Supporting information for

Planar Three-Coordinate Iron(II) Complexes Supported by Sterically Demanding -$Si(SiMe_3)_2(SiMe_2{}^tBu)$ ligands

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Contents

General. Manipulation of air and moisture sensitive compounds was carried out under a dry nitrogen atmosphere using Schlenk tube techniques associated with a high-vacuum line or in the glove box which was filled with dry nitrogen. All solvents were purchased from Kanto Chemical Co. Inc., and was dried over activated molecular sieves 4Å prior to use. ^{1}H NMR spectrum was recorded using a JEOL Lambda 400 spectrometer and ECZ 600 spectrometer at ambient temperature. ^{1}H NMR chemical shifts (δ values) were given in ppm relative to the solvent signal. Elemental analyses were performed by a Thermo Scientific FLASH 2000 Organic Elemental Analyzer. Starting materials, $Si(SiMe_3)_3(Si^tBuMe_2)$[1], $MeIM^{Me}$ [2] were synthesized by the method reported in the literature. Other reagents were purchased from Tokyo Chemical Industries Co., Ltd. or FUJIFILM Wako Pure Chemical Co., Inc. or Kanto Chemical Co., Inc. or Sigma Aldrich, and were used without further purification.

Synthesis of $Fe[Si(SiMe_3)_2(Si^tBuMe_2)]_2(THF)$ (2). In a 50 mL vial, $Si(SiMe_3)_3(Si^tBuMe_2)$ (5.45 g, 15.0 mmol) was dissolved in THF (15 mL), then KO^tBu (1.69 g, 15.1 mmol) was added to this solution. The solution was stirred at room temperature for 15 h to prepare the solution of silyl anion $K[Si(SiMe_3)_2(Si^tBuMe_2)]$. Subsequently, $FeBr_2$ (1.64 g, 7.59 mmol) was suspended in THF (10 mL) in a 50 mL vial, and the solution of the silyl anion, $K[Si(SiMe_3)_2(Si^tBuMe_2)]$, was added dropwise. After stirring at room temperature for 30 min, insoluble materials were removed by centrifugation. The mother liquid was evaporated in vacuo, and the obtained solid was dissolved in pentane (20 mL). The supernatant was again centrifuged to remove the insoluble materials. The solvent was concentrated to ca. 4 mL, and the remaining solution was cooled at -78 °C. Complex **2** was obtained as green crystals in 83% yield (4.41 g). ^{1}H NMR (400 MHz, r.t., C_6D_6): δ = -47.08 (brs, 18H, ^{t}Bu), 0.28 (m, 4H, THF), 1.01 (m, 4H, THF), 11.09 (brs, 36H, $SiMe_3$), 23.99 (brs, 12H, $SiMe_3$). Magnetic susceptibility (Evans): μ_{eff} = 4.49 (C_6D_6, 20 °C). Anal calcd for calcd for $C_{28}H_{74}OSi_8Fe$; C 47.54, H 10.54; found: C 47.24, H 10.71. Melting point: 103 °C. (then decomposed at 125 °C)

Synthesis of $Fe[Si(SiMe_3)_2(Si^tBuMe_2)]_2(MeIM^{Me})$ (3). In a 50 mL Schlenk tube, $Fe[Si(SiMe_3)_2(Si^tBuMe_2)]_2(THF)$ (**2**) (1.06 g, 1.50 mmol) was dissolved in toluene (10 mL) and the solution was cooled at -78 °C. Then toluene (10 mL) solution of $MeIM^{Me}$ (188 mg, 1.51 mmol) was slowly added to this solution. The solution was stirred to room temperature for 30 min. The color of the solution turned from dark green to dark brown. The reaction solution was evaporated *in vacuo*, and the obtained solid was dissolved in pentane (10 mL), then the solution was centrifuged to remove the insoluble materials. The solvent was concentrated to ca. 2 mL, and the remaining solution was cooled at -78 °C, from which complex **3** was obtained as dark brown crystals in 69% yield (785 mg). ^{1}H NMR (400 MHz, r.t., C_6D_6): δ = -26.32 (brs, 18H, ^{t}Bu), 0.28 (brs, 6H, $MeIM^{Me}$), 9.99 (brs, 36H, $SiMe_3$), 26.78 (brs, 12H, $SiMe_3$), 73.13 (brs, 6H, $MeIM^{Me}$). Magnetic susceptibility (Evans): μ_{eff} = 5.32 (C_6D_6, 20 °C). Anal calcd for calcd for $C_{31}H_{78}N_2Si_8Fe$; C 49.02, H 10.35, N 3.69; found: C 48.63, H 10.05, N 3.88. Melting point: 107°C. (then decomposed at 150 °C).

General Procedure for the hydrosilylation of acetophenone with Ph_2SiH_2 catalyzed by iron(II) complexes. Acetophenone (360 μL, 3.0 mmol) and Ph_2SiH_2 (1.21 mL, 6.6 mmol) were placed in a 4 mL vial, then an iron(II)

complexes **2** or **3** (0.003 mmol, 0.1 mol%) was added to this mixture. The resulting mixture was stirred at r.t. for 1 h, then conversion of acetophenone and the yield of the product was estimated by ^{1}H NMR analysis in comparison with internal standard 1,4-dioxane.

General Procedure for the hydrosilylation of acetophenone with TMDS catalyzed by iron(II) complexes. Acetophenone (120 μL, 1.0 mmol) and 1,1,3,3-tetramethyldisiloxane (TMDS) (390 μL, 2.2 mmol) were placed in a 4 mL vial, then an iron(II) complexes **2** or **3** (0.005 mmol, 0.5 mol%) was added. The resulting mixture was stirred at r.t. for 24 h, then conversion of acetophenone and the yield of the product was estimated by ^{1}H NMR analysis in comparison with internal standard 1,4-dioxane.

Time course of the Hydrosilylation of acetophenone with Ph_2SiH_2 catalyzed by iron(II) complexes. Acetophenone (360 μL, 3.0 mmol), Ph_2SiH_2 (1.21 mL, 6.6 mmol), hexamethylbenzene (1.5 mmol, as internal standard) and benzene (3 mL) were placed in a 4 mL vial, then an iron(II) complexes **1**, **2** or **3** (0.003 mmol, 0.1 mol%) was added. The resulting mixture was stirred at r.t. for 24 h, then conversion of acetophenone and the yield of the product was estimated by ^{1}H NMR analysis in comparison with hexamethylbenzene. Time course of the reactions were described in Figure S1.

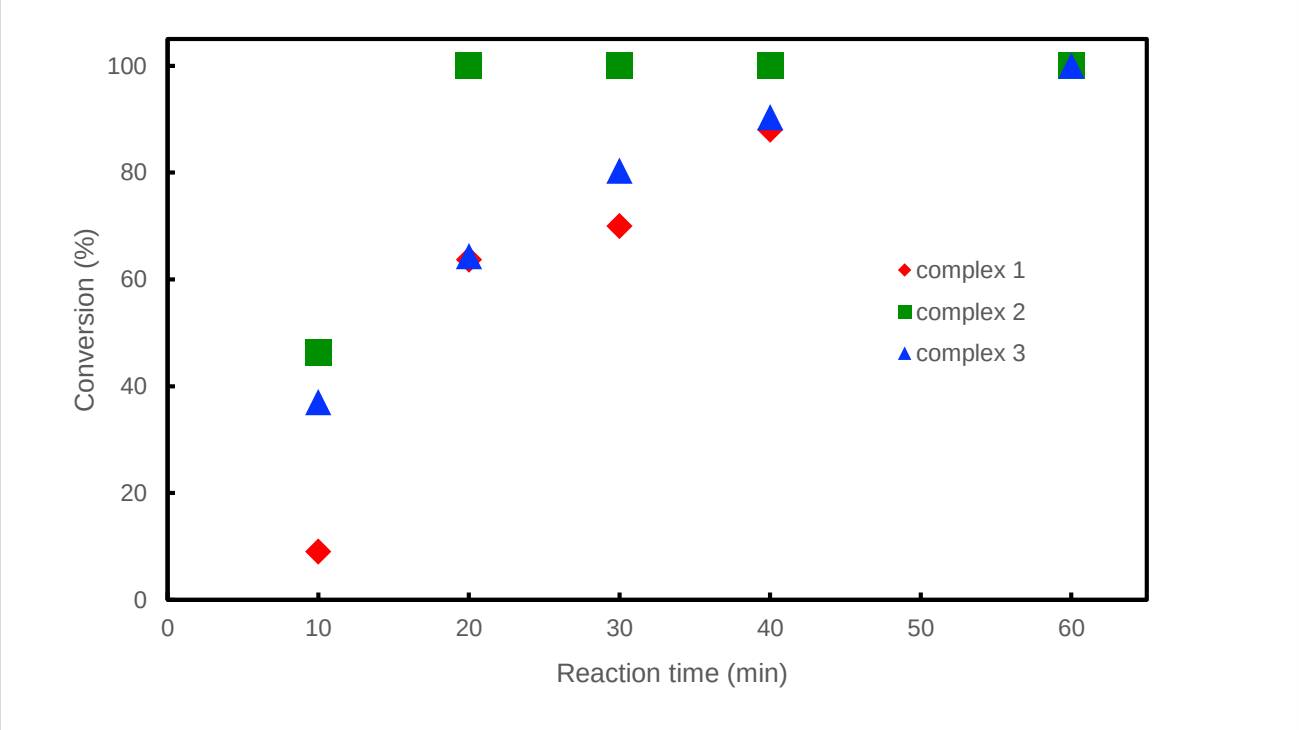


Figure S1. Time profile for the hydrosilylation of acetophenone with Ph2SiH2 catalyzed by iron catalysts.

