Synthesis, Resolution, and Aldol Reactions of a Planar-Chiral Lewis Acid Complex

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Supporting Information

I. General

All oxygen- and moisture-sensitive manipulations were carried out under an inert atmosphere using either standard Schlenk techniques or a glove box.

All chemicals and solvents were purchased from Aldrich or Strem Chemicals and used as received. Iron complex (+)-**2**¹ was prepared according to a literature procedure.

THF, Et₂O, CH₂Cl₂, and toluene were purified by passing through a neutral alumina column under argon. Anhydrous pentane and benzene (Aldrich) were used as received.

Silica gel (230-400 mesh; SiliCycle) was heated under vacuum in a 200 °C sand bath for 12 h. Flash chromatography was performed with this pre-treated silica gel under an inert atmosphere.

¹¹B NMR spectra were recorded on a Varian Unity 300 or on a Varian Unity 500 spectrometer at ambient temperature and are referenced to boron trifluoride diethyl etherate (δ 0).

II. Synthesis and Resolution of Planar-Chiral Lewis Acid **1** (Figure 2)

In a glove box, eight vials were each charged with ($\pm$)-**2** (100 mg, 0.253 mmol) and sodium amalgam (10% Na content; 570 mg, 2.53 mmol Na). THF (1.0 mL) was added to each vial, and the resulting heterogeneous mixtures were stirred vigorously for 25 min. Then, the dark reaction mixtures were combined and filtered through an acrodisc. The residue was extracted with additional THF (24 mL) and then filtered. TMSCl (550 mg, 5.06 mmol) was added dropwise to the combined THF solutions, with stirring. After 30 min, the reaction mixture was concentrated, and then the crude mixture was subjected to flash chromatography (pentane). The desired product eluted as the first yellow band. Yellow solid (440 mg, 64%).

This reaction was run in eight vials, rather than one, because the results were not always reproducible on a larger scale.

^1H NMR (500 MHz, CD_2Cl_2): δ 5.72 (s, 1H), 4.79 (d, $^3J_{\text{HH}} = 3.5$ Hz, 1H), 3.40 (d, $^3J_{\text{HH}} = 4.5$ Hz, 1H), 1.45 (s, 9H), 0.26 (s, 9H).

^{13}C NMR (125 MHz, CD_2Cl_2): δ 215.2, 214.0, 90.4, 86.0, 71.4 (br), 57.7, 31.0, 7.7.

^{11}B NMR (160 MHz, CD_2Cl_2): δ 19.9.

FTIR (thin film) 3157, 2947, 2889, 1980, 1921, 1470, 1434, 1401, 1371, 1325, 1268, 1241, 1203, 1174, 1130 cm^{-1} .

HRMS (EI) calcd for $\text{C}_{12}\text{H}_{21}\text{BClFeNO}_2\text{Si}$ (M^+) 341.0473, found 341.0467.

mp 65–66 $^\circ\text{C}$.

In a glove box, a vial was charged with ($\pm$)-**3** (480 mg, 1.41 mmol) and K_3PO_4 monohydrate (971 mg, 4.22 mmol). THF (19.0 mL) was added, and the reaction mixture was stirred vigorously for 9 h. Then, pentane was added, and the reaction mixture was filtered through an acrodisc. The filtrate was concentrated under vacuum, and the resulting residue was purified by flash chromatography (pentane/ Et_2O), which furnished the desired product as a yellow oil (294 mg, 65%).

^1H NMR (500 MHz, CD_2Cl_2): δ 5.54 (s, 1H), 4.62 (d, $^3J_{\text{HH}} = 4.5$ Hz, 1H), 3.44 (s, 1H), 2.78 (d, $^3J_{\text{HH}} = 5.0$ Hz, 1H), 1.36 (s, 9H), 0.21 (s, 9H).

^{13}C NMR (125 MHz, CD_2Cl_2): δ 216.6, 215.0, 88.2, 82.8, 58.5 (br), 55.6, 30.5, 7.4.

^{11}B NMR (160 MHz, CD_2Cl_2): δ 21.5.

FTIR (thin film) 3625, 2947, 2889, 1968, 1895, 1470, 1434, 1410, 1367, 1280, 1239, 1208, 1169 cm^{-1} .

HRMS (EI) calcd for $\text{C}_{12}\text{H}_{22}\text{BFeNO}_3\text{Si}$ (M^+) 323.0806, found 323.0811.

This compound can be assayed via chiral HPLC (Daicel Chiralpak OD, hexanes:*i*-PrOH = 95:5, 1.0 mL/min, (R) isomer: 5.6 min, (S) isomer: 7.3 min).

Preparative Chiral HPLC: Separation of the Enantiomers of 4. A hexane solution of (+)-**4** was prepared (290 mg in 18 mL of hexanes) and subjected to chiral preparative HPLC separation using the following conditions: Daicel Chiralpak OD (semi-preparative column), hexanes:*i*-PrOH = 90:10, 2.0 mL/min, 300 nm, 0.5 mL/injection, ((R) isomer: 9.8-11.5 min, (S) isomer: 12.0-14.5 min). The separated enantiomers of **4** were re-purified by flash chromatography (pentane/Et₂O) under an inert atmosphere.

The separation procedure furnished the (-) enantiomer in 45% isolated yield as a yellow solid. The optical purity was determined to be 99% by analytical HPLC (Daicel Chiralpak OD, hexanes:*i*-PrOH = 95:5, 1.0 mL/min, (R) isomer: 5.6 min). Crystals suitable for X-ray analysis were obtained from a slowly evaporating, cold (-30 °C) pentane/benzene solution. Thus, the absolute configuration of (-)-**4** is as illustrated above.

$[\alpha]_{\text{D}}^{20} = -30^\circ$ ($c=0.33$, CH_2Cl_2 ; 99% ee).

mp 43-44 °C.

The separation procedure furnished the (+) enantiomer in 42% isolated yield as a yellow solid. The optical purity was determined to be 99% by analytical HPLC (Daicel Chiralpak OD, hexanes:*i*-PrOH = 95:5, 1.0 mL/min, (S) isomer: 7.2 min).

In a glove box, a 100-mL Schlenk tube was charged with a solution of (-)-4 (120 mg, 0.371 mmol) in THF (50.0 mL). Oxalyl chloride (321 μ L, 3.68 mmol) was added via syringe, followed by a catalytic amount of *N,N*-dimethylformamide (11.4 μ L, 0.147 mmol). The reaction mixture was allowed to sit at room temperature with occasional release of the pressure. After 48 h, ^{11}B NMR established that the reaction had proceeded to completion. The reaction mixture was diluted with hexanes (35 mL) and concentrated under vacuum. When the volume was $\sim$ 5 mL, more hexanes were added ($\sim$ 35 mL), and the solution was concentrated to dryness under vacuum. The resulting residue was then purified by flash chromatography (pentane), which furnished the desired product as a yellow solid (84 mg, 66%). The spectral data are identical to those reported above for the racemic product.

$[\alpha]_{\text{D}}^{20} = -8.8^\circ$ ($c=1.0$, CH_2Cl_2 ; 99% ee).

mp 102-103 $^\circ\text{C}$.

In a glove box, a vial was charged with (-)-3 (83.0 mg, 0.243 mmol) and silver *p*-toluenesulfonate (150 mg, 0.535 mmol). Benzene (2.4 mL) was added, and the reaction mixture was stirred vigorously for 23 h. Then, pentane was added, the reaction mixture was filtered through an acrodisc, and the filtrate was concentrated under vacuum. The residue was then purified by flash chromatography (pentane/ Et_2O), which furnished the desired product as yellow needles (97 mg, 83%).

^1H NMR (500 MHz, CD_2Cl_2): δ 7.88 (d, $^3J_{\text{HH}} = 7.0$ Hz, 2H), 7.38 (d, $^3J_{\text{HH}} = 8.0$ Hz, 2H), 5.53 (s, 1H), 4.70 (d, $^3J_{\text{HH}} = 4.5$ Hz, 1H), 3.21 (d, $^3J_{\text{HH}} = 5.0$ Hz, 1H), 2.44 (s, 3H), 1.30 (s, 9H), 0.22 (s, 9H).

^{13}C NMR (125 MHz, CD_2Cl_2): δ 214.4, 214.2, 145.8, 135.3, 130.5, 128.1, 89.2, 83.2, 62.8 (br), 56.8, 30.9, 22.1, 7.7.

^{11}B NMR (160 MHz, CD_2Cl_2): δ 18.6.

FTIR (thin film) 3189, 2981, 2947, 2889, 1986, 1926, 1600, 1434, 1359, 1278, 1240, 1189, 1178, 1098, 1090 cm^{-1} .

HRMS (EI) calcd for $\text{C}_{19}\text{H}_{28}\text{BFeNO}_5\text{SSi}$ (M^+) 477.0894, found 477.0906.

$[\alpha]_{\text{D}}^{20} = +67^\circ$ ($c=0.41$, CH_2Cl_2 ; 99% ee).

mp 90-91 $^\circ\text{C}$.

III. Synthesis of Silyl Ketene Acetals

A round-bottomed flask was charged with a solution of diisopropylamine (1.98 g, 19.6 mmol) in THF (45 mL) and then cooled to 0 °C. *n*-BuLi (2.8 M in hexanes; 7.0 mL, 20 mmol) was added to this solution dropwise at 0 °C, and the resulting mixture was stirred for 20 min. The solution was then cooled to -78 °C, and DMPU (9.5 mL) and methyl isobutyrate (2.25 mL, 19.6 mmol) were added. After 30 min of stirring at -78 °C, a solution of triisopropylsilyl triflate (6.0 g, 20 mmol) in THF (5 mL) was added. The mixture was stirred for 30 min at -78 °C, then warmed to room temperature and stirred for 30 min. The reaction was quenched with a mixture of hexanes/water. The organic layer was washed with brine, dried over sodium sulfate, and concentrated under vacuum. The crude product was fractionally distilled under reduced pressure to furnish the desired product as a colorless liquid. The product was further purified by flash chromatography (pentane) (2.7 g, 53%).

¹H NMR (500 MHz, CD₂Cl₂): δ 3.53 (s, 3H), 1.55 (apparent s, 6H), 1.20-1.08 (m, 21H).

¹³C NMR (125 MHz, CD₂Cl₂): δ 151.4, 91.3, 58.6, 18.2, 17.4, 16.6, 13.3.

FTIR (thin film) 2946, 2867, 1703, 1465, 1256, 1200, 1183, 1142 cm⁻¹.

bp 62-65 °C (300 mtorr).

214287-10-2. This compound was prepared according to a literature procedure.²

¹H NMR (500 MHz, C₆D₆): δ 4.86 (s, 1H), 4.71 (s, 1H), 1.42 (s, 9H), 1.18-1.12 (m, 21H).

FTIR (thin film) 2946, 2895, 2868, 1593, 1464, 1384, 1364, 1189, 1151, 1014, 883 cm⁻¹.

HRMS (ESI) calcd for C₁₅H₃₂NaSSiO (M⁺+Na) 311.1835, found 311.1831.

IV. Mukaiyama Aldol Additions (Table 1)

Table 1, entry 1. In a glove box, a vial was charged with a solution of (+)-**1** (46.0 mg, 0.0960 mmol) in CD₂Cl₂ (1.0 mL). 4-Methoxybenzaldehyde (24.0 μ L, 0.192 mmol) was added via a syringe at room temperature, followed by the silyl ketene acetal (54.7 mg, 0.212 mmol). The reaction was monitored by ¹H NMR spectroscopy. After seven days, the reaction mixture was concentrated under vacuum. The resulting residue was purified by flash chromatography (pentane/Et₂O), which furnished the desired product as a yellow oil (39 mg, 74%). ¹H NMR indicated a de >95%.

¹H NMR (500 MHz, CD₂Cl₂): δ 7.27 (d, ³J_{HH} = 8.5 Hz, 2H), 6.87 (d, ³J_{HH} = 8.5 Hz, 2H), 5.48 (s, 1H), 5.20 (s, 1H), 4.57 (d, ³J_{HH} = 5.0 Hz, 1H), 3.79 (s, 3H), 3.57 (s, 3H), 2.70 (d, ³J_{HH} = 5.0 Hz, 1H), 1.37 (s, 9H), 1.16 (s, 3H), 1.01 (s, 3H), 0.06 (s, 9H).

¹³C NMR (125 MHz, CD₂Cl₂): δ 215.1, 214.8, 177.1, 159.9, 130.7, 129.9, 113.5, 88.1, 84.8, 82.5, 57.2 (br), 55.7, 55.5, 52.1, 49.2, 30.5, 22.7, 19.4, 7.2.

¹¹B NMR (160 MHz, CD₂Cl₂): δ 22.0.

FTIR (thin film) 2949, 1978, 1917, 1736, 1614, 1514, 1435, 1405, 1366, 1249, 1133 cm⁻¹.

HRMS (EI) calcd for C₂₅H₃₈BF₂NO₆Si (M⁺) 543.1905, found 543.1921.

[α]_D²⁰ = -7.6° (c=0.42, CH₂Cl₂).

Table 1, entry 2. In a glove box, a vial was charged with a solution of (+)-**1** (44.0 mg, 0.0920 mmol) in CD₂Cl₂ (1.0 mL). 4-Dimethylaminobenzaldehyde (27.5 mg, 0.184 mmol) was added at room temperature, followed by the silyl ketene acetal (52.0 mg, 0.200 mmol). The reaction was monitored by ¹H NMR spectroscopy. After three days, the reaction mixture was concentrated under vacuum. The resulting residue was purified by flash chromatography (pentane/Et₂O), which furnished the desired product as a yellow solid (36 mg, 70%). ¹H NMR indicated a de >95%.

¹H NMR (500 MHz, CD₂Cl₂): δ 7.19 (d, ³J_{HH} = 6.5 Hz, 2H), 6.69 (d, ³J_{HH} = 6.5 Hz, 2H), 5.48 (s, 1H), 5.15 (s, 1H), 4.56 (d, ³J_{HH} = 5.0 Hz, 1H), 3.57 (s, 3H), 2.93 (s, 6H), 2.69 (d, ³J_{HH} = 5.0 Hz, 1H), 1.37 (s, 9H), 1.16 (s, 3H), 1.01 (s, 3H), 0.06 (s, 9H).

¹³C NMR (125 MHz, CD₂Cl₂): δ 215.2, 214.8, 177.3, 150.9, 129.5, 126.2, 112.0, 88.1, 85.1, 82.4, 57.4 (br), 55.5, 52.0, 49.4, 40.9, 30.4, 22.7, 19.4, 7.2.

¹¹B NMR (160 MHz, CD₂Cl₂): δ 21.9.

FTIR (thin film) 2980, 2947, 2808, 1972, 1909, 1735, 1616, 1525, 1436, 1405, 1394, 1367, 1253, 1134, 1045 cm⁻¹.

HRMS (EI) calcd for C₂₆H₄₁BF₂N₂O₅Si (M⁺) 556.2222, found 556.2216.

[α]_D²⁰ = -17° (c=0.50, CH₂Cl₂).

mp 120-121 °C.

Table 1, entry 3. In a glove box, a vial was charged with a solution of (±)-**1** (30.0 mg, 0.0600 mmol) in CD₂Cl₂ (0.7 mL). Indole-3-carboxaldehyde (20.0 mg, 0.125 mmol) was added at room temperature, followed by the silyl ketene acetal (35.7 mg, 0.138 mmol). The reaction was monitored by ