For Supporting Information

2,6-Diiminopyridine Iron(II) Dialkyl Complexes. Interaction with Aluminum Alkyls and Ethylene Polymerization Catalysis

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General Information

All preparations and other operations were carried out under oxygen-free nitrogen by conventional Schlenk techniques. Solvents were rigorously dried and degassed before use. Microanalyses were performed by the Microanalytical Service of the Instituto de Investigaciones Químicas (Sevilla, Spain). Infrared spectra were recorded on a Bruker Vector 22 spectrometer, and NMR spectra on Bruker 300, 400 and 500 MHz spectrometers. The ^{1}H and $^{13}C\{^{1}H\}$ resonances of the solvent were used as the internal standard but the chemical shifts are reported with respect to TMS. Complexes $FeCl_2(Py)_4$[1] and $MeAl(OC_6H_2Bu^t_3\text{-}2,4,6)_2$[2] were prepared according to the literature procedure. Imine ligands were synthesized by condensation of 2,6-Diacetylpyridine with the appropriate anilines in a Dean-Stark aparatus. Magnetic susceptibilities were measured on a Sherwood Scientific "AUTO" Magnetic Susceptibility Balance. Molecular weights of the polymers were determined by gel permeation chromatography employing universal calibration in a Waters 150c instrument with differential refractive index (DRI) detector and a Viscotek 150R DV detector. The terminal group analysis was done by NMR methods.[3,4]

Synthesis of $Fe(CH_2Ph)_2(Py)_2$ (1)

A yellow suspension of $FeCl_2(Py)_4$ (0.89 g, 4 mmol) and 0.5 mL of Py in 40 mL of Et_2O cooled at -40 °C was treated with 4.1 mL of a 0.97 M solution of $Mg(CH_2Ph)Cl$ (4 mmol) in Et_2O. The mixture turned dark red. It was stirred at this temperature for 15 min. and at room temperature for 1 h. Then it was filtered through celite and the filter washed with Et_2O (3 x 40 mL). The liquids were reunited with the filtrante, and after partial evaporation of the solvent, addition of some hexane and cooling at -20 °C complex **1** was isolated as deep red crystals in 20% yield.
^{1}H NMR (C_6D_6, 298 K, 400 MHz): δ -80.28 ($\Delta\nu_{1/2}$ = 116 Hz, 2H, *p*-CH_{ar}), -58.03 ($\Delta\nu_{1/2}$ = 456 Hz, 4H, *m*-CH_{ar}), 34.04 ($\Delta\nu_{1/2}$ = 132 Hz, 4H, H3-py), 11.02 (2H, $H2_{py}$). *IR (Nujol mull):* 1587 cm^{-1} (ν (C=N)) . Anal. Calcd for $C_{24}H_{24}FeN_2$: C, 72.74; H, 6.10; N, 7.07. Found: C, 71.91; H, 5.98; N, 6.74.

Synthesis of $Fe(CH_2CMe_2Ph)_2(Py)_2$, (2).

To a cooled (-40 °C) suspension of $FeCl_2(Py)_4$ (1.78 g, 4 mmol) in 50 mL of Et_2O was added 1 mL of Py and 7.4 mL of 1.08 M solution of $Mg(CH_2CMe_2Ph)Cl$ (8 mmol) in Et_2O. The mixture turned deep red. After stirring at this temperature for 30 min it was allowed to reach room temperature and was stirred for 2 h. The solvent was evaporated under reduced pressure, the residue extracted with hexane (3 x 50 mL) and the suspension filtered through celite. After concentration and cooling to 0° C, the product was isolated as red crystals in 78% yield. ^{1}H NMR (C_6D_6, 298 K, 300 MHz): δ 5.42 ($\Delta\nu_{1/2}$ = 48 Hz, 4H, *m*-CH_{ar}) 11.77 ($\Delta\nu_{1/2}$ = 330 Hz, 2H, *p*-CH_{ar}), 12.92 ($\Delta\nu_{1/2}$ = 117 Hz, 2H, $H4_{py}$), 25.23 ($\Delta\nu_{1/2}$ = 462 Hz, 12H, CMe_2), 35.27 ($\Delta\nu_{1/2}$ = 174 Hz, 4H, $H3_{py}$), 119.99 ($\Delta\nu_{1/2}$ = 1350 Hz, 4H, *o*-CH_{ar}). IR (Nujol mull): ν (C=N) 1595 cm^{-1}. UV-vis (hexane): λ_{max} = 492 nm (ε = 970). μ_{eff}= 5.2 μ_B (magnetic balance, 25 °C).

Synthesis of $Fe(CH_2SiMe_3)_2(Py)_2$, 3.

To a cooled (-40 °C) suspension of $FeCl_2(Py)_4$ (0.89 g, 2 mmol) in 40 mL of Et_2O was added 0.5 mL of Py and 3.8 mL of 1.06 M solution of $Mg(CH_2SiMe_3)Cl$ (4 mmol) in Et_2O. The mixture turned deep red. After stirring at this temperature for 15 min it was allowed to reach room temperature and was stirred for 1 h. The solvent was evaporated under reduced pressure, the residue extracted with hexane (3 x 40 mL) and the suspension filtered. NMR analysis of the solution showed that complex **3** was formed in 80% yield. ^{1}H NMR (C_6D_6, 25 °C, 300 MHz): δ 11.37 ($\Delta\nu_{1/2}$ = 318 Hz, 18 H, SiMe_3), 17.37 ($\Delta\nu_{1/2}$ = 348 Hz, 2 H, $H4_{py}$), 35.53 ($\Delta\nu_{1/2}$ = 657 Hz, 4 H, $H3_{py}$). UV-vis (hexane): λ_{max} = 528 nm

Synthesis of 4a, 4b and 4c

A solution of 1.6 mmol of the iminopyridine ligand in 15 mL of hexane was added dropwise to a solution of a solution of complex **3** (2 mmol) prepared as previously described in the same scale, at room temperature. The mixture turned violet. It was stirred at room temperature for 45 min. Afterwads, it was filtered, and the solution partially concentrated and cooled at -20 °C. Compound **4a-c** were obtained as deep violet crystals in 70% (**4a**), 66% (**4b**) and 50% (**4c**) yield.

Analytical and Spectroscopic Data for (4a).- *^{1}H NMR (C_6D_6, 25 °C): δ -148.28 ($\Delta\nu_{1/2}$ =460 Hz, 6H, CH_3-C=N), 11.74 ($\Delta\nu_{1/2}$ =412 Hz, 18H, SiMe_3), 12.14 (overlaping signal, 4H,* m-CH_{ar}*), 23.21 ($\Delta\nu_{1/2}$ = 836 Hz, 12H,* o-CH_3*), 29.44 ($\Delta\nu_{1/2}$ =36 Hz, 6H,* p-CH_3*), 57.55 ($\Delta\nu_{1/2}$ =192 Hz, 2H, C*H3*(py)), 283.07 ($\Delta\nu_{1/2}$ =656 Hz, 1 H, C*H4*(py)). UV-vis (hexane), λ_{max} (nm): 547 (ε = 2540), 400 (ε =2850), 694 (ε =1100). μ_{eff}= 5.1 μ_B (magnetic balance, 25 °C). Anal. Calcd for $C_{35}H_{53}FeN_3Si_2$: C, 66.96; H, 8.51; N, 6.69. Found: C, 66.50; H, 8.10; N, 6.70.*