Figure S2. ^{1}H NMR spectrum of solution of **2** in C_6D_6 at room temperature.

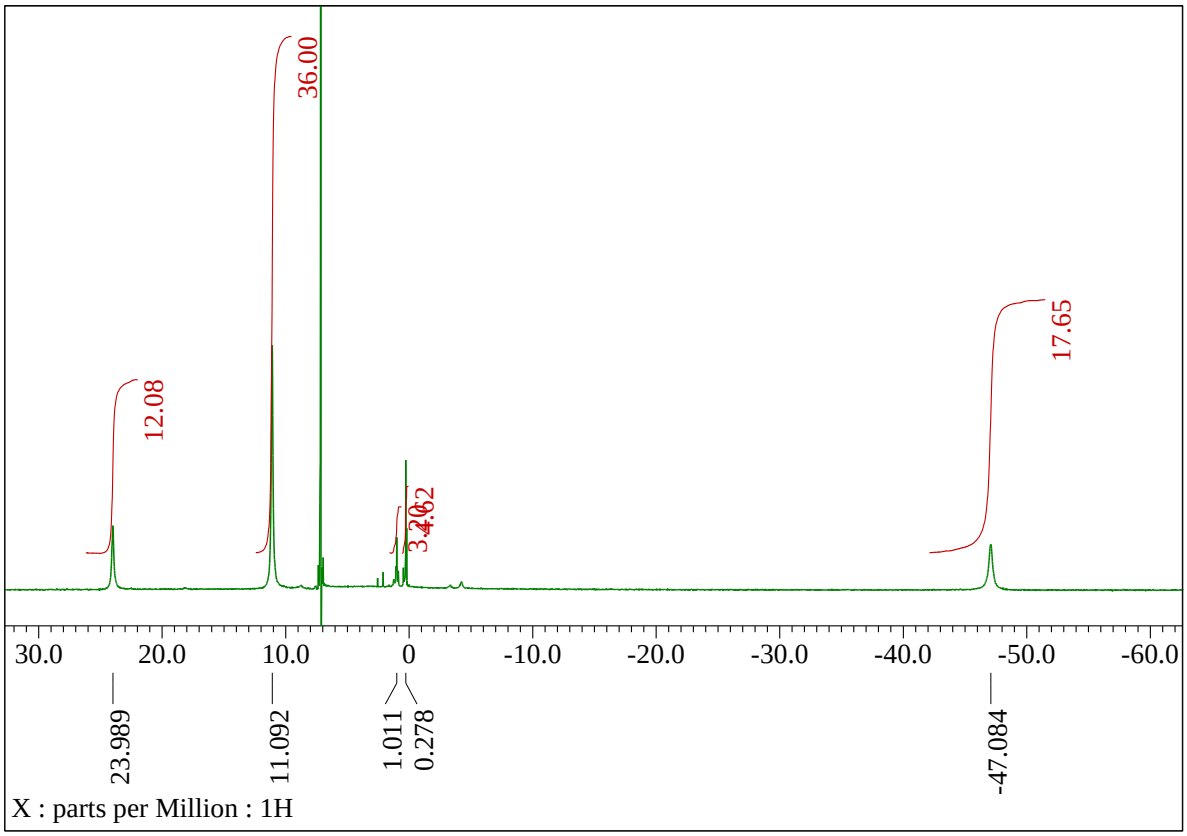
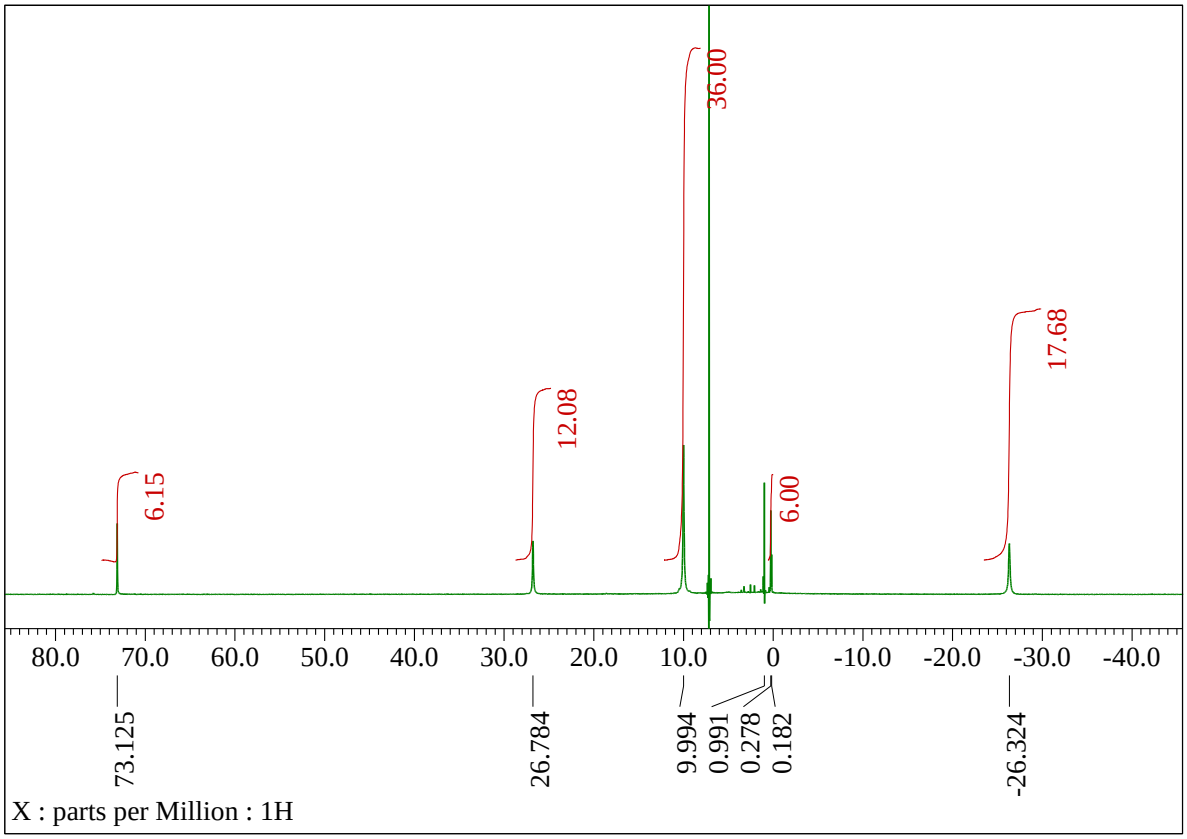


Figure S3. ^{1}H NMR spectrum of solution of **3** in C_6D_6 at room temperature.



X-ray data collection and reduction

X-ray crystallography for compounds **2** was performed on a Rigaku Saturn CCD area detector with graphite monochromated Mo-Kα radiation (λ=0.71075 Å) and single crystals of **3** suitable for X-ray crystallography were analyzed by synchrotron radiation at beam line BL02B1 (λ=0.41440 Å) of Spring-8 (Hyogo, Japan) using PILATUS3 X CdTe 1M detector. The data were collected at 133 K for **2** and 100 K for **3** and using ω scan in the θ range of $2.09 \leq \theta \leq 31.34$ deg (**2**), $7.69 \leq \theta \leq 15.69$ deg (**3**). The data obtained were processed using Crystal-Clear (Rigaku) on a Pentium computer, and were corrected for Lorentz and polarization effects. The structures were solved by direct methods[3], and expanded using Fourier techniques. Hydrogen atoms were refined using the riding model. The final cycle of full-matrix least-squares refinement on F^2 was based on 12894 observed reflections and 365 variable parameters for **2**, 10859 observed reflections and 405 variable parameters for **3**. Neutral atom scattering factors were taken from International Tables for Crystallography (IT), Vol. C, Table 6.1.1.4[4]. Anomalous dispersion effects were included in F_{calc}[5]; the values for Δf' and Δf'' were those of Creagh and McAuley[6]. The values for the mass attenuation coefficients are those of Creagh and Hubbell[7]. All calculations were performed using the CrystalStructure[8] crystallographic software package except for refinement, which was performed using SHELXL Version 2017/1[9]. Details of final refinement as well as the bond lengths and angle are summarized in Tables S1 and S2, and the numbering scheme employed is also shown in Figures S4 and S5 which were drawn with ORTEP at 50% probability ellipsoids. CCDC 2300423 (**2**), 2300424 (**3**) contain the supplementary crystallographic data for this paper.

Figure S4. ORTEP drawing of **2** (50% probability of the thermal ellipsoids). Hydrogen atoms were omitted for clarity.

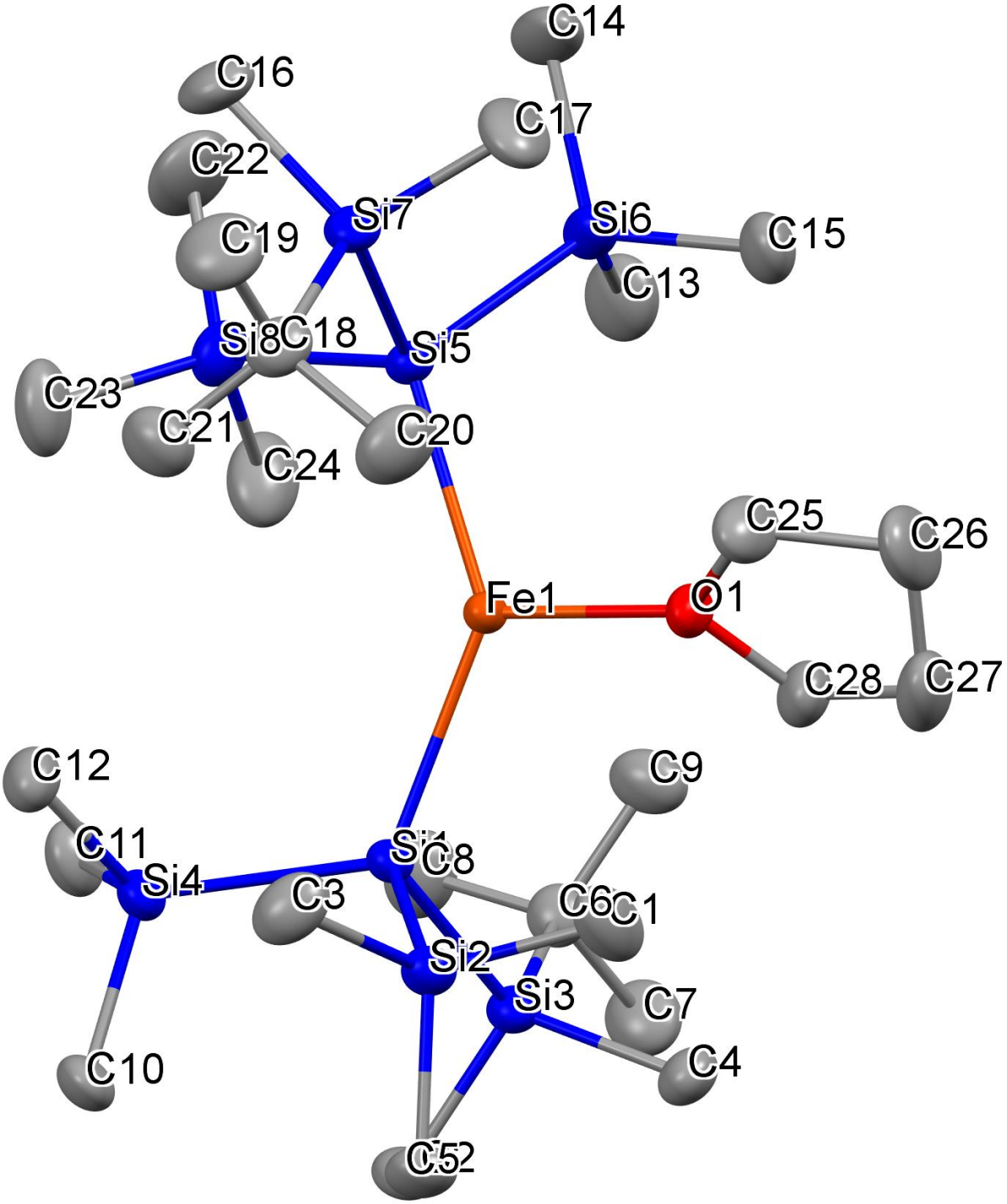


Table S1. Crystal data and structure refinement for **2**.

Empirical Formula	$C_{28}H_{74}FeOSi_8$
Formula Weight	707.42
Crystal Color, Habit	green, platelet
Crystal Dimensions	0.200 X 0.200 X 0.200 mm
Crystal System	monoclinic
Lattice Type	Primitive
Lattice Parameters	a = 10.5191(2) Å
	b = 22.8961(4) Å
	c = 18.6336(3) Å
	β = 99.1085(19) °
	V = 4431.24(14) Å^3
Space Group	$P2_1/n$ (#14)
Z value	4
D_{calc}	1.060 g/cm^3
F_{000}	1552.00
μ(MoKα)	5.745 cm^{-1}
Diffractometer	Saturn724
Radiation	MoKα (λ = 0.71075 Å)
	graphite monochromated
Voltage, Current	50kV, 24mA
Temperature	-140.0°C
Detector Aperture	72.8 x 72.8 mm
Data Images	720 exposures
ω oscillation Range (χ=45.0, ϕ=0.0)	-70.0 - 110.0°
Exposure Rate	6.0 sec./°
Detector Swing Angle	20.00°
ω oscillation Range (χ=45.0, ϕ=90.0)	-70.0 - 110.0°
Exposure Rate	6.0 sec./°
Detector Swing Angle	20.00°
Detector Position	45.00 mm
Pixel Size	0.035 mm
$2\theta_{max}$	62.4°
No. of Reflections Measured	Total: 40566
	Unique: 12894 (R_{int} = 0.0179)
Corrections	Lorentz-polarization
	Absorption
	(trans. factors: 0.717 - 0.891)

Structure Solution	Direct Methods (SHELXT Version 2014/5)
Refinement	Full-matrix least-squares on F^2
Function Minimized	$\Sigma\ w\ (Fo^2 - Fc^2)^2$
Least Squares Weights	$w = 1/ [\ \sigma^2(Fo^2) + (0.0408 \cdot P)^2 + 1.2983 \cdot P\ ]$
	where $P = (Max(Fo^2,0) + 2Fc^2)/3$
$2\theta_{max}$ cutoff	62.4^o
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	12894
No. Variables	365
Reflection/Parameter Ratio	35.33
Residuals: R1(I>2.00σ(I))	0.0295
Residuals: R (All reflections)	0.0341
Residuals: wR2 (All reflections)	0.0795
Goodness of Fit Indicator	1.036
Max Shift/Error in Final Cycle	0.002
Maximum peak in Final Diff. Map	1.10 $e^-/Å^3$
Minimum peak in Final Diff. Map	-0.36 $e^-/Å^3$

