(2)-C(3)-H(3)	119.0
C(3)-C(4)-C(5)	118.9(11)
C(3)-C(4)-H(4)	120.5
C(5)-C(4)-H(4)	120.5
C(6)-C(5)-C(4)	121.4(10)
C(6)-C(5)-H(5)	119.3
C(4)-C(5)-H(5)	119.3
C(5)-C(6)-C(1)	119.0(10)
C(5)-C(6)-C(10)	120.5(10)
C(1)-C(6)-C(10)	120.5(9)
C(9)-C(7)-C(8)	110.7(9)
C(9)-C(7)-C(2)	111.6(10)
C(8)-C(7)-C(2)	112.4(9)
C(9)-C(7)-H(7)	107.3
C(8)-C(7)-H(7)	107.3
C(2)-C(7)-H(7)	107.3
C(7)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(7)-C(9)-H(9A)	109.5
C(7)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(7)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(12)-C(10)-C(11)	111.0(11)
C(12)-C(10)-C(6)	113.5(10)
C(11)-C(10)-C(6)	108.3(10)
C(12)-C(10)-H(10)	108.0
C(11)-C(10)-H(10)	108.0
C(6)-C(10)-H(10)	108.0
C(10)-C(11)-H(11A)	109.5
C(10)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(10)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(10)-C(12)-H(12A)	109.5
C(10)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(10)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
Si(1A)-C(13)-H(13A)	109.5
Si(1A)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
Si(1A)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
Si(1A)-C(14)-H(14A)	109.5
Si(1A)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
Si(1A)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
P(1A)-C(15)-Si(1A)	109.8(6)
P(1A)-C(15)-H(15A)	109.7
Si(1A)-C(15)-H(15A)	109.7
P(1A)-C(15)-H(15B)	109.7
Si(1A)-C(15)-H(15B)	109.7
H(15A)-C(15)-H(15B)	108.2
C(17)-C(16)-C(21)	118.8(10)
C(17)-C(16)-P(1A)	120.3(9)
C(21)-C(16)-P(1A)	120.9(8)
C(18)-C(17)-C(16)	123.1(11)
C(18)-C(17)-H(17)	118.5
C(16)-C(17)-H(17)	118.5
C(17)-C(18)-C(19)	118.3(11)
C(17)-C(18)-H(18)	120.8
C(19)-C(18)-H(18)	120.8
C(18)-C(19)-C(20)	120.0(11)
C(18)-C(19)-H(19)	120.0
C(20)-C(19)-H(19)	120.0
C(21)-C(20)-C(19)	121.5(11)
C(21)-C(20)-H(20)	119.3
C(19)-C(20)-H(20)	119.3
C(20)-C(21)-C(16)	118.4(10)
C(20)-C(21)-P(2A)	121.7(9)
C(16)-C(21)-P(2A)	119.9(8)
C(27)-C(22)-C(23)	117.9(11)
C(27)-C(22)-P(2A)	119.8(9)
C(23)-C(22)-P(2A)	122.1(9)
C(24)-C(23)-C(22)	125.2(13)
C(24)-C(23)-H(23)	117.4
C(22)-C(23)-H(23)	117.4
C(25)-C(24)-C(23)	106.8(14)
C(25)-C(24)-H(24)	126.6
C(23)-C(24)-H(24)	126.6
C(24)-C(25)-C(26)	136.1(14)
C(24)-C(25)-H(25)	111.9
C(26)-C(25)-H(25)	111.9
C(25)-C(26)-C(27)	109.8(12)
C(25)-C(26)-H(26)	125.1
C(27)-C(26)-H(26)	125.1
C(26)-C(27)-C(22)	121.9(13)
C(26)-C(27)-H(27)	119.0
C(22)-C(27)-H(27)	119.0
C(29)-C(28)-C(33)	118.5(11)
C(29)-C(28)-P(2A)	122.5(9)
C(33)-C(28)-P(2A)	119.0(9)
C(30)-C(29)-C(28)	121.2(13)
C(30)-C(29)-H(29)	119.4
C(28)-C(29)-H(29)	119.4
C(29)-C(30)-C(31)	119.5(13)
C(29)-C(30)-H(30)	120.3
C(31)-C(30)-H(30)	120.3
C(32)-C(31)-C(30)	118.9(12)

C(32)-C(31)-H(31)	120.6
C(30)-C(31)-H(31)	120.6
C(31)-C(32)-C(33)	121.9(13)
C(31)-C(32)-H(32)	119.1
C(33)-C(32)-H(32)	119.1
C(32)-C(33)-C(28)	119.9(12)
C(32)-C(33)-H(33)	120.0
C(28)-C(33)-H(33)	120.0
C(35)-C(34)-C(39)	119.6(11)
C(35)-C(34)-P(1A)	121.6(9)
C(39)-C(34)-P(1A)	118.8(9)
C(34)-C(35)-C(36)	119.0(13)
C(34)-C(35)-H(35)	120.5
C(36)-C(35)-H(35)	120.5
C(37)-C(36)-C(35)	121.3(14)
C(37)-C(36)-H(36)	119.4
C(35)-C(36)-H(36)	119.4
C(36)-C(37)-C(38)	120.0(13)
C(36)-C(37)-H(37)	120.0
C(38)-C(37)-H(37)	120.0
C(39)-C(38)-C(37)	121.5(14)
C(39)-C(38)-H(38)	119.2
C(37)-C(38)-H(38)	119.2
C(38)-C(39)-C(34)	118.5(12)
C(38)-C(39)-P(3A)	124.4(11)
C(34)-C(39)-P(3A)	117.0(9)
C(45)-C(40)-C(41)	116.9(13)
C(45)-C(40)-P(3A)	119.4(11)
C(41)-C(40)-P(3A)	123.3(11)
C(40)-C(41)-C(42)	120.7(15)
C(40)-C(41)-H(41)	119.7
C(42)-C(41)-H(41)	119.7
C(43)-C(42)-C(41)	119.5(16)
C(43)-C(42)-H(42)	120.3
C(41)-C(42)-H(42)	120.3
C(42)-C(43)-C(44)	121.2(14)
C(42)-C(43)-H(43)	119.4
C(44)-C(43)-H(43)	119.4
C(45)-C(44)-C(43)	119.4(15)
C(45)-C(44)-H(44)	120.3
C(43)-C(44)-H(44)	120.3
C(44)-C(45)-C(40)	122.1(15)
C(44)-C(45)-H(45)	118.9
C(40)-C(45)-H(45)	118.9
C(47)-C(46)-C(51)	118.1(13)
C(47)-C(46)-P(3A)	125.8(11)
C(51)-C(46)-P(3A)	116.1(10)
C(46)-C(47)-C(48)	119.5(15)
C(46)-C(47)-H(47)	120.3
C(48)-C(47)-H(47)	120.2
C(49)-C(48)-C(47)	122.4(16)
C(49)-C(48)-H(48)	118.8
C(47)-C(48)-H(48)	118.8
C(48)-C(49)-C(50)	119.5(15)
C(48)-C(49)-H(49)	120.2
C(50)-C(49)-H(49)	120.2
C(49)-C(50)-C(51)	118.9(17)
C(49)-C(50)-H(50)	120.6
C(51)-C(50)-H(50)	120.6
C(46)-C(51)-C(50)	120.7(16)
C(46)-C(51)-H(51)	119.7
C(50)-C(51)-H(51)	119.7
C(56)-C(52)-C(53)	129(3)
C(56)-C(52)-H(52A)	105.2
C(53)-C(52)-H(52A)	105.2
C(56)-C(52)-H(52B)	105.2
C(53)-C(52)-H(52B)	105.2
H(52A)-C(52)-H(52B)	105.9
C(52)-C(53)-C(54)	97(3)
C(52)-C(53)-H(53A)	112.3
C(54)-C(53)-H(53A)	112.3
C(52)-C(53)-H(53B)	112.3
C(54)-C(53)-H(53B)	112.3
H(53A)-C(53)-H(53B)	109.9
C(55)-C(54)-C(53)	104(2)
C(55)-C(54)-H(54A)	110.9
C(53)-C(54)-H(54A)	110.9
C(55)-C(54)-H(54B)	110.9
C(53)-C(54)-H(54B)	110.9
H(54A)-C(54)-H(54B)	108.9
C(54)-C(55)-C(56)	102(2)
C(54)-C(55)-H(55A)	111.3
C(56)-C(55)-H(55A)	111.3
C(54)-C(55)-H(55B)	111.3
C(56)-C(55)-H(55B)	111.3
H(55A)-C(55)-H(55B)	109.2
C(52)-C(56)-C(55)	88(2)
C(52)-C(56)-H(56A)	114.1
C(55)-C(56)-H(56A)	114.1
C(52)-C(56)-H(56B)	114.1
C(55)-C(56)-H(56B)	114.1
H(56A)-C(56)-H(56B)	111.2
C(62)-C(57)-C(58)	123(3)
C(62)-C(57)-H(57)	118.3
C(58)-C(57)-H(57)	118.3
C(59)-C(58)-C(57)	123(2)
C(59)-C(58)-H(58)	118.7
C(57)-C(58)-H(58)	118.7
C(58)-C(59)-C(60)	120(2)
C(58)-C(59)-H(59)	120.1
C(60)-C(59)-H(59)	120.1
C(59)-C(60)-C(61)	115(3)
C(59)-C(60)-H(60)	122.7
C(61)-C(60)-H(60)	122.7
C(62)-C(61)-C(60)	127(3)
C(62)-C(61)-H(61)	116.6
C(60)-C(61)-H(61)	116.6
C(57)-C(62)-C(61)	112(2)
C(57)-C(62)-H(62)	124.1
C(61)-C(62)-H(62)	124.1
N(1B)-C(63)-C(64)	121.6(9)
N(1B)-C(63)-C(68)	119.4(9)

C(64)-C(63)-C(68)	118.9(9)
C(65)-C(64)-C(63)	120.1(10)
C(65)-C(64)-C(69)	118.4(9)
C(63)-C(64)-C(69)	121.5(9)
C(64)-C(65)-C(66)	120.9(10)
C(64)-C(65)-H(65)	119.6
C(66)-C(65)-H(65)	119.6
C(67)-C(66)-C(65)	119.3(10)
C(67)-C(66)-H(66)	120.3
C(65)-C(66)-H(66)	120.3
C(66)-C(67)-C(68)	122.7(10)
C(66)-C(67)-H(67)	118.7
C(68)-C(67)-H(67)	118.7
C(67)-C(68)-C(63)	117.7(10)
C(67)-C(68)-C(72)	119.5(10)
C(63)-C(68)-C(72)	122.8(10)
C(71)-C(69)-C(64)	114.3(10)
C(71)-C(69)-C(70)	112.6(11)
C(64)-C(69)-C(70)	107.5(10)
C(71)-C(69)-H(69)	107.4
C(64)-C(69)-H(69)	107.4
C(70)-C(69)-H(69)	107.4
C(69)-C(70)-H(70A)	109.5
C(69)-C(70)-H(70B)	109.5
H(70A)-C(70)-H(70B)	109.5
C(69)-C(70)-H(70C)	109.5
H(70A)-C(70)-H(70C)	109.5
H(70B)-C(70)-H(70C)	109.5
C(69)-C(71)-H(71A)	109.5
C(69)-C(71)-H(71B)	109.5
H(71A)-C(71)-H(71B)	109.5
C(69)-C(71)-H(71C)	109.5
H(71A)-C(71)-H(71C)	109.5
H(71B)-C(71)-H(71C)	109.5
C(73)-C(72)-C(68)	113.2(9)
C(73)-C(72)-C(74)	111.0(10)
C(68)-C(72)-C(74)	110.2(10)
C(73)-C(72)-H(72)	107.4
C(68)-C(72)-H(72)	107.4
C(74)-C(72)-H(72)	107.4
C(72)-C(73)-H(73A)	109.5
C(72)-C(73)-H(73B)	109.5
H(73A)-C(73)-H(73B)	109.5
C(72)-C(73)-H(73C)	109.5
H(73A)-C(73)-H(73C)	109.5
H(73B)-C(73)-H(73C)	109.5
C(72)-C(74)-H(74A)	109.5
C(72)-C(74)-H(74B)	109.5
H(74A)-C(74)-H(74B)	109.5
C(72)-C(74)-H(74C)	109.5
H(74A)-C(74)-H(74C)	109.5
H(74B)-C(74)-H(74C)	109.5
Si(1B)-C(75)-H(75A)	109.5
Si(1B)-C(75)-H(75B)	109.5
H(75A)-C(75)-H(75B)	109.5
Si(1B)-C(75)-H(75C)	109.5
H(75A)-C(75)-H(75C)	109.5
H(75B)-C(75)-H(75C)	109.5
Si(1B)-C(76)-H(76A)	109.5
Si(1B)-C(76)-H(76B)	109.5
H(76A)-C(76)-H(76B)	109.5
Si(1B)-C(76)-H(76C)	109.5
H(76A)-C(76)-H(76C)	109.5
H(76B)-C(76)-H(76C)	109.5
P(1B)-C(77)-Si(1B)	109.7(6)
P(1B)-C(77)-H(77A)	109.7
Si(1B)-C(77)-H(77A)	109.7
P(1B)-C(77)-H(77B)	109.7
Si(1B)-C(77)-H(77B)	109.7
H(77A)-C(77)-H(77B)	108.2
C(79)-C(78)-C(83)	119.3(10)
C(79)-C(78)-P(1B)	119.4(8)
C(83)-C(78)-P(1B)	121.3(8)
C(78)-C(79)-C(80)	121.7(11)
C(78)-C(79)-H(79)	119.1
C(80)-C(79)-H(79)	119.1
C(81)-C(80)-C(79)	119.3(11)
C(81)-C(80)-H(80)	120.3
C(79)-C(80)-H(80)	120.3
C(80)-C(81)-C(82)	119.7(10)
C(80)-C(81)-H(81)	120.1
C(82)-C(81)-H(81)	120.1
C(83)-C(82)-C(81)	120.8(10)
C(83)-C(82)-H(82)	119.6
C(81)-C(82)-H(82)	119.6
C(82)-C(83)-C(78)	119.2(10)
C(82)-C(83)-P(2B)	121.5(8)
C(78)-C(83)-P(2B)	119.4(8)
C(85)-C(84)-C(89)	119.8(12)
C(85)-C(84)-P(2B)	123.0(9)
C(89)-C(84)-P(2B)	117.0(10)
C(84)-C(85)-C(86)	122.5(13)
C(84)-C(85)-H(85)	118.8
C(86)-C(85)-H(85)	118.7
C(87)-C(86)-C(85)	112.3(14)
C(87)-C(86)-H(86)	123.9
C(85)-C(86)-H(86)	123.9
C(86)-C(87)-C(88)	129.3(14)
C(86)-C(87)-H(87)	115.3
C(88)-C(87)-H(87)	115.3
C(89)-C(88)-C(87)	114.7(14)
C(89)-C(88)-H(88)	122.7
C(87)-C(88)-H(88)	122.7
C(88)-C(89)-C(84)	120.9(13)
C(88)-C(89)-H(89)	119.6
C(84)-C(89)-H(89)	119.6
C(91)-C(90)-C(95)	119.9(11)
C(91)-C(90)-P(2B)	119.0(9)
C(95)-C(90)-P(2B)	121.0(9)
C(90)-C(91)-C(92)	119.5(12)
C(90)-C(91)-H(91)	120.2
C(92)-C(91)-H(91)	120.2

C(93)-C(92)-C(91)	120.9(13)	C(102)-C(103)-C(104)	120.7(13)
C(93)-C(92)-H(92)	119.5	C(102)-C(103)-H(103)	119.6
C(91)-C(92)-H(92)	119.5	C(104)-C(103)-H(103)	119.6
C(92)-C(93)-C(94)	121.1(13)	C(105)-C(104)-C(103)	120.4(14)
C(92)-C(93)-H(93)	119.5	C(105)-C(104)-H(104)	119.8
C(94)-C(93)-H(93)	119.5	C(103)-C(104)-H(104)	119.8
C(93)-C(94)-C(95)	120.4(12)	C(106)-C(105)-C(104)	118.4(14)
C(93)-C(94)-H(94)	119.8	C(106)-C(105)-H(105)	120.8
C(95)-C(94)-H(94)	119.8	C(104)-C(105)-H(105)	120.8
C(94)-C(95)-C(90)	118.1(11)	C(105)-C(106)-C(107)	121.0(14)
C(94)-C(95)-H(95)	121.0	C(105)-C(106)-H(106)	119.5
C(90)-C(95)-H(95)	121.0	C(107)-C(106)-H(106)	119.5
C(97)-C(96)-C(101)	118.9(11)	C(102)-C(107)-C(106)	120.9(14)
C(97)-C(96)-P(1B)	121.4(10)	C(102)-C(107)-H(107)	119.5
C(101)-C(96)-P(1B)	119.7(9)	C(106)-C(107)-H(107)	119.5
C(98)-C(97)-C(96)	121.4(14)	C(113)-C(108)-C(109)	114.5(17)
C(98)-C(97)-H(97)	119.3	C(113)-C(108)-P(3B)	119.9(12)
C(96)-C(97)-H(97)	119.3	C(109)-C(108)-P(3B)	125.6(16)
C(99)-C(98)-C(97)	120.8(14)	C(108)-C(109)-C(110)	120(3)
C(99)-C(98)-H(98)	119.6	C(108)-C(109)-H(109)	120.2
C(97)-C(98)-H(98)	119.6	C(110)-C(109)-H(109)	120.2
C(98)-C(99)-C(100)	119.4(12)	C(111)-C(110)-C(109)	125(3)
C(98)-C(99)-H(99)	120.3	C(111)-C(110)-H(110)	117.5
C(100)-C(99)-H(99)	120.3	C(109)-C(110)-H(110)	117.5
C(101)-C(100)-C(99)	121.1(14)	C(112)-C(111)-C(110)	114(2)
C(101)-C(100)-H(100)	119.4	C(112)-C(111)-H(111)	122.8
C(99)-C(100)-H(100)	119.4	C(110)-C(111)-H(111)	122.8
C(100)-C(101)-C(96)	118.1(12)	C(111)-C(112)-C(113)	123.9(19)
C(100)-C(101)-P(3B)	124.5(11)	C(111)-C(112)-H(112)	118.0
C(96)-C(101)-P(3B)	117.3(8)	C(113)-C(112)-H(112)	118.0
C(107)-C(102)-C(103)	118.4(13)	C(108)-C(113)-C(112)	122.1(17)
C(107)-C(102)-P(3B)	117.8(11)	C(108)-C(113)-H(113)	118.9
C(103)-C(102)-P(3B)	123.4(10)	C(112)-C(113)-H(113)	118.9

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for [$^{Si}NP_3$]FeCl (**1**). The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Fe(1A)	8(1)	11(1)	12(1)	-7(1)	2(1)	-2(1)
Fe(1B)	8(1)	11(1)	14(1)	-8(1)	-1(1)	0(1)
Cl(1A)	23(2)	15(2)	22(2)	-9(1)	4(1)	-8(1)
Cl(1B)	25(2)	16(2)	22(2)	-7(1)	-6(1)	8(1)
N(1A)	14(5)	17(5)	12(5)	-14(4)	2(4)	-6(4)
N(1B)	5(5)	19(5)	15(5)	-14(4)	-2(4)	2(4)
P(1A)	9(2)	9(2)	18(2)	-7(1)	-4(1)	1(1)
P(2A)	9(2)	12(2)	17(2)	-8(1)	-3(1)	0(1)
P(3A)	14(2)	35(2)	26(2)	-20(2)	7(1)	-7(1)
P(1B)	8(1)	11(2)	18(2)	-9(1)	3(1)	-3(1)
P(2B)	11(2)	12(2)	15(2)	-6(1)	1(1)	-1(1)
P(3B)	21(2)	26(2)	26(2)	-16(2)	-11(1)	7(1)
Si(1A)	17(2)	17(2)	11(2)	-6(1)	2(1)	-4(1)
Si(1B)	18(2)	15(2)	13(2)	-6(1)	-3(1)	-1(1)
C(1)	14(6)	13(6)	5(6)	-1(5)	3(4)	-1(5)
C(2)	9(6)	19(7)	17(6)	-9(5)	3(5)	-1(5)
C(3)	17(6)	30(7)	22(7)	-17(6)	-12(5)	5(5)
C(4)	27(7)	23(7)	22(7)	-17(6)	1(5)	3(6)
C(5)	10(6)	29(7)	18(6)	-16(6)	0(5)	9(5)
C(6)	15(6)	9(6)	12(6)	-4(5)	-3(5)	-7(5)
C(7)	11(6)	19(7)	28(7)	-17(6)	-13(5)	5(5)
C(8)	6(5)	28(6)	30(6)	-6(5)	-1(5)	5(5)
C(9)	28(7)	26(7)	24(7)	-14(6)	-11(6)	-2(6)
C(10)	10(6)	26(7)	25(7)	-19(6)	-8(5)	6(5)
C(11)	28(8)	46(9)	43(9)	-12(8)	-16(7)	-5(7)
C(12)	20(7)	52(10)	39(9)	-27(8)	10(6)	-9(7)
C(13)	25(7)	25(7)	34(8)	-11(6)	13(6)	-12(6)
C(14)	34(8)	25(7)	10(6)	-3(5)	3(5)	0(6)
C(15)	23(7)	15(6)	20(7)	-7(5)	-14(5)	-1(5)
C(16)	7(6)	28(7)	9(6)	-10(5)	4(4)	-5(5)
C(17)	11(4)	7(4)	11(4)	-4(3)	3(3)	4(3)
C(18)	11(6)	8(6)	36(8)	-7(6)	7(5)	-3(5)
C(19)	5(6)	22(7)	33(7)	-12(6)	-2(5)	0(5)
C(20)	6(6)	14(6)	26(7)	-5(5)	-4(5)	-1(5)
C(21)	13(6)	10(6)	17(6)	-5(5)	0(5)	-1(5)
C(22)	7(6)	17(6)	18(6)	-12(5)	-7(5)	1(5)
C(23)	13(7)	52(9)	48(9)	-37(8)	-10(6)	5(6)
C(24)	29(7)	48(7)	62(8)	-37(6)	-3(6)	-4(6)
C(25)	59(6)	27(5)	36(5)	-24(4)	25(4)	1(4)
C(26)	114(17)	72(13)	40(10)	-24(10)	-47(11)	83(13)
C(27)	35(9)	30(8)	40(9)	-8(7)	-9(7)	17(7)
C(28)	10(6)	14(6)	20(7)	-5(5)	-1(5)	6(5)
C(29)	37(8)	34(8)	15(7)	-3(6)	-5(6)	-1(6)
C(30)	48(9)	35(9)	25(8)	-5(7)	-19(7)	-7(7)
C(31)	96(14)	28(8)	5(7)	-2(6)	7(7)	-22(8)
C(32)	49(9)	21(7)	21(8)	5(6)	-12(6)	-9(6)
C(33)	36(8)	12(7)	27(8)	-3(6)	-3(6)	-8(6)
C(34)	10(6)	17(6)	25(7)	-13(5)	-8(5)	-3(5)
C(35)	20(7)	17(7)	50(9)	-22(7)	-9(6)	-3(5)
C(36)	26(8)	22(8)	75(12)	-20(8)	-31(8)	0(6)
C(37)	1(6)	53(10)	108(15)	-61(11)	2(8)	-2(6)