Analytical and Spectroscopic Data for (4b).- *^{1}H NMR (C_6D_6, 25 °C): δ -148.71 ($\Delta\nu_{1/2}$ = 456 Hz, 6H, CH_3-C=N), -16.53 ($\Delta\nu_{1/2}$ = 64 Hz, 2H,* p-CH_{ar}*), 11.65 ($\Delta\nu_{1/2}$ = 392 Hz, 18H, Si*Me_3*), 12.92 ($\Delta\nu_{1/2}$ =116 Hz, 4H,* m-CH_{ar}*), 23.04 ($\Delta\nu_{1/2}$ = 784 Hz, 12H,* o-CH_3*), 58.12 (184 Hz, 2H, C*H3*(py)), 279.42 ($\Delta\nu_{1/2}$ = 660 Hz, 1 H, C*H4*(py)). UV-vis (hexane), λ_{max} (nm): 546 (ε = 3635), 398 (ε =2920), 693 (ε =1510). μ_{eff}= 5.2 μ_B (magnetic balance, 25 °C) .Anal. Calcd for $C_{33}H_{49}FeN_3Si_2$: C, 66.08; H, 8.23; N, 7.01. Found: C, 65.98; H, 8.33; N, 7.15.*

Analytical and Spectroscopic Data for (4c).- *^{1}H (C_6D_6, 25 °C): δ -153.35 ($\Delta\nu_{1/2}$ =549 Hz, 6H, CH_3-C=N), -18.37 ($\Delta\nu_{1/2}$ =81 Hz, 1H,* p-C$H_{ar'}$*), 11.79 ($\Delta\nu_{1/2}$ = 468 Hz, 20H, Si*Me_3 *and* m-CH_{ar}*), 14.23 ($\Delta\nu_{1/2}$ = 144 Hz, 1H,* m-C$H_{ar'}$*), 16.12 ($\Delta\nu_{1/2}$ = 93 Hz, 1H,* m-C$H_{ar'}$*), 24.76 ($\Delta\nu_{1/2}$ =963 Hz, 6H,* o-CH_3*), 29.85 $\Delta\nu_{1/2}$ =(42 Hz, 3H,* p-CH_3*), 53.32, 52.39 ($\Delta\nu_{1/2}$ = 486 Hz, 2H, C*H3*(py)), 306.41 ($\Delta\nu_{1/2}$ = 693 Hz, 1 H, C*H4*(py)). UV-vis (hexane), λ_{max} (nm): 540 (ε = 2500), 403 (ε =1860), 687 (ε =810). μ_{eff}= 5.1 μ_B (magnetic balance, 25 °C). Anal. Calcd for $C_{35}H_{53}FeN_3Si_2$: C, 66.96; H, 8.51; N, 6.69. Found: C, 66.50; H, 8.32; N, 6.77.*

Reaction of 4a with TMA.

In a glove box, a NMR tube was charged with a weighed amount (9 mg, 0.014 mmol) of **4a,** and the apropriate solvent (C_6D_6 or toluene-d_8) and capped with a septum. After checking the purity of the complex by ^{1}H NMR, a solution of TMA in the same deuterated solvent (0.013 mmol, 0.9 equiv; ca 7 μL) was added under inert atmosphere. The mixture turned from the initial deep-violet colour to greenish yellow. ^{1}H NMR were measured immediately.

A similar procedure was followed to investigate the interaction of **4a** with increasing amounts of TMA (1:2.6, 1:4.4, 1:6.1). Below is shown the NMR spectrum of the mixture obtained with a Fe/Al ratio of 2.6. The remaining spectra show no significant changes other than the increase of the signal at ca. 1 ppm (TMA).

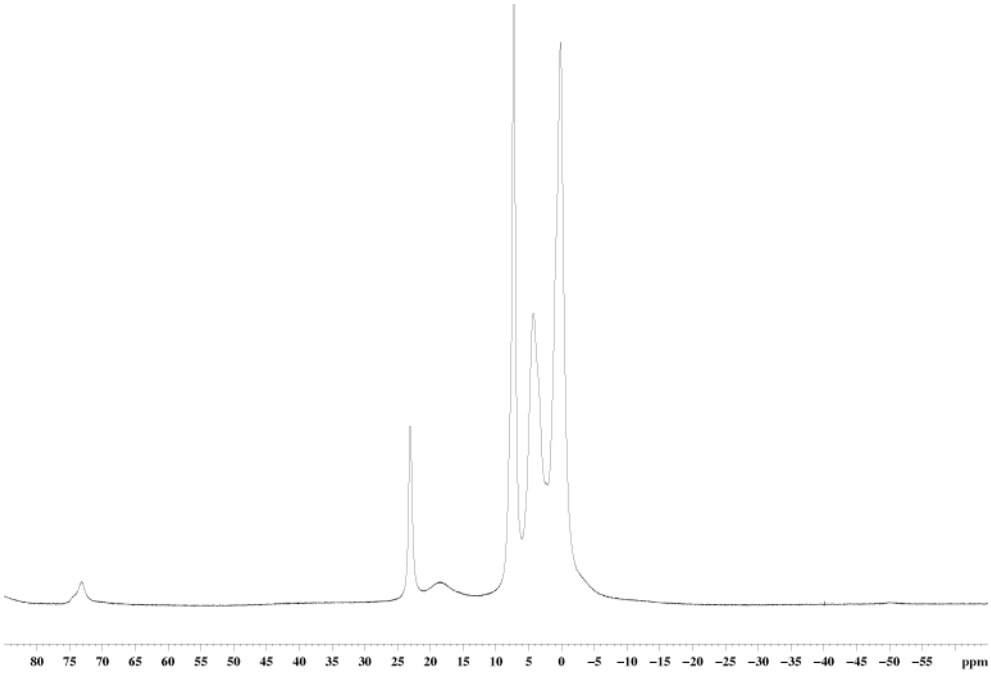
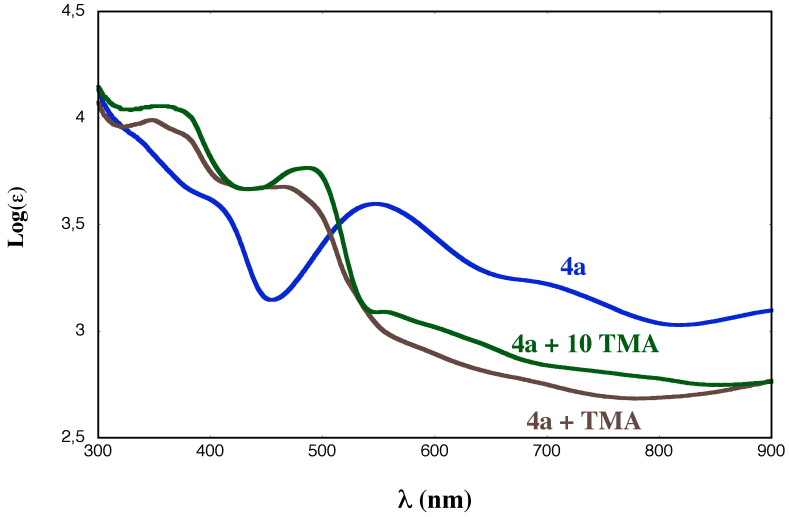


Figure 1. ^{1}H NMR spectrum of **4a** + 2.6 Eq. TMA.