Atomic coordinates and B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}
Fe1	0.59360(2)	0.27549(2)	0.40843(2)	1.558(3)
Si1	0.54837(3)	0.17119(2)	0.37637(2)	1.567(5)
Si2	0.33693(3)	0.15384(2)	0.39753(2)	1.977(6)
Si3	0.67431(3)	0.10267(2)	0.45125(2)	1.978(6)
Si4	0.53657(3)	0.14148(2)	0.25446(2)	2.020(6)
Si5	0.67865(3)	0.36394(2)	0.35616(2)	1.681(5)
Si6	0.82999(4)	0.41215(2)	0.44152(2)	2.664(6)
Si7	0.52235(3)	0.43443(2)	0.31452(2)	2.182(6)
Si8	0.79659(3)	0.34043(2)	0.26379(2)	2.497(6)
O1	0.55045(9)	0.29535(4)	0.50884(4)	2.430(14)
C1	0.30423(15)	0.18984(8)	0.48284(9)	3.70(3)
C2	0.29582(14)	0.07473(6)	0.40602(8)	3.04(2)
C3	0.21840(13)	0.18479(7)	0.32159(9)	3.48(3)
C4	0.61565(14)	0.09389(6)	0.54098(7)	2.83(2)
C5	0.66358(15)	0.02840(5)	0.40802(8)	3.05(2)
C6	0.85235(12)	0.12311(6)	0.47168(7)	2.57(2)
C7	0.92470(15)	0.07752(7)	0.52306(9)	3.82(3)
C8	0.90966(15)	0.12403(9)	0.40192(9)	4.08(3)
C9	0.87187(13)	0.18266(6)	0.50836(9)	3.39(3)
C10	0.45079(15)	0.07002(6)	0.23714(7)	3.10(2)
C11	0.69586(14)	0.13312(7)	0.22302(8)	3.35(3)
C12	0.44058(15)	0.19373(6)	0.18960(7)	3.13(2)
C13	0.98137(15)	0.36878(9)	0.46542(10)	4.37(3)
C14	0.8746(2)	0.48547(8)	0.40792(10)	4.84(4)
C15	0.76885(17)	0.42505(7)	0.52907(8)	3.73(3)
C16	0.57061(16)	0.47867(7)	0.23844(9)	3.56(3)
C17	0.49990(19)	0.48801(7)	0.38803(9)	4.23(3)
C18	0.35813(12)	0.40041(6)	0.28157(7)	2.61(2)
C19	0.26703(16)	0.44687(8)	0.24373(11)	4.33(3)
C20	0.30024(15)	0.37483(8)	0.34499(10)	4.08(3)
C21	0.36975(14)	0.35134(7)	0.22810(9)	3.52(3)
C22	0.90238(18)	0.40066(10)	0.23990(11)	4.94(4)
C23	0.69487(16)	0.31820(9)	0.17701(8)	4.21(3)
C24	0.90422(19)	0.27796(9)	0.29683(10)	4.68(4)
C25	0.47178(18)	0.34250(7)	0.52922(8)	3.72(3)
C26	0.5040(2)	0.34214(9)	0.61306(10)	5.19(4)

C27	0.5303(2)	0.28049(9)	0.63066(9)	4.62(4)
C28	0.60350(16)	0.26218(7)	0.57278(7)	3.34(3)

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{2}3(bb^*cc^*)\cos\alpha)$

Anisotropic displacement parameters

atom	U11	U22	U33	U12	U13	U23
Fe1	0.02421(8)	0.01728(7)	0.01851(7)	-0.00199(5)	0.00588(5)	-0.00056(5)
Si1	0.02070(13)	0.01743(13)	0.02144(13)	-0.00082(10)	0.00338(10)	-0.00131(10)
Si2	0.02175(14)	0.02505(15)	0.02866(15)	-0.00302(11)	0.00506(11)	0.00013(11)
Si3	0.02671(15)	0.02059(14)	0.02724(15)	0.00170(11)	0.00242(12)	0.00206(11)
Si4	0.03062(16)	0.02297(14)	0.02319(14)	-0.00045(12)	0.00436(12)	-0.00434(11)
Si5	0.02257(14)	0.01959(13)	0.02178(13)	-0.00245(10)	0.00376(10)	0.00231(10)
Si6	0.03626(18)	0.03556(18)	0.02728(16)	-0.01450(14)	-0.00156(13)	0.00279(13)
Si7	0.03405(17)	0.01910(14)	0.02955(15)	0.00322(12)	0.00435(13)	0.00301(11)
Si8	0.02514(15)	0.04305(19)	0.02836(16)	0.00200(14)	0.00943(12)	0.00471(14)
O1	0.0465(5)	0.0263(4)	0.0220(4)	0.0003(4)	0.0127(4)	-0.0016(3)
C1	0.0359(7)	0.0577(9)	0.0517(9)	-0.0132(7)	0.0220(6)	-0.0195(7)
C2	0.0362(7)	0.0315(6)	0.0480(8)	-0.0106(5)	0.0076(6)	0.0035(5)
C3	0.0264(6)	0.0541(9)	0.0511(8)	0.0053(6)	0.0046(6)	0.0172(7)
C4	0.0408(7)	0.0355(6)	0.0309(6)	-0.0014(5)	0.0049(5)	0.0089(5)
C5	0.0493(8)	0.0218(6)	0.0428(7)	0.0047(5)	0.0016(6)	0.0004(5)
C6	0.0248(5)	0.0357(6)	0.0356(6)	0.0063(5)	-0.0002(5)	0.0021(5)
C7	0.0386(7)	0.0481(8)	0.0535(9)	0.0156(6)	-0.0082(7)	0.0046(7)
C8	0.0293(7)	0.0771(12)	0.0495(9)	-0.0005(7)	0.0092(6)	0.0015(8)
C9	0.0283(6)	0.0388(7)	0.0572(9)	-0.0012(5)	-0.0067(6)	-0.0016(6)
C10	0.0538(8)	0.0292(6)	0.0333(6)	-0.0082(6)	0.0018(6)	-0.0086(5)
C11	0.0408(7)	0.0525(9)	0.0366(7)	0.0027(6)	0.0136(6)	-0.0124(6)
C12	0.0503(8)	0.0376(7)	0.0300(6)	0.0051(6)	0.0034(6)	0.0027(5)
C13	0.0348(8)	0.0760(12)	0.0507(9)	-0.0067(8)	-0.0078(7)	-0.0024(8)
C14	0.0796(13)	0.0514(10)	0.0473(9)	-0.0408(9)	-0.0075(8)	0.0067(7)
C15	0.0573(9)	0.0518(9)	0.0303(7)	-0.0117(7)	-0.0001(6)	-0.0057(6)
C16	0.0489(8)	0.0358(7)	0.0491(8)	-0.0040(6)	0.0036(7)	0.0200(6)
C17	0.0773(12)	0.0309(7)	0.0509(9)	0.0172(7)	0.0051(8)	-0.0102(6)
C18	0.0257(6)	0.0338(6)	0.0398(7)	0.0074(5)	0.0049(5)	0.0077(5)
C19	0.0389(8)	0.0526(9)	0.0699(11)	0.0173(7)	-0.0010(8)	0.0157(8)
C20	0.0355(7)	0.0650(11)	0.0574(10)	0.0032(7)	0.0168(7)	0.0150(8)
C21	0.0345(7)	0.0461(8)	0.0498(8)	-0.0030(6)	-0.0036(6)	-0.0060(6)

C22	0.0447(9)	0.0874(14)	0.0607(11)	-0.0186(9)	0.0237(8)	0.0175(10)
C23	0.0418(8)	0.0873(13)	0.0321(7)	0.0050(8)	0.0095(6)	-0.0125(8)
C24	0.0600(11)	0.0690(12)	0.0498(9)	0.0319(9)	0.0118(8)	-0.0037(8)
C25	0.0678(10)	0.0357(7)	0.0432(8)	0.0109(7)	0.0258(7)	-0.0035(6)
C26	0.0946(15)	0.0676(12)	0.0436(9)	-0.0125(11)	0.0378(10)	-0.0237(8)
C27	0.0746(12)	0.0737(12)	0.0296(7)	-0.0232(10)	0.0151(7)	-0.0031(7)
C28	0.0551(9)	0.0444(8)	0.0259(6)	-0.0042(7)	0.0023(6)	0.0039(5)

The general temperature factor expression: $\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Bond lengths (Å)

atom	atom	distance	atom	atom	distance
Fe1	Si1	2.4892(6)	Fe1	Si5	2.4751(6)
Fe1	O1	2.0451(9)	Si1	Si2	2.3533(5)
Si1	Si3	2.3618(5)	Si1	Si4	2.3557(5)
Si2	C1	1.8702(18)	Si2	C2	1.8747(15)
Si2	C3	1.8710(15)	Si3	C4	1.8824(15)
Si3	C5	1.8774(13)	Si3	C6	1.9094(13)
Si4	C10	1.8717(15)	Si4	C11	1.8704(16)
Si4	C12	1.8775(14)	Si5	Si6	2.3411(5)
Si5	Si7	2.3465(5)	Si5	Si8	2.3383(5)
Si6	C13	1.8696(18)	Si6	C14	1.877(2)
Si6	C15	1.8693(17)	Si7	C16	1.8765(18)
Si7	C17	1.8813(18)	Si7	C18	1.9058(13)
Si8	C22	1.870(2)	Si8	C23	1.8630(15)
Si8	C24	1.867(2)	O1	C25	1.447(2)
O1	C28	1.4482(16)	C6	C7	1.535(2)
C6	C8	1.517(2)	C6	C9	1.524(2)
C18	C19	1.527(2)	C18	C20	1.529(2)
C18	C21	1.519(2)	C25	C26	1.545(2)
C26	C27	1.465(3)	C27	C28	1.482(3)

Bond angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
Si1	Fe1	Si5	139.27(2)	Si1	Fe1	O1	111.79(3)
Si5	Fe1	O1	108.93(3)	Fe1	Si1	Si2	105.76(2)
Fe1	Si1	Si3	115.307(18)	Fe1	Si1	Si4	119.17(2)

Si2	Si1	Si3	104.21(2)	Si2	Si1	Si4	101.883(18)
Si3	Si1	Si4	108.47(2)	Si1	Si2	C1	111.96(5)
Si1	Si2	C2	114.46(5)	Si1	Si2	C3	110.10(5)
C1	Si2	C2	106.15(8)	C1	Si2	C3	106.60(7)
C2	Si2	C3	107.14(7)	Si1	Si3	C4	111.32(5)
Si1	Si3	C5	110.99(5)	Si1	Si3	C6	113.31(5)
C4	Si3	C5	106.17(7)	C4	Si3	C6	107.35(6)
C5	Si3	C6	107.34(7)	Si1	Si4	C10	111.66(5)
Si1	Si4	C11	114.74(5)	Si1	Si4	C12	112.19(5)
C10	Si4	C11	106.73(7)	C10	Si4	C12	104.51(6)
C11	Si4	C12	106.31(7)	Fe1	Si5	Si6	111.574(19)
Fe1	Si5	Si7	114.513(17)	Fe1	Si5	Si8	111.61(2)
Si6	Si5	Si7	105.42(2)	Si6	Si5	Si8	103.043(18)
Si7	Si5	Si8	109.91(2)	Si5	Si6	C13	111.92(6)
Si5	Si6	C14	111.97(6)	Si5	Si6	C15	112.12(6)
C13	Si6	C14	107.81(9)	C13	Si6	C15	105.89(8)
C14	Si6	C15	106.77(8)	Si5	Si7	C16	111.22(5)
Si5	Si7	C17	111.71(5)	Si5	Si7	C18	112.17(5)
C16	Si7	C17	106.15(8)	C16	Si7	C18	108.49(6)
C17	Si7	C18	106.81(7)	Si5	Si8	C22	114.25(7)
Si5	Si8	C23	113.77(6)	Si5	Si8	C24	107.36(6)
C22	Si8	C23	106.06(8)	C22	Si8	C24	106.91(9)
C23	Si8	C24	108.17(9)	Fe1	O1	C25	128.68(8)
Fe1	O1	C28	121.58(8)	C25	O1	C28	109.71(10)
Si3	C6	C7	109.37(10)	Si3	C6	C8	110.05(9)
Si3	C6	C9	111.52(9)	C7	C6	C8	108.60(12)
C7	C6	C9	108.08(11)	C8	C6	C9	109.16(13)
Si7	C18	C19	109.54(10)	Si7	C18	C20	111.05(9)
Si7	C18	C21	110.52(9)	C19	C18	C20	109.03(13)
C19	C18	C21	108.78(12)	C20	C18	C21	107.87(13)
O1	C25	C26	102.60(13)	C25	C26	C27	103.58(15)
C26	C27	C28	102.17(16)	O1	C28	C27	105.87(13)

Torsion Angles(°)

(Those having bond angles > 160 or < 20 degrees are excluded.)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
Si1	Fe1	Si5	Si6	-133.84(2)	Si1	Fe1	Si5	Si7	106.52(2)
Si1	Fe1	Si5	Si8	-19.16(3)	Si5	Fe1	Si1	Si2	-130.56(2)

Si5	Fe1	Si1	Si3	114.88(2)	Si5	Fe1	Si1	Si4	-16.83(3)
Si1	Fe1	O1	C25	-128.49(6)	Si1	Fe1	O1	C28	53.91(7)
O1	Fe1	Si1	Si2	50.44(3)	O1	Fe1	Si1	Si3	-64.11(3)
O1	Fe1	Si1	Si4	164.18(3)	Si5	Fe1	O1	C25	52.20(7)
Si5	Fe1	O1	C28	-125.39(6)	O1	Fe1	Si5	Si6	45.17(3)
O1	Fe1	Si5	Si7	-74.47(3)	O1	Fe1	Si5	Si8	159.85(3)
Fe1	Si1	Si2	C1	-40.92(3)	Fe1	Si1	Si2	C2	-161.776(18)
Fe1	Si1	Si2	C3	77.47(2)	Fe1	Si1	Si3	C4	77.03(2)
Fe1	Si1	Si3	C5	-164.943(17)	Fe1	Si1	Si3	C6	-44.09(3)
Fe1	Si1	Si4	C10	-161.314(16)	Fe1	Si1	Si4	C11	77.08(3)
Fe1	Si1	Si4	C12	-44.37(2)	Si2	Si1	Si3	C4	-38.42(3)
Si2	Si1	Si3	C5	79.61(2)	Si2	Si1	Si3	C6	-159.53(2)
Si3	Si1	Si2	C1	81.06(3)	Si3	Si1	Si2	C2	-39.79(3)
Si3	Si1	Si2	C3	-160.54(2)	Si2	Si1	Si4	C10	-45.51(3)
Si2	Si1	Si4	C11	-167.12(2)	Si2	Si1	Si4	C12	71.43(3)
Si4	Si1	Si2	C1	-166.15(2)	Si4	Si1	Si2	C2	72.99(2)
Si4	Si1	Si2	C3	-47.76(3)	Si3	Si1	Si4	C10	64.05(2)
Si3	Si1	Si4	C11	-57.56(3)	Si3	Si1	Si4	C12	-179.009(18)
Si4	Si1	Si3	C4	-146.39(2)	Si4	Si1	Si3	C5	-28.36(3)
Si4	Si1	Si3	C6	92.50(2)	Si1	Si3	C6	C7	177.60(5)
Si1	Si3	C6	C8	-63.18(8)	Si1	Si3	C6	C9	58.11(8)
C4	Si3	C6	C7	54.28(9)	C4	Si3	C6	C8	173.50(7)
C4	Si3	C6	C9	-65.21(9)	C5	Si3	C6	C7	-59.50(9)
C5	Si3	C6	C8	59.72(9)	C5	Si3	C6	C9	-178.99(7)
Fe1	Si5	Si6	C13	68.35(3)	Fe1	Si5	Si6	C14	-170.460(19)
Fe1	Si5	Si6	C15	-50.47(3)	Fe1	Si5	Si7	C16	-151.68(2)
Fe1	Si5	Si7	C17	89.91(2)	Fe1	Si5	Si7	C18	-29.98(3)
Fe1	Si5	Si8	C22	-163.281(16)	Fe1	Si5	Si8	C23	74.73(3)
Fe1	Si5	Si8	C24	-44.92(2)	Si6	Si5	Si7	C16	85.30(2)
Si6	Si5	Si7	C17	-33.11(3)	Si6	Si5	Si7	C18	-153.00(2)
Si7	Si5	Si6	C13	-166.77(2)	Si7	Si5	Si6	C14	-45.58(3)
Si7	Si5	Si6	C15	74.41(3)	Si6	Si5	Si8	C22	-43.43(3)
Si6	Si5	Si8	C23	-165.42(2)	Si6	Si5	Si8	C24	74.93(2)
Si8	Si5	Si6	C13	-51.52(3)	Si8	Si5	Si6	C14	69.67(3)
Si8	Si5	Si6	C15	-170.35(2)	Si7	Si5	Si8	C22	68.54(2)
Si7	Si5	Si8	C23	-53.45(3)	Si7	Si5	Si8	C24	-173.099(19)
Si8	Si5	Si7	C16	-25.12(3)	Si8	Si5	Si7	C17	-143.53(2)
Si8	Si5	Si7	C18	96.58(2)	Si5	Si7	C18	C19	-170.58(5)

Si5	Si7	C18	C20	68.94(8)	Si5	Si7	C18	C21	-50.73(8)
C16	Si7	C18	C19	-47.33(10)	C16	Si7	C18	C20	-167.81(8)
C16	Si7	C18	C21	72.51(9)	C17	Si7	C18	C19	66.71(9)
C17	Si7	C18	C20	-53.77(10)	C17	Si7	C18	C21	-173.44(8)
Fe1	O1	C25	C26	-167.01(6)	Fe1	O1	C28	C27	-168.12(6)
C25	O1	C28	C27	13.88(14)	C28	O1	C25	C26	10.81(14)
O1	C25	C26	C27	-31.79(18)	C25	C26	C27	C28	40.03(19)
C26	C27	C28	O1	-33.81(17)					

Figure S5. ORTEP drawing of **3** (50% probability of the thermal ellipsoids). Hydrogen atoms were omitted for clarity.

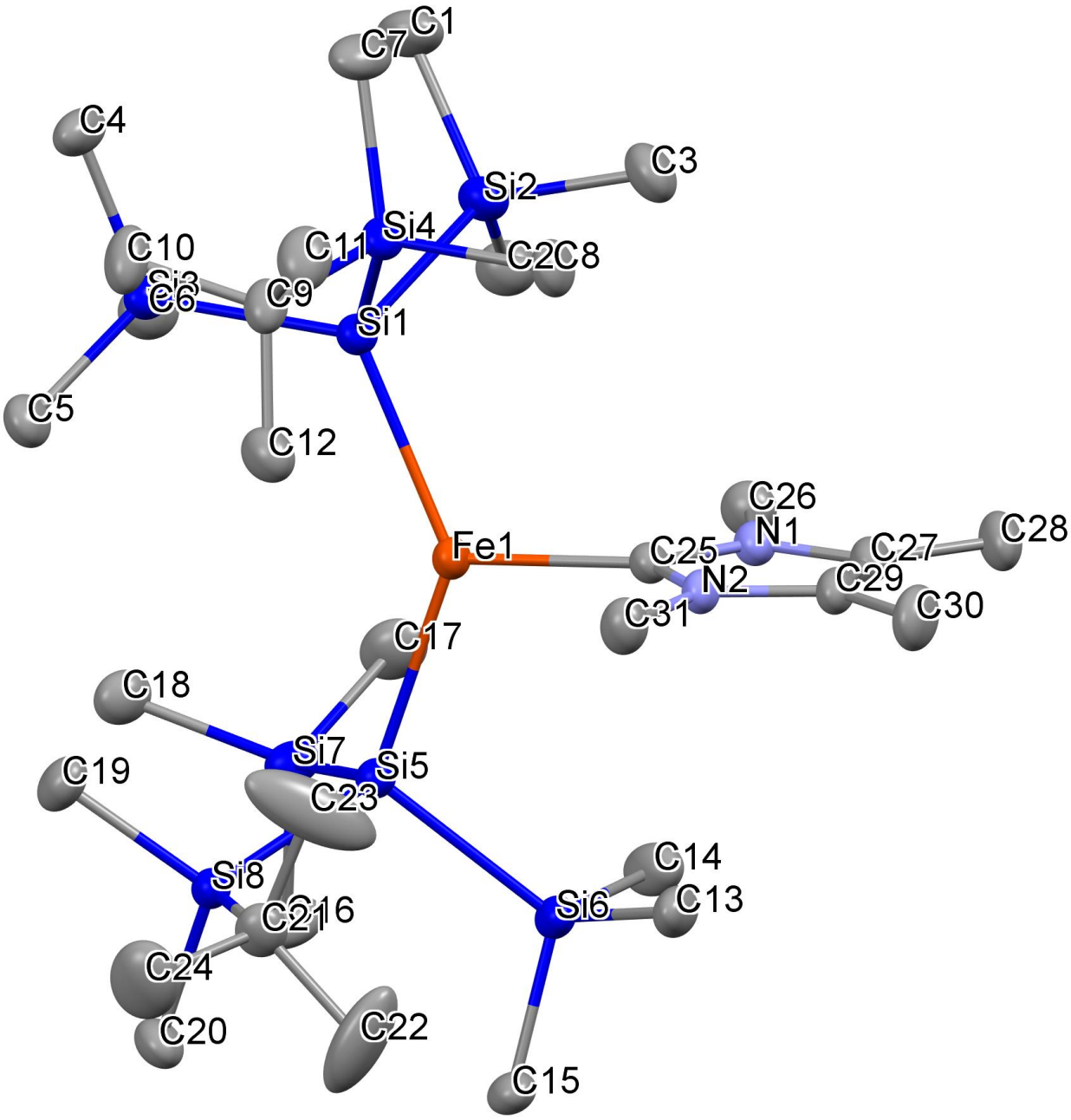


Table S2. Crystal data and structure refinement for **3**.

Empirical Formula	$C_{31}H_{78}FeN_2Si_8$
Formula Weight	759.50
Crystal Color, Habit	green, block
Crystal Dimensions	0.300 X 0.300 X 0.300 mm
Crystal System	triclinic
Lattice Type	Primitive
Lattice Parameters	a = 10.4392(16) Å
	b = 11.7999(18) Å
	c = 20.072(3) Å
	α = 100.822(7) ^{o}
	β = 94.290(7) ^{o}
	γ = 101.043(7) ^{o}
	V = 2367.8(6) Å^3
Space Group	P-1 (#2)
Z value	2
D_{calc}	1.065 g/cm^3
F_{000}	832.00
μ (synchrotron radiation, λ = 0.41440Å)	0.000 cm^{-1}
Diffractometer	R-AXIS IV
Radiation	synchrotron (λ = 0.41440Å)
Voltage, Current	8 kV, 100 mA
Temperature	-173.0 ^{o}C
Detector Aperture	300.0 x 300.0 mm
Data Images	1080 exposures
ω oscillation Range (χ=45.0, ϕ=0.0)	0.0 - 180.0^{o}
Exposure Rate	120.0 sec./^{o}
Detector Swing Angle	0.00^{o}
ω oscillation Range (χ=45.0, ϕ=90.0)	0.0 - 180.0^{o}
Exposure Rate	120.0 sec./^{o}
Detector Swing Angle	0.00^{o}
Detector Position	130.00 mm
Pixel Size	0.172 mm
$2\theta_{max}$	31.2^{o}
No. of Reflections Measured	Total: 52887
	Unique: 10859 (R_{int} = 0.0466)
Corrections	Lorentz-polarization
	Absorption

	(trans. factors: 0.6740 – 1.000)
Structure Solution	Direct Methods (SHELXT Version 2014/5)
Refinement	Full-matrix least-squares on F^2
Function Minimized	Σ w $(Fo^2 - Fc^2)^2$
Least Squares Weights	$w = 1/ [\sigma^2(Fo^2) + (0.0367 \cdot P)^2 + 1.0374 \cdot P]$
	where $P = (Max(Fo^2,0) + 2Fc^2)/3$
$2\theta_{max}$ cutoff	31.2°
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	10859
No. Variables	405
Reflection/Parameter Ratio	26.81
Residuals: R1(I>2.00σ(I))	0.0308
Residuals: R (All reflections)	0.0335
Residuals: wR2 (All reflections)	0.0815
Goodness of Fit Indicator	1.026
Max Shift/Error in Final Cycle	0.002
Maximum peak in Final Diff. Map	0.81 $e^-/Å^3$
Minimum peak in Final Diff. Map	-0.51 $e^-/Å^3$

Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
Fe1	0.75344(2)	0.75190(2)	0.76460(2)	1.502(4)
Si1	0.83350(4)	0.81354(3)	0.65977(2)	1.641(6)
Si2	0.99736(4)	0.98700(4)	0.69234(2)	2.151(7)
Si3	0.93803(4)	0.69057(3)	0.58552(2)	1.981(7)
Si4	0.66659(4)	0.87605(3)	0.59829(2)	1.833(6)
Si5	0.75377(3)	0.57624(3)	0.81828(2)	1.471(6)
Si6	0.72140(4)	0.62452(3)	0.93431(2)	1.950(7)
Si7	0.96630(4)	0.53699(4)	0.82465(2)	1.974(7)
Si8	0.61723(3)	0.39150(3)	0.76694(2)	1.523(6)
N1	0.75745(12)	0.97503(10)	0.87833(6)	1.847(18)
N2	0.56067(11)	0.89942(10)	0.83402(6)	1.714(17)
C1	1.08352(18)	1.03123(16)	0.61919(9)	3.26(3)
C2	1.13237(15)	0.97207(16)	0.75597(9)	2.83(3)
C3	0.92872(18)	1.11595(14)	0.73337(9)	3.02(3)
C4	0.96129(19)	0.73616(16)	0.50150(8)	2.97(3)
C5	0.84716(17)	0.53290(13)	0.56650(8)	2.57(3)
C6	1.10691(15)	0.69341(16)	0.62695(9)	2.90(3)
C7	0.73407(18)	0.96417(16)	0.53506(9)	3.01(3)
C8	0.58610(16)	0.97552(13)	0.65916(8)	2.49(3)
C9	0.53043(15)	0.74841(13)	0.54968(7)	2.17(2)
C10	0.58143(17)	0.67881(16)	0.48858(8)	2.92(3)
C11	0.41425(17)	0.79592(16)	0.52243(9)	2.92(3)
C12	0.48102(16)	0.66495(14)	0.59639(8)	2.63(3)
C13	0.58351(19)	0.70540(15)	0.95011(9)	3.10(3)
C14	0.8707(2)	0.72864(16)	0.98606(8)	3.45(3)
C15	0.68798(16)	0.49440(13)	0.97676(7)	2.28(2)
C16	0.99829(16)	0.44632(18)	0.88959(9)	3.21(3)
C17	1.09376(16)	0.67885(17)	0.84802(10)	3.34(3)
C18	1.00298(15)	0.45541(15)	0.74109(8)	2.60(3)
C19	0.65169(16)	0.34613(15)	0.67638(8)	2.59(3)
C20	0.64658(17)	0.27015(13)	0.81141(8)	2.61(3)
C21	0.43414(14)	0.39418(14)	0.76377(8)	2.32(2)
C22	0.38995(19)	0.4013(3)	0.83457(11)	6.00(7)
C23	0.4080(2)	0.4941(2)	0.7319(2)	7.84(10)
C24	0.35242(18)	0.28016(19)	0.71989(12)	4.32(4)
C25	0.68552(13)	0.88556(11)	0.82929(7)	1.66(2)

C26	0.89987(15)	0.99746(15)	0.89279(8)	2.61(3)
C27	0.67858(15)	1.04324(12)	0.91296(7)	2.04(2)
C28	0.73340(18)	1.14870(14)	0.96824(8)	2.91(3)
C29	0.55375(15)	0.99489(12)	0.88492(7)	2.01(2)
C30	0.42742(17)	1.02977(16)	0.89980(9)	3.04(3)
C31	0.44591(14)	0.82006(14)	0.79298(8)	2.37(2)

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Anisotropic displacement parameters

atom	U11	U22	U33	U12	U13	U23
Fe1	0.01930(10)	0.01866(10)	0.01905(9)	0.00491(7)	0.00305(7)	0.00245(7)
Si1	0.02277(17)	0.01943(17)	0.02174(17)	0.00652(13)	0.00507(14)	0.00510(13)
Si2	0.0284(2)	0.02358(19)	0.0288(2)	0.00154(15)	0.00305(16)	0.00715(15)
Si3	0.0286(2)	0.02483(19)	0.02692(19)	0.01203(15)	0.01029(15)	0.00861(15)
Si4	0.02882(19)	0.02149(18)	0.02308(18)	0.01132(15)	0.00564(15)	0.00670(14)
Si5	0.01802(16)	0.01906(17)	0.01792(16)	0.00237(13)	0.00222(13)	0.00308(13)
Si6	0.0317(2)	0.02163(18)	0.01798(17)	0.00088(15)	0.00451(15)	0.00135(14)
Si7	0.01718(17)	0.0340(2)	0.02492(19)	0.00395(15)	0.00129(14)	0.01086(16)
Si8	0.02051(17)	0.01859(17)	0.01775(16)	0.00266(13)	0.00257(13)	0.00256(13)
N1	0.0273(6)	0.0212(6)	0.0207(5)	0.0044(5)	0.0018(4)	0.0030(4)
N2	0.0254(6)	0.0197(5)	0.0202(5)	0.0065(4)	0.0046(4)	0.0020(4)
C1	0.0413(9)	0.0395(9)	0.0394(9)	-0.0072(7)	0.0059(7)	0.0149(7)
C2	0.0277(8)	0.0396(9)	0.0384(9)	0.0021(6)	0.0006(6)	0.0100(7)
C3	0.0473(10)	0.0232(7)	0.0411(9)	0.0066(7)	-0.0019(7)	0.0025(6)
C4	0.0518(10)	0.0389(9)	0.0330(8)	0.0221(8)	0.0218(7)	0.0149(7)
C5	0.0411(8)	0.0248(7)	0.0349(8)	0.0138(6)	0.0071(7)	0.0059(6)
C6	0.0284(8)	0.0415(9)	0.0464(9)	0.0148(7)	0.0114(7)	0.0143(7)
C7	0.0454(9)	0.0395(9)	0.0415(9)	0.0202(7)	0.0146(7)	0.0234(7)
C8	0.0352(8)	0.0263(7)	0.0347(8)	0.0139(6)	0.0065(6)	0.0015(6)
C9	0.0323(7)	0.0288(7)	0.0219(6)	0.0133(6)	-0.0023(6)	0.0018(5)
C10	0.0423(9)	0.0422(9)	0.0259(7)	0.0207(7)	-0.0030(7)	-0.0037(7)
C11	0.0367(8)	0.0425(9)	0.0334(8)	0.0188(7)	-0.0039(7)	0.0047(7)
C12	0.0350(8)	0.0276(8)	0.0332(8)	0.0018(6)	-0.0042(6)	0.0039(6)
C13	0.0581(11)	0.0306(8)	0.0346(8)	0.0167(8)	0.0229(8)	0.0064(7)
C14	0.0560(11)	0.0377(9)	0.0253(8)	-0.0126(8)	-0.0034(7)	0.0027(7)
C15	0.0365(8)	0.0293(7)	0.0204(6)	0.0031(6)	0.0062(6)	0.0066(5)
C16	0.0282(8)	0.0644(12)	0.0392(9)	0.0168(8)	0.0030(7)	0.0279(8)

C17	0.0256(8)	0.0521(11)	0.0412(9)	-0.0079(7)	0.0008(7)	0.0072(8)
C18	0.0252(7)	0.0415(9)	0.0361(8)	0.0123(6)	0.0084(6)	0.0110(7)
C19	0.0319(8)	0.0399(9)	0.0218(7)	0.0017(6)	0.0050(6)	0.0002(6)
C20	0.0466(9)	0.0216(7)	0.0309(8)	0.0074(6)	0.0008(7)	0.0059(6)
C21	0.0191(6)	0.0312(8)	0.0335(8)	-0.0013(5)	0.0030(6)	0.0028(6)
C22	0.0256(9)	0.142(3)	0.0426(11)	0.0123(12)	0.0095(8)	-0.0221(13)
C23	0.0205(9)	0.0766(17)	0.222(4)	0.0093(10)	-0.0013(14)	0.091(2)
C24	0.0299(9)	0.0544(12)	0.0631(13)	-0.0124(8)	-0.0027(9)	-0.0047(10)
C25	0.0250(6)	0.0179(6)	0.0198(6)	0.0043(5)	0.0032(5)	0.0035(5)
C26	0.0281(7)	0.0341(8)	0.0329(8)	0.0009(6)	-0.0021(6)	0.0045(6)
C27	0.0368(8)	0.0205(6)	0.0210(6)	0.0087(6)	0.0040(6)	0.0029(5)
C28	0.0523(10)	0.0257(8)	0.0278(8)	0.0077(7)	-0.0008(7)	-0.0034(6)
C29	0.0345(7)	0.0226(7)	0.0213(6)	0.0109(6)	0.0063(5)	0.0028(5)
C30	0.0412(9)	0.0399(9)	0.0366(9)	0.0199(7)	0.0104(7)	-0.0005(7)
C31	0.0245(7)	0.0311(8)	0.0303(7)	0.0028(6)	0.0020(6)	-0.0007(6)

The general temperature factor expression: $\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Bond lengths (Å)

atom	atom	distance	atom	atom	distance
Fe1	Si1	2.5020(7)	Fe1	Si5	2.5096(6)
Fe1	C25	2.1150(14)	Si1	Si2	2.3520(6)
Si1	Si3	2.3570(6)	Si1	Si4	2.3697(7)
Si2	C1	1.882(2)	Si2	C2	1.8865(18)
Si2	C3	1.8821(19)	Si3	C4	1.8827(18)
Si3	C5	1.8735(15)	Si3	C6	1.8837(17)
Si4	C7	1.881(2)	Si4	C8	1.8893(17)
Si4	C9	1.9135(13)	Si5	Si6	2.3572(7)
Si5	Si7	2.3509(7)	Si5	Si8	2.3648(5)
Si6	C13	1.888(2)	Si6	C14	1.8873(17)
Si6	C15	1.8804(17)	Si7	C16	1.884(2)
Si7	C17	1.8844(17)	Si7	C18	1.8755(17)
Si8	C19	1.8779(17)	Si8	C20	1.8836(18)
Si8	C21	1.9141(16)	N1	C25	1.3575(15)
N1	C26	1.456(2)	N1	C27	1.392(2)
N2	C25	1.3523(19)	N2	C29	1.3886(17)
N2	C31	1.4573(16)	C9	C10	1.533(2)

C9	C11	1.536(3)	C9	C12	1.530(2)
C21	C22	1.519(3)	C21	C23	1.502(4)
C21	C24	1.522(2)	C27	C28	1.4903(19)
C27	C29	1.351(2)	C29	C30	1.489(3)

Bond angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
Si1	Fe1	Si5	135.434(18)	Si1	Fe1	C25	113.13(4)
Si5	Fe1	C25	111.11(5)	Fe1	Si1	Si2	109.09(2)
Fe1	Si1	Si3	120.22(2)	Fe1	Si1	Si4	110.38(2)
Si2	Si1	Si3	101.89(2)	Si2	Si1	Si4	102.53(2)
Si3	Si1	Si4	110.92(2)	Si1	Si2	C1	113.53(5)
Si1	Si2	C2	112.37(6)	Si1	Si2	C3	111.69(6)
C1	Si2	C2	104.93(8)	C1	Si2	C3	107.16(9)
C2	Si2	C3	106.64(8)	Si1	Si3	C4	114.05(7)
Si1	Si3	C5	112.07(6)	Si1	Si3	C6	109.52(6)
C4	Si3	C5	107.60(7)	C4	Si3	C6	106.47(9)
C5	Si3	C6	106.73(8)	Si1	Si4	C7	112.00(6)
Si1	Si4	C8	109.81(6)	Si1	Si4	C9	113.33(6)
C7	Si4	C8	106.62(8)	C7	Si4	C9	107.71(7)
C8	Si4	C9	107.04(7)	Fe1	Si5	Si6	109.87(2)
Fe1	Si5	Si7	109.312(19)	Fe1	Si5	Si8	120.30(2)
Si6	Si5	Si7	102.32(2)	Si6	Si5	Si8	109.49(2)
Si7	Si5	Si8	103.92(2)	Si5	Si6	C13	113.79(6)
Si5	Si6	C14	111.20(6)	Si5	Si6	C15	114.37(5)
C13	Si6	C14	104.16(8)	C13	Si6	C15	106.59(8)
C14	Si6	C15	105.93(8)	Si5	Si7	C16	114.07(6)
Si5	Si7	C17	110.53(7)	Si5	Si7	C18	112.34(5)
C16	Si7	C17	106.80(8)	C16	Si7	C18	106.19(9)
C17	Si7	C18	106.45(8)	Si5	Si8	C19	109.99(5)
Si5	Si8	C20	112.56(5)	Si5	Si8	C21	112.85(5)
C19	Si8	C20	106.37(8)	C19	Si8	C21	106.83(7)
C20	Si8	C21	107.88(8)	C25	N1	C26	124.18(13)
C25	N1	C27	111.79(12)	C26	N1	C27	124.03(11)
C25	N2	C29	112.14(11)	C25	N2	C31	124.07(12)
C29	N2	C31	123.73(12)	Si4	C9	C10	110.31(11)
Si4	C9	C11	110.24(11)	Si4	C9	C12	110.64(9)
C10	C9	C11	108.01(13)	C10	C9	C12	109.00(13)

C11	C9	C12	108.58(13)	Si8	C21	C22	110.55(12)
Si8	C21	C23	109.47(12)	Si8	C21	C24	110.41(12)
C22	C21	C23	112.6(2)	C22	C21	C24	106.14(16)
C23	C21	C24	107.64(17)	Fe1	C25	N1	127.75(10)
Fe1	C25	N2	128.61(8)	N1	C25	N2	103.58(11)
N1	C27	C28	122.61(14)	N1	C27	C29	106.24(11)
C28	C27	C29	131.13(15)	N2	C29	C27	106.26(13)
N2	C29	C30	122.61(12)	C27	C29	C30	131.12(13)

Torsion Angles(°)

(Those having bond angles > 160 or < 20 degrees are excluded.)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
Si1	Fe1	Si5	Si6	160.834(17)	Si1	Fe1	Si5	Si7	49.30(3)
Si1	Fe1	Si5	Si8	-70.69(3)	Si5	Fe1	Si1	Si2	-117.00(2)
Si5	Fe1	Si1	Si3	-0.01(3)	Si5	Fe1	Si1	Si4	131.073(19)
Si1	Fe1	C25	N1	-85.20(11)	Si1	Fe1	C25	N2	98.15(11)
C25	Fe1	Si1	Si2	55.63(4)	C25	Fe1	Si1	Si3	172.62(4)
C25	Fe1	Si1	Si4	-56.29(4)	Si5	Fe1	C25	N1	89.26(11)
Si5	Fe1	C25	N2	-87.38(12)	C25	Fe1	Si5	Si6	-11.90(4)
C25	Fe1	Si5	Si7	-123.44(4)	C25	Fe1	Si5	Si8	116.57(4)
Fe1	Si1	Si2	C1	171.66(2)	Fe1	Si1	Si2	C2	52.77(3)
Fe1	Si1	Si2	C3	-67.03(3)	Fe1	Si1	Si3	C4	168.562(17)
Fe1	Si1	Si3	C5	46.00(3)	Fe1	Si1	Si3	C6	-72.25(3)
Fe1	Si1	Si4	C7	163.023(15)	Fe1	Si1	Si4	C8	44.77(2)
Fe1	Si1	Si4	C9	-74.87(2)	Si2	Si1	Si3	C4	-70.82(3)
Si2	Si1	Si3	C5	166.62(2)	Si2	Si1	Si3	C6	48.37(3)
Si3	Si1	Si2	C1	43.56(3)	Si3	Si1	Si2	C2	-75.33(3)
Si3	Si1	Si2	C3	164.86(2)	Si2	Si1	Si4	C7	46.92(3)
Si2	Si1	Si4	C8	-71.33(3)	Si2	Si1	Si4	C9	169.03(2)
Si4	Si1	Si2	C1	-71.31(3)	Si4	Si1	Si2	C2	169.80(2)
Si4	Si1	Si2	C3	49.99(3)	Si3	Si1	Si4	C7	-61.19(2)
Si3	Si1	Si4	C8	-179.440(18)	Si3	Si1	Si4	C9	60.92(3)
Si4	Si1	Si3	C4	37.72(3)	Si4	Si1	Si3	C5	-84.85(3)
Si4	Si1	Si3	C6	156.906(19)	Si1	Si4	C9	C10	-71.36(9)
Si1	Si4	C9	C11	169.44(6)	Si1	Si4	C9	C12	49.33(10)
C7	Si4	C9	C10	53.11(12)	C7	Si4	C9	C11	-66.09(11)
C7	Si4	C9	C12	173.80(10)	C8	Si4	C9	C10	167.44(9)
C8	Si4	C9	C11	48.24(10)	C8	Si4	C9	C12	-71.88(11)

Fe1	Si5	Si6	C13	46.30(2)	Fe1	Si5	Si6	C14	-70.94(2)
Fe1	Si5	Si6	C15	169.141(17)	Fe1	Si5	Si7	C16	159.437(19)
Fe1	Si5	Si7	C17	39.08(3)	Fe1	Si5	Si7	C18	-79.65(3)
Fe1	Si5	Si8	C19	55.88(3)	Fe1	Si5	Si8	C20	174.301(17)
Fe1	Si5	Si8	C21	-63.30(3)	Si6	Si5	Si7	C16	43.00(3)
Si6	Si5	Si7	C17	-77.35(2)	Si6	Si5	Si7	C18	163.91(2)
Si7	Si5	Si6	C13	162.333(19)	Si7	Si5	Si6	C14	45.09(3)
Si7	Si5	Si6	C15	-74.83(3)	Si6	Si5	Si8	C19	-175.476(19)
Si6	Si5	Si8	C20	-57.06(3)	Si6	Si5	Si8	C21	65.34(3)
Si8	Si5	Si6	C13	-87.88(3)	Si8	Si5	Si6	C14	154.880(19)
Si8	Si5	Si6	C15	34.96(3)	Si7	Si5	Si8	C19	-66.76(3)
Si7	Si5	Si8	C20	51.66(3)	Si7	Si5	Si8	C21	174.06(2)
Si8	Si5	Si7	C16	-70.95(3)	Si8	Si5	Si7	C17	168.69(2)
Si8	Si5	Si7	C18	49.96(3)	Si5	Si8	C21	C22	-72.45(10)
Si5	Si8	C21	C23	52.09(9)	Si5	Si8	C21	C24	170.41(7)
C19	Si8	C21	C22	166.55(9)	C19	Si8	C21	C23	-68.91(10)
C19	Si8	C21	C24	49.41(12)	C20	Si8	C21	C22	52.53(10)
C20	Si8	C21	C23	177.07(8)	C20	Si8	C21	C24	-64.60(11)
C26	N1	C25	Fe1	3.0(2)	C26	N1	C25	N2	-179.65(13)
C25	N1	C27	C28	-178.60(12)	C25	N1	C27	C29	0.17(16)
C27	N1	C25	Fe1	-177.26(11)	C27	N1	C25	N2	0.04(15)
C26	N1	C27	C28	1.1(2)	C26	N1	C27	C29	179.86(13)
C25	N2	C29	C27	0.35(16)	C25	N2	C29	C30	179.22(12)
C29	N2	C25	Fe1	177.03(11)	C29	N2	C25	N1	-0.24(16)
C31	N2	C25	Fe1	-0.0(2)	C31	N2	C25	N1	-177.29(13)
C31	N2	C29	C27	177.41(12)	C31	N2	C29	C30	-3.7(2)
N1	C27	C29	N2	-0.30(16)	N1	C27	C29	C30	-179.04(13)
C28	C27	C29	N2	178.32(15)	C28	C27	C29	C30	-0.4(3)

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