C(38)	4(6)	46(9)	69(11)	-47(8)	1(6)	5(6)
C(39)	10(6)	25(7)	41(8)	-20(6)	-8(6)	-4(5)
C(40)	10(6)	36(8)	33(8)	-19(7)	10(5)	-1(6)
C(41)	33(9)	53(11)	51(10)	-27(9)	1(7)	-4(7)
C(42)	47(10)	41(10)	83(13)	-43(10)	-35(9)	8(8)
C(43)	44(10)	71(13)	87(14)	-65(12)	-18(10)	3(9)
C(44)	58(11)	54(11)	50(10)	-43(9)	-25(8)	12(8)
C(45)	33(8)	45(9)	46(10)	-29(8)	-6(7)	1(7)
C(46)	12(6)	39(8)	23(7)	-20(6)	3(5)	-7(6)
C(47)	92(15)	85(14)	52(12)	-52(11)	35(10)	-52(12)
C(48)	76(14)	75(14)	41(11)	-26(10)	27(9)	-23(11)
C(49)	31(9)	45(10)	45(10)	-12(8)	19(7)	-14(7)
C(50)	99(16)	79(14)	53(12)	-26(11)	16(11)	-63(13)
C(51)	89(15)	125(18)	48(11)	-55(12)	47(10)	-99(14)
C(52)	86(18)	59(15)	140(20)	-25(15)	87(17)	-26(13)
C(53)	92(17)	130(20)	170(30)	-120(20)	82(18)	-88(16)
C(54)	410(30)	700(50)	60(20)	-130(30)	110(30)	-515
C(55)	810(120)	61(18)	80(20)	25(15)	-220(50)	-120(40)
C(56)	130(20)	71(15)	39(12)	-39(11)	8(12)	-34(14)
C(57)	110(20)	72(16)	120(20)	6(15)	-99(18)	19(14)
C(58)	70(16)	120(20)	160(30)	100(20)	-67(17)	-55(15)
C(59)	81(15)	86(16)	38(11)	-24(11)	4(9)	-15(12)
C(60)	92(18)	65(15)	106(19)	-37(14)	49(15)	-22(13)
C(61)	160(30)	140(30)	90(20)	55(19)	50(20)	110(30)
C(62)	90(20)	190(30)	40(13)	-17(17)	-8(13)	90(20)
C(63)	12(6)	4(5)	12(6)	-4(5)	-1(4)	1(4)
C(64)	7(6)	16(6)	10(6)	-3(5)	2(4)	-5(5)
C(65)	19(6)	20(7)	11(6)	-7(5)	-2(5)	-11(5)
C(66)	29(7)	17(7)	18(7)	-17(5)	3(5)	-6(5)
C(67)	18(5)	16(5)	22(6)	-16(5)	5(4)	4(4)
C(68)	12(6)	19(6)	11(6)	-7(5)	-1(5)	2(5)
C(69)	2(5)	23(7)	26(7)	-15(6)	-1(5)	-2(5)
C(70)	29(8)	32(8)	48(10)	-10(7)	18(7)	1(6)
C(71)	20(7)	52(10)	35(8)	-22(7)	-13(6)	8(6)
C(72)	11(5)	12(5)	29(6)	-15(5)	11(4)	-7(4)
C(73)	12(6)	39(8)	37(8)	-19(7)	-11(6)	2(6)
C(74)	9(6)	28(7)	37(8)	-15(6)	6(5)	-8(5)
C(75)	27(7)	26(7)	25(7)	-7(6)	-11(6)	9(6)
C(76)	29(7)	30(8)	12(6)	-5(6)	-7(5)	0(6)
C(77)	12(6)	12(6)	17(6)	-5(5)	6(5)	4(5)
C(78)	4(5)	18(6)	14(5)	-6(4)	0(4)	3(4)
C(79)	10(6)	21(7)	36(8)	-12(6)	4(5)	-2(5)
C(80)	12(6)	14(6)	34(7)	-12(6)	-7(5)	0(5)
C(81)	13(6)	19(7)	23(7)	-14(6)	-1(5)	2(5)
C(82)	10(6)	16(6)	12(6)	0(5)	2(4)	-1(5)
C(83)	6(5)	5(5)	20(6)	-3(5)	-7(5)	1(4)
C(84)	13(6)	29(7)	18(7)	-11(6)	-2(5)	-6(5)
C(85)	16(6)	41(7)	44(7)	-29(6)	-1(5)	-2(5)
C(86)	17(6)	66(8)	48(7)	-29(6)	-7(5)	0(6)
C(87)	40(4)	36(4)	37(4)	-14(2)	-13(2)	2(2)
C(88)	82(9)	68(9)	59(9)	-17(7)	-7(7)	-57(7)
C(89)	42(7)	31(7)	21(6)	6(5)	-10(5)	-17(6)
C(90)	9(6)	15(6)	20(7)	-7(5)	3(5)	-1(5)
C(91)	31(8)	18(7)	27(8)	-10(6)	0(6)	4(6)
C(92)	51(9)	17(7)	24(8)	-1(6)	-17(7)	6(6)
C(93)	38(9)	51(10)	11(7)	2(7)	-7(6)	-13(7)

C(94)	41(9)	54(10)	22(8)	-22(7)	9(6)	7(7)
C(95)	12(6)	17(6)	19(7)	-4(5)	4(5)	5(5)
C(96)	9(6)	9(6)	31(7)	-11(5)	1(5)	1(5)
C(97)	27(8)	22(7)	44(9)	-20(7)	7(6)	0(6)
C(98)	7(6)	28(8)	77(12)	-27(8)	7(7)	-12(6)
C(99)	8(7)	37(9)	92(13)	-49(9)	-21(8)	11(6)
C(100)	21(8)	44(9)	62(11)	-37(8)	-13(7)	7(7)
C(101)	9(5)	18(6)	37(6)	-12(5)	-1(5)	6(4)
C(102)	16(6)	34(8)	26(7)	-16(6)	-14(5)	5(6)
C(103)	16(7)	23(8)	47(9)	-17(7)	2(6)	-2(5)
C(104)	38(9)	33(8)	41(9)	-15(7)	-2(7)	9(7)
C(105)	50(10)	47(10)	34(9)	-30(8)	0(7)	-4(8)
C(106)	88(14)	57(12)	40(10)	-22(9)	31(9)	-34(10)
C(107)	79(13)	41(10)	30(9)	-15(8)	11(8)	-14(9)
C(108)	25(8)	81(12)	36(9)	-41(9)	-26(6)	41(8)
C(109)	450(70)	420(60)	250(40)	-320(50)	-320(50)	400(60)
C(110)	710(110)	690(100)	300(50)	-430(70)	-460(70)	670(100)
C(111)	73(14)	140(20)	41(12)	-22(13)	-23(10)	78(14)
C(112)	120(20)	93(17)	97(19)	-61(15)	-43(16)	84(16)
C(113)	170(20)	123(19)	103(18)	-90(16)	-105(18)	136(19)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for mtw06.

	x	y	z	U(eq)
H(3)	9619	2699	4536	24
H(4)	7711	3115	4758	26
H(5)	5951	2774	4415	21
H(7)	10268	1577	3667	20
H(8A)	11379	2637	3989	33
H(8B)	10947	2724	3345	33
H(8C)	12054	2238	3565	33
H(9A)	11633	1198	4407	36
H(9B)	10241	912	4650	36
H(9C)	10773	1523	4839	36
H(10)	5891	1549	3627	21
H(11A)	5229	2914	3460	58
H(11B)	4528	2426	3184	58
H(11C)	5968	2622	2970	58
H(12A)	4211	2036	4400	53
H(12B)	4853	1327	4628	53
H(12C)	3950	1448	4119	53
H(13A)	5547	341	4149	43
H(13B)	5991	-352	4577	43
H(13C)	6296	-173	3865	43
H(14A)	8439	656	5076	36
H(14B)	7639	-39	5295	36
H(14C)	6956	664	5147	36
H(15A)	9719	-33	4170	22
H(15B)	8688	-568	4141	22
H(17)	8804	-1211	3331	11
H(18)	7449	-1859	3027	23
H(19)	5966	-1322	2417	23
H(20)	5847	-147	2140	19
H(23)	5054	196	3156	39
H(24)	2930	382	3402	50
H(25)	2520	1492	2995	48
H(26)	3397	2212	2097	85
H(27)	5551	2022	1910	42
H(29)	5854	817	1375	35
H(30)	6177	1217	347	43
H(31)	8040	1854	-137	54
H(32)	9342	2167	431	39
H(33)	9025	1773	1462	31
H(35)	10979	-741	3879	31
H(36)	12874	-1229	3632	45
H(37)	13756	-987	2661	56
H(38)	12782	-275	1887	40
H(41)	10382	-1063	2102	52
H(42)	9554	-1831	1665	60
H(43)	8734	-1429	775	69
H(44)	8526	-274	338	56
H(45)	9207	485	793	46
H(47)	11831	413	662	88
H(48)	13221	1201	-60	78

H(49)	14052	2049	147	51
H(50)	13054	2404	919	93
H(51)	11648	1640	1659	103
H(52A)	2184	3012	1586	124
H(52B)	2223	3578	1904	124
H(53A)	4063	3145	1303	146
H(53B)	4115	3672	1683	146
H(54A)	3729	4581	879	478
H(54B)	4518	4139	521	478
H(55A)	2827	3667	368	374
H(55B)	2517	4454	234	374
H(56A)	1225	4219	1309	93
H(56B)	847	3534	1158	93
H(57)	2879	8202	1160	124
H(58)	4636	7872	1592	170
H(59)	6360	8542	1333	82
H(60)	6153	9700	933	108
H(61)	4283	10039	546	188
H(62)	2535	9321	710	136
H(65)	9343	7793	4399	20
H(66)	7416	8113	4755	23
H(67)	5624	7699	4533	20
H(69)	9858	6578	3609	18
H(70A)	10694	7918	3509	58
H(70B)	10044	7716	3010	58
H(70C)	11390	7450	3156	58
H(71A)	11504	6456	4120	50
H(71B)	10303	6285	4609	50
H(71C)	11028	6998	4444	50
H(72)	5412	6573	3666	20
H(73A)	4144	7613	4000	41
H(73B)	3654	7196	3597	41
H(73C)	4853	7691	3348	41
H(74A)	4353	6503	4854	36
H(74B)	4997	5899	4659	36
H(74C)	3702	6167	4434	36
H(75A)	9439	4930	3779	38
H(75B)	9278	4598	4492	38
H(75C)	9973	5319	4193	38
H(76A)	8113	5643	5135	35
H(76B)	7320	4954	5278	35
H(76C)	6661	5661	5073	35
H(77A)	6852	4424	4158	17
H(77B)	5785	4944	4207	17
H(79)	7049	3777	3360	26
H(80)	8572	3135	3035	22
H(81)	10319	3674	2395	20
H(82)	10546	4859	2100	17
H(85)	10998	5197	3055	37
H(86)	12988	5467	3260	49
H(87)	13597	6584	2861	43
H(88)	12726	7366	2102	84
H(89)	10785	7072	1911	41
H(91)	7635	6733	1481	30
H(92)	7769	7106	431	36
H(93)	9339	6789	-135	43

H(94)	10981	6201	298	45
H(95)	10927	5814	1350	20
H(97)	4630	4257	3956	35
H(98)	2850	3753	3799	43
H(99)	2344	3926	2852	45
H(100)	3658	4630	2014	44
H(103)	6013	3853	2189	34
H(104)	7046	3070	1787	44
H(105)	8475	3443	910	48
H(106)	8799	4592	445	76
H(107)	7823	5376	875	61
H(109)	5068	5189	821	366
H(110)	3906	5878	119	563
H(111)	3335	6902	130	101
H(112)	3647	7176	921	114
H(113)	4822	6529	1647	133

Figure 7. Fully labeled drawing of ($^{Si}NP_3$)CoI (**2b**).

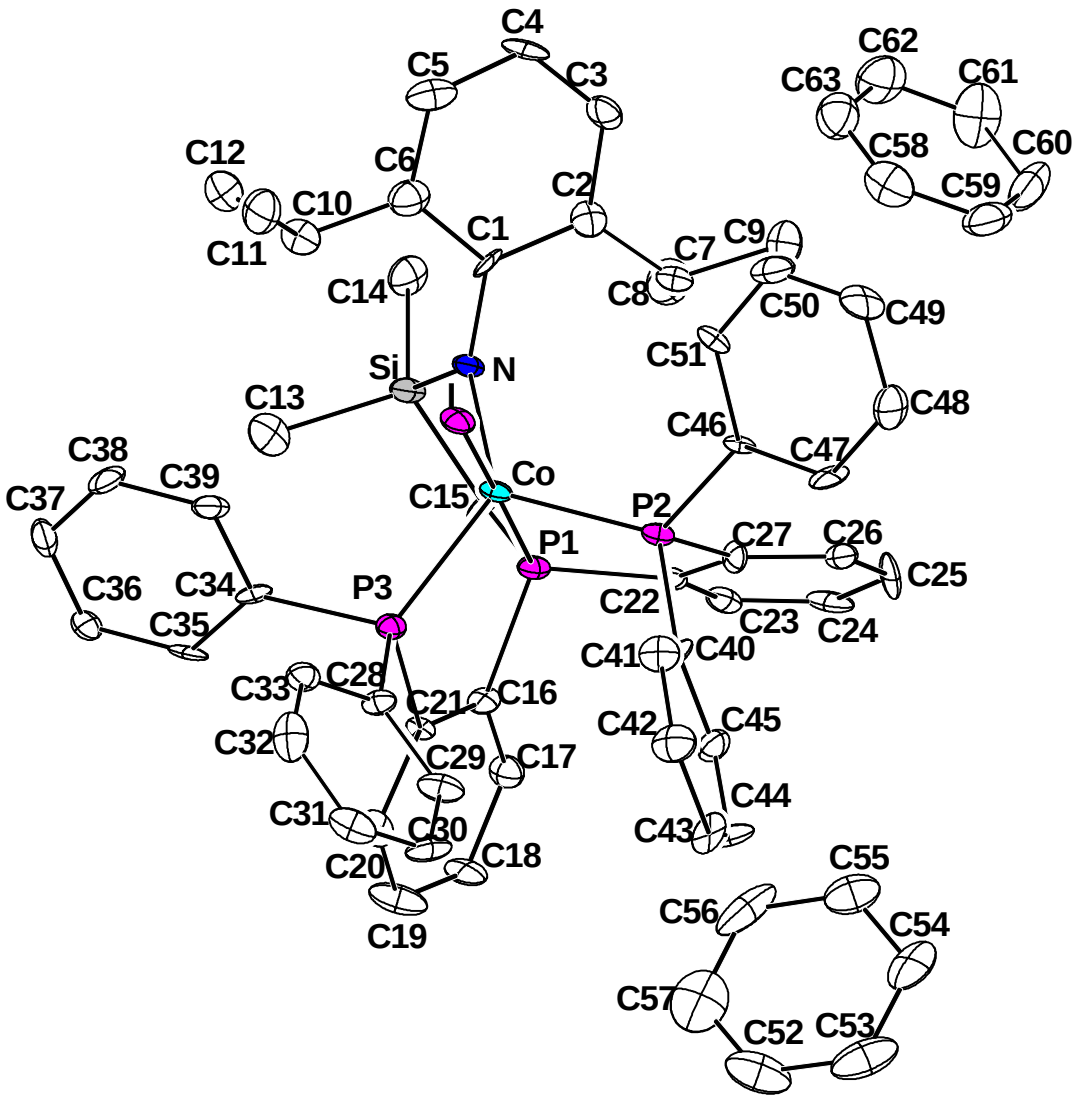

Table 6. Crystal data and structure refinement for ($^{Si}NP_3$)CoI (**2b**).

Identification code	ear13	
Empirical formula	C63 H64 Co I N P3 Si	
Formula weight	1141.98	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 13.0701(10) Å	α= 90°.
	b = 19.1387(15) Å	β= 102.943(3)°.
	c = 22.1493(16) Å	γ = 90°.
Volume	5399.8(7) Å^3	
Z	4	
Density (calculated)	1.405 Mg/m^3	
Absorption coefficient	1.042 mm^{-1}	
F(000)	2352	
Crystal size	0.30 x 0.15 x 0.11 mm^3	
Theta range for data collection	1.42 to 27.06°.	
Index ranges	-16<=h<=16, -23<=k<=23, -28<=l<=28	
Reflections collected	44992	
Independent reflections	10823 [R(int) = 0.1666]	
Completeness to theta = 27.06°	91.1 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	10823 / 18 / 637	
Goodness-of-fit on F^2	1.254	
Final R indices [I>2sigma(I)]	R1 = 0.0717, wR2 = 0.1089	
R indices (all data)	R1 = 0.1635, wR2 = 0.1243	
Largest diff. peak and hole	2.181 and -1.397 e.Å^{-3}	

Special Refinement Details.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full convariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles, and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes. The following atoms were restrained so that their U_{ij} components approximated isotropic behavior: C16, C21, C46.

Table 7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for ($^{Si}NP_3$)CoI (**2b**). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
I	2575(1)	8020(1)	1512(1)	17(1)
Co	2309(1)	6918(1)	2178(1)	14(1)
N	1238(4)	6381(3)	1576(3)	16(2)
P(1)	2271(2)	6083(1)	2815(1)	14(1)
P(3)	2096(2)	7646(1)	2938(1)	14(1)
P(2)	4043(2)	6684(1)	2327(1)	13(1)
Si	299(2)	5965(1)	1894(1)	17(1)
C(1)	1141(5)	6337(4)	939(3)	15(2)
C(2)	1734(6)	5823(4)	692(3)	20(2)
C(3)	1574(6)	5759(4)	40(4)	22(2)
C(4)	863(6)	6185(4)	-366(4)	26(2)
C(5)	338(6)	6676(4)	-111(4)	25(2)
C(6)	445(6)	6778(4)	516(4)	26(2)
C(7)	2448(6)	5319(4)	1089(3)	22(2)
C(8)	1873(7)	4677(4)	1274(4)	38(2)
C(9)	3342(6)	5034(4)	829(4)	28(2)
C(10)	-217(6)	7319(4)	735(4)	21(2)
C(11)	-147(6)	8035(4)	442(4)	32(2)
C(12)	-1375(6)	7087(4)	595(4)	30(2)
C(13)	-678(6)	6512(4)	2176(4)	26(2)
C(14)	-516(6)	5326(4)	1355(4)	25(2)
C(15)	1116(5)	5539(4)	2617(3)	16(2)
C(16)	2344(6)	6416(4)	3598(3)	15(2)
C(17)	2431(6)	5970(4)	4117(3)	20(2)
C(18)	2492(6)	6275(4)	4697(3)	21(2)
C(19)	2396(7)	7007(5)	4751(4)	36(2)
C(20)	2307(5)	7432(4)	4238(4)	19(2)
C(21)	2288(5)	7133(3)	3655(3)	11(2)
C(22)	3406(5)	5530(4)	2870(3)	15(2)
C(23)	3487(6)	4851(4)	3117(3)	17(2)
C(24)	4345(6)	4443(4)	3114(3)	23(2)
C(25)	5136(6)	4690(4)	2831(4)	22(2)
C(26)	5071(6)	5352(4)	2598(3)	20(2)
C(27)	4235(5)	5782(3)	2609(3)	15(2)
C(28)	2812(6)	8453(4)	3212(3)	15(2)
C(29)	3719(6)	8444(4)	3669(3)	21(2)
C(30)	4232(6)	9049(4)	3909(3)	21(2)
C(31)	3836(6)	9688(4)	3683(4)	23(2)
C(32)	2938(6)	9718(4)	3201(4)	27(2)
C(33)	2418(6)	9101(4)	2975(3)	19(2)
C(34)	736(5)	7954(4)	2810(3)	13(2)
C(35)	120(6)	7897(3)	3251(3)	16(2)
C(36)	-897(5)	8125(4)	3136(3)	19(2)
C(37)	-1365(6)	8423(4)	2571(4)	21(2)
C(38)	-770(6)	8498(4)	2131(4)	24(2)
C(39)	263(6)	8261(3)	2245(3)	19(2)
C(40)	4974(5)	7172(3)	2911(3)	14(2)
C(41)	5290(6)	7825(3)	2772(4)	20(2)
C(42)	6005(6)	8212(4)	3206(4)	27(2)
C(43)	6413(5)	7941(4)	3783(4)	24(2)
C(44)	6122(6)	7282(4)	3941(4)	27(2)

C(45)	5403(5)	6903(4)	3503(3)	19(2)
C(46)	4716(5)	6699(3)	1686(3)	10(2)
C(47)	5799(6)	6706(4)	1788(3)	19(2)
C(48)	6300(6)	6715(4)	1292(4)	29(2)
C(49)	5698(6)	6713(4)	685(4)	26(2)
C(50)	4619(6)	6709(4)	582(4)	25(2)
C(51)	4144(6)	6699(3)	1073(3)	15(2)
C(52)	6372(8)	6395(5)	5577(4)	42(3)
C(53)	7274(7)	6101(5)	5450(4)	44(3)
C(54)	7187(7)	5646(4)	4947(4)	37(2)
C(55)	6203(7)	5483(4)	4616(4)	36(2)
C(56)	5300(7)	5769(5)	4754(5)	46(3)
C(57)	5404(8)	6237(5)	5245(5)	52(3)
C(58)	1317(7)	1242(4)	1300(4)	33(2)
C(59)	2127(7)	783(5)	1523(4)	37(2)
C(60)	1947(7)	83(5)	1454(4)	39(2)
C(61)	987(7)	-158(5)	1137(5)	44(3)
C(62)	196(7)	309(5)	905(4)	40(2)
C(63)	381(7)	1015(5)	996(4)	35(2)

Table 8. Bond lengths [Å] and angles [°] for ($^{Si}NP_3$)CoI (**2b**).

I-Co	2.6415(10)	C(15)-H(15)	0.9500
Co-N	1.990(6)	C(16)-C(21)	1.380(9)
Co-P(1)	2.139(2)	C(16)-C(17)	1.417(9)
Co-P(3)	2.250(2)	C(17)-C(18)	1.396(10)
Co-P(2)	2.260(2)	C(17)-H(17)	0.9500
N-C(1)	1.391(8)	C(18)-C(19)	1.413(10)
N-Si	1.739(6)	C(18)-H(18)	0.9500
P(1)-C(22)	1.804(7)	C(19)-C(20)	1.380(10)
P(1)-C(15)	1.806(7)	C(19)-H(19)	0.9500
P(1)-C(16)	1.830(7)	C(20)-C(21)	1.409(10)
P(3)-C(34)	1.833(7)	C(20)-H(20)	0.9500
P(3)-C(21)	1.836(7)	C(22)-C(23)	1.405(9)
P(3)-C(28)	1.837(7)	C(22)-C(27)	1.423(9)
P(2)-C(40)	1.823(7)	C(23)-C(24)	1.367(10)
P(2)-C(46)	1.830(7)	C(23)-H(23)	0.9500
P(2)-C(27)	1.834(7)	C(24)-C(25)	1.406(10)
Si-C(13)	1.863(7)	C(24)-H(24)	0.9500
Si-C(14)	1.867(7)	C(25)-C(26)	1.364(9)
Si-C(15)	1.899(7)	C(25)-H(25)	0.9500
C(1)-C(6)	1.426(10)	C(26)-C(27)	1.371(9)
C(1)-C(2)	1.433(10)	C(26)-H(26)	0.9500
C(2)-C(3)	1.418(10)	C(28)-C(29)	1.375(9)
C(2)-C(7)	1.486(10)	C(28)-C(33)	1.400(9)
C(3)-C(4)	1.401(10)	C(29)-C(30)	1.383(9)
C(3)-H(3)	0.9500	C(29)-H(29)	0.9500
C(4)-C(5)	1.360(10)	C(30)-C(31)	1.379(10)
C(4)-H(4)	0.9500	C(30)-H(30)	0.9500
C(5)-C(6)	1.379(10)	C(31)-C(32)	1.399(10)
C(5)-H(5)	0.9500	C(31)-H(31)	0.9500
C(6)-C(10)	1.498(10)	C(32)-C(33)	1.399(10)
C(7)-C(9)	1.516(10)	C(32)-H(32)	0.9500
C(7)-C(8)	1.541(10)	C(33)-H(33)	0.9500
C(7)-H(7)	1.0000	C(34)-C(39)	1.396(9)
C(8)-H(8A)	0.9800	C(34)-C(35)	1.403(9)
C(8)-H(8B)	0.9800	C(35)-C(36)	1.368(9)
C(8)-H(8C)	0.9800	C(35)-H(35)	0.9500
C(9)-H(9A)	0.9800	C(36)-C(37)	1.387(9)
C(9)-H(9B)	0.9800	C(36)-H(36)	0.9500
C(9)-H(9C)	0.9800	C(37)-C(38)	1.384(10)
C(10)-C(11)	1.528(10)	C(37)-H(37)	0.9500
C(10)-C(12)	1.540(9)	C(38)-C(39)	1.393(9)
C(10)-H(10)	1.0000	C(38)-H(38)	0.9500
C(11)-H(11A)	0.9800	C(39)-H(39)	0.9500
C(11)-H(11B)	0.9800	C(40)-C(41)	1.372(9)
C(11)-H(11C)	0.9800	C(40)-C(45)	1.404(9)
C(12)-H(12A)	0.9800	C(41)-C(42)	1.395(10)
C(12)-H(12B)	0.9800	C(41)-H(41)	0.9500
C(12)-H(12C)	0.9800	C(42)-C(43)	1.371(10)
C(13)-H(13A)	0.9800	C(42)-H(42)	0.9500
C(13)-H(13B)	0.9800	C(43)-C(44)	1.384(10)
C(13)-H(13C)	0.9800	C(43)-H(43)	0.9500
C(14)-H(14A)	0.9800	C(44)-C(45)	1.394(9)
C(14)-H(14B)	0.9800	C(44)-H(44)	0.9500
C(14)-H(14C)	0.9800	C(45)-H(45)	0.9500

C(46)-C(47)	1.383(9)	C(34)-P(3)-C(28)	100.7(3)
C(46)-C(51)	1.395(9)	C(21)-P(3)-C(28)	101.7(3)
C(47)-C(48)	1.400(11)	C(34)-P(3)-Co	111.2(2)
C(47)-H(47)	0.9500	C(21)-P(3)-Co	107.4(2)
C(48)-C(49)	1.397(10)	C(28)-P(3)-Co	129.0(3)
C(48)-H(48)	0.9500	C(40)-P(2)-C(46)	100.5(3)
C(49)-C(50)	1.377(10)	C(40)-P(2)-C(27)	102.8(3)
C(49)-H(49)	0.9500	C(46)-P(2)-C(27)	103.1(3)
C(50)-C(51)	1.368(10)	C(40)-P(2)-Co	119.4(2)
C(50)-H(50)	0.9500	C(46)-P(2)-Co	121.6(2)
C(51)-H(51)	0.9500	C(27)-P(2)-Co	107.0(2)
C(52)-C(57)	1.347(12)	N-Si-C(13)	118.5(3)
C(52)-C(53)	1.391(12)	N-Si-C(14)	113.2(3)
C(52)-H(52)	0.9500	C(13)-Si-C(14)	104.3(3)
C(53)-C(54)	1.399(12)	N-Si-C(15)	103.0(3)
C(53)-H(53)	0.9500	C(13)-Si-C(15)	104.9(3)
C(54)-C(55)	1.365(11)	C(14)-Si-C(15)	113.0(3)
C(54)-H(54)	0.9500	N-C(1)-C(6)	121.9(7)
C(55)-C(56)	1.396(12)	N-C(1)-C(2)	119.6(6)
C(55)-H(55)	0.9500	C(6)-C(1)-C(2)	118.4(7)
C(56)-C(57)	1.392(13)	C(3)-C(2)-C(1)	118.6(7)
C(56)-H(56)	0.9500	C(3)-C(2)-C(7)	118.5(7)
C(57)-H(57)	0.9500	C(1)-C(2)-C(7)	122.8(7)
C(58)-C(63)	1.330(11)	C(4)-C(3)-C(2)	121.9(7)
C(58)-C(59)	1.380(11)	C(4)-C(3)-H(3)	119.0
C(58)-H(58)	0.9500	C(2)-C(3)-H(3)	119.0
C(59)-C(60)	1.363(11)	C(5)-C(4)-C(3)	117.4(7)
C(59)-H(59)	0.9500	C(5)-C(4)-H(4)	121.3
C(60)-C(61)	1.373(11)	C(3)-C(4)-H(4)	121.3
C(60)-H(60)	0.9500	C(4)-C(5)-C(6)	124.7(8)
C(61)-C(62)	1.376(11)	C(4)-C(5)-H(5)	117.6
C(61)-H(61)	0.9500	C(6)-C(5)-H(5)	117.6
C(62)-C(63)	1.380(11)	C(5)-C(6)-C(1)	118.9(8)
C(62)-H(62)	0.9500	C(5)-C(6)-C(10)	119.1(7)
C(63)-H(63)	0.9500	C(1)-C(6)-C(10)	121.8(7)
		C(2)-C(7)-C(9)	116.3(7)
N-Co-P(1)	86.54(18)	C(2)-C(7)-C(8)	113.3(6)
N-Co-P(3)	129.39(17)	C(9)-C(7)-C(8)	106.1(6)
P(1)-Co-P(3)	86.78(8)	C(2)-C(7)-H(7)	106.9
N-Co-P(2)	121.84(17)	C(9)-C(7)-H(7)	106.9
P(1)-Co-P(2)	85.81(8)	C(8)-C(7)-H(7)	106.9
P(3)-Co-P(2)	107.57(8)	C(7)-C(8)-H(8A)	109.5
N-Co-I	101.49(17)	C(7)-C(8)-H(8B)	109.5
P(1)-Co-I	171.93(7)	H(8A)-C(8)-H(8B)	109.5
P(3)-Co-I	88.66(6)	C(7)-C(8)-H(8C)	109.5
P(2)-Co-I	89.24(6)	H(8A)-C(8)-H(8C)	109.5
C(1)-N-Si	118.1(5)	H(8B)-C(8)-H(8C)	109.5
C(1)-N-Co	127.0(5)	C(7)-C(9)-H(9A)	109.5
Si-N-Co	114.8(3)	C(7)-C(9)-H(9B)	109.5
C(22)-P(1)-C(15)	107.9(3)	H(9A)-C(9)-H(9B)	109.5
C(22)-P(1)-C(16)	105.8(3)	C(7)-C(9)-H(9C)	109.5
C(15)-P(1)-C(16)	107.1(3)	H(9A)-C(9)-H(9C)	109.5
C(22)-P(1)-Co	110.0(3)	H(9B)-C(9)-H(9C)	109.5
C(15)-P(1)-Co	114.4(2)	C(6)-C(10)-C(11)	112.9(7)
C(16)-P(1)-Co	111.2(2)	C(6)-C(10)-C(12)	110.5(6)
C(34)-P(3)-C(21)	104.2(3)	C(11)-C(10)-C(12)	108.9(6)

C(6)-C(10)-H(10)	108.2	C(25)-C(24)-H(24)	120.2
C(11)-C(10)-H(10)	108.2	C(26)-C(25)-C(24)	119.5(7)
C(12)-C(10)-H(10)	108.2	C(26)-C(25)-H(25)	120.2
C(10)-C(11)-H(11A)	109.5	C(24)-C(25)-H(25)	120.2
C(10)-C(11)-H(11B)	109.5	C(25)-C(26)-C(27)	122.1(7)
H(11A)-C(11)-H(11B)	109.5	C(25)-C(26)-H(26)	118.9
C(10)-C(11)-H(11C)	109.5	C(27)-C(26)-H(26)	118.9
H(11A)-C(11)-H(11C)	109.5	C(26)-C(27)-C(22)	119.1(6)
H(11B)-C(11)-H(11C)	109.5	C(26)-C(27)-P(2)	127.4(6)
C(10)-C(12)-H(12A)	109.5	C(22)-C(27)-P(2)	113.5(5)
C(10)-C(12)-H(12B)	109.5	C(29)-C(28)-C(33)	118.1(6)
H(12A)-C(12)-H(12B)	109.5	C(29)-C(28)-P(3)	121.7(5)
C(10)-C(12)-H(12C)	109.5	C(33)-C(28)-P(3)	120.2(6)
H(12A)-C(12)-H(12C)	109.5	C(28)-C(29)-C(30)	122.5(7)
H(12B)-C(12)-H(12C)	109.5	C(28)-C(29)-H(29)	118.8
Si-C(13)-H(13A)	109.5	C(30)-C(29)-H(29)	118.8
Si-C(13)-H(13B)	109.5	C(31)-C(30)-C(29)	119.5(7)
H(13A)-C(13)-H(13B)	109.5	C(31)-C(30)-H(30)	120.2
Si-C(13)-H(13C)	109.5	C(29)-C(30)-H(30)	120.2
H(13A)-C(13)-H(13C)	109.5	C(30)-C(31)-C(32)	119.7(7)
H(13B)-C(13)-H(13C)	109.5	C(30)-C(31)-H(31)	120.2
Si-C(14)-H(14A)	109.5	C(32)-C(31)-H(31)	120.2
Si-C(14)-H(14B)	109.5	C(33)-C(32)-C(31)	119.8(7)
H(14A)-C(14)-H(14B)	109.5	C(33)-C(32)-H(32)	120.1
Si-C(14)-H(14C)	109.5	C(31)-C(32)-H(32)	120.1
H(14A)-C(14)-H(14C)	109.5	C(32)-C(33)-C(28)	120.3(7)
H(14B)-C(14)-H(14C)	109.5	C(32)-C(33)-H(33)	119.8
P(1)-C(15)-Si	103.8(4)	C(28)-C(33)-H(33)	119.8
P(1)-C(15)-H(15)	128.1	C(39)-C(34)-C(35)	116.7(6)
Si-C(15)-H(15)	128.1	C(39)-C(34)-P(3)	119.6(5)
C(21)-C(16)-C(17)	121.4(6)	C(35)-C(34)-P(3)	123.7(5)
C(21)-C(16)-P(1)	116.1(5)	C(36)-C(35)-C(34)	122.1(7)
C(17)-C(16)-P(1)	122.5(5)	C(36)-C(35)-H(35)	119.0
C(18)-C(17)-C(16)	118.2(7)	C(34)-C(35)-H(35)	119.0
C(18)-C(17)-H(17)	120.9	C(35)-C(36)-C(37)	120.9(7)
C(16)-C(17)-H(17)	120.9	C(35)-C(36)-H(36)	119.6
C(17)-C(18)-C(19)	120.3(7)	C(37)-C(36)-H(36)	119.6
C(17)-C(18)-H(18)	119.8	C(38)-C(37)-C(36)	118.4(7)
C(19)-C(18)-H(18)	119.8	C(38)-C(37)-H(37)	120.8
C(20)-C(19)-C(18)	120.5(7)	C(36)-C(37)-H(37)	120.8
C(20)-C(19)-H(19)	119.8	C(37)-C(38)-C(39)	120.8(7)
C(18)-C(19)-H(19)	119.8	C(37)-C(38)-H(38)	119.6
C(19)-C(20)-C(21)	119.8(7)	C(39)-C(38)-H(38)	119.6
C(19)-C(20)-H(20)	120.1	C(38)-C(39)-C(34)	121.1(7)
C(21)-C(20)-H(20)	120.1	C(38)-C(39)-H(39)	119.4
C(16)-C(21)-C(20)	119.8(6)	C(34)-C(39)-H(39)	119.4
C(16)-C(21)-P(3)	116.9(5)	C(41)-C(40)-C(45)	117.8(7)
C(20)-C(21)-P(3)	123.2(5)	C(41)-C(40)-P(2)	119.6(5)
C(23)-C(22)-C(27)	118.3(6)	C(45)-C(40)-P(2)	122.6(5)
C(23)-C(22)-P(1)	124.0(6)	C(40)-C(41)-C(42)	121.2(7)
C(27)-C(22)-P(1)	117.6(5)	C(40)-C(41)-H(41)	119.4
C(24)-C(23)-C(22)	121.2(7)	C(42)-C(41)-H(41)	119.4
C(24)-C(23)-H(23)	119.4	C(43)-C(42)-C(41)	120.2(7)
C(22)-C(23)-H(23)	119.4	C(43)-C(42)-H(42)	119.9
C(23)-C(24)-C(25)	119.7(7)	C(41)-C(42)-H(42)	119.9
C(23)-C(24)-H(24)	120.2	C(42)-C(43)-C(44)	120.5(7)

C(42)-C(43)-H(43)	119.7	C(54)-C(53)-H(53)	120.3
C(44)-C(43)-H(43)	119.7	C(55)-C(54)-C(53)	118.0(9)
C(43)-C(44)-C(45)	118.7(7)	C(55)-C(54)-H(54)	121.0
C(43)-C(44)-H(44)	120.7	C(53)-C(54)-H(54)	121.0
C(45)-C(44)-H(44)	120.7	C(54)-C(55)-C(56)	122.2(9)
C(44)-C(45)-C(40)	121.6(7)	C(54)-C(55)-H(55)	118.9
C(44)-C(45)-H(45)	119.2	C(56)-C(55)-H(55)	118.9
C(40)-C(45)-H(45)	119.2	C(57)-C(56)-C(55)	119.0(9)
C(47)-C(46)-C(51)	117.8(6)	C(57)-C(56)-H(56)	120.5
C(47)-C(46)-P(2)	121.7(5)	C(55)-C(56)-H(56)	120.5
C(51)-C(46)-P(2)	120.5(5)	C(52)-C(57)-C(56)	119.0(10)
C(46)-C(47)-C(48)	120.8(7)	C(52)-C(57)-H(57)	120.5
C(46)-C(47)-H(47)	119.6	C(56)-C(57)-H(57)	120.5
C(48)-C(47)-H(47)	119.6	C(63)-C(58)-C(59)	121.2(8)
C(49)-C(48)-C(47)	119.6(7)	C(63)-C(58)-H(58)	119.4
C(49)-C(48)-H(48)	120.2	C(59)-C(58)-H(58)	119.4
C(47)-C(48)-H(48)	120.2	C(60)-C(59)-C(58)	119.1(8)
C(50)-C(49)-C(48)	119.6(7)	C(60)-C(59)-H(59)	120.5
C(50)-C(49)-H(49)	120.2	C(58)-C(59)-H(59)	120.5
C(48)-C(49)-H(49)	120.2	C(59)-C(60)-C(61)	120.2(8)
C(51)-C(50)-C(49)	120.0(7)	C(59)-C(60)-H(60)	119.9
C(51)-C(50)-H(50)	120.0	C(61)-C(60)-H(60)	119.9
C(49)-C(50)-H(50)	120.0	C(60)-C(61)-C(62)	119.8(9)
C(50)-C(51)-C(46)	122.2(7)	C(60)-C(61)-H(61)	120.1
C(50)-C(51)-H(51)	118.9	C(62)-C(61)-H(61)	120.1
C(46)-C(51)-H(51)	118.9	C(61)-C(62)-C(63)	119.3(8)
C(57)-C(52)-C(53)	122.3(9)	C(61)-C(62)-H(62)	120.3
C(57)-C(52)-H(52)	118.8	C(63)-C(62)-H(62)	120.3
C(53)-C(52)-H(52)	118.8	C(58)-C(63)-C(62)	120.3(8)
C(52)-C(53)-C(54)	119.4(9)	C(58)-C(63)-H(63)	119.8
C(52)-C(53)-H(53)	120.3	C(62)-C(63)-H(63)	119.8

Symmetry transformations used to generate equivalent atoms:

Table 9. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for ($^{Si}NP_3$)CoI (**2b**). The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
I	25(1)	18(1)	9(1)	3(1)	6(1)	2(1)
Co	19(1)	16(1)	6(1)	0(1)	4(1)	-1(1)
N	11(3)	27(4)	10(4)	-7(3)	3(3)	-4(3)
P(1)	17(1)	18(1)	9(1)	0(1)	3(1)	-2(1)
P(3)	16(1)	15(1)	10(1)	1(1)	4(1)	0(1)
P(2)	17(1)	15(1)	8(1)	0(1)	4(1)	-2(1)
Si	18(1)	22(1)	11(1)	-3(1)	3(1)	-4(1)
C(1)	4(4)	28(5)	12(4)	7(4)	-3(3)	1(3)
C(2)	23(5)	20(5)	19(5)	5(4)	9(4)	-1(4)
C(3)	22(5)	20(5)	23(5)	-11(4)	5(4)	-3(4)
C(4)	40(6)	34(5)	5(4)	-3(4)	8(4)	-3(4)
C(5)	28(5)	30(5)	16(5)	4(4)	1(4)	-14(4)
C(6)	24(5)	33(6)	21(5)	3(4)	4(4)	-2(4)
C(7)	24(5)	27(5)	13(5)	-8(4)	1(4)	1(4)
C(8)	43(6)	41(6)	31(6)	11(4)	9(5)	14(5)
C(9)	21(5)	28(5)	36(6)	3(4)	9(4)	2(4)
C(10)	29(5)	15(4)	20(5)	2(3)	8(4)	-2(4)
C(11)	36(5)	27(5)	33(5)	5(5)	6(4)	12(5)
C(12)	29(5)	37(6)	27(5)	-2(4)	10(4)	5(4)
C(13)	24(5)	28(5)	29(5)	0(4)	15(4)	-8(4)
C(14)	17(5)	31(5)	27(5)	2(4)	5(4)	-5(4)
C(15)	5(4)	22(4)	17(4)	6(3)	-5(3)	-6(3)
C(16)	16(3)	23(3)	8(3)	7(3)	5(3)	0(3)
C(17)	24(5)	16(4)	18(5)	0(4)	5(4)	1(4)
C(18)	38(5)	18(5)	8(4)	4(3)	8(4)	1(4)
C(19)	57(6)	42(6)	14(5)	-3(5)	16(4)	-11(5)
C(20)	13(4)	23(5)	24(5)	-4(4)	11(4)	-8(4)
C(21)	14(4)	16(4)	5(4)	4(3)	7(3)	-1(3)
C(22)	10(4)	22(5)	11(4)	-8(3)	1(3)	-2(3)
C(23)	20(5)	19(5)	13(4)	-6(3)	4(4)	-4(4)
C(24)	43(6)	18(5)	6(4)	0(3)	4(4)	-3(4)
C(25)	18(5)	11(5)	39(6)	-6(4)	13(4)	5(4)
C(26)	15(4)	32(5)	11(5)	-2(4)	1(4)	2(4)
C(27)	15(4)	9(4)	19(5)	-1(3)	2(4)	4(3)
C(28)	17(4)	13(4)	12(4)	-1(3)	-1(4)	-3(3)
C(29)	35(5)	17(4)	12(4)	1(3)	8(4)	-9(4)
C(30)	20(5)	30(5)	11(4)	-1(4)	-3(4)	-13(4)
C(31)	39(6)	9(4)	23(5)	-6(4)	11(4)	-11(4)
C(32)	27(5)	19(5)	38(6)	11(4)	15(5)	4(4)
C(33)	14(4)	25(5)	16(5)	-5(4)	3(4)	-4(4)
C(34)	14(4)	13(4)	9(4)	-2(3)	-5(3)	-7(3)
C(35)	31(5)	14(4)	3(4)	-2(3)	3(3)	-2(4)
C(36)	16(4)	28(5)	13(4)	-1(4)	8(3)	1(4)
C(37)	18(5)	20(5)	27(5)	-5(4)	9(4)	5(4)
C(38)	18(5)	40(5)	10(5)	7(4)	-2(4)	5(4)
C(39)	19(4)	26(5)	10(4)	-4(3)	1(3)	-4(4)
C(40)	12(4)	16(5)	12(4)	8(3)	-3(3)	3(3)
C(41)	26(5)	14(5)	20(5)	5(3)	6(4)	-5(3)
C(42)	35(5)	20(5)	24(5)	3(4)	2(4)	0(4)
C(43)	4(4)	27(5)	37(5)	-9(4)	-4(4)	-8(4)
C(44)	33(5)	35(5)	9(5)	5(4)	-7(4)	-3(4)

C(45)	15(4)	19(4)	21(5)	-3(4)	-3(3)	1(4)
C(46)	16(4)	13(4)	3(4)	2(3)	5(3)	-3(3)
C(47)	22(5)	28(5)	6(4)	9(3)	-2(4)	1(4)
C(48)	14(5)	38(6)	34(6)	0(4)	8(4)	0(4)
C(49)	32(5)	36(5)	15(5)	3(4)	15(4)	-5(4)
C(50)	30(5)	29(5)	13(5)	1(4)	-3(4)	0(4)
C(51)	21(4)	13(4)	13(4)	-6(3)	8(4)	-2(3)
C(52)	67(8)	40(6)	26(6)	-2(4)	25(6)	-23(6)
C(53)	43(7)	51(7)	29(6)	18(5)	-8(5)	-23(5)
C(54)	33(6)	45(6)	31(6)	28(5)	3(5)	5(5)
C(55)	45(6)	39(6)	23(5)	13(4)	1(5)	-5(5)
C(56)	22(6)	65(8)	43(7)	28(6)	-12(5)	-13(5)
C(57)	51(7)	56(7)	54(8)	29(6)	23(6)	-3(6)
C(58)	48(6)	18(5)	34(6)	0(4)	14(5)	-4(5)
C(59)	29(5)	62(7)	17(5)	3(5)	0(4)	-1(5)
C(60)	20(5)	54(7)	40(6)	12(5)	-2(5)	7(5)
C(61)	31(6)	30(6)	72(8)	6(5)	17(6)	-9(5)
C(62)	26(6)	50(7)	43(7)	-4(5)	4(5)	-10(5)
C(63)	34(6)	36(6)	35(6)	5(5)	9(5)	5(5)

Table 10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for ($^{Si}NP_3$)CoI (**2b**).

	x	y	z	U(eq)
H(3)	1961	5418	-127	26
H(4)	751	6132	-802	31
H(5)	-137	6971	-385	30
H(7)	2772	5570	1481	26
H(8A)	1351	4831	1501	57
H(8B)	2382	4368	1537	57
H(8C)	1521	4425	900	57
H(9A)	3063	4712	488	42
H(9B)	3839	4785	1155	42
H(9C)	3703	5421	675	42
H(10)	32	7367	1194	25
H(11A)	592	8160	481	49
H(11B)	-486	8385	654	49
H(11C)	-502	8019	3	49
H(12A)	-1658	7088	147	45
H(12B)	-1780	7410	794	45
H(12C)	-1423	6614	757	45
H(13A)	-333	6747	2560	38
H(13B)	-1245	6214	2253	38
H(13C)	-969	6863	1861	38
H(14A)	-259	5297	973	37
H(14B)	-1249	5480	1257	37
H(14C)	-467	4865	1553	37
H(15)	954	5134	2826	19
H(17)	2448	5477	4072	23
H(18)	2597	5990	5056	25
H(19)	2394	7208	5143	44
H(20)	2258	7924	4279	23
H(23)	2936	4672	3289	21
H(24)	4406	3994	3303	27
H(25)	5711	4398	2803	26
H(26)	5622	5522	2422	23
H(29)	4004	8006	3825	25
H(30)	4854	9024	4227	26
H(31)	4171	10107	3854	27
H(32)	2683	10156	3029	32
H(33)	1794	9121	2658	23
H(35)	419	7693	3642	19
H(36)	-1288	8078	3448	22
H(37)	-2076	8572	2488	25
H(38)	-1071	8714	1746	28
H(39)	652	8309	1933	22
H(41)	5017	8016	2373	24
H(42)	6211	8664	3102	33
H(43)	6900	8207	4077	29
H(44)	6406	7093	4340	33
H(45)	5197	6450	3608	23
H(47)	6209	6705	2201	23
H(48)	7044	6722	1367	34
H(49)	6031	6714	345	31

H(50)	4205	6713	171	30
H(51)	3399	6691	994	18
H(52)	6441	6718	5909	51
H(53)	7944	6208	5703	53
H(54)	7793	5456	4839	44
H(55)	6131	5164	4280	44
H(56)	4625	5647	4516	55
H(57)	4801	6442	5345	62
H(58)	1429	1729	1365	39
H(59)	2802	952	1722	44
H(60)	2487	-240	1625	47
H(61)	869	-646	1077	52
H(62)	-471	147	686	48
H(63)	-162	1341	839	42

Figure 8. Fully labeled drawing of ($^{Si}NP_2$)FeCl (**3**).

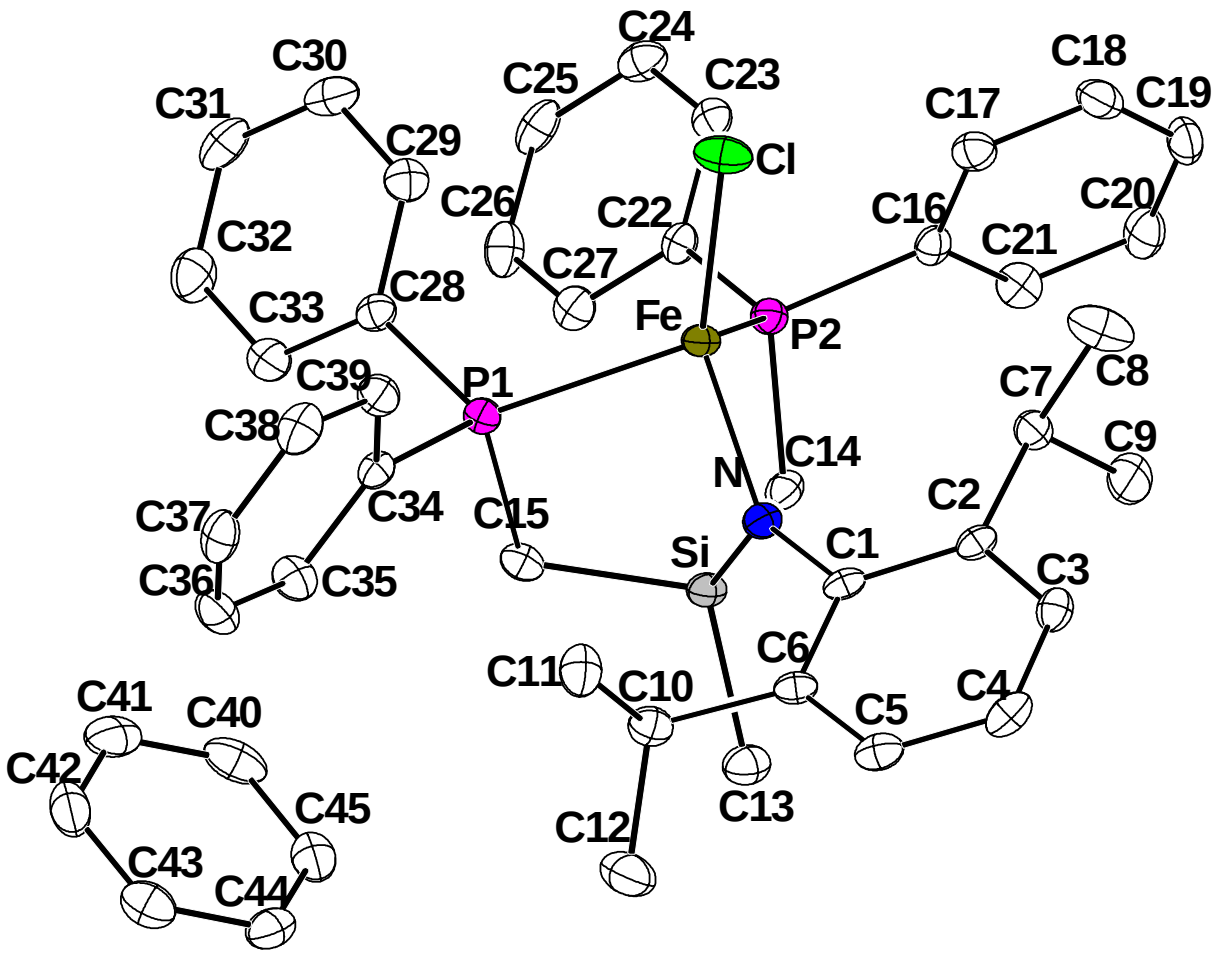

Table 11. Crystal data and structure refinement for ($^{Si}NP_2$)FeCl (**3**).

Identification code	mtw07	
Empirical formula	C45 H50 Cl Fe N P2 Si	
Formula weight	786.19	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 9.793(3) Å	α= 90°.
	b = 9.371(3) Å	β= 94.581(4)°.
	c = 44.610(12) Å	γ = 90°.
Volume	4080.9(19) Å^3	
Z	4	
Density (calculated)	1.280 Mg/m^3	
Absorption coefficient	0.575 mm^{-1}	
F(000)	1656	
Crystal size	0.33 x 0.20 x 0.17 mm^3	
Theta range for data collection	1.83 to 28.24°.	
Index ranges	-12<=h<=12, -12<=k<=11, -58<=l<=50	
Reflections collected	34419	
Independent reflections	8533 [R(int) = 0.0769]	
Completeness to theta = 28.24°	84.7 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8533 / 0 / 465	
Goodness-of-fit on F^2	1.305	
Final R indices [I>2sigma(I)]	R1 = 0.0456, wR2 = 0.0682	
R indices (all data)	R1 = 0.0713, wR2 = 0.0710	
Largest diff. peak and hole	0.794 and -0.466 e.Å^{-3}	

Special Refinement Details.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full convariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles, and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table 12. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for ($^{Si}NP_2$)FeCl (**3**). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Fe	3097(1)	2188(1)	1398(1)	14(1)
Cl	2009(1)	308(1)	1579(1)	25(1)
P(1)	1765(1)	4280(1)	1250(1)	15(1)
P(2)	4588(1)	3434(1)	1794(1)	15(1)
N	4372(2)	2640(2)	1097(1)	15(1)
Si	4812(1)	4406(1)	1153(1)	15(1)
C(1)	4928(2)	1715(2)	884(1)	13(1)
C(2)	5800(2)	563(2)	983(1)	15(1)
C(3)	6357(2)	-293(2)	767(1)	17(1)
C(4)	6098(2)	-61(2)	464(1)	19(1)
C(5)	5218(2)	1032(2)	368(1)	18(1)
C(6)	4615(2)	1910(2)	571(1)	15(1)
C(7)	6138(2)	264(2)	1313(1)	17(1)
C(8)	5901(3)	-1304(2)	1397(1)	33(1)
C(9)	7621(2)	704(3)	1411(1)	28(1)
C(10)	3546(2)	3000(2)	449(1)	19(1)
C(11)	2192(2)	2255(2)	353(1)	25(1)
C(12)	4003(3)	3882(3)	186(1)	31(1)
C(13)	6007(2)	5189(2)	894(1)	21(1)
C(14)	5641(2)	4487(2)	1550(1)	17(1)
C(15)	3145(2)	5461(2)	1139(1)	16(1)
C(16)	5759(2)	2224(2)	2008(1)	15(1)
C(17)	5327(2)	844(2)	2066(1)	19(1)
C(18)	6210(2)	-117(2)	2219(1)	22(1)
C(19)	7533(2)	300(3)	2314(1)	23(1)
C(20)	7965(2)	1672(3)	2261(1)	23(1)
C(21)	7090(2)	2632(2)	2108(1)	20(1)
C(22)	4116(2)	4694(2)	2082(1)	15(1)
C(23)	4063(2)	4257(2)	2380(1)	17(1)
C(24)	3670(2)	5193(3)	2598(1)	21(1)
C(25)	3303(2)	6585(3)	2521(1)	23(1)
C(26)	3333(2)	7021(3)	2226(1)	24(1)
C(27)	3739(2)	6093(2)	2007(1)	19(1)
C(28)	865(2)	5219(2)	1534(1)	16(1)
C(29)	596(2)	4466(2)	1792(1)	20(1)
C(30)	-61(2)	5114(3)	2019(1)	25(1)
C(31)	-472(2)	6528(3)	1989(1)	26(1)
C(32)	-210(2)	7287(3)	1734(1)	27(1)
C(33)	460(2)	6641(2)	1508(1)	22(1)
C(34)	511(2)	4165(2)	924(1)	15(1)
C(35)	294(2)	5216(2)	706(1)	20(1)
C(36)	-688(2)	5034(3)	466(1)	23(1)
C(37)	-1465(2)	3810(2)	446(1)	21(1)
C(38)	-1271(2)	2760(3)	661(1)	23(1)
C(39)	-282(2)	2927(2)	899(1)	20(1)
C(40)	1966(3)	8913(2)	811(1)	28(1)
C(41)	586(3)	9144(2)	732(1)	31(1)
C(42)	68(3)	8936(2)	437(1)	30(1)
C(43)	906(3)	8498(2)	223(1)	26(1)
C(44)	2282(2)	8270(2)	304(1)	23(1)
C(45)	2807(2)	8479(2)	596(1)	24(1)

Table 13. Bond lengths [Å] and angles [°] for ($^{Si}NP_2$)FeCl (**3**).

Fe-N	1.9532(17)	C(17)-H(17)	0.9500
Fe-Cl	2.2418(8)	C(18)-C(19)	1.387(3)
Fe-P(1)	2.4180(8)	C(18)-H(18)	0.9500
Fe-P(2)	2.4903(8)	C(19)-C(20)	1.381(3)
P(1)-C(28)	1.828(2)	C(19)-H(19)	0.9500
P(1)-C(34)	1.829(2)	C(20)-C(21)	1.384(3)
P(1)-C(15)	1.844(2)	C(20)-H(20)	0.9500
P(2)-C(16)	1.827(2)	C(21)-H(21)	0.9500
P(2)-C(22)	1.832(2)	C(22)-C(23)	1.396(3)
P(2)-C(14)	1.842(2)	C(22)-C(27)	1.396(3)
N-C(1)	1.424(3)	C(23)-C(24)	1.387(3)
N-Si	1.7228(19)	C(23)-H(23)	0.9500
Si-C(13)	1.858(2)	C(24)-C(25)	1.388(3)
Si-C(14)	1.893(2)	C(24)-H(24)	0.9500
Si-C(15)	1.906(2)	C(25)-C(26)	1.381(3)
C(1)-C(6)	1.416(3)	C(25)-H(25)	0.9500
C(1)-C(2)	1.425(3)	C(26)-C(27)	1.389(3)
C(2)-C(3)	1.396(3)	C(26)-H(26)	0.9500
C(2)-C(7)	1.511(3)	C(27)-H(27)	0.9500
C(3)-C(4)	1.376(3)	C(28)-C(29)	1.391(3)
C(3)-H(3)	0.9500	C(28)-C(33)	1.393(3)
C(4)-C(5)	1.384(3)	C(29)-C(30)	1.385(3)
C(4)-H(4)	0.9500	C(29)-H(29)	0.9500
C(5)-C(6)	1.391(3)	C(30)-C(31)	1.387(3)
C(5)-H(5)	0.9500	C(30)-H(30)	0.9500
C(6)-C(10)	1.532(3)	C(31)-C(32)	1.385(3)
C(7)-C(8)	1.538(3)	C(31)-H(31)	0.9500
C(7)-C(9)	1.539(3)	C(32)-C(33)	1.387(3)
C(7)-H(7)	1.0000	C(32)-H(32)	0.9500
C(8)-H(8A)	0.9800	C(33)-H(33)	0.9500
C(8)-H(8B)	0.9800	C(34)-C(35)	1.389(3)
C(8)-H(8C)	0.9800	C(34)-C(39)	1.396(3)
C(9)-H(9A)	0.9800	C(35)-C(36)	1.391(3)
C(9)-H(9B)	0.9800	C(35)-H(35)	0.9500
C(9)-H(9C)	0.9800	C(36)-C(37)	1.376(3)
C(10)-C(11)	1.529(3)	C(36)-H(36)	0.9500
C(10)-C(12)	1.531(3)	C(37)-C(38)	1.376(3)
C(10)-H(10)	1.0000	C(37)-H(37)	0.9500
C(11)-H(11A)	0.9800	C(38)-C(39)	1.389(3)
C(11)-H(11B)	0.9800	C(38)-H(38)	0.9500
C(11)-H(11C)	0.9800	C(39)-H(39)	0.9500
C(12)-H(12A)	0.9800	C(40)-C(45)	1.377(3)
C(12)-H(12B)	0.9800	C(40)-C(41)	1.387(4)
C(12)-H(12C)	0.9800	C(40)-H(40)	0.9500
C(13)-H(13A)	0.9800	C(41)-C(42)	1.384(4)
C(13)-H(13B)	0.9800	C(41)-H(41)	0.9500
C(13)-H(13C)	0.9800	C(42)-C(43)	1.370(3)
C(14)-H(14A)	0.9900	C(42)-H(42)	0.9500
C(14)-H(14B)	0.9900	C(43)-C(44)	1.384(3)
C(15)-H(15A)	0.9900	C(43)-H(43)	0.9500
C(15)-H(15B)	0.9900	C(44)-C(45)	1.375(3)
C(16)-C(17)	1.392(3)	C(44)-H(44)	0.9500
C(16)-C(21)	1.397(3)	C(45)-H(45)	0.9500
C(17)-C(18)	1.389(3)		

N-Fe-Cl	140.03(6)	H(8B)-C(8)-H(8C)	109.5
N-Fe-P(1)	89.76(5)	C(7)-C(9)-H(9A)	109.5
Cl-Fe-P(1)	118.30(3)	C(7)-C(9)-H(9B)	109.5
N-Fe-P(2)	90.91(6)	H(9A)-C(9)-H(9B)	109.5
Cl-Fe-P(2)	112.48(3)	C(7)-C(9)-H(9C)	109.5
P(1)-Fe-P(2)	94.98(3)	H(9A)-C(9)-H(9C)	109.5
C(28)-P(1)-C(34)	104.45(10)	H(9B)-C(9)-H(9C)	109.5
C(28)-P(1)-C(15)	107.54(10)	C(11)-C(10)-C(12)	109.4(2)
C(34)-P(1)-C(15)	106.43(10)	C(11)-C(10)-C(6)	110.38(18)
C(28)-P(1)-Fe	118.67(8)	C(12)-C(10)-C(6)	113.55(19)
C(34)-P(1)-Fe	118.87(7)	C(11)-C(10)-H(10)	107.8
C(15)-P(1)-Fe	99.74(7)	C(12)-C(10)-H(10)	107.8
C(16)-P(2)-C(22)	102.51(10)	C(6)-C(10)-H(10)	107.8
C(16)-P(2)-C(14)	106.42(10)	C(10)-C(11)-H(11A)	109.5
C(22)-P(2)-C(14)	104.64(10)	C(10)-C(11)-H(11B)	109.5
C(16)-P(2)-Fe	112.78(8)	H(11A)-C(11)-H(11B)	109.5
C(22)-P(2)-Fe	129.31(7)	C(10)-C(11)-H(11C)	109.5
C(14)-P(2)-Fe	99.05(8)	H(11A)-C(11)-H(11C)	109.5
C(1)-N-Si	125.21(14)	H(11B)-C(11)-H(11C)	109.5
C(1)-N-Fe	128.71(14)	C(10)-C(12)-H(12A)	109.5
Si-N-Fe	105.93(9)	C(10)-C(12)-H(12B)	109.5
N-Si-C(13)	116.88(10)	H(12A)-C(12)-H(12B)	109.5
N-Si-C(14)	105.00(9)	C(10)-C(12)-H(12C)	109.5
C(13)-Si-C(14)	108.73(10)	H(12A)-C(12)-H(12C)	109.5
N-Si-C(15)	106.84(9)	H(12B)-C(12)-H(12C)	109.5
C(13)-Si-C(15)	110.82(10)	Si-C(13)-H(13A)	109.5
C(14)-Si-C(15)	108.14(10)	Si-C(13)-H(13B)	109.5
C(6)-C(1)-N	120.85(19)	H(13A)-C(13)-H(13B)	109.5
C(6)-C(1)-C(2)	118.7(2)	Si-C(13)-H(13C)	109.5
N-C(1)-C(2)	120.5(2)	H(13A)-C(13)-H(13C)	109.5
C(3)-C(2)-C(1)	118.7(2)	H(13B)-C(13)-H(13C)	109.5
C(3)-C(2)-C(7)	119.9(2)	P(2)-C(14)-Si	108.21(11)
C(1)-C(2)-C(7)	121.4(2)	P(2)-C(14)-H(14A)	110.1
C(4)-C(3)-C(2)	122.4(2)	Si-C(14)-H(14A)	110.1
C(4)-C(3)-H(3)	118.8	P(2)-C(14)-H(14B)	110.1
C(2)-C(3)-H(3)	118.8	Si-C(14)-H(14B)	110.1
C(3)-C(4)-C(5)	118.8(2)	H(14A)-C(14)-H(14B)	108.4
C(3)-C(4)-H(4)	120.6	P(1)-C(15)-Si	108.92(11)
C(5)-C(4)-H(4)	120.6	P(1)-C(15)-H(15A)	109.9
C(4)-C(5)-C(6)	121.5(2)	Si-C(15)-H(15A)	109.9
C(4)-C(5)-H(5)	119.3	P(1)-C(15)-H(15B)	109.9
C(6)-C(5)-H(5)	119.3	Si-C(15)-H(15B)	109.9
C(5)-C(6)-C(1)	119.8(2)	H(15A)-C(15)-H(15B)	108.3
C(5)-C(6)-C(10)	118.4(2)	C(17)-C(16)-C(21)	119.0(2)
C(1)-C(6)-C(10)	121.7(2)	C(17)-C(16)-P(2)	119.12(17)
C(2)-C(7)-C(8)	112.87(19)	C(21)-C(16)-P(2)	121.87(17)
C(2)-C(7)-C(9)	110.70(18)	C(18)-C(17)-C(16)	120.5(2)
C(8)-C(7)-C(9)	110.18(19)	C(18)-C(17)-H(17)	119.8
C(2)-C(7)-H(7)	107.6	C(16)-C(17)-H(17)	119.8
C(8)-C(7)-H(7)	107.6	C(19)-C(18)-C(17)	119.8(2)
C(9)-C(7)-H(7)	107.6	C(19)-C(18)-H(18)	120.1
C(7)-C(8)-H(8A)	109.5	C(17)-C(18)-H(18)	120.1
C(7)-C(8)-H(8B)	109.5	C(20)-C(19)-C(18)	120.1(2)
H(8A)-C(8)-H(8B)	109.5	C(20)-C(19)-H(19)	120.0
C(7)-C(8)-H(8C)	109.5	C(18)-C(19)-H(19)	120.0
H(8A)-C(8)-H(8C)	109.5	C(19)-C(20)-C(21)	120.2(2)

C(19)-C(20)-H(20)	119.9	C(32)-C(33)-H(33)	119.9
C(21)-C(20)-H(20)	119.9	C(28)-C(33)-H(33)	119.9
C(20)-C(21)-C(16)	120.3(2)	C(35)-C(34)-C(39)	118.7(2)
C(20)-C(21)-H(21)	119.8	C(35)-C(34)-P(1)	124.73(17)
C(16)-C(21)-H(21)	119.8	C(39)-C(34)-P(1)	116.59(18)
C(23)-C(22)-C(27)	118.4(2)	C(34)-C(35)-C(36)	120.6(2)
C(23)-C(22)-P(2)	120.66(17)	C(34)-C(35)-H(35)	119.7
C(27)-C(22)-P(2)	120.85(18)	C(36)-C(35)-H(35)	119.7
C(24)-C(23)-C(22)	121.1(2)	C(37)-C(36)-C(35)	119.8(2)
C(24)-C(23)-H(23)	119.5	C(37)-C(36)-H(36)	120.1
C(22)-C(23)-H(23)	119.5	C(35)-C(36)-H(36)	120.1
C(23)-C(24)-C(25)	120.0(2)	C(38)-C(37)-C(36)	120.4(2)
C(23)-C(24)-H(24)	120.0	C(38)-C(37)-H(37)	119.8
C(25)-C(24)-H(24)	120.0	C(36)-C(37)-H(37)	119.8
C(26)-C(25)-C(24)	119.3(2)	C(37)-C(38)-C(39)	120.1(2)
C(26)-C(25)-H(25)	120.3	C(37)-C(38)-H(38)	120.0
C(24)-C(25)-H(25)	120.3	C(39)-C(38)-H(38)	120.0
C(25)-C(26)-C(27)	120.9(2)	C(38)-C(39)-C(34)	120.3(2)
C(25)-C(26)-H(26)	119.5	C(38)-C(39)-H(39)	119.8
C(27)-C(26)-H(26)	119.5	C(34)-C(39)-H(39)	119.8
C(26)-C(27)-C(22)	120.2(2)	C(45)-C(40)-C(41)	119.5(2)
C(26)-C(27)-H(27)	119.9	C(45)-C(40)-H(40)	120.3
C(22)-C(27)-H(27)	119.9	C(41)-C(40)-H(40)	120.3
C(29)-C(28)-C(33)	119.0(2)	C(42)-C(41)-C(40)	119.8(2)
C(29)-C(28)-P(1)	117.57(17)	C(42)-C(41)-H(41)	120.1
C(33)-C(28)-P(1)	123.46(18)	C(40)-C(41)-H(41)	120.1
C(30)-C(29)-C(28)	120.8(2)	C(43)-C(42)-C(41)	120.6(2)
C(30)-C(29)-H(29)	119.6	C(43)-C(42)-H(42)	119.7
C(28)-C(29)-H(29)	119.6	C(41)-C(42)-H(42)	119.7
C(29)-C(30)-C(31)	119.8(2)	C(42)-C(43)-C(44)	119.4(2)
C(29)-C(30)-H(30)	120.1	C(42)-C(43)-H(43)	120.3
C(31)-C(30)-H(30)	120.1	C(44)-C(43)-H(43)	120.3
C(32)-C(31)-C(30)	119.8(2)	C(45)-C(44)-C(43)	120.4(2)
C(32)-C(31)-H(31)	120.1	C(45)-C(44)-H(44)	119.8
C(30)-C(31)-H(31)	120.1	C(43)-C(44)-H(44)	119.8
C(31)-C(32)-C(33)	120.3(2)	C(44)-C(45)-C(40)	120.3(2)
C(31)-C(32)-H(32)	119.8	C(44)-C(45)-H(45)	119.8
C(33)-C(32)-H(32)	119.8	C(40)-C(45)-H(45)	119.8
C(32)-C(33)-C(28)	120.2(2)		

Symmetry transformations used to generate equivalent atoms:

Table 14. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for ($^{Si}NP_2$)FeCl (**3**). The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Fe	16(1)	14(1)	13(1)	1(1)	3(1)	-1(1)
Cl	31(1)	23(1)	20(1)	3(1)	3(1)	-11(1)
P(1)	15(1)	14(1)	16(1)	1(1)	2(1)	0(1)
P(2)	15(1)	15(1)	14(1)	0(1)	1(1)	0(1)
N	16(1)	13(1)	17(1)	-1(1)	4(1)	-1(1)
Si	18(1)	13(1)	15(1)	0(1)	4(1)	-1(1)
C(1)	11(1)	14(1)	16(2)	-2(1)	4(1)	-7(1)
C(2)	12(1)	16(1)	17(2)	-2(1)	3(1)	-4(1)
C(3)	13(1)	16(1)	21(2)	-2(1)	0(1)	0(1)
C(4)	15(1)	23(1)	18(2)	-10(1)	4(1)	-4(1)
C(5)	17(1)	23(1)	15(1)	-2(1)	2(1)	-7(1)
C(6)	16(1)	14(1)	16(2)	1(1)	4(1)	-6(1)
C(7)	20(1)	16(1)	15(2)	-1(1)	2(1)	2(1)
C(8)	50(2)	25(2)	25(2)	5(1)	3(1)	-8(1)
C(9)	25(2)	34(2)	24(2)	1(1)	2(1)	3(1)
C(10)	23(1)	19(1)	15(1)	-1(1)	2(1)	-1(1)
C(11)	20(1)	23(1)	31(2)	-1(1)	-1(1)	2(1)
C(12)	34(2)	30(2)	29(2)	10(1)	1(1)	-4(1)
C(13)	24(1)	19(1)	22(2)	0(1)	6(1)	-3(1)
C(14)	14(1)	15(1)	24(2)	0(1)	5(1)	-1(1)
C(15)	21(1)	14(1)	14(1)	0(1)	0(1)	-2(1)
C(16)	15(1)	19(1)	12(1)	-3(1)	2(1)	3(1)
C(17)	20(1)	22(1)	15(2)	0(1)	2(1)	-1(1)
C(18)	30(2)	18(1)	19(2)	4(1)	4(1)	2(1)
C(19)	21(1)	28(2)	19(2)	3(1)	-1(1)	9(1)
C(20)	16(1)	30(2)	23(2)	-3(1)	-4(1)	2(1)
C(21)	23(1)	17(1)	19(2)	-4(1)	0(1)	-2(1)
C(22)	10(1)	17(1)	16(2)	-3(1)	-1(1)	-2(1)
C(23)	13(1)	18(1)	20(2)	-1(1)	-1(1)	-3(1)
C(24)	19(1)	30(2)	16(2)	-3(1)	2(1)	-5(1)
C(25)	15(1)	30(2)	25(2)	-14(1)	3(1)	0(1)
C(26)	17(1)	22(1)	31(2)	-5(1)	-3(1)	2(1)
C(27)	17(1)	23(1)	16(2)	-3(1)	-2(1)	0(1)
C(28)	14(1)	17(1)	16(2)	-1(1)	1(1)	-2(1)
C(29)	21(1)	18(1)	21(2)	-1(1)	2(1)	-1(1)
C(30)	23(2)	32(2)	20(2)	1(1)	6(1)	-7(1)
C(31)	19(1)	33(2)	26(2)	-12(1)	8(1)	-1(1)
C(32)	27(2)	19(1)	36(2)	-4(1)	6(1)	3(1)
C(33)	24(1)	21(1)	22(2)	3(1)	4(1)	2(1)
C(34)	14(1)	15(1)	17(1)	-2(1)	3(1)	1(1)
C(35)	22(1)	14(1)	24(2)	0(1)	-1(1)	-3(1)
C(36)	26(1)	24(1)	19(2)	5(1)	-2(1)	3(1)
C(37)	15(1)	28(2)	21(2)	-7(1)	-4(1)	3(1)
C(38)	18(1)	19(1)	32(2)	-7(1)	2(1)	-4(1)
C(39)	21(1)	16(1)	23(2)	2(1)	3(1)	0(1)
C(40)	46(2)	16(1)	20(2)	1(1)	-2(1)	-9(1)
C(41)	46(2)	14(1)	35(2)	3(1)	21(2)	2(1)
C(42)	19(1)	22(1)	46(2)	10(1)	-2(1)	1(1)
C(43)	32(2)	24(1)	20(2)	1(1)	-3(1)	-5(1)
C(44)	23(2)	22(1)	25(2)	0(1)	8(1)	-4(1)
C(45)	19(1)	18(1)	35(2)	4(1)	-2(1)	-5(1)

Table 15. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for ($^{Si}NP_2$)FeCl (**3**).

	x	y	z	U(eq)
H(3)	6935	-1064	833	20
H(4)	6515	-641	322	22
H(5)	5021	1187	158	22
H(7)	5517	864	1429	20
H(8A)	4960	-1579	1330	50
H(8B)	6047	-1418	1616	50
H(8C)	6545	-1914	1299	50
H(9A)	8254	144	1298	41
H(9B)	7812	528	1627	41
H(9C)	7742	1722	1369	41
H(10)	3377	3674	616	23
H(11A)	1514	2967	279	37
H(11B)	1861	1752	526	37
H(11C)	2335	1568	193	37
H(12A)	4052	3266	10	46
H(12B)	4908	4294	242	46
H(12C)	3342	4650	139	46
H(13A)	6901	4721	926	32
H(13B)	6110	6213	935	32
H(13C)	5639	5047	686	32
H(14A)	6580	4092	1558	21
H(14B)	5698	5490	1620	21
H(15A)	3248	6285	1278	20
H(15B)	2916	5828	933	20
H(17)	4421	557	2001	23
H(18)	5908	-1057	2258	26
H(19)	8143	-361	2416	27
H(20)	8867	1960	2330	28
H(21)	7396	3572	2070	23
H(23)	4299	3303	2434	21
H(24)	3652	4883	2800	26
H(25)	3034	7230	2669	28
H(26)	3073	7969	2172	28
H(27)	3760	6412	1805	22
H(29)	866	3495	1812	24
H(30)	-231	4593	2195	30
H(31)	-932	6974	2144	31
H(32)	-490	8255	1714	33
H(33)	643	7171	1334	27
H(35)	820	6068	721	24
H(36)	-820	5753	316	28
H(37)	-2141	3690	283	26
H(38)	-1814	1919	646	27
H(39)	-145	2195	1045	24
H(40)	2328	9054	1013	33
H(41)	-3	9443	879	37
H(42)	-877	9099	383	35
H(43)	545	8353	22	31
H(44)	2869	7966	157	28
H(45)	3754	8323	649	29

Figure 9. Fully labeled drawing of ($^{Si}NP_2$)CoI (**4b**)

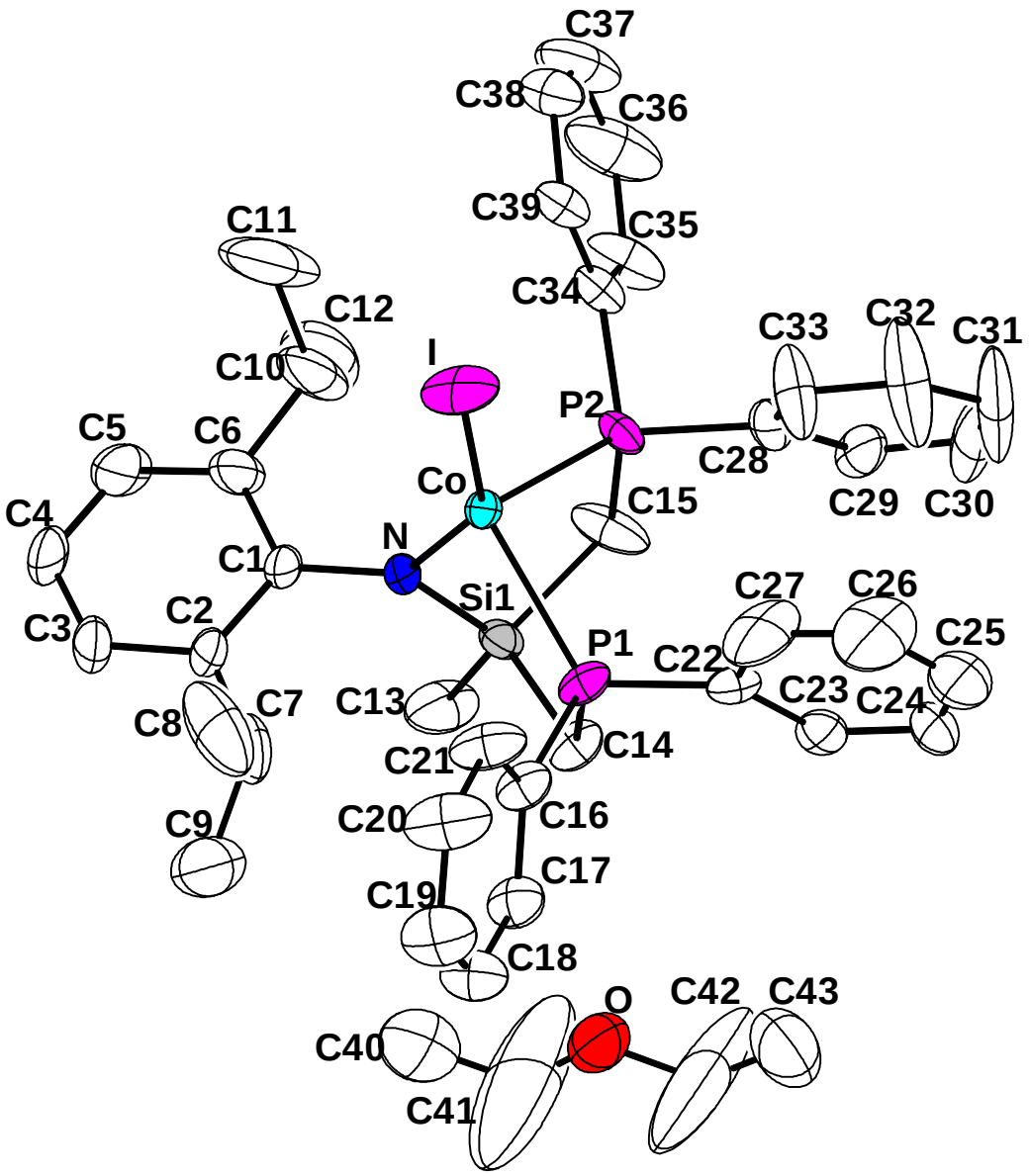

Table 16. Crystal data and structure refinement for ($^{Si}NP_2$)CoI (**4b**).

Identification code	mtw12	
Empirical formula	C43 H54 Co I N O P2 Si	
Formula weight	876.73	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 11.6071(8) Å	α= 90°.
	b = 21.6762(15) Å	β= 92.988(2)°.
	c = 16.8895(12) Å	γ = 90°.
Volume	4243.6(5) Å^3	
Z	4	
Density (calculated)	1.372 Mg/m^3	
Absorption coefficient	1.268 mm^{-1}	
F(000)	1804	
Crystal size	0.52 x 0.33 x 0.31 mm^3	
Theta range for data collection	1.76 to 32.82°.	
Index ranges	-17<=h<=16, -32<=k<=33, -25<=l<=24	
Reflections collected	77696	
Independent reflections	14707 [R(int) = 0.0791]	
Completeness to theta = 32.82°	93.3 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	14707 / 0 / 458	
Goodness-of-fit on F^2	3.006	
Final R indices [I>2sigma(I)]	R1 = 0.0700, wR2 = 0.1290	
R indices (all data)	R1 = 0.1074, wR2 = 0.1386	
Largest diff. peak and hole	3.111 and -2.974 e.Å^{-3}	

Special Refinement Details.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of F^2 > 2σ(F^2) is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full convariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles, and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes. The diethyl ether molecule suffers from rather severe disorder in the atomic positions.

Table 17. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for ($^{Si}NP_2$)CoI (**4b**). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
I	9201(1)	2019(1)	-1197(1)	56(1)
Co	8124(1)	2321(1)	5(1)	24(1)
P(1)	8761(1)	3247(1)	652(1)	29(1)
P(2)	8624(1)	1695(1)	1123(1)	29(1)
Si(1)	6789(1)	2627(1)	1364(1)	27(1)
N	6618(2)	2445(1)	382(2)	34(1)
C(1)	5553(3)	2386(2)	-64(3)	48(1)
C(14)	7742(3)	3322(2)	1429(2)	34(1)
C(2)	5035(4)	2905(2)	-441(2)	47(1)
C(20)	9114(5)	4467(2)	-1156(3)	63(1)
C(16)	8678(3)	3951(2)	62(2)	35(1)
C(34)	8376(3)	866(2)	1047(2)	37(1)
C(28)	10077(3)	1710(2)	1570(2)	38(1)
C(15)	7640(4)	1979(2)	1851(2)	52(1)
C(21)	9083(4)	3933(2)	-695(2)	49(1)
C(29)	10324(4)	1711(2)	2384(2)	48(1)
C(17)	8271(3)	4511(2)	347(2)	40(1)
C(22)	10213(3)	3314(1)	1104(2)	33(1)
C(7)	5636(4)	3523(2)	-453(3)	57(1)
C(18)	8285(4)	5030(2)	-121(3)	49(1)
C(38)	8571(4)	-74(2)	296(3)	60(1)
C(23)	10456(3)	3438(1)	1898(2)	34(1)
C(33)	10983(4)	1729(3)	1070(3)	74(2)
C(39)	8664(3)	563(2)	360(3)	44(1)
C(37)	8177(5)	-403(2)	914(4)	78(2)
C(8)	6146(5)	3637(3)	-1252(3)	94(2)
C(27)	11145(5)	3226(3)	617(3)	79(2)
C(13)	5418(4)	2756(2)	1867(3)	63(1)
C(19)	8696(4)	5012(2)	-873(3)	57(1)
C(30)	11452(5)	1703(2)	2683(3)	75(2)
C(9)	4861(6)	4067(2)	-244(3)	81(2)
C(35)	7966(4)	525(2)	1673(3)	59(1)
C(6)	5017(4)	1807(2)	-154(5)	104(3)
C(11)	5804(6)	769(2)	-505(7)	179(5)
C(10)	5591(6)	1232(2)	184(7)	164(5)
C(5)	3960(5)	1769(2)	-561(6)	138(4)
C(36)	7862(5)	-113(2)	1600(4)	85(2)
C(24)	11591(4)	3473(2)	2207(3)	50(1)
C(25)	12483(5)	3396(2)	1729(4)	84(2)
C(31)	12330(6)	1702(3)	2186(4)	109(3)
C(32)	12116(5)	1727(4)	1383(4)	119(3)
C(26)	12276(5)	3281(3)	931(5)	102(2)
C(12)	4929(9)	939(3)	819(8)	216(8)
C(3)	3965(4)	2832(2)	-847(3)	66(2)
C(4)	3414(4)	2273(3)	-901(4)	103(3)
O	7055(3)	4746(1)	2344(2)	61(1)
C(43)	8919(6)	4862(3)	2869(4)	94(2)
C(40)	5106(6)	4633(3)	1967(4)	103(2)
C(41)	5981(11)	4846(9)	2400(7)	303(12)
C(42)	7868(9)	4945(7)	2820(8)	287(10)

Table 18. Bond lengths [Å] and angles [°] for ($^{Si}NP_2$)CoI (**4b**).

I-Co	2.5258(5)	C(8)-H(8A)	0.9800
Co-N	1.910(3)	C(8)-H(8B)	0.9800
Co-P(2)	2.3731(8)	C(8)-H(8C)	0.9800
Co-P(1)	2.3849(9)	C(27)-C(26)	1.395(8)
P(1)-C(14)	1.820(4)	C(27)-H(27)	0.9500
P(1)-C(22)	1.820(4)	C(13)-H(13A)	0.9800
P(1)-C(16)	1.822(3)	C(13)-H(13B)	0.9800
P(2)-C(28)	1.813(4)	C(13)-H(13C)	0.9800
P(2)-C(34)	1.821(3)	C(19)-H(19)	0.9500
P(2)-C(15)	1.829(4)	C(30)-C(31)	1.354(9)
Si(1)-N	1.706(3)	C(30)-H(30)	0.9500
Si(1)-C(13)	1.863(4)	C(9)-H(9A)	0.9800
Si(1)-C(14)	1.869(3)	C(9)-H(9B)	0.9800
Si(1)-C(15)	1.883(4)	C(9)-H(9C)	0.9800
N-C(1)	1.419(4)	C(35)-C(36)	1.392(6)
C(1)-C(6)	1.405(6)	C(35)-H(35)	0.9500
C(1)-C(2)	1.413(5)	C(6)-C(5)	1.377(6)
C(14)-H(14A)	0.9900	C(6)-C(10)	1.511(8)
C(14)-H(14B)	0.9900	C(11)-C(10)	1.566(13)
C(2)-C(3)	1.396(5)	C(11)-H(11A)	0.9800
C(2)-C(7)	1.511(6)	C(11)-H(11B)	0.9800
C(20)-C(19)	1.372(6)	C(11)-H(11C)	0.9800
C(20)-C(21)	1.396(5)	C(10)-C(12)	1.494(16)
C(20)-H(20)	0.9500	C(10)-H(10)	1.0000
C(16)-C(21)	1.386(5)	C(5)-C(4)	1.375(8)
C(16)-C(17)	1.396(5)	C(5)-H(5)	0.9500
C(34)-C(39)	1.390(5)	C(36)-H(36)	0.9500
C(34)-C(35)	1.395(5)	C(24)-C(25)	1.355(7)
C(28)-C(33)	1.382(6)	C(24)-H(24)	0.9500
C(28)-C(29)	1.389(5)	C(25)-C(26)	1.380(9)
C(15)-H(15A)	0.9900	C(25)-H(25)	0.9500
C(15)-H(15B)	0.9900	C(31)-C(32)	1.366(8)
C(21)-H(21)	0.9500	C(31)-H(31)	0.9500
C(29)-C(30)	1.379(7)	C(32)-H(32)	0.9500
C(29)-H(29)	0.9500	C(26)-H(26)	0.9500
C(17)-C(18)	1.377(5)	C(12)-H(12A)	0.9800
C(17)-H(17)	0.9500	C(12)-H(12B)	0.9800
C(22)-C(23)	1.382(5)	C(12)-H(12C)	0.9800
C(22)-C(27)	1.405(6)	C(3)-C(4)	1.370(7)
C(7)-C(8)	1.521(7)	C(3)-H(3)	0.9500
C(7)-C(9)	1.536(7)	C(4)-H(4)	0.9500
C(7)-H(7)	1.0000	O-C(41)	1.275(12)
C(18)-C(19)	1.380(6)	O-C(42)	1.282(8)
C(18)-H(18)	0.9500	C(43)-C(42)	1.232(11)
C(38)-C(37)	1.363(7)	C(43)-H(43A)	0.9800
C(38)-C(39)	1.388(5)	C(43)-H(43B)	0.9800
C(38)-H(38)	0.9500	C(43)-H(43C)	0.9800
C(23)-C(24)	1.394(5)	C(40)-C(41)	1.304(11)
C(23)-H(23)	0.9500	C(40)-H(40A)	0.9800
C(33)-C(32)	1.391(7)	C(40)-H(40B)	0.9800
C(33)-H(33)	0.9500	C(40)-H(40C)	0.9800
C(39)-H(39)	0.9500	C(41)-H(41A)	0.9900
C(37)-C(36)	1.384(8)	C(41)-H(41B)	0.9900
C(37)-H(37)	0.9500	C(42)-H(42A)	0.9900

C(42)-H(42B)	0.9900
N-Co-P(2)	90.29(9)
N-Co-P(1)	89.78(8)
P(2)-Co-P(1)	93.44(3)
N-Co-I	143.57(8)
P(2)-Co-I	112.33(3)
P(1)-Co-I	115.61(3)
C(14)-P(1)-C(22)	108.27(16)
C(14)-P(1)-C(16)	107.59(17)
C(22)-P(1)-C(16)	100.57(16)
C(14)-P(1)-Co	101.99(11)
C(22)-P(1)-Co	121.20(10)
C(16)-P(1)-Co	116.62(11)
C(28)-P(2)-C(34)	100.83(15)
C(28)-P(2)-C(15)	108.3(2)
C(34)-P(2)-C(15)	106.12(19)
C(28)-P(2)-Co	120.31(12)
C(34)-P(2)-Co	118.49(12)
C(15)-P(2)-Co	101.95(11)
N-Si(1)-C(13)	114.82(19)
N-Si(1)-C(14)	106.41(15)
C(13)-Si(1)-C(14)	111.65(17)
N-Si(1)-C(15)	106.51(16)
C(13)-Si(1)-C(15)	110.7(2)
C(14)-Si(1)-C(15)	106.3(2)
C(1)-N-Si(1)	126.2(3)
C(1)-N-Co	126.7(3)
Si(1)-N-Co	107.15(13)
C(6)-C(1)-C(2)	119.1(3)
C(6)-C(1)-N	120.5(3)
C(2)-C(1)-N	120.4(3)
P(1)-C(14)-Si(1)	106.90(16)
P(1)-C(14)-H(14A)	110.3
Si(1)-C(14)-H(14A)	110.3
P(1)-C(14)-H(14B)	110.3
Si(1)-C(14)-H(14B)	110.3
H(14A)-C(14)-H(14B)	108.6
C(3)-C(2)-C(1)	118.6(4)
C(3)-C(2)-C(7)	119.5(4)
C(1)-C(2)-C(7)	121.8(3)
C(19)-C(20)-C(21)	119.9(4)
C(19)-C(20)-H(20)	120.0
C(21)-C(20)-H(20)	120.0
C(21)-C(16)-C(17)	118.7(3)
C(21)-C(16)-P(1)	118.0(3)
C(17)-C(16)-P(1)	123.2(3)
C(39)-C(34)-C(35)	119.2(3)
C(39)-C(34)-P(2)	118.7(3)
C(35)-C(34)-P(2)	121.9(3)
C(33)-C(28)-C(29)	118.7(4)
C(33)-C(28)-P(2)	117.9(3)
C(29)-C(28)-P(2)	123.5(3)
P(2)-C(15)-Si(1)	106.79(18)
P(2)-C(15)-H(15A)	110.4
Si(1)-C(15)-H(15A)	110.4
P(2)-C(15)-H(15B)	110.4
Si(1)-C(15)-H(15B)	110.4
H(15A)-C(15)-H(15B)	108.6
C(16)-C(21)-C(20)	120.7(4)
C(16)-C(21)-H(21)	119.6
C(20)-C(21)-H(21)	119.6
C(30)-C(29)-C(28)	120.3(5)
C(30)-C(29)-H(29)	119.8
C(28)-C(29)-H(29)	119.8
C(18)-C(17)-C(16)	119.8(4)
C(18)-C(17)-H(17)	120.1
C(16)-C(17)-H(17)	120.1
C(23)-C(22)-C(27)	118.0(4)
C(23)-C(22)-P(1)	124.1(3)
C(27)-C(22)-P(1)	117.9(3)
C(2)-C(7)-C(8)	110.9(4)
C(2)-C(7)-C(9)	113.7(4)
C(8)-C(7)-C(9)	109.8(4)
C(2)-C(7)-H(7)	107.4
C(8)-C(7)-H(7)	107.4
C(9)-C(7)-H(7)	107.4
C(17)-C(18)-C(19)	121.3(4)
C(17)-C(18)-H(18)	119.3
C(19)-C(18)-H(18)	119.3
C(37)-C(38)-C(39)	119.3(5)
C(37)-C(38)-H(38)	120.4
C(39)-C(38)-H(38)	120.4
C(22)-C(23)-C(24)	121.0(4)
C(22)-C(23)-H(23)	119.5
C(24)-C(23)-H(23)	119.5
C(28)-C(33)-C(32)	120.1(5)
C(28)-C(33)-H(33)	119.9
C(32)-C(33)-H(33)	119.9
C(38)-C(39)-C(34)	120.9(4)
C(38)-C(39)-H(39)	119.5
C(34)-C(39)-H(39)	119.5
C(38)-C(37)-C(36)	121.1(4)
C(38)-C(37)-H(37)	119.5
C(36)-C(37)-H(37)	119.5
C(7)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(26)-C(27)-C(22)	120.3(5)
C(26)-C(27)-H(27)	119.9
C(22)-C(27)-H(27)	119.9
Si(1)-C(13)-H(13A)	109.5
Si(1)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
Si(1)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(20)-C(19)-C(18)	119.4(4)
C(20)-C(19)-H(19)	120.3

C(18)-C(19)-H(19)	120.3	C(31)-C(32)-C(33)	119.8(6)
C(31)-C(30)-C(29)	120.3(5)	C(31)-C(32)-H(32)	120.1
C(31)-C(30)-H(30)	119.8	C(33)-C(32)-H(32)	120.1
C(29)-C(30)-H(30)	119.8	C(25)-C(26)-C(27)	119.9(5)
C(7)-C(9)-H(9A)	109.5	C(25)-C(26)-H(26)	120.1
C(7)-C(9)-H(9B)	109.5	C(27)-C(26)-H(26)	120.1
H(9A)-C(9)-H(9B)	109.5	C(10)-C(12)-H(12A)	109.5
C(7)-C(9)-H(9C)	109.5	C(10)-C(12)-H(12B)	109.5
H(9A)-C(9)-H(9C)	109.5	H(12A)-C(12)-H(12B)	109.5
H(9B)-C(9)-H(9C)	109.5	C(10)-C(12)-H(12C)	109.5
C(36)-C(35)-C(34)	119.4(5)	H(12A)-C(12)-H(12C)	109.5
C(36)-C(35)-H(35)	120.3	H(12B)-C(12)-H(12C)	109.5
C(34)-C(35)-H(35)	120.3	C(4)-C(3)-C(2)	122.2(4)
C(5)-C(6)-C(1)	119.1(5)	C(4)-C(3)-H(3)	118.9
C(5)-C(6)-C(10)	120.2(5)	C(2)-C(3)-H(3)	118.9
C(1)-C(6)-C(10)	120.7(4)	C(3)-C(4)-C(5)	118.2(4)
C(10)-C(11)-H(11A)	109.5	C(3)-C(4)-H(4)	120.9
C(10)-C(11)-H(11B)	109.5	C(5)-C(4)-H(4)	120.9
H(11A)-C(11)-H(11B)	109.5	C(41)-O-C(42)	125.9(7)
C(10)-C(11)-H(11C)	109.5	C(42)-C(43)-H(43A)	109.5
H(11A)-C(11)-H(11C)	109.5	C(42)-C(43)-H(43B)	109.5
H(11B)-C(11)-H(11C)	109.5	H(43A)-C(43)-H(43B)	109.5
C(12)-C(10)-C(6)	112.9(7)	C(42)-C(43)-H(43C)	109.5
C(12)-C(10)-C(11)	111.6(6)	H(43A)-C(43)-H(43C)	109.5
C(6)-C(10)-C(11)	109.4(8)	H(43B)-C(43)-H(43C)	109.5
C(12)-C(10)-H(10)	107.6	C(41)-C(40)-H(40A)	109.5
C(6)-C(10)-H(10)	107.6	C(41)-C(40)-H(40B)	109.5
C(11)-C(10)-H(10)	107.6	H(40A)-C(40)-H(40B)	109.5
C(4)-C(5)-C(6)	122.7(5)	C(41)-C(40)-H(40C)	109.5
C(4)-C(5)-H(5)	118.7	H(40A)-C(40)-H(40C)	109.5
C(6)-C(5)-H(5)	118.7	H(40B)-C(40)-H(40C)	109.5
C(37)-C(36)-C(35)	120.0(5)	O-C(41)-C(40)	129.4(10)
C(37)-C(36)-H(36)	120.0	O-C(41)-H(41A)	104.9
C(35)-C(36)-H(36)	120.0	C(40)-C(41)-H(41A)	104.9
C(25)-C(24)-C(23)	120.5(4)	O-C(41)-H(41B)	104.9
C(25)-C(24)-H(24)	119.8	C(40)-C(41)-H(41B)	104.9
C(23)-C(24)-H(24)	119.8	H(41A)-C(41)-H(41B)	105.8
C(24)-C(25)-C(26)	120.3(5)	C(43)-C(42)-O	133.3(9)
C(24)-C(25)-H(25)	119.8	C(43)-C(42)-H(42A)	103.9
C(26)-C(25)-H(25)	119.8	O-C(42)-H(42A)	103.9
C(30)-C(31)-C(32)	120.7(5)	C(43)-C(42)-H(42B)	103.9
C(30)-C(31)-H(31)	119.7	O-C(42)-H(42B)	103.9
C(32)-C(31)-H(31)	119.7	H(42A)-C(42)-H(42B)	105.4

Symmetry transformations used to generate equivalent atoms:

Table 19. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for ($^{Si}NP_2$)CoI (**4b**). The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
I	111(1)	40(1)	17(1)	-4(1)	18(1)	7(1)
Co	33(1)	23(1)	16(1)	-1(1)	-6(1)	4(1)
P(1)	42(1)	30(1)	16(1)	-6(1)	8(1)	-7(1)
P(2)	36(1)	32(1)	20(1)	4(1)	2(1)	17(1)
Si(1)	23(1)	24(1)	34(1)	-1(1)	3(1)	5(1)
N	25(1)	32(1)	42(2)	-14(1)	-12(1)	10(1)
C(1)	28(2)	43(2)	69(3)	-30(2)	-24(2)	14(2)
C(14)	44(2)	39(2)	19(2)	-6(1)	9(1)	-8(2)
C(2)	46(2)	50(2)	41(2)	-23(2)	-24(2)	15(2)
C(20)	109(4)	42(2)	40(2)	5(2)	36(3)	-9(2)
C(16)	47(2)	35(2)	24(2)	-3(1)	9(2)	-7(2)
C(34)	34(2)	32(2)	44(2)	8(2)	1(2)	12(1)
C(28)	45(2)	38(2)	29(2)	5(1)	-10(2)	9(2)
C(15)	79(3)	43(2)	38(2)	18(2)	31(2)	34(2)
C(21)	80(3)	34(2)	37(2)	-5(2)	27(2)	-9(2)
C(29)	77(3)	33(2)	31(2)	5(2)	-19(2)	-3(2)
C(17)	52(2)	41(2)	28(2)	-3(2)	7(2)	-1(2)
C(22)	39(2)	25(1)	36(2)	-9(1)	7(2)	1(1)
C(7)	61(3)	65(3)	42(2)	12(2)	-28(2)	4(2)
C(18)	62(3)	37(2)	50(3)	1(2)	13(2)	3(2)
C(38)	58(3)	39(2)	81(3)	-11(2)	-3(3)	15(2)
C(23)	45(2)	24(1)	33(2)	7(1)	0(2)	-2(1)
C(33)	42(3)	129(4)	48(3)	24(3)	-16(2)	9(3)
C(39)	44(2)	34(2)	54(3)	1(2)	-2(2)	16(2)
C(37)	67(3)	31(2)	137(6)	12(3)	18(3)	8(2)
C(8)	88(4)	134(5)	59(3)	38(3)	1(3)	46(4)
C(27)	57(3)	101(4)	81(4)	-63(3)	22(3)	0(3)
C(13)	36(2)	56(2)	98(4)	-32(3)	23(2)	-4(2)
C(19)	80(3)	44(2)	47(3)	12(2)	19(2)	-8(2)
C(30)	89(4)	75(3)	56(3)	27(2)	-47(3)	-34(3)
C(9)	118(5)	54(3)	69(4)	-9(2)	-15(3)	7(3)
C(35)	59(3)	45(2)	74(3)	18(2)	30(2)	20(2)
C(6)	54(3)	39(2)	211(7)	-46(3)	-71(4)	18(2)
C(11)	68(4)	46(3)	417(16)	-69(6)	-52(7)	25(3)
C(10)	82(5)	27(2)	368(14)	-37(5)	-121(7)	15(3)
C(5)	62(4)	60(3)	281(10)	-79(5)	-96(5)	19(3)
C(36)	73(4)	49(3)	136(6)	29(3)	47(4)	14(2)
C(24)	57(3)	34(2)	56(3)	8(2)	-21(2)	7(2)
C(25)	45(3)	83(3)	123(5)	-51(3)	-15(3)	33(3)
C(31)	66(4)	157(6)	97(5)	60(5)	-60(4)	-33(4)
C(32)	40(3)	223(8)	91(5)	66(5)	-25(3)	-6(4)
C(26)	44(3)	129(5)	134(6)	-73(5)	26(3)	16(3)
C(12)	177(10)	42(3)	410(19)	-15(6)	-180(12)	7(5)
C(3)	56(3)	75(3)	61(3)	-37(2)	-37(2)	32(2)
C(4)	55(3)	92(4)	155(6)	-77(4)	-72(4)	37(3)
O	78(2)	46(2)	56(2)	-1(1)	-12(2)	-8(2)
C(43)	82(5)	76(3)	122(6)	22(4)	-23(4)	8(3)
C(40)	121(6)	76(4)	108(5)	-1(4)	-16(5)	15(4)
C(41)	145(11)	590(30)	177(12)	-239(17)	6(9)	-48(14)
C(42)	102(8)	470(20)	286(16)	-302(17)	-15(9)	-36(11)

Table 20. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for ($^{Si}NP_2$)CoI (**4b**).

	x	y	z	U(eq)
H(14A)	7278	3703	1351	41
H(14B)	8157	3342	1956	41
H(20)	9425	4453	-1665	75
H(15A)	8080	2130	2331	63
H(15B)	7117	1645	2009	63
H(21)	9342	3553	-903	59
H(29)	9712	1716	2736	57
H(17)	7984	4533	863	48
H(7)	6291	3509	-45	69
H(18)	8007	5409	78	59
H(38)	8781	-278	-173	72
H(23)	9840	3499	2238	41
H(33)	10832	1743	512	88
H(39)	8928	795	-73	53
H(37)	8118	-839	873	94
H(8A)	6702	3310	-1357	141
H(8B)	6538	4037	-1244	141
H(8C)	5528	3636	-1670	141
H(27)	11003	3127	73	94
H(13A)	5006	3107	1623	94
H(13B)	5593	2841	2431	94
H(13C)	4935	2386	1814	94
H(19)	8689	5373	-1191	68
H(30)	11614	1698	3240	90
H(9A)	4234	4111	-652	122
H(9B)	5319	4447	-217	122
H(9C)	4535	3992	271	122
H(35)	7759	725	2145	70
H(11A)	6191	399	-289	269
H(11B)	6289	965	-891	269
H(11C)	5063	652	-768	269
H(10)	6362	1355	426	196
H(5)	3593	1378	-608	165
H(36)	7575	-348	2020	102
H(24)	11741	3552	2756	60
H(25)	13254	3422	1945	101
H(31)	13104	1684	2398	131
H(32)	12738	1743	1040	143
H(26)	12903	3239	595	122
H(12A)	4905	1220	1272	324
H(12B)	5307	553	988	324
H(12C)	4141	852	613	324
H(3)	3607	3182	-1094	79
H(4)	2676	2236	-1167	124
H(43A)	9082	4419	2860	141
H(43B)	9242	5040	3366	141
H(43C)	9270	5062	2420	141
H(40A)	5364	4513	1446	154
H(40B)	4514	4954	1902	154
H(40C)	4784	4273	2228	154

H(41A)	5899	5300	2376	363
H(41B)	5821	4728	2950	363
H(42A)	7787	5400	2790	345
H(42B)	7616	4829	3351	345

Figure 10. Fully labeled drawing of [$^{Si}NP_3$]CoCl (**2a**).

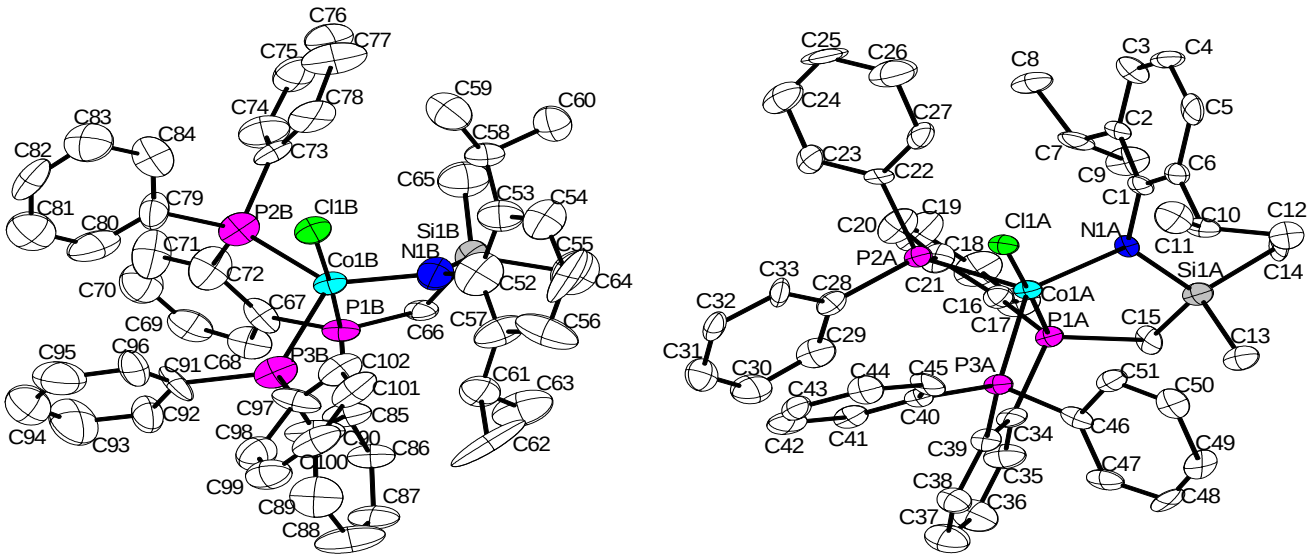

Table 21. Crystal data and structure refinement for $Co(^{Si}NP_3)Cl$ (**2a**).

Identification code	mtw21	
Empirical formula	C51 H52 Cl Co N P3 Si	
Formula weight	894.32	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 12.8058(15) Å	α= 93.701(4)°.
	b = 17.612(2) Å	β= 91.736(4)°.
	c = 20.505(3) Å	γ = 103.463(4)°.
Volume	4483.4(10) $Å^3$	
Z	4	
Density (calculated)	1.325 Mg/m^3	
Absorption coefficient	0.613 mm^{-1}	
F(000)	1872	
Crystal size	0.19 x 0.081 x 0.074 mm^3	
Theta range for data collection	1.00 to 23.01°.	
Index ranges	-13<=h<=13, -19<=k<=18, -20<=l<=21	
Reflections collected	17435	
Independent reflections	9939 [R(int) = 0.1319]	
Completeness to theta = 23.01°	79.5 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9939 / 17 / 1057	
Goodness-of-fit on F^2	0.970	
Final R indices [I>2sigma(I)]	R1 = 0.0935, wR2 = 0.2331	
R indices (all data)	R1 = 0.1835, wR2 = 0.2813	
Largest diff. peak and hole	2.294 and -0.767 $e.Å^{-3}$	

Special Refinement Details.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full convariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles, and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes. The phenyl ring defined by C52 to C56, with respect to deviations away from the plane of the ring, was treated with a FLAT command. The following atoms were restrained so that their U_{ij} components approximated isotropic behavior: C22, C55.

Table 22. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Co($^{Si}NP_3$)Cl (**2a**). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Co(1A)	7491(1)	9398(1)	2561(1)	20(1)
Co(1B)	7843(1)	4416(1)	2481(1)	28(1)
Cl(1A)	7125(2)	8108(2)	2745(2)	24(1)
Cl(1B)	8197(3)	3212(2)	2311(2)	37(1)
P(1A)	7903(3)	10620(2)	2428(2)	22(1)
P(2A)	8322(3)	9271(2)	1595(2)	23(1)
P(3A)	8835(3)	9630(2)	3313(2)	23(1)
P(1B)	7538(3)	5539(2)	2697(2)	31(1)
P(2B)	8565(4)	4524(2)	3512(2)	49(1)
P(3B)	6036(4)	3947(2)	2585(2)	51(1)
Si(1A)	5811(3)	10362(2)	3015(2)	28(1)
Si(1B)	9214(3)	5813(2)	1768(2)	40(1)
N(1A)	5976(8)	9522(5)	2586(5)	21(3)
N(1B)	8438(10)	4838(7)	1690(6)	50(4)
C(1)	5111(10)	8919(7)	2368(6)	22(3)
C(2)	4770(10)	8786(7)	1690(7)	22(3)
C(3)	3902(11)	8188(8)	1481(7)	30(4)
C(4)	3352(11)	7704(8)	1892(7)	34(4)
C(5)	3615(11)	7784(8)	2560(7)	34(4)
C(6)	4532(10)	8390(7)	2807(7)	28(4)
C(7)	5397(11)	9309(8)	1212(7)	38(4)
C(8)	5228(11)	8977(8)	496(6)	38(4)
C(9)	5153(12)	10133(7)	1215(7)	42(4)
C(10)	4822(10)	8444(7)	3542(6)	28(4)
C(11)	4934(12)	7658(8)	3769(7)	44(4)
C(12)	4031(11)	8729(9)	3956(7)	48(4)
C(13)	6029(11)	10497(7)	3924(6)	33(4)
C(14)	4450(10)	10541(8)	2840(7)	34(4)
C(15)	6923(10)	11151(7)	2725(7)	31(4)
C(16)	8063(10)	10777(7)	1556(6)	27(3)
C(17)	7980(12)	11461(8)	1286(8)	41(4)
C(18)	8075(13)	11502(9)	633(8)	49(5)
C(19)	8248(14)	10911(9)	232(7)	56(5)
C(20)	8339(12)	10209(9)	502(7)	46(4)
C(21)	8238(11)	10139(7)	1161(7)	35(4)
C(22)	7805(10)	8431(7)	992(6)	19(3)
C(23)	8356(12)	8326(8)	446(7)	37(4)
C(24)	7934(15)	7711(10)	-22(8)	56(5)
C(25)	6985(15)	7203(10)	91(9)	56(5)
C(26)	6428(15)	7288(10)	646(9)	63(5)
C(27)	6862(11)	7922(8)	1113(7)	33(4)
C(28)	9760(11)	9311(7)	1573(6)	26(3)
C(29)	10534(13)	10013(8)	1587(7)	42(4)
C(30)	11620(13)	10026(9)	1599(7)	48(4)
C(31)	11923(13)	9330(10)	1589(7)	45(4)
C(32)	11184(12)	8632(9)	1571(6)	31(4)
C(33)	10123(11)	8623(8)	1586(6)	31(4)
C(34)	9217(10)	11079(7)	2822(6)	26(3)
C(35)	9793(12)	11823(8)	2735(7)	41(4)
C(36)	10776(12)	12132(9)	3022(9)	54(5)
C(37)	11259(12)	11677(9)	3417(8)	52(5)

C(38)	10691(11)	10919(7)	3524(7)	35(4)
C(39)	9673(10)	10607(7)	3231(6)	23(3)
C(40)	9763(11)	8980(7)	3409(6)	21(3)
C(41)	10714(12)	9125(8)	3114(7)	31(4)
C(42)	11406(13)	8569(10)	3160(7)	45(4)
C(43)	11065(13)	7918(9)	3476(7)	36(4)
C(44)	10105(12)	7783(8)	3778(7)	37(4)
C(45)	9443(11)	8338(8)	3731(7)	34(4)
C(46)	8338(10)	9696(7)	4133(7)	24(3)
C(47)	8754(11)	10308(8)	4610(7)	34(4)
C(48)	8295(13)	10335(9)	5208(7)	35(4)
C(49)	7494(12)	9761(10)	5375(6)	36(4)
C(50)	7079(11)	9143(8)	4916(7)	35(4)
C(51)	7496(11)	9110(8)	4303(7)	32(4)
C(52)	8346(16)	4362(9)	1097(9)	73(6)
C(53)	9226(13)	4012(8)	907(8)	58(5)
C(54)	9082(12)	3545(9)	307(8)	64(5)
C(55)	8149(13)	3421(9)	-95(7)	75(7)
C(56)	7302(13)	3739(9)	78(11)	83(7)
C(57)	7366(14)	4195(10)	695(8)	62(5)
C(58)	10267(11)	4173(8)	1272(8)	40(4)
C(59)	10597(14)	3426(10)	1422(9)	72(6)
C(60)	11160(12)	4679(9)	913(7)	54(5)
C(61)	6461(12)	4535(9)	860(9)	57(5)
C(62)	5459(18)	4141(11)	499(10)	119(10)
C(63)	6631(14)	5403(9)	756(10)	83(7)
C(64)	9371(15)	6251(10)	939(8)	81(6)
C(65)	10572(13)	6070(10)	2142(9)	70(6)
C(66)	8392(10)	6330(8)	2305(7)	34(4)
C(67)	7698(12)	5806(7)	3580(7)	39(4)
C(68)	7485(12)	6475(8)	3883(9)	48(5)
C(69)	7686(12)	6634(10)	4543(9)	53(5)
C(70)	8072(15)	6144(11)	4916(10)	70(6)
C(71)	8319(16)	5494(9)	4641(8)	73(6)
C(72)	8153(15)	5294(10)	3982(8)	64(5)
C(73)	10047(12)	4835(9)	3509(8)	44(4)
C(74)	10628(15)	5467(10)	3889(9)	64(5)
C(75)	11750(15)	5695(11)	3843(9)	62(5)
C(76)	12253(16)	5256(13)	3437(11)	83(6)
C(77)	11673(14)	4605(9)	3085(9)	71(6)
C(78)	10599(15)	4476(11)	3096(8)	66(6)
C(79)	8325(16)	3700(10)	4030(8)	54(5)
C(80)	7529(17)	3542(13)	4444(11)	74(6)
C(81)	7357(16)	2891(13)	4812(10)	75(6)
C(82)	8026(18)	2415(10)	4755(9)	60(5)
C(83)	8830(17)	2538(10)	4360(11)	72(6)
C(84)	9014(14)	3187(9)	3980(8)	57(5)
C(85)	6150(11)	5539(8)	2431(8)	44(4)
C(86)	5780(11)	6189(7)	2352(7)	40(4)
C(87)	4740(12)	6117(9)	2145(8)	54(5)
C(88)	4024(14)	5398(10)	2034(10)	81(7)
C(89)	4369(14)	4707(9)	2187(9)	68(6)
C(90)	5468(12)	4769(9)	2388(9)	63(6)
C(91)	5499(12)	3695(9)	3387(8)	46(4)
C(92)	5130(14)	4225(10)	3784(9)	56(5)
C(93)	4727(18)	3999(14)	4367(12)	99(8)

C(94)	4598(17)	3252(15)	4543(11)	97(7)
C(95)	4897(16)	2697(13)	4102(12)	86(7)
C(96)	5342(13)	2937(9)	3526(8)	48(4)
C(97)	5293(12)	3143(8)	2008(9)	48(5)
C(98)	4178(14)	2817(10)	2123(8)	58(5)
C(99)	3600(14)	2172(10)	1704(9)	57(5)
C(100)	4163(15)	1898(8)	1236(10)	56(5)
C(101)	5241(16)	2214(10)	1135(9)	65(5)
C(102)	5776(14)	2806(9)	1547(8)	48(5)

Table 23. Bond lengths [Å] and angles [°] for Co($^{Si}NP_3$)Cl (**2a**).

Co(1A)-N(1A)	2.004(9)	C(8)-H(8C)	0.9800
Co(1A)-P(1A)	2.132(4)	C(9)-H(9A)	0.9800
Co(1A)-P(3A)	2.222(4)	C(9)-H(9B)	0.9800
Co(1A)-Cl(1A)	2.269(3)	C(9)-H(9C)	0.9800
Co(1A)-P(2A)	2.301(4)	C(10)-C(12)	1.495(18)
Co(1B)-N(1B)	1.931(13)	C(10)-C(11)	1.526(18)
Co(1B)-P(1B)	2.125(4)	C(10)-H(10)	1.0000
Co(1B)-P(2B)	2.260(5)	C(11)-H(11A)	0.9800
Co(1B)-Cl(1B)	2.277(3)	C(11)-H(11B)	0.9800
Co(1B)-P(3B)	2.291(5)	C(11)-H(11C)	0.9800
P(1A)-C(34)	1.827(13)	C(12)-H(12A)	0.9800
P(1A)-C(15)	1.827(12)	C(12)-H(12B)	0.9800
P(1A)-C(16)	1.838(14)	C(12)-H(12C)	0.9800
P(2A)-C(28)	1.828(14)	C(13)-H(13A)	0.9800
P(2A)-C(21)	1.841(14)	C(13)-H(13B)	0.9800
P(2A)-C(22)	1.846(12)	C(13)-H(13C)	0.9800
P(3A)-C(46)	1.821(14)	C(14)-H(14A)	0.9800
P(3A)-C(39)	1.824(12)	C(14)-H(14B)	0.9800
P(3A)-C(40)	1.847(12)	C(14)-H(14C)	0.9800
P(1B)-C(66)	1.810(14)	C(15)-H(15)	0.9500
P(1B)-C(67)	1.833(15)	C(16)-C(17)	1.382(18)
P(1B)-C(85)	1.843(13)	C(16)-C(21)	1.407(18)
P(2B)-C(72)	1.800(15)	C(17)-C(18)	1.352(19)
P(2B)-C(79)	1.828(17)	C(17)-H(17)	0.9500
P(2B)-C(73)	1.849(16)	C(18)-C(19)	1.35(2)
P(3B)-C(90)	1.826(16)	C(18)-H(18)	0.9500
P(3B)-C(91)	1.843(16)	C(19)-C(20)	1.41(2)
P(3B)-C(97)	1.845(16)	C(19)-H(19)	0.9500
Si(1A)-N(1A)	1.730(10)	C(20)-C(21)	1.371(19)
Si(1A)-C(13)	1.868(13)	C(20)-H(20)	0.9500
Si(1A)-C(14)	1.870(12)	C(22)-C(23)	1.366(18)
Si(1A)-C(15)	1.884(14)	C(22)-C(27)	1.366(18)
Si(1B)-N(1B)	1.766(13)	C(23)-C(24)	1.40(2)
Si(1B)-C(65)	1.823(16)	C(23)-H(23)	0.9500
Si(1B)-C(66)	1.881(14)	C(24)-C(25)	1.37(2)
Si(1B)-C(64)	1.909(18)	C(24)-H(24)	0.9500
N(1A)-C(1)	1.385(15)	C(25)-C(26)	1.38(2)
N(1B)-C(52)	1.42(2)	C(25)-H(25)	0.9500
C(1)-C(2)	1.432(17)	C(26)-C(27)	1.419(19)
C(1)-C(6)	1.433(18)	C(26)-H(26)	0.9500
C(2)-C(3)	1.378(17)	C(27)-H(27)	0.9500
C(2)-C(7)	1.508(19)	C(28)-C(29)	1.392(18)
C(3)-C(4)	1.334(18)	C(28)-C(33)	1.396(17)
C(3)-H(3)	0.9500	C(29)-C(30)	1.39(2)
C(4)-C(5)	1.392(19)	C(29)-H(29)	0.9500
C(4)-H(4)	0.9500	C(30)-C(31)	1.37(2)
C(5)-C(6)	1.444(18)	C(30)-H(30)	0.9500
C(5)-H(5)	0.9500	C(31)-C(32)	1.364(19)
C(6)-C(10)	1.533(18)	C(31)-H(31)	0.9500
C(7)-C(8)	1.535(18)	C(32)-C(33)	1.356(17)
C(7)-C(9)	1.553(18)	C(32)-H(32)	0.9500
C(7)-H(7)	1.0000	C(33)-H(33)	0.9500
C(8)-H(8A)	0.9800	C(34)-C(35)	1.372(18)
C(8)-H(8B)	0.9800	C(34)-C(39)	1.422(17)

C(35)-C(36)	1.349(19)	C(63)-H(63A)	0.9800
C(35)-H(35)	0.9500	C(63)-H(63B)	0.9800
C(36)-C(37)	1.40(2)	C(63)-H(63C)	0.9800
C(36)-H(36)	0.9500	C(64)-H(64A)	0.9800
C(37)-C(38)	1.397(18)	C(64)-H(64B)	0.9800
C(37)-H(37)	0.9500	C(64)-H(64C)	0.9800
C(38)-C(39)	1.392(17)	C(65)-H(65A)	0.9800
C(38)-H(38)	0.9500	C(65)-H(65B)	0.9800
C(40)-C(45)	1.333(18)	C(65)-H(65C)	0.9800
C(40)-C(41)	1.354(18)	C(66)-H(66)	0.9500
C(41)-C(42)	1.471(19)	C(67)-C(68)	1.384(19)
C(41)-H(41)	0.9500	C(67)-C(72)	1.46(2)
C(42)-C(43)	1.34(2)	C(68)-C(69)	1.37(2)
C(42)-H(42)	0.9500	C(68)-H(68)	0.9500
C(43)-C(44)	1.371(19)	C(69)-C(70)	1.35(2)
C(43)-H(43)	0.9500	C(69)-H(69)	0.9500
C(44)-C(45)	1.441(18)	C(70)-C(71)	1.35(2)
C(44)-H(44)	0.9500	C(70)-H(70)	0.9500
C(45)-H(45)	0.9500	C(71)-C(72)	1.37(2)
C(46)-C(51)	1.379(18)	C(71)-H(71)	0.9500
C(46)-C(47)	1.403(18)	C(73)-C(78)	1.34(2)
C(47)-C(48)	1.379(19)	C(73)-C(74)	1.37(2)
C(47)-H(47)	0.9500	C(74)-C(75)	1.41(2)
C(48)-C(49)	1.332(19)	C(74)-H(74)	0.9500
C(48)-H(48)	0.9500	C(75)-C(76)	1.37(2)
C(49)-C(50)	1.387(19)	C(75)-H(75)	0.9500
C(49)-H(49)	0.9500	C(76)-C(77)	1.36(2)
C(50)-C(51)	1.382(19)	C(76)-H(76)	0.9500
C(50)-H(50)	0.9500	C(77)-C(78)	1.34(2)
C(51)-H(51)	0.9500	C(77)-H(77)	0.9500
C(52)-C(57)	1.44(2)	C(78)-H(78)	0.9500
C(52)-C(53)	1.46(2)	C(79)-C(80)	1.34(2)
C(53)-C(54)	1.42(2)	C(79)-C(84)	1.40(2)
C(53)-C(58)	1.47(2)	C(80)-C(81)	1.39(3)
C(54)-C(55)	1.396(10)	C(80)-H(80)	0.9500
C(54)-H(54)	0.9500	C(81)-C(82)	1.33(2)
C(55)-C(56)	1.378(10)	C(81)-H(81)	0.9500
C(55)-H(55)	0.9500	C(82)-C(83)	1.32(2)
C(56)-C(57)	1.44(2)	C(82)-H(82)	0.9500
C(56)-H(56)	0.9500	C(83)-C(84)	1.40(2)
C(57)-C(61)	1.46(2)	C(83)-H(83)	0.9500
C(58)-C(59)	1.52(2)	C(84)-H(84)	0.9500
C(58)-C(60)	1.519(19)	C(85)-C(86)	1.354(18)
C(58)-H(58)	1.0000	C(85)-C(90)	1.428(19)
C(59)-H(59A)	0.9800	C(86)-C(87)	1.361(19)
C(59)-H(59B)	0.9800	C(86)-H(86)	0.9500
C(59)-H(59C)	0.9800	C(87)-C(88)	1.38(2)
C(60)-H(60A)	0.9800	C(87)-H(87)	0.9500
C(60)-H(60B)	0.9800	C(88)-C(89)	1.44(2)
C(60)-H(60C)	0.9800	C(88)-H(88)	0.9500
C(61)-C(62)	1.46(2)	C(89)-C(90)	1.43(2)
C(61)-C(63)	1.52(2)	C(89)-H(89)	0.9500
C(61)-H(61)	1.0000	C(91)-C(96)	1.35(2)
C(62)-H(62A)	0.9800	C(91)-C(92)	1.37(2)
C(62)-H(62B)	0.9800	C(92)-C(93)	1.36(2)
C(62)-H(62C)	0.9800	C(92)-H(92)	0.9500

C(93)-C(94)	1.36(3)
C(93)-H(93)	0.9500
C(94)-C(95)	1.41(3)
C(94)-H(94)	0.9500
C(95)-C(96)	1.38(2)
C(95)-H(95)	0.9500
C(96)-H(96)	0.9500
C(97)-C(102)	1.33(2)
C(97)-C(98)	1.44(2)
C(98)-C(99)	1.42(2)
C(98)-H(98)	0.9500
C(99)-C(100)	1.35(2)
C(99)-H(99)	0.9500
C(100)-C(101)	1.39(2)
C(100)-H(100)	0.9500
C(101)-C(102)	1.34(2)
C(101)-H(101)	0.9500
C(102)-H(102)	0.9500

N(1A)-Co(1A)-P(1A)	85.2(3)
N(1A)-Co(1A)-P(3A)	132.5(3)
P(1A)-Co(1A)-P(3A)	87.12(13)
N(1A)-Co(1A)-Cl(1A)	96.9(3)
P(1A)-Co(1A)-Cl(1A)	176.93(15)
P(3A)-Co(1A)-Cl(1A)	89.81(13)
N(1A)-Co(1A)-P(2A)	122.2(3)
P(1A)-Co(1A)-P(2A)	85.00(14)
P(3A)-Co(1A)-P(2A)	103.56(14)
Cl(1A)-Co(1A)-P(2A)	95.75(13)
N(1B)-Co(1B)-P(1B)	85.4(4)
N(1B)-Co(1B)-P(2B)	131.0(4)
P(1B)-Co(1B)-P(2B)	86.65(16)
N(1B)-Co(1B)-Cl(1B)	97.1(4)
P(1B)-Co(1B)-Cl(1B)	176.72(17)
P(2B)-Co(1B)-Cl(1B)	90.12(15)
N(1B)-Co(1B)-P(3B)	122.7(4)
P(1B)-Co(1B)-P(3B)	85.42(15)
P(2B)-Co(1B)-P(3B)	104.68(18)
Cl(1B)-Co(1B)-P(3B)	94.88(15)
C(34)-P(1A)-C(15)	108.8(6)
C(34)-P(1A)-C(16)	104.8(6)
C(15)-P(1A)-C(16)	107.7(6)
C(34)-P(1A)-Co(1A)	110.5(4)
C(15)-P(1A)-Co(1A)	114.4(4)
C(16)-P(1A)-Co(1A)	110.0(4)
C(28)-P(2A)-C(21)	101.1(6)
C(28)-P(2A)-C(22)	99.5(6)
C(21)-P(2A)-C(22)	104.9(6)
C(28)-P(2A)-Co(1A)	122.0(4)
C(21)-P(2A)-Co(1A)	105.4(5)
C(22)-P(2A)-Co(1A)	121.2(5)
C(46)-P(3A)-C(39)	103.6(6)
C(46)-P(3A)-C(40)	101.9(6)
C(39)-P(3A)-C(40)	106.4(6)
C(46)-P(3A)-Co(1A)	110.9(4)
C(39)-P(3A)-Co(1A)	108.6(4)
C(40)-P(3A)-Co(1A)	123.6(4)
C(66)-P(1B)-C(67)	106.7(6)
C(66)-P(1B)-C(85)	105.7(6)
C(67)-P(1B)-C(85)	108.0(7)
C(66)-P(1B)-Co(1B)	115.1(5)
C(67)-P(1B)-Co(1B)	110.7(5)
C(85)-P(1B)-Co(1B)	110.3(4)
C(72)-P(2B)-C(79)	104.8(9)
C(72)-P(2B)-C(73)	105.4(8)
C(79)-P(2B)-C(73)	103.8(8)
C(72)-P(2B)-Co(1B)	109.3(6)
C(79)-P(2B)-Co(1B)	122.0(6)
C(73)-P(2B)-Co(1B)	110.2(5)
C(90)-P(3B)-C(91)	103.5(8)
C(90)-P(3B)-C(97)	103.1(7)
C(91)-P(3B)-C(97)	104.5(7)
C(90)-P(3B)-Co(1B)	103.5(6)
C(91)-P(3B)-Co(1B)	120.6(6)
C(97)-P(3B)-Co(1B)	119.1(6)
N(1A)-Si(1A)-C(13)	120.9(5)
N(1A)-Si(1A)-C(14)	111.7(5)
C(13)-Si(1A)-C(14)	105.5(6)
N(1A)-Si(1A)-C(15)	103.2(6)
C(13)-Si(1A)-C(15)	102.9(6)
C(14)-Si(1A)-C(15)	112.4(6)
N(1B)-Si(1B)-C(65)	122.1(7)
N(1B)-Si(1B)-C(66)	103.0(6)
C(65)-Si(1B)-C(66)	106.0(7)
N(1B)-Si(1B)-C(64)	111.3(7)
C(65)-Si(1B)-C(64)	104.0(8)
C(66)-Si(1B)-C(64)	110.3(7)
C(1)-N(1A)-Si(1A)	122.1(8)
C(1)-N(1A)-Co(1A)	121.6(7)
Si(1A)-N(1A)-Co(1A)	115.5(5)
C(52)-N(1B)-Si(1B)	122.1(11)
C(52)-N(1B)-Co(1B)	121.2(10)
Si(1B)-N(1B)-Co(1B)	116.4(7)
N(1A)-C(1)-C(2)	121.4(12)
N(1A)-C(1)-C(6)	121.6(11)
C(2)-C(1)-C(6)	117.1(11)
C(3)-C(2)-C(1)	120.7(13)
C(3)-C(2)-C(7)	121.1(12)
C(1)-C(2)-C(7)	118.3(11)
C(4)-C(3)-C(2)	122.2(14)
C(4)-C(3)-H(3)	118.9
C(2)-C(3)-H(3)	118.9
C(3)-C(4)-C(5)	121.7(14)
C(3)-C(4)-H(4)	119.1
C(5)-C(4)-H(4)	119.1
C(4)-C(5)-C(6)	118.6(14)
C(4)-C(5)-H(5)	120.7
C(6)-C(5)-H(5)	120.7
C(1)-C(6)-C(5)	119.7(12)
C(1)-C(6)-C(10)	123.0(11)
C(5)-C(6)-C(10)	117.3(13)
C(2)-C(7)-C(8)	114.6(11)

C(2)-C(7)-C(9)	114.1(12)
C(8)-C(7)-C(9)	105.5(11)
C(2)-C(7)-H(7)	107.4
C(8)-C(7)-H(7)	107.4
C(9)-C(7)-H(7)	107.4
C(7)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(7)-C(9)-H(9A)	109.5
C(7)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(7)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(12)-C(10)-C(11)	108.3(12)
C(12)-C(10)-C(6)	113.5(11)
C(11)-C(10)-C(6)	111.6(11)
C(12)-C(10)-H(10)	107.7
C(11)-C(10)-H(10)	107.7
C(6)-C(10)-H(10)	107.7
C(10)-C(11)-H(11A)	109.5
C(10)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(10)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(10)-C(12)-H(12A)	109.5
C(10)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(10)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
Si(1A)-C(13)-H(13A)	109.5
Si(1A)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
Si(1A)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
Si(1A)-C(14)-H(14A)	109.5
Si(1A)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
Si(1A)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
P(1A)-C(15)-Si(1A)	103.8(6)
P(1A)-C(15)-H(15)	128.1
Si(1A)-C(15)-H(15)	128.1
C(17)-C(16)-C(21)	120.8(13)
C(17)-C(16)-P(1A)	123.4(11)
C(21)-C(16)-P(1A)	115.7(10)
C(18)-C(17)-C(16)	118.3(14)
C(18)-C(17)-H(17)	120.8
C(16)-C(17)-H(17)	120.8
C(19)-C(18)-C(17)	123.4(14)
C(19)-C(18)-H(18)	118.3
C(17)-C(18)-H(18)	118.3
C(18)-C(19)-C(20)	118.8(14)
C(18)-C(19)-H(19)	120.6
C(20)-C(19)-H(19)	120.6
C(21)-C(20)-C(19)	119.8(14)
C(21)-C(20)-H(20)	120.1
C(19)-C(20)-H(20)	120.1
C(20)-C(21)-C(16)	118.8(13)
C(20)-C(21)-P(2A)	125.7(11)
C(16)-C(21)-P(2A)	115.4(11)
C(23)-C(22)-C(27)	121.5(12)
C(23)-C(22)-P(2A)	120.7(11)
C(27)-C(22)-P(2A)	117.8(10)
C(22)-C(23)-C(24)	120.3(15)
C(22)-C(23)-H(23)	119.8
C(24)-C(23)-H(23)	119.8
C(25)-C(24)-C(23)	118.5(16)
C(25)-C(24)-H(24)	120.7
C(23)-C(24)-H(24)	120.7
C(24)-C(25)-C(26)	122.1(15)
C(24)-C(25)-H(25)	119.0
C(26)-C(25)-H(25)	119.0
C(25)-C(26)-C(27)	118.6(16)
C(25)-C(26)-H(26)	120.7
C(27)-C(26)-H(26)	120.7
C(22)-C(27)-C(26)	118.9(14)
C(22)-C(27)-H(27)	120.5
C(26)-C(27)-H(27)	120.5
C(29)-C(28)-C(33)	117.4(13)
C(29)-C(28)-P(2A)	122.5(10)
C(33)-C(28)-P(2A)	120.0(10)
C(30)-C(29)-C(28)	121.1(13)
C(30)-C(29)-H(29)	119.4
C(28)-C(29)-H(29)	119.4
C(31)-C(30)-C(29)	118.6(14)
C(31)-C(30)-H(30)	120.7
C(29)-C(30)-H(30)	120.7
C(32)-C(31)-C(30)	121.5(15)
C(32)-C(31)-H(31)	119.2
C(30)-C(31)-H(31)	119.2
C(33)-C(32)-C(31)	119.6(13)
C(33)-C(32)-H(32)	120.2
C(31)-C(32)-H(32)	120.2
C(32)-C(33)-C(28)	121.5(13)
C(32)-C(33)-H(33)	119.2
C(28)-C(33)-H(33)	119.2
C(35)-C(34)-C(39)	118.8(12)
C(35)-C(34)-P(1A)	125.0(10)
C(39)-C(34)-P(1A)	116.2(9)
C(36)-C(35)-C(34)	123.1(14)
C(36)-C(35)-H(35)	118.5
C(34)-C(35)-H(35)	118.5
C(35)-C(36)-C(37)	119.6(14)
C(35)-C(36)-H(36)	120.2

C(37)-C(36)-H(36)	120.2
C(38)-C(37)-C(36)	118.9(14)
C(38)-C(37)-H(37)	120.5
C(36)-C(37)-H(37)	120.5
C(39)-C(38)-C(37)	121.1(13)
C(39)-C(38)-H(38)	119.4
C(37)-C(38)-H(38)	119.4
C(38)-C(39)-C(34)	118.4(11)
C(38)-C(39)-P(3A)	126.5(10)
C(34)-C(39)-P(3A)	115.1(9)
C(45)-C(40)-C(41)	121.0(12)
C(45)-C(40)-P(3A)	118.7(11)
C(41)-C(40)-P(3A)	120.1(10)
C(40)-C(41)-C(42)	119.1(14)
C(40)-C(41)-H(41)	120.5
C(42)-C(41)-H(41)	120.5
C(43)-C(42)-C(41)	119.3(15)
C(43)-C(42)-H(42)	120.4
C(41)-C(42)-H(42)	120.4
C(42)-C(43)-C(44)	120.9(13)
C(42)-C(43)-H(43)	119.5
C(44)-C(43)-H(43)	119.5
C(43)-C(44)-C(45)	118.9(14)
C(43)-C(44)-H(44)	120.6
C(45)-C(44)-H(44)	120.6
C(40)-C(45)-C(44)	120.8(14)
C(40)-C(45)-H(45)	119.6
C(44)-C(45)-H(45)	119.6
C(51)-C(46)-C(47)	117.0(13)
C(51)-C(46)-P(3A)	118.6(10)
C(47)-C(46)-P(3A)	124.4(11)
C(48)-C(47)-C(46)	120.8(14)
C(48)-C(47)-H(47)	119.6
C(46)-C(47)-H(47)	119.6
C(49)-C(48)-C(47)	121.9(14)
C(49)-C(48)-H(48)	119.0
C(47)-C(48)-H(48)	119.0
C(48)-C(49)-C(50)	118.3(14)
C(48)-C(49)-H(49)	120.9
C(50)-C(49)-H(49)	120.9
C(51)-C(50)-C(49)	121.3(14)
C(51)-C(50)-H(50)	119.4
C(49)-C(50)-H(50)	119.4
C(46)-C(51)-C(50)	120.6(13)
C(46)-C(51)-H(51)	119.7
C(50)-C(51)-H(51)	119.7
N(1B)-C(52)-C(57)	120.2(17)
N(1B)-C(52)-C(53)	120.0(17)
C(57)-C(52)-C(53)	119.7(16)
C(54)-C(53)-C(52)	117.0(15)
C(54)-C(53)-C(58)	119.2(15)
C(52)-C(53)-C(58)	123.5(16)
C(55)-C(54)-C(53)	122.6(15)
C(55)-C(54)-H(54)	118.7
C(53)-C(54)-H(54)	118.7
C(56)-C(55)-C(54)	121.4(16)
C(56)-C(55)-H(55)	119.3
C(54)-C(55)-H(55)	119.3
C(55)-C(56)-C(57)	119.5(18)
C(55)-C(56)-H(56)	120.3
C(57)-C(56)-H(56)	120.3
C(52)-C(57)-C(56)	119.6(17)
C(52)-C(57)-C(61)	122.1(15)
C(56)-C(57)-C(61)	118.1(15)
C(53)-C(58)-C(59)	112.1(13)
C(53)-C(58)-C(60)	112.3(13)
C(59)-C(58)-C(60)	108.6(12)
C(53)-C(58)-H(58)	107.9
C(59)-C(58)-H(58)	107.9
C(60)-C(58)-H(58)	107.9
C(58)-C(59)-H(59A)	109.5
C(58)-C(59)-H(59B)	109.5
H(59A)-C(59)-H(59B)	109.5
C(58)-C(59)-H(59C)	109.5
H(59A)-C(59)-H(59C)	109.5
H(59B)-C(59)-H(59C)	109.5
C(58)-C(60)-H(60A)	109.5
C(58)-C(60)-H(60B)	109.5
H(60A)-C(60)-H(60B)	109.5
C(58)-C(60)-H(60C)	109.5
H(60A)-C(60)-H(60C)	109.5
H(60B)-C(60)-H(60C)	109.5
C(62)-C(61)-C(57)	113.2(16)
C(62)-C(61)-C(63)	106.4(14)
C(57)-C(61)-C(63)	114.8(15)
C(62)-C(61)-H(61)	107.3
C(57)-C(61)-H(61)	107.3
C(63)-C(61)-H(61)	107.3
C(61)-C(62)-H(62A)	109.5
C(61)-C(62)-H(62B)	109.5
H(62A)-C(62)-H(62B)	109.5
C(61)-C(62)-H(62C)	109.5
H(62A)-C(62)-H(62C)	109.5
H(62B)-C(62)-H(62C)	109.5
C(61)-C(63)-H(63A)	109.5
C(61)-C(63)-H(63B)	109.5
H(63A)-C(63)-H(63B)	109.5
C(61)-C(63)-H(63C)	109.5
H(63A)-C(63)-H(63C)	109.5
H(63B)-C(63)-H(63C)	109.5
Si(1B)-C(64)-H(64A)	109.5
Si(1B)-C(64)-H(64B)	109.5
H(64A)-C(64)-H(64B)	109.5
Si(1B)-C(64)-H(64C)	109.5
H(64A)-C(64)-H(64C)	109.5
H(64B)-C(64)-H(64C)	109.5
Si(1B)-C(65)-H(65A)	109.5
Si(1B)-C(65)-H(65B)	109.5
H(65A)-C(65)-H(65B)	109.5
Si(1B)-C(65)-H(65C)	109.5
H(65A)-C(65)-H(65C)	109.5
H(65B)-C(65)-H(65C)	109.5

P(1B)-C(66)-Si(1B)	103.1(7)
P(1B)-C(66)-H(66)	128.5
Si(1B)-C(66)-H(66)	128.5
C(68)-C(67)-C(72)	118.2(14)
C(68)-C(67)-P(1B)	124.9(13)
C(72)-C(67)-P(1B)	116.8(10)
C(69)-C(68)-C(67)	119.7(16)
C(69)-C(68)-H(68)	120.1
C(67)-C(68)-H(68)	120.1
C(70)-C(69)-C(68)	121.8(17)
C(70)-C(69)-H(69)	119.1
C(68)-C(69)-H(69)	119.1
C(71)-C(70)-C(69)	120.7(18)
C(71)-C(70)-H(70)	119.6
C(69)-C(70)-H(70)	119.6
C(70)-C(71)-C(72)	121.3(18)
C(70)-C(71)-H(71)	119.3
C(72)-C(71)-H(71)	119.4
C(71)-C(72)-C(67)	118.2(14)
C(71)-C(72)-P(2B)	127.9(15)
C(67)-C(72)-P(2B)	113.5(11)
C(78)-C(73)-C(74)	116.5(16)
C(78)-C(73)-P(2B)	120.8(13)
C(74)-C(73)-P(2B)	122.5(14)
C(73)-C(74)-C(75)	119.8(17)
C(73)-C(74)-H(74)	120.1
C(75)-C(74)-H(74)	120.1
C(76)-C(75)-C(74)	119.4(18)
C(76)-C(75)-H(75)	120.3
C(74)-C(75)-H(75)	120.3
C(77)-C(76)-C(75)	120.3(19)
C(77)-C(76)-H(76)	119.8
C(75)-C(76)-H(76)	119.8
C(78)-C(77)-C(76)	116.7(17)
C(78)-C(77)-H(77)	121.6
C(76)-C(77)-H(77)	121.6
C(73)-C(78)-C(77)	126.1(16)
C(73)-C(78)-H(78)	116.9
C(77)-C(78)-H(78)	116.9
C(80)-C(79)-C(84)	117.7(16)
C(80)-C(79)-P(2B)	124.8(16)
C(84)-C(79)-P(2B)	117.6(15)
C(79)-C(80)-C(81)	122.6(17)
C(79)-C(80)-H(80)	118.7
C(81)-C(80)-H(80)	118.7
C(82)-C(81)-C(80)	118(2)
C(82)-C(81)-H(81)	120.8
C(80)-C(81)-H(81)	120.8
C(83)-C(82)-C(81)	122.1(19)
C(83)-C(82)-H(82)	118.9
C(81)-C(82)-H(82)	118.9
C(82)-C(83)-C(84)	120.5(18)
C(82)-C(83)-H(83)	119.7
C(84)-C(83)-H(83)	119.7
C(83)-C(84)-C(79)	118.6(17)
C(83)-C(84)-H(84)	120.7
C(79)-C(84)-H(84)	120.7
C(86)-C(85)-C(90)	123.0(13)
C(86)-C(85)-P(1B)	125.0(10)
C(90)-C(85)-P(1B)	111.7(10)
C(85)-C(86)-C(87)	119.7(13)
C(85)-C(86)-H(86)	120.1
C(87)-C(86)-H(86)	120.1
C(86)-C(87)-C(88)	122.3(14)
C(86)-C(87)-H(87)	118.9
C(88)-C(87)-H(87)	118.9
C(87)-C(88)-C(89)	118.7(15)
C(87)-C(88)-H(88)	120.7
C(89)-C(88)-H(88)	120.7
C(90)-C(89)-C(88)	119.6(15)
C(90)-C(89)-H(89)	120.2
C(88)-C(89)-H(89)	120.2
C(85)-C(90)-C(89)	116.0(14)
C(85)-C(90)-P(3B)	119.1(11)
C(89)-C(90)-P(3B)	124.9(12)
C(96)-C(91)-C(92)	121.2(15)
C(96)-C(91)-P(3B)	116.9(12)
C(92)-C(91)-P(3B)	121.3(13)
C(93)-C(92)-C(91)	118.5(16)
C(93)-C(92)-H(92)	120.8
C(91)-C(92)-H(92)	120.8
C(94)-C(93)-C(92)	122(2)
C(94)-C(93)-H(93)	118.9
C(92)-C(93)-H(93)	118.9
C(93)-C(94)-C(95)	118(2)
C(93)-C(94)-H(94)	120.9
C(95)-C(94)-H(94)	120.9
C(96)-C(95)-C(94)	119(2)
C(96)-C(95)-H(95)	120.4
C(94)-C(95)-H(95)	120.4
C(91)-C(96)-C(95)	120.3(17)
C(91)-C(96)-H(96)	119.9
C(95)-C(96)-H(96)	119.9
C(102)-C(97)-C(98)	119.9(15)
C(102)-C(97)-P(3B)	122.2(12)
C(98)-C(97)-P(3B)	117.5(13)
C(99)-C(98)-C(97)	118.6(16)
C(99)-C(98)-H(98)	120.7
C(97)-C(98)-H(98)	120.7
C(100)-C(99)-C(98)	116.2(16)
C(100)-C(99)-H(99)	121.9
C(98)-C(99)-H(99)	121.9
C(99)-C(100)-C(101)	124.5(17)
C(99)-C(100)-H(100)	117.8
C(101)-C(100)-H(100)	117.8
C(102)-C(101)-C(100)	118.2(18)
C(102)-C(101)-H(101)	120.9
C(100)-C(101)-H(101)	120.9
C(97)-C(102)-C(101)	122.3(18)
C(97)-C(102)-H(102)	118.9
C(101)-C(102)-H(102)	118.9

Symmetry transformations used to generate equivalent atoms:

Table 24. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for Co($^{Si}NP_3$)Cl (**2a**). The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Co(1A)	24(1)	16(1)	21(1)	1(1)	-10(1)	10(1)
Co(1B)	29(1)	16(1)	39(1)	0(1)	-5(1)	7(1)
Cl(1A)	25(2)	16(2)	31(2)	-1(2)	-9(2)	6(1)
Cl(1B)	46(2)	23(2)	48(3)	2(2)	0(2)	18(2)
P(1A)	27(2)	18(2)	23(2)	0(2)	-7(2)	12(2)
P(2A)	27(2)	19(2)	24(2)	-1(2)	-7(2)	12(2)
P(3A)	26(2)	17(2)	27(2)	-2(2)	-9(2)	10(2)
P(1B)	26(2)	15(2)	52(3)	-2(2)	-4(2)	6(2)
P(2B)	56(3)	36(3)	51(3)	-4(2)	-8(2)	9(2)
P(3B)	53(3)	37(3)	61(3)	0(2)	-12(2)	9(2)
Si(1A)	33(2)	25(2)	30(2)	-3(2)	-12(2)	18(2)
Si(1B)	45(3)	25(2)	47(3)	7(2)	-1(2)	0(2)
N(1A)	20(6)	22(6)	27(7)	0(5)	-10(5)	18(5)
N(1B)	63(10)	51(9)	44(9)	3(7)	6(7)	27(7)
C(1)	16(8)	25(8)	27(9)	-1(7)	-9(7)	10(7)
C(2)	16(8)	12(7)	42(10)	-5(7)	-12(7)	11(6)
C(3)	23(9)	39(9)	32(9)	15(8)	-8(8)	13(7)
C(4)	33(10)	32(9)	38(11)	-17(8)	-22(8)	15(7)
C(5)	28(9)	32(9)	49(11)	1(8)	6(8)	22(7)
C(6)	20(8)	25(8)	40(10)	-10(7)	-6(8)	12(7)
C(7)	23(9)	46(10)	41(10)	-7(8)	-21(8)	7(7)
C(8)	51(10)	32(9)	30(9)	-6(7)	-19(8)	10(7)
C(9)	59(11)	30(9)	40(10)	8(7)	-20(8)	21(8)
C(10)	27(9)	19(8)	33(9)	3(7)	-10(7)	-1(6)
C(11)	43(10)	44(10)	42(10)	14(8)	5(8)	5(8)
C(12)	39(10)	56(11)	45(11)	-12(9)	-3(9)	11(8)
C(13)	44(9)	21(8)	35(9)	-2(7)	-12(8)	15(7)
C(14)	29(9)	50(9)	34(9)	-4(7)	-1(7)	33(7)
C(15)	26(8)	18(7)	53(10)	2(7)	-1(7)	17(6)
C(16)	30(9)	29(9)	24(8)	0(7)	-5(7)	11(7)
C(17)	64(11)	23(9)	42(11)	10(8)	-19(9)	22(7)
C(18)	86(13)	39(10)	33(11)	17(9)	-16(10)	31(9)
C(19)	108(15)	53(11)	19(9)	17(9)	-5(9)	41(10)
C(20)	74(13)	43(10)	28(10)	8(8)	1(9)	27(9)
C(21)	44(10)	12(8)	46(11)	4(7)	8(8)	2(7)
C(22)	24(7)	17(6)	19(7)	-1(5)	-17(6)	12(5)
C(23)	38(10)	49(10)	35(10)	-7(8)	-10(8)	34(8)
C(24)	76(14)	54(12)	49(12)	-19(10)	-23(11)	47(11)
C(25)	64(13)	46(11)	49(13)	-33(9)	-31(11)	9(10)
C(26)	72(14)	49(11)	59(13)	-19(10)	-14(11)	5(10)
C(27)	39(10)	35(9)	32(9)	-9(8)	-4(8)	24(8)
C(28)	37(9)	22(8)	18(8)	3(6)	4(7)	7(7)
C(29)	54(12)	33(10)	41(10)	3(8)	-7(9)	16(8)
C(30)	51(12)	36(10)	53(12)	-2(8)	-1(9)	1(8)
C(31)	38(10)	64(12)	31(10)	7(9)	15(8)	5(10)
C(32)	39(10)	46(10)	15(8)	-1(7)	5(7)	25(8)
C(33)	31(10)	40(9)	28(9)	-4(7)	8(7)	21(7)
C(34)	31(9)	10(8)	36(9)	-8(7)	-7(7)	5(6)
C(35)	51(11)	29(9)	41(10)	-1(8)	-18(9)	10(8)
C(36)	49(11)	26(9)	86(14)	9(9)	-15(11)	8(8)
C(37)	45(11)	38(10)	67(13)	2(9)	-9(9)	-3(8)

C(38)	32(9)	21(8)	51(10)	-1(7)	-6(8)	6(7)
C(39)	30(9)	7(7)	34(9)	2(6)	-5(7)	8(6)
C(40)	25(9)	18(8)	23(8)	-2(7)	-15(7)	15(6)
C(41)	43(10)	32(8)	25(9)	-4(7)	-20(8)	26(8)
C(42)	49(11)	59(12)	26(10)	-11(9)	-18(8)	15(9)
C(43)	38(11)	41(10)	34(10)	-14(8)	-14(8)	27(8)
C(44)	43(11)	31(9)	42(10)	4(7)	-13(9)	23(8)
C(45)	24(9)	34(9)	46(10)	1(8)	-20(8)	15(7)
C(46)	20(8)	12(7)	43(10)	8(7)	-11(7)	6(6)
C(47)	30(9)	24(8)	48(11)	-2(8)	-23(8)	12(7)
C(48)	53(12)	47(11)	11(9)	-12(8)	-19(8)	31(9)
C(49)	48(11)	61(11)	4(8)	7(8)	-1(8)	22(9)
C(50)	35(9)	37(9)	40(11)	10(8)	-10(9)	24(7)
C(51)	37(10)	34(9)	29(10)	-10(7)	-16(8)	24(8)
C(52)	96(17)	42(11)	79(15)	-4(11)	-4(13)	16(11)
C(53)	45(11)	56(11)	70(14)	-3(10)	-8(10)	8(9)
C(54)	88(15)	50(11)	57(13)	-2(10)	-2(12)	25(10)
C(55)	140(20)	38(11)	24(10)	-4(8)	-55(12)	-10(12)
C(56)	36(12)	37(11)	160(20)	-12(13)	23(13)	-10(9)
C(57)	69(14)	60(12)	55(12)	-22(10)	-37(11)	24(10)
C(58)	34(10)	40(10)	50(11)	-4(8)	-5(9)	17(8)
C(59)	63(13)	68(13)	86(15)	8(11)	18(11)	14(10)
C(60)	51(12)	54(11)	50(11)	-1(9)	2(9)	0(9)
C(61)	35(11)	63(12)	67(13)	14(10)	-6(10)	-5(9)
C(62)	180(20)	69(14)	115(19)	-26(13)	-121(18)	66(15)
C(63)	85(15)	37(11)	126(19)	5(11)	-33(13)	20(10)
C(64)	98(16)	71(14)	69(14)	-5(11)	-13(12)	14(11)
C(65)	64(13)	69(13)	74(14)	-15(11)	-16(11)	15(10)
C(66)	25(8)	28(8)	55(11)	17(8)	3(8)	13(7)
C(67)	45(10)	14(8)	54(11)	-8(8)	22(9)	-4(7)
C(68)	46(11)	21(9)	74(14)	-3(9)	2(10)	1(7)
C(69)	36(11)	42(11)	70(14)	-13(11)	3(10)	-6(8)
C(70)	81(15)	71(14)	61(14)	-5(12)	12(11)	26(12)
C(71)	136(19)	45(11)	50(13)	-2(10)	23(12)	45(12)
C(72)	101(15)	50(11)	38(11)	-25(9)	-4(11)	25(11)
C(73)	43(11)	53(11)	40(11)	6(9)	-20(9)	20(9)
C(74)	63(14)	47(11)	85(15)	-3(11)	-13(12)	23(10)
C(75)	54(14)	65(13)	56(13)	4(10)	-20(10)	-2(10)
C(76)	62(14)	105(18)	97(17)	32(15)	0(14)	43(14)
C(77)	56(14)	30(10)	115(17)	-39(11)	-51(12)	3(9)
C(78)	54(14)	107(16)	30(11)	-30(11)	-35(10)	17(12)
C(79)	78(14)	59(12)	33(11)	12(9)	14(10)	30(11)
C(80)	76(16)	80(16)	77(16)	-7(13)	-21(13)	49(12)
C(81)	64(15)	76(15)	77(16)	-8(13)	-4(12)	4(13)
C(82)	86(16)	42(11)	43(12)	11(9)	-32(12)	-1(12)
C(83)	76(16)	45(13)	99(17)	15(12)	2(14)	18(11)
C(84)	66(13)	33(10)	64(13)	-8(10)	12(10)	-2(9)
C(85)	28(9)	17(8)	79(13)	-6(8)	-24(9)	-4(7)
C(86)	32(10)	15(8)	71(12)	-14(8)	-13(9)	9(7)
C(87)	39(11)	36(10)	95(15)	0(10)	-6(10)	25(9)
C(88)	60(13)	46(12)	135(19)	-37(12)	-54(12)	27(10)
C(89)	76(14)	24(10)	98(16)	-12(10)	-4(12)	2(9)
C(90)	37(11)	38(10)	112(16)	-21(10)	-27(11)	16(8)
C(91)	46(11)	34(10)	60(12)	2(9)	40(9)	11(8)
C(92)	69(13)	53(11)	55(12)	22(10)	25(11)	23(10)
C(93)	120(20)	91(18)	110(20)	19(16)	55(17)	63(15)

C(94)	93(18)	130(20)	91(18)	32(17)	33(14)	56(16)
C(95)	61(14)	90(16)	120(20)	22(16)	11(14)	32(12)
C(96)	48(11)	43(11)	47(12)	10(9)	15(9)	-5(8)
C(97)	22(10)	21(8)	96(15)	-5(9)	8(9)	1(7)
C(98)	61(14)	65(12)	48(12)	-2(10)	-7(10)	18(10)
C(99)	42(11)	48(11)	80(14)	8(11)	-12(11)	5(9)
C(100)	57(14)	18(9)	87(16)	12(9)	-31(12)	0(9)
C(101)	76(16)	54(12)	63(14)	13(11)	-27(12)	17(11)
C(102)	67(12)	33(10)	49(11)	-11(9)	-13(10)	25(9)

Table 25. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for Co(^{Si}NP$_3$)Cl (**2a**).

	x	y	z	U(eq)
H(3)	3688	8117	1029	36
H(4)	2765	7295	1724	41
H(5)	3199	7446	2848	40
H(7)	6178	9385	1337	45
H(8A)	5262	8425	470	58
H(8B)	5792	9273	237	58
H(8C)	4523	9019	324	58
H(9A)	4398	10079	1079	62
H(9B)	5615	10447	911	62
H(9C)	5292	10392	1657	62
H(10)	5534	8824	3623	33
H(11A)	5118	7713	4240	65
H(11B)	5504	7487	3534	65
H(11C)	4253	7268	3680	65
H(12A)	3871	9195	3779	71
H(12B)	4335	8861	4405	71
H(12C)	3367	8317	3957	71
H(13A)	5616	10035	4121	49
H(13B)	5790	10961	4088	49
H(13C)	6795	10567	4041	49
H(14A)	4497	10919	2506	51
H(14B)	4187	10749	3241	51
H(14C)	3952	10047	2681	51
H(15)	6964	11697	2731	37
H(17)	7859	11891	1552	49
H(18)	8018	11972	448	59
H(19)	8307	10964	-225	67
H(20)	8470	9788	229	55
H(23)	9029	8672	386	45
H(24)	8299	7648	-411	67
H(25)	6700	6778	-222	67
H(26)	5768	6929	714	76
H(27)	6503	7990	1503	40
H(29)	10313	10493	1589	50
H(30)	12144	10509	1615	58
H(31)	12666	9333	1595	54
H(32)	11410	8154	1547	37
H(33)	9615	8138	1605	37
H(35)	9487	12135	2460	49
H(36)	11138	12655	2957	65
H(37)	11962	11880	3609	63
H(38)	11004	10612	3801	42
H(41)	10931	9581	2881	37
H(42)	12086	8669	2968	54
H(43)	11495	7546	3491	43
H(44)	9880	7331	4014	44
H(45)	8770	8245	3931	41
H(47)	9358	10708	4520	41
H(48)	8557	10776	5510	42
H(49)	7214	9775	5799	43

H(50)	6497	8735	5024	42
H(51)	7199	8680	3997	38
H(54)	9642	3307	173	76
H(55)	8098	3111	-497	90
H(56)	6680	3658	-206	99
H(58)	10196	4463	1698	49
H(59A)	10024	3091	1649	108
H(59B)	11259	3557	1701	108
H(59C)	10722	3149	1013	108
H(60A)	11223	4418	484	80
H(60B)	11841	4761	1169	80
H(60C)	10992	5187	854	80
H(61)	6341	4473	1336	69
H(62A)	5513	4255	38	178
H(62B)	4861	4329	683	178
H(62C)	5334	3575	532	178
H(63A)	7251	5700	1030	124
H(63B)	5988	5581	877	124
H(63C)	6764	5486	295	124
H(64A)	9216	5829	589	121
H(64B)	10108	6561	911	121
H(64C)	8868	6589	891	121
H(65A)	10551	5933	2597	105
H(65B)	10871	6634	2128	105
H(65C)	11025	5782	1900	105
H(66)	8419	6875	2358	41
H(68)	7200	6823	3634	58
H(69)	7552	7100	4745	63
H(70)	8169	6259	5376	84
H(71)	8615	5170	4910	88
H(74)	10276	5752	4183	77
H(75)	12156	6148	4090	74
H(76)	13011	5408	3403	100
H(77)	12012	4260	2843	85
H(78)	10192	4093	2781	79
H(80)	7063	3888	4489	88
H(81)	6776	2788	5096	90
H(82)	7919	1973	5009	72
H(83)	9288	2185	4331	87
H(84)	9594	3277	3694	69
H(86)	6245	6693	2441	48
H(87)	4498	6577	2074	65
H(88)	3316	5361	1859	97
H(89)	3871	4212	2154	82
H(92)	5156	4738	3655	67
H(93)	4530	4376	4661	119
H(94)	4314	3107	4952	116
H(95)	4793	2167	4203	104
H(96)	5540	2569	3224	58
H(98)	3837	3029	2472	70
H(99)	2859	1947	1751	69
H(100)	3798	1460	957	67
H(101)	5588	2015	782	78
H(102)	6528	2993	1508	58