UV-Vis Spectra of 4a and 4a+TMA



The above figure shows the UV-Vis spectra of **4a** and **4a** + TMA in toluene (concentration of **4a** is 10^{-4} M in all cases), with Fe:Al = 1:1 and

1:10, respectively. Under these highly diluted conditions, the reaction of **4a** with one equiv. of TMA becomes sluggish. Therefore the 1:1 mixture was prepared at by dilution of a 10^{-2} M solution of **4a** and TMA.

Ethylene polymerization reactions.

Polymerizations activated with aluminum cocatalysts or $ZnMe_2$

A 250 mL glass reactor was degassed and charged with a solution of the cocatalyst in 50 mL of toluene. The system was flushed with ethylene three times (to remove the initial argon atsmophere) and the solution was stirred at 30 ° C under 4 bar of ethylene until equilibrium was reached. Then a solution of the catalyst in toluene was added and the mixture was stirred for 20 min. The reactor was depressurized and the mixture treated with 150 mL of MeOH and some drops of HCl (37%) and stirred. The polimer was collected by filtration and dried under vacuum.

Polymerizations activated with $B(C_6F_5)_3$

These were performed similarly, but in this case the co-catalyst was added over the presurized reactor containing a catalyst solution in 50 mL of toluene, previously stabilized at the working temperature.

Crystal structure determination for 2

A summary of the conditions for data collection is given in Table 1 for the compound 2. A red irregular crystal was coated with perfluoropolyether oil (FOMBLIN® 140/13, Aldrich) and cooled at 173 K. The crystal was mounted on a Brucker-Siemens Smart CCD diffractometer equipped with a normal focus, 2.4 kW sealed tube X-ray source (Molybdenum radiation, _ = 0.71073 Å) operating at 50 kV and 20 mA. Data were collected by a combination of three sets of exposures. Each set had a different _ angle for the crystal and each exposure of 20 s covered 0.3º in _ , with a detector distance of 49.6 mm. Unit cell dimensions were determined by a least-squares fit of 40 reflections with I>20_ (I) and 5.71º < 2_ > 54.14. The first 30 frames of data were collected at the end of the data collection to monitor crystal decay. The data were reduced (SAINT)[5] and corrected for Lorentz polarisation effects and absorption by multi-scan method applied by (SADABS)[6] . The structure was solved by direct methods (SIR-2002)[7] and refined against all F^2 data by full-matrix least-squares techniques (SHELXTL-6.12)[8] minimizing $w[Fo^2-Fc^2]^2$. All the non-hydrogen atoms were refined

with anisotropic displacement parameters. The hydrogen atoms were included from calculated positions and refined riding on their respective carbon atoms with isotropic displacement parameters. Weighted *R* factors (*Rw*) and all goodness of fit *S* are based on F^2, conventional *R* factors (*R*) are based on *F*.

Crystal structure determination for 4a:

A summary of the conditions for data collection is given in Table 1 for the compound 4a. A representative single red plate crystal of suitable size was mounted on glass fibre with perfluoropolyether oil (FOMBLIN® 140/13, Aldrich) and attached the goniometer head on a Bruker-Nonius X8Apex-II CCD diffractometer using graphite monochrotomator _(Mo K_1) = 0.71073 Å, and equipped with a Bruker-Nonius Kryo-Flex low temperature device cooled at 100 K. Data collection was performed by using _ and _ scans with a width of 0.30 and 20 s (in the range 4.34 < 2_ < 57.26°) exposure times with a detector distance of 37.5 mm. The data were reduced (SAINT)[5] and corrected for Lorentz polarisation effects and absorption by multi-scan method applied by (SADABS)[6] . The structure was solved by direct methods (SIR-2002)[7] and refined against all F^2 data by full-matrix least-squares techniques (SHELXTL-6.12)[8] minimizing $w[Fo^2-Fc^2]^2$. All the non-hydrogen atoms were refined with anisotropic displacement parameters. The hydrogen atoms were included from calculated positions and refined riding on their respective carbon atoms with isotropic displacement parameters. Weighted *R* factors (*Rw*) and all goodness of fit *S* are based on F^2, conventional *R* factors (*R*) are based on *F*.

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TABLE S1. Crystal and Refinement Data for $Fe(CH_2CMe_2Ph)_2(Py)_2$ (**2**).

Table 1. Crystal data and structure refinement for ear45svs.

Empirical formula	$C_{30}\ H_{36}\ Fe\ N_2$	
Formula weight	480.46	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 11.6538(12) Å	α= 108.971(2)°.
	b = 11.8197(12) Å	β= 105.834(2)°.
	c = 12.0936(13) Å	γ = 108.571(2)°.
Volume	1355.3(2) $Å^3$	
Z	2	
Density (calculated)	1.177 Mg/m^3	
Absorption coefficient	0.575 mm^{-1}	
F(000)	512	
Crystal size	0.43 x 0.21 x 0.15 mm^3	
Theta range for data collection	1.96 to 28.03°.	
Index ranges	-15<=h<=14, -15<=k<=14, -14<=l<=15	
Reflections collected	8424	
Independent reflections	6382 [R(int) = 0.0242]	
Completeness to theta = 28.03°	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9187 and 0.7901	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6382 / 0 / 302	
Goodness-of-fit on F^2	1.016	
Final R indices [I>2sigma(I)]	R1 = 0.0395, wR2 = 0.0754	
R indices (all data)	R1 = 0.0615, wR2 = 0.0798	
Largest diff. peak and hole	0.296 and -0.378 $e.Å^{-3}$	

TABLE S2 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $Fe(CH_2CMe_2Ph)_2(Py)_2$ (**2**). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Fe(1)	6138(1)	9283(1)	7435(1)	25(1)
N(1)	4003(2)	8206(2)	6720(2)	26(1)
N(2)	6450(2)	8026(2)	8301(2)	29(1)
C(1)	6787(2)	11118(2)	9002(2)	29(1)
C(2)	6385(2)	12176(2)	8756(2)	29(1)
C(3)	4864(2)	11627(2)	8256(2)	51(1)
C(4)	6780(3)	12413(2)	7714(2)	52(1)
C(5)	7090(2)	13497(2)	9993(2)	25(1)
C(6)	6422(2)	13980(2)	10677(2)	31(1)
C(7)	7097(2)	15184(2)	11801(2)	38(1)
C(8)	8441(2)	15939(2)	12266(2)	39(1)
C(9)	9126(2)	15485(2)	11605(2)	37(1)
C(10)	8461(2)	14283(2)	10501(2)	33(1)
C(11)	6489(2)	8815(2)	5776(2)	28(1)
C(12)	7906(2)	9007(2)	5917(2)	28(1)
C(13)	8918(2)	10446(2)	6925(2)	42(1)
C(14)	8058(2)	8830(2)	4647(2)	41(1)
C(15)	8188(2)	7977(2)	6299(2)	28(1)
C(16)	7494(2)	6623(2)	5411(2)	37(1)
C(17)	7696(2)	5643(2)	5702(3)	47(1)
C(18)	8597(2)	5984(3)	6905(3)	52(1)
C(19)	9293(2)	7310(3)	7808(3)	50(1)
C(20)	9092(2)	8292(2)	7503(2)	38(1)
C(21)	3194(2)	8008(2)	5580(2)	31(1)
C(22)	1829(2)	7470(2)	5142(2)	40(1)
C(23)	1254(2)	7108(2)	5908(2)	45(1)
C(24)	2073(2)	7292(2)	7074(2)	47(1)
C(25)	3424(2)	7839(2)	7443(2)	36(1)
C(26)	5965(2)	6708(2)	7562(2)	34(1)
C(27)	6208(2)	5853(2)	8033(3)	42(1)
C(28)	6970(2)	6348(3)	9311(3)	51(1)
C(29)	7480(2)	7707(3)	10100(2)	49(1)
C(30)	7194(2)	8500(2)	9559(2)	38(1)

Table S3. Bond lengths [Å] and angles [°] for $Fe(CH_2CMe_2Ph)_2(Py)_2$ (**2**)

Fe(1)-C(11)	2.0895(19)	C(12)-C(14)	1.548(3)
Fe(1)-C(1)	2.0905(18)	C(13)-H(13A)	0.9800
Fe(1)-N(2)	2.1414(16)	C(13)-H(13B)	0.9800
Fe(1)-N(1)	2.1569(16)	C(13)-H(13C)	0.9800
N(1)-C(21)	1.335(2)	C(14)-H(14A)	0.9800
N(1)-C(25)	1.339(3)	C(14)-H(14B)	0.9800
N(2)-C(30)	1.340(3)	C(14)-H(14C)	0.9800
N(2)-C(26)	1.343(2)	C(15)-C(20)	1.389(3)
C(1)-C(2)	1.552(3)	C(15)-C(16)	1.397(3)
C(1)-H(1A)	0.9900	C(16)-C(17)	1.384(3)
C(1)-H(1B)	0.9900	C(16)-H(16)	0.9500
C(2)-C(5)	1.531(3)	C(17)-C(18)	1.378(3)
C(2)-C(4)	1.531(3)	C(17)-H(17)	0.9500
C(2)-C(3)	1.535(3)	C(18)-C(19)	1.379(3)
C(3)-H(3A)	0.9800	C(18)-H(18)	0.9500
C(3)-H(3B)	0.9800	C(19)-C(20)	1.393(3)
C(3)-H(3C)	0.9800	C(19)-H(19)	0.9500
C(4)-H(4A)	0.9800	C(20)-H(20)	0.9500
C(4)-H(4B)	0.9800	C(21)-C(22)	1.376(3)
C(4)-H(4C)	0.9800	C(21)-H(21)	0.9500
C(5)-C(10)	1.394(3)	C(22)-C(23)	1.379(3)
C(5)-C(6)	1.394(3)	C(22)-H(22)	0.9500
C(6)-C(7)	1.392(3)	C(23)-C(24)	1.372(3)
C(6)-H(6)	0.9500	C(23)-H(23)	0.9500
C(7)-C(8)	1.367(3)	C(24)-C(25)	1.370(3)
C(7)-H(7)	0.9500	C(24)-H(24)	0.9500
C(8)-C(9)	1.381(3)	C(25)-H(25)	0.9500
C(8)-H(8)	0.9500	C(26)-C(27)	1.376(3)
C(9)-C(10)	1.379(3)	C(26)-H(26)	0.9500
C(9)-H(9)	0.9500	C(27)-C(28)	1.361(3)
C(10)-H(10)	0.9500	C(27)-H(27)	0.9500
C(11)-C(12)	1.547(3)	C(28)-C(29)	1.389(3)
C(11)-H(11A)	0.9900	C(28)-H(28)	0.9500
C(11)-H(11B)	0.9900	C(29)-C(30)	1.377(3)
C(12)-C(15)	1.530(3)	C(29)-H(29)	0.9500
C(12)-C(13)	1.536(3)	C(30)-H(30)	0.9500

		C(10)-C(5)-C(2)	120.73(17)
C(11)-Fe(1)-C(1)	131.31(8)	C(6)-C(5)-C(2)	122.99(18)
C(11)-Fe(1)-N(2)	110.57(7)	C(7)-C(6)-C(5)	121.4(2)
C(1)-Fe(1)-N(2)	104.00(7)	C(7)-C(6)-H(6)	119.3
C(11)-Fe(1)-N(1)	104.16(7)	C(5)-C(6)-H(6)	119.3
C(1)-Fe(1)-N(1)	108.06(7)	C(8)-C(7)-C(6)	121.0(2)
N(2)-Fe(1)-N(1)	91.70(6)	C(8)-C(7)-H(7)	119.5
C(21)-N(1)-C(25)	116.78(18)	C(6)-C(7)-H(7)	119.5
C(21)-N(1)-Fe(1)	120.74(14)	C(7)-C(8)-C(9)	118.84(19)
C(25)-N(1)-Fe(1)	122.07(14)	C(7)-C(8)-H(8)	120.6
C(30)-N(2)-C(26)	116.82(18)	C(9)-C(8)-H(8)	120.6
C(30)-N(2)-Fe(1)	123.11(14)	C(10)-C(9)-C(8)	120.3(2)
C(26)-N(2)-Fe(1)	119.92(14)	C(10)-C(9)-H(9)	119.9
C(2)-C(1)-Fe(1)	118.72(13)	C(8)-C(9)-H(9)	119.9
C(2)-C(1)-H(1A)	107.6	C(9)-C(10)-C(5)	122.27(19)
Fe(1)-C(1)-H(1A)	107.6	C(9)-C(10)-H(10)	118.9
C(2)-C(1)-H(1B)	107.6	C(5)-C(10)-H(10)	118.9
Fe(1)-C(1)-H(1B)	107.6	C(12)-C(11)-Fe(1)	118.31(13)
H(1A)-C(1)-H(1B)	107.1	C(12)-C(11)-H(11A)	107.7
C(5)-C(2)-C(4)	109.29(17)	Fe(1)-C(11)-H(11A)	107.7
C(5)-C(2)-C(3)	110.93(16)	C(12)-C(11)-H(11B)	107.7
C(4)-C(2)-C(3)	108.03(19)	Fe(1)-C(11)-H(11B)	107.7
C(5)-C(2)-C(1)	110.42(16)	H(11A)-C(11)-H(11B)	107.1
C(4)-C(2)-C(1)	109.27(17)	C(15)-C(12)-C(13)	111.77(17)
C(3)-C(2)-C(1)	108.85(18)	C(15)-C(12)-C(11)	109.02(16)
C(2)-C(3)-H(3A)	109.5	C(13)-C(12)-C(11)	108.98(16)
C(2)-C(3)-H(3B)	109.5	C(15)-C(12)-C(14)	108.93(16)
H(3A)-C(3)-H(3B)	109.5	C(13)-C(12)-C(14)	106.37(17)
C(2)-C(3)-H(3C)	109.5	C(11)-C(12)-C(14)	111.77(16)
H(3A)-C(3)-H(3C)	109.5	C(12)-C(13)-H(13A)	109.5
H(3B)-C(3)-H(3C)	109.5	C(12)-C(13)-H(13B)	109.5
C(2)-C(4)-H(4A)	109.5	H(13A)-C(13)-H(13B)	109.5
C(2)-C(4)-H(4B)	109.5	C(12)-C(13)-H(13C)	109.5
H(4A)-C(4)-H(4B)	109.5	H(13A)-C(13)-H(13C)	109.5
C(2)-C(4)-H(4C)	109.5	H(13B)-C(13)-H(13C)	109.5
H(4A)-C(4)-H(4C)	109.5	C(12)-C(14)-H(14A)	109.5
H(4B)-C(4)-H(4C)	109.5	C(12)-C(14)-H(14B)	109.5
C(10)-C(5)-C(6)	116.28(18)	H(14A)-C(14)-H(14B)	109.5

C(12)-C(14)-H(14C)	109.5	C(27)-C(26)-H(26)	118.3
H(14A)-C(14)-H(14C)	109.5	C(28)-C(27)-C(26)	119.3(2)
H(14B)-C(14)-H(14C)	109.5	C(28)-C(27)-H(27)	120.4
C(20)-C(15)-C(16)	116.3(2)	C(26)-C(27)-H(27)	120.4
C(20)-C(15)-C(12)	124.12(18)	C(27)-C(28)-C(29)	118.7(2)
C(16)-C(15)-C(12)	119.53(19)	C(27)-C(28)-H(28)	120.7
C(17)-C(16)-C(15)	122.3(2)	C(29)-C(28)-H(28)	120.7
C(17)-C(16)-H(16)	118.9	C(30)-C(29)-C(28)	118.7(2)
C(15)-C(16)-H(16)	118.9	C(30)-C(29)-H(29)	120.6
C(18)-C(17)-C(16)	120.1(2)	C(28)-C(29)-H(29)	120.6
C(18)-C(17)-H(17)	119.9	N(2)-C(30)-C(29)	123.2(2)
C(16)-C(17)-H(17)	119.9	N(2)-C(30)-H(30)	118.4
C(17)-C(18)-C(19)	119.2(2)	C(29)-C(30)-H(30)	118.4
C(17)-C(18)-H(18)	120.4		
C(19)-C(18)-H(18)	120.4		
C(18)-C(19)-C(20)	120.3(2)		
C(18)-C(19)-H(19)	119.8		
C(20)-C(19)-H(19)	119.8		
C(15)-C(20)-C(19)	121.8(2)		
C(15)-C(20)-H(20)	119.1		
C(19)-C(20)-H(20)	119.1		
N(1)-C(21)-C(22)	123.3(2)		
N(1)-C(21)-H(21)	118.4		
C(22)-C(21)-H(21)	118.4		
C(21)-C(22)-C(23)	119.0(2)		
C(21)-C(22)-H(22)	120.5		
C(23)-C(22)-H(22)	120.5		
C(24)-C(23)-C(22)	118.3(2)		
C(24)-C(23)-H(23)	120.9		
C(22)-C(23)-H(23)	120.9		
C(25)-C(24)-C(23)	119.2(2)		
C(25)-C(24)-H(24)	120.4		
C(23)-C(24)-H(24)	120.4		
N(1)-C(25)-C(24)	123.4(2)		
N(1)-C(25)-H(25)	118.3		
C(24)-C(25)-H(25)	118.3		
N(2)-C(26)-C(27)	123.3(2)		
N(2)-C(26)-H(26)	118.3		

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $Fe(CH_2CMe_2Ph)_2(Py)_2$. (**2**). 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(1)	30(1)	23(1)	25(1)	11(1)	12(1)	12(1)
N(1)	29(1)	24(1)	26(1)	12(1)	11(1)	11(1)
N(2)	28(1)	29(1)	33(1)	17(1)	12(1)	14(1)
C(1)	33(1)	29(1)	24(1)	12(1)	10(1)	17(1)
C(2)	37(1)	26(1)	23(1)	10(1)	9(1)	16(1)
C(3)	43(1)	37(1)	43(2)	-4(1)	-3(1)	23(1)
C(4)	102(2)	34(1)	25(1)	17(1)	27(1)	35(2)
C(5)	33(1)	23(1)	23(1)	13(1)	11(1)	15(1)
C(6)	33(1)	26(1)	28(1)	10(1)	13(1)	9(1)
C(7)	43(1)	33(1)	33(1)	8(1)	21(1)	15(1)
C(8)	42(1)	29(1)	30(1)	3(1)	9(1)	13(1)
C(9)	28(1)	32(1)	38(1)	10(1)	7(1)	9(1)
C(10)	35(1)	34(1)	33(1)	14(1)	17(1)	20(1)
C(11)	31(1)	25(1)	28(1)	12(1)	11(1)	15(1)
C(12)	28(1)	27(1)	25(1)	9(1)	12(1)	10(1)
C(13)	37(1)	30(1)	49(2)	14(1)	19(1)	8(1)
C(14)	48(1)	47(2)	39(1)	21(1)	27(1)	25(1)
C(15)	24(1)	34(1)	29(1)	13(1)	14(1)	14(1)
C(16)	36(1)	35(1)	39(1)	13(1)	17(1)	18(1)
C(17)	51(2)	38(1)	63(2)	23(1)	30(1)	27(1)
C(18)	53(2)	59(2)	79(2)	46(2)	38(2)	39(2)
C(19)	36(1)	84(2)	50(2)	42(2)	21(1)	36(2)
C(20)	29(1)	46(1)	41(1)	20(1)	16(1)	17(1)
C(21)	37(1)	30(1)	28(1)	15(1)	13(1)	14(1)
C(22)	36(1)	43(1)	34(1)	19(1)	7(1)	15(1)
C(23)	29(1)	57(2)	54(2)	31(1)	15(1)	18(1)
C(24)	39(1)	69(2)	55(2)	42(1)	28(1)	26(1)
C(25)	35(1)	49(1)	32(1)	25(1)	16(1)	21(1)
C(26)	33(1)	31(1)	44(1)	20(1)	19(1)	16(1)
C(27)	40(1)	35(1)	65(2)	30(1)	25(1)	21(1)
C(28)	49(2)	54(2)	78(2)	51(2)	31(2)	30(1)
C(29)	43(2)	64(2)	47(2)	38(1)	12(1)	24(1)
C(30)	34(1)	41(1)	35(1)	20(1)	10(1)	15(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{-3}) for $Fe(CH_2CMe_2Ph)_2(Py)_2$ (**2**).

	x	y	z	U(eq)
H(1A)	6459	10931	9627	34
H(1B)	7773	11532	9426	34
H(3A)	4579	11387	8873	77
H(3B)	4436	10832	7422	77
H(3C)	4606	12312	8155	77
H(4A)	6605	13140	7613	77
H(4B)	6257	11594	6895	77
H(4C)	7732	12657	7965	77
H(6)	5487	13476	10370	37
H(7)	6617	15485	12251	45
H(8)	8896	16762	13032	47
H(9)	10058	16003	11911	45
H(10)	8956	13980	10073	39
H(11A)	5860	7867	5168	33
H(11B)	6259	9363	5369	33
H(13A)	8865	10605	7753	62
H(13B)	8714	11076	6644	62
H(13C)	9820	10574	7023	62
H(14A)	8953	8920	4761	61
H(14B)	7926	9517	4419	61
H(14C)	7390	7942	3956	61
H(16)	6862	6367	4579	44
H(17)	7213	4733	5070	56
H(18)	8736	5314	7110	63
H(19)	9914	7556	8642	60
H(20)	9586	9201	8135	46
H(21)	3581	8251	5045	38
H(22)	1292	7348	4325	48
H(23)	315	6742	5634	55
H(24)	1707	7043	7619	57
H(25)	3978	7964	8255	43
H(26)	5426	6347	6669	41

H(27)	5849	4928	7472	51
H(28)	7148	5775	9657	61
H(29)	8017	8082	10996	59
H(30)	7541	9428	10103	45

Table S6. Torsion angles [°] for $Fe(CH_2CMe_2Ph)_2(Py)_2$ (**2**).

C(11)-Fe(1)-N(1)-C(21)	-32.57(16)
C(1)-Fe(1)-N(1)-C(21)	110.40(15)
N(2)-Fe(1)-N(1)-C(21)	-144.28(15)
C(11)-Fe(1)-N(1)-C(25)	154.99(16)
C(1)-Fe(1)-N(1)-C(25)	-62.04(17)
N(2)-Fe(1)-N(1)-C(25)	43.28(16)
C(11)-Fe(1)-N(2)-C(30)	131.16(16)
C(1)-Fe(1)-N(2)-C(30)	-13.95(17)
N(1)-Fe(1)-N(2)-C(30)	-123.03(16)
C(11)-Fe(1)-N(2)-C(26)	-44.23(16)
C(1)-Fe(1)-N(2)-C(26)	170.67(15)
N(1)-Fe(1)-N(2)-C(26)	61.58(15)
C(11)-Fe(1)-C(1)-C(2)	60.99(19)
N(2)-Fe(1)-C(1)-C(2)	-164.50(15)
N(1)-Fe(1)-C(1)-C(2)	-67.99(17)
Fe(1)-C(1)-C(2)-C(5)	-173.42(13)
Fe(1)-C(1)-C(2)-C(4)	-53.2(2)
Fe(1)-C(1)-C(2)-C(3)	64.6(2)
C(4)-C(2)-C(5)-C(10)	-50.6(3)
C(3)-C(2)-C(5)-C(10)	-169.57(19)
C(1)-C(2)-C(5)-C(10)	69.7(3)
C(4)-C(2)-C(5)-C(6)	130.0(2)
C(3)-C(2)-C(5)-C(6)	10.9(3)
C(1)-C(2)-C(5)-C(6)	-109.8(2)
C(10)-C(5)-C(6)-C(7)	0.3(3)
C(2)-C(5)-C(6)-C(7)	179.8(2)
C(5)-C(6)-C(7)-C(8)	0.4(4)
C(6)-C(7)-C(8)-C(9)	-0.3(4)
C(7)-C(8)-C(9)-C(10)	-0.6(4)
C(8)-C(9)-C(10)-C(5)	1.5(4)
C(6)-C(5)-C(10)-C(9)	-1.3(3)
C(2)-C(5)-C(10)-C(9)	179.2(2)
C(1)-Fe(1)-C(11)-C(12)	69.98(17)
N(2)-Fe(1)-C(11)-C(12)	-62.37(16)
N(1)-Fe(1)-C(11)-C(12)	-159.68(14)
Fe(1)-C(11)-C(12)-C(15)	68.39(18)

Fe(1)-C(11)-C(12)-C(13)	-53.9(2)
Fe(1)-C(11)-C(12)-C(14)	-171.13(13)
C(13)-C(12)-C(15)-C(20)	10.5(3)
C(11)-C(12)-C(15)-C(20)	-110.0(2)
C(14)-C(12)-C(15)-C(20)	127.8(2)
C(13)-C(12)-C(15)-C(16)	-170.53(18)
C(11)-C(12)-C(15)-C(16)	68.9(2)
C(14)-C(12)-C(15)-C(16)	-53.3(2)
C(20)-C(15)-C(16)-C(17)	-0.5(3)
C(12)-C(15)-C(16)-C(17)	-179.5(2)
C(15)-C(16)-C(17)-C(18)	0.7(4)
C(16)-C(17)-C(18)-C(19)	-0.3(4)
C(17)-C(18)-C(19)-C(20)	-0.3(4)
C(16)-C(15)-C(20)-C(19)	-0.1(3)
C(12)-C(15)-C(20)-C(19)	178.86(19)
C(18)-C(19)-C(20)-C(15)	0.5(4)
C(25)-N(1)-C(21)-C(22)	0.7(3)
Fe(1)-N(1)-C(21)-C(22)	-172.15(16)
N(1)-C(21)-C(22)-C(23)	-0.2(3)
C(21)-C(22)-C(23)-C(24)	-0.6(4)
C(22)-C(23)-C(24)-C(25)	0.8(4)
C(21)-N(1)-C(25)-C(24)	-0.4(3)
Fe(1)-N(1)-C(25)-C(24)	172.29(17)
C(23)-C(24)-C(25)-N(1)	-0.3(4)
C(30)-N(2)-C(26)-C(27)	-0.7(3)
Fe(1)-N(2)-C(26)-C(27)	174.97(16)
N(2)-C(26)-C(27)-C(28)	0.5(3)
C(26)-C(27)-C(28)-C(29)	-0.2(4)
C(27)-C(28)-C(29)-C(30)	0.2(4)
C(26)-N(2)-C(30)-C(29)	0.7(3)
Fe(1)-N(2)-C(30)-C(29)	-174.85(17)
C(28)-C(29)-C(30)-N(2)	-0.4(4)

Table S7. Crystal data and structure refinement for compound **4a**.

Empirical formula	C_{35} H_{53} Fe N_3 Si_2	
Formula weight	627.83	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 11.2970(8) Å	α= 90°.
	b = 16.9829(12) Å	β= 95.2160(10)°.
	c = 18.6068(13) Å	γ = 90°.
Volume	3555.0(4) $Å^3$	
Z	4	
Density (calculated)	1.173 Mg/m^3	
Absorption coefficient	0.518 mm^{-1}	
F(000)	1352	
Crystal size	0.45 x 0.35 x 0.31 mm^3	
Theta range for data collection	2.17 to 28.63°.	
Index ranges	-15<=h<=14, -22<=k<=22, -21<=l<=23	
Reflections collected	22463	
Independent reflections	8838 [R(int) = 0.0527]	
Completeness to theta = 28.63°	98.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8559 and 0.8003	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8838 / 0 / 370	
Goodness-of-fit on F^2	1.012	
Final R indices [I>2sigma(I)]	R1 = 0.0461, wR2 = 0.0947	
R indices (all data)	R1 = 0.0937, wR2 = 0.1050	
Largest diff. peak and hole	0.488 and -0.508 $e.Å^{-3}$	

Table S8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for compound **4a**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Fe(1)	7298(1)	8372(1)	1266(1)	18(1)
Si(1)	9983(1)	7408(1)	1319(1)	23(1)
Si(2)	5674(1)	8045(1)	2749(1)	23(1)
N(1)	6153(1)	7708(1)	436(1)	19(1)
N(2)	5896(1)	9065(1)	980(1)	18(1)
N(3)	7816(2)	9561(1)	1653(1)	19(1)
C(1)	4925(2)	8784(1)	561(1)	20(1)
C(2)	3894(2)	9227(2)	438(1)	26(1)
C(3)	3839(2)	9979(2)	730(1)	29(1)
C(4)	4829(2)	10272(1)	1132(1)	25(1)
C(5)	5845(2)	9815(1)	1252(1)	19(1)
C(6)	6954(2)	10079(1)	1631(1)	20(1)
C(7)	5111(2)	8015(1)	253(1)	22(1)
C(8)	7066(2)	10885(1)	1954(1)	26(1)
C(9)	4168(2)	7628(2)	-251(1)	28(1)
C(10)	6487(2)	6969(1)	134(1)	20(1)
C(11)	6193(2)	6254(2)	441(1)	24(1)
C(12)	6669(2)	5565(2)	185(1)	27(1)
C(13)	7424(2)	5570(2)	-361(1)	27(1)
C(14)	7629(2)	6284(2)	-692(1)	27(1)
C(15)	7156(2)	6987(1)	-463(1)	23(1)
C(16)	5364(2)	6207(2)	1039(1)	32(1)
C(17)	8024(2)	4818(2)	-573(2)	38(1)
C(18)	7322(2)	7744(2)	-864(1)	28(1)
C(19)	9014(2)	9823(1)	1865(1)	20(1)
C(20)	9605(2)	10225(1)	1343(1)	21(1)
C(21)	10779(2)	10461(1)	1524(1)	24(1)
C(22)	11369(2)	10304(1)	2196(1)	24(1)
C(23)	10760(2)	9893(1)	2696(1)	24(1)
C(24)	9581(2)	9654(1)	2542(1)	23(1)
C(25)	9000(2)	10421(2)	617(1)	25(1)
C(26)	12626(2)	10584(2)	2387(2)	36(1)
C(27)	8941(2)	9257(2)	3119(1)	29(1)

C(28)	8935(2)	8141(1)	887(1)	22(1)
C(29)	10412(2)	7605(2)	2301(1)	35(1)
C(30)	11413(2)	7414(2)	875(1)	33(1)
C(31)	9339(2)	6393(2)	1232(2)	32(1)
C(32)	6900(2)	7781(1)	2191(1)	21(1)
C(33)	5607(2)	9108(2)	3001(2)	40(1)
C(34)	4194(2)	7780(2)	2267(2)	46(1)
C(35)	5806(2)	7503(2)	3628(1)	36(1)

Table S9. Bond lengths [Å] and angles [°] for compound **4a.**

Fe(1)-N(2)	2.0056(18)	C(10)-C(11)	1.394(3)
Fe(1)-C(28)	2.075(2)	C(10)-C(15)	1.401(3)
Fe(1)-C(32)	2.077(2)	C(11)-C(12)	1.390(3)
Fe(1)-N(3)	2.2044(19)	C(11)-C(16)	1.519(3)
Fe(1)-N(1)	2.2284(19)	C(12)-C(13)	1.385(3)
Si(1)-C(28)	1.851(2)	C(12)-H(12)	0.9500
Si(1)-C(31)	1.873(3)	C(13)-C(14)	1.388(3)
Si(1)-C(29)	1.878(3)	C(13)-C(17)	1.516(3)
Si(1)-C(30)	1.879(2)	C(14)-C(15)	1.391(3)
Si(2)-C(32)	1.859(2)	C(14)-H(14)	0.9500
Si(2)-C(33)	1.869(3)	C(15)-C(18)	1.506(3)
Si(2)-C(35)	1.872(3)	C(16)-H(16A)	0.9800
Si(2)-C(34)	1.878(3)	C(16)-H(16B)	0.9800
N(1)-C(7)	1.304(3)	C(16)-H(16C)	0.9800
N(1)-C(10)	1.438(3)	C(17)-H(17A)	0.9800
N(2)-C(1)	1.372(3)	C(17)-H(17B)	0.9800
N(2)-C(5)	1.374(3)	C(17)-H(17C)	0.9800
N(3)-C(6)	1.312(3)	C(18)-H(18A)	0.9800
N(3)-C(19)	1.445(3)	C(18)-H(18B)	0.9800
C(1)-C(2)	1.388(3)	C(18)-H(18C)	0.9800
C(1)-C(7)	1.450(3)	C(19)-C(24)	1.390(3)
C(2)-C(3)	1.390(3)	C(19)-C(20)	1.405(3)
C(2)-H(2)	0.9500	C(20)-C(21)	1.398(3)
C(3)-C(4)	1.381(3)	C(20)-C(25)	1.496(3)
C(3)-H(3)	0.9500	C(21)-C(22)	1.388(3)
C(4)-C(5)	1.386(3)	C(21)-H(21)	0.9500
C(4)-H(4)	0.9500	C(22)-C(23)	1.393(3)
C(5)-C(6)	1.451(3)	C(22)-C(26)	1.509(3)
C(6)-C(8)	1.495(3)	C(23)-C(24)	1.397(3)
C(7)-C(9)	1.504(3)	C(23)-H(23)	0.9500
C(8)-H(8A)	0.9800	C(24)-C(27)	1.507(3)
C(8)-H(8B)	0.9800	C(25)-H(25A)	0.9800
C(8)-H(8C)	0.9800	C(25)-H(25B)	0.9800
C(9)-H(9A)	0.9800	C(25)-H(25C)	0.9800
C(9)-H(9B)	0.9800	C(26)-H(26A)	0.9800
C(9)-H(9C)	0.9800	C(26)-H(26B)	0.9800

C(26)-H(26C)	0.9800	C(28)-Si(1)-C(29)	113.66(11)
C(27)-H(27A)	0.9800	C(31)-Si(1)-C(29)	108.17(13)
C(27)-H(27B)	0.9800	C(28)-Si(1)-C(30)	110.33(11)
C(27)-H(27C)	0.9800	C(31)-Si(1)-C(30)	108.04(11)
C(28)-H(28A)	0.9900	C(29)-Si(1)-C(30)	105.70(11)
C(28)-H(28B)	0.9900	C(32)-Si(2)-C(33)	114.98(11)
C(29)-H(29A)	0.9800	C(32)-Si(2)-C(35)	111.39(11)
C(29)-H(29B)	0.9800	C(33)-Si(2)-C(35)	104.93(13)
C(29)-H(29C)	0.9800	C(32)-Si(2)-C(34)	110.61(12)
C(30)-H(30A)	0.9800	C(33)-Si(2)-C(34)	107.28(14)
C(30)-H(30B)	0.9800	C(35)-Si(2)-C(34)	107.19(13)
C(30)-H(30C)	0.9800	C(7)-N(1)-C(10)	120.59(19)
C(31)-H(31A)	0.9800	C(7)-N(1)-Fe(1)	115.59(15)
C(31)-H(31B)	0.9800	C(10)-N(1)-Fe(1)	123.76(13)
C(31)-H(31C)	0.9800	C(1)-N(2)-C(5)	118.23(18)
C(32)-H(32A)	0.9900	C(1)-N(2)-Fe(1)	121.20(15)
C(32)-H(32B)	0.9900	C(5)-N(2)-Fe(1)	120.35(14)
C(33)-H(33A)	0.9800	C(6)-N(3)-C(19)	118.44(19)
C(33)-H(33B)	0.9800	C(6)-N(3)-Fe(1)	115.51(15)
C(33)-H(33C)	0.9800	C(19)-N(3)-Fe(1)	125.84(13)
C(34)-H(34A)	0.9800	N(2)-C(1)-C(2)	121.4(2)
C(34)-H(34B)	0.9800	N(2)-C(1)-C(7)	113.63(18)
C(34)-H(34C)	0.9800	C(2)-C(1)-C(7)	124.9(2)
C(35)-H(35A)	0.9800	C(1)-C(2)-C(3)	120.0(2)
C(35)-H(35B)	0.9800	C(1)-C(2)-H(2)	120.0
C(35)-H(35C)	0.9800	C(3)-C(2)-H(2)	120.0
		C(4)-C(3)-C(2)	118.6(2)
N(2)-Fe(1)-C(28)	136.66(8)	C(4)-C(3)-H(3)	120.7
N(2)-Fe(1)-C(32)	106.11(8)	C(2)-C(3)-H(3)	120.7
C(28)-Fe(1)-C(32)	117.23(9)	C(3)-C(4)-C(5)	120.3(2)
N(2)-Fe(1)-N(3)	74.28(7)	C(3)-C(4)-H(4)	119.8
C(28)-Fe(1)-N(3)	93.76(8)	C(5)-C(4)-H(4)	119.9
C(32)-Fe(1)-N(3)	104.03(8)	N(2)-C(5)-C(4)	121.4(2)
N(2)-Fe(1)-N(1)	73.68(7)	N(2)-C(5)-C(6)	113.71(18)
C(28)-Fe(1)-N(1)	98.52(8)	C(4)-C(5)-C(6)	124.8(2)
C(32)-Fe(1)-N(1)	100.00(8)	N(3)-C(6)-C(5)	114.4(2)
N(3)-Fe(1)-N(1)	144.11(7)	N(3)-C(6)-C(8)	124.5(2)
C(28)-Si(1)-C(31)	110.68(11)	C(5)-C(6)-C(8)	121.08(19)

N(1)-C(7)-C(1)	114.6(2)	H(16B)-C(16)-H(16C)	109.5
N(1)-C(7)-C(9)	124.0(2)	C(13)-C(17)-H(17A)	109.5
C(1)-C(7)-C(9)	121.4(2)	C(13)-C(17)-H(17B)	109.5
C(6)-C(8)-H(8A)	109.5	H(17A)-C(17)-H(17B)	109.5
C(6)-C(8)-H(8B)	109.5	C(13)-C(17)-H(17C)	109.5
H(8A)-C(8)-H(8B)	109.5	H(17A)-C(17)-H(17C)	109.5
C(6)-C(8)-H(8C)	109.4	H(17B)-C(17)-H(17C)	109.5
H(8A)-C(8)-H(8C)	109.5	C(15)-C(18)-H(18A)	109.6
H(8B)-C(8)-H(8C)	109.5	C(15)-C(18)-H(18B)	109.2
C(7)-C(9)-H(9A)	109.4	H(18A)-C(18)-H(18B)	109.5
C(7)-C(9)-H(9B)	109.6	C(15)-C(18)-H(18C)	109.6
H(9A)-C(9)-H(9B)	109.5	H(18A)-C(18)-H(18C)	109.5
C(7)-C(9)-H(9C)	109.4	H(18B)-C(18)-H(18C)	109.5
H(9A)-C(9)-H(9C)	109.5	C(24)-C(19)-C(20)	121.2(2)
H(9B)-C(9)-H(9C)	109.5	C(24)-C(19)-N(3)	121.82(19)
C(11)-C(10)-C(15)	120.7(2)	C(20)-C(19)-N(3)	116.9(2)
C(11)-C(10)-N(1)	121.25(19)	C(21)-C(20)-C(19)	118.2(2)
C(15)-C(10)-N(1)	118.1(2)	C(21)-C(20)-C(25)	120.0(2)
C(12)-C(11)-C(10)	118.6(2)	C(19)-C(20)-C(25)	121.78(19)
C(12)-C(11)-C(16)	119.3(2)	C(22)-C(21)-C(20)	122.0(2)
C(10)-C(11)-C(16)	122.1(2)	C(22)-C(21)-H(21)	119.0
C(13)-C(12)-C(11)	122.0(2)	C(20)-C(21)-H(21)	119.0
C(13)-C(12)-H(12)	119.0	C(21)-C(22)-C(23)	118.1(2)
C(11)-C(12)-H(12)	119.0	C(21)-C(22)-C(26)	121.1(2)
C(12)-C(13)-C(14)	117.9(2)	C(23)-C(22)-C(26)	120.7(2)
C(12)-C(13)-C(17)	120.4(2)	C(22)-C(23)-C(24)	121.9(2)
C(14)-C(13)-C(17)	121.6(2)	C(22)-C(23)-H(23)	119.0
C(13)-C(14)-C(15)	122.1(2)	C(24)-C(23)-H(23)	119.1
C(13)-C(14)-H(14)	118.9	C(19)-C(24)-C(23)	118.5(2)
C(15)-C(14)-H(14)	119.1	C(19)-C(24)-C(27)	121.8(2)
C(14)-C(15)-C(10)	118.3(2)	C(23)-C(24)-C(27)	119.7(2)
C(14)-C(15)-C(18)	120.9(2)	C(20)-C(25)-H(25A)	109.4
C(10)-C(15)-C(18)	120.8(2)	C(20)-C(25)-H(25B)	109.5
C(11)-C(16)-H(16A)	109.7	H(25A)-C(25)-H(25B)	109.5
C(11)-C(16)-H(16B)	109.3	C(20)-C(25)-H(25C)	109.5
H(16A)-C(16)-H(16B)	109.5	H(25A)-C(25)-H(25C)	109.5
C(11)-C(16)-H(16C)	109.5	H(25B)-C(25)-H(25C)	109.5
H(16A)-C(16)-H(16C)	109.5	C(22)-C(26)-H(26A)	109.6

C(22)-C(26)-H(26B)	109.6	Si(2)-C(32)-H(32B)	106.1
H(26A)-C(26)-H(26B)	109.5	Fe(1)-C(32)-H(32B)	106.1
C(22)-C(26)-H(26C)	109.2	H(32A)-C(32)-H(32B)	106.3
H(26A)-C(26)-H(26C)	109.5	Si(2)-C(33)-H(33A)	109.5
H(26B)-C(26)-H(26C)	109.5	Si(2)-C(33)-H(33B)	109.4
C(24)-C(27)-H(27A)	109.3	H(33A)-C(33)-H(33B)	109.5
C(24)-C(27)-H(27B)	109.4	Si(2)-C(33)-H(33C)	109.6
H(27A)-C(27)-H(27B)	109.5	H(33A)-C(33)-H(33C)	109.5
C(24)-C(27)-H(27C)	109.7	H(33B)-C(33)-H(33C)	109.5
H(27A)-C(27)-H(27C)	109.5	Si(2)-C(34)-H(34A)	109.3
H(27B)-C(27)-H(27C)	109.5	Si(2)-C(34)-H(34B)	109.6
Si(1)-C(28)-Fe(1)	122.28(12)	H(34A)-C(34)-H(34B)	109.5
Si(1)-C(28)-H(28A)	106.8	Si(2)-C(34)-H(34C)	109.5
Fe(1)-C(28)-H(28A)	106.8	H(34A)-C(34)-H(34C)	109.5
Si(1)-C(28)-H(28B)	106.7	H(34B)-C(34)-H(34C)	109.5
Fe(1)-C(28)-H(28B)	106.7	Si(2)-C(35)-H(35A)	109.7
H(28A)-C(28)-H(28B)	106.7	Si(2)-C(35)-H(35B)	109.3
Si(1)-C(29)-H(29A)	109.4	H(35A)-C(35)-H(35B)	109.5
Si(1)-C(29)-H(29B)	109.5	Si(2)-C(35)-H(35C)	109.4
H(29A)-C(29)-H(29B)	109.5	H(35A)-C(35)-H(35C)	109.5
Si(1)-C(29)-H(29C)	109.5	H(35B)-C(35)-H(35C)	109.5
H(29A)-C(29)-H(29C)	109.5		
H(29B)-C(29)-H(29C)	109.5		
Si(1)-C(30)-H(30A)	109.3		
Si(1)-C(30)-H(30B)	109.5		
H(30A)-C(30)-H(30B)	109.5		
Si(1)-C(30)-H(30C)	109.5		
H(30A)-C(30)-H(30C)	109.5		
H(30B)-C(30)-H(30C)	109.5		
Si(1)-C(31)-H(31A)	109.7		
Si(1)-C(31)-H(31B)	109.4		
H(31A)-C(31)-H(31B)	109.5		
Si(1)-C(31)-H(31C)	109.3		
H(31A)-C(31)-H(31C)	109.5		
H(31B)-C(31)-H(31C)	109.5		
Si(2)-C(32)-Fe(1)	125.07(12)		
Si(2)-C(32)-H(32A)	106.1		
Fe(1)-C(32)-H(32A)	106.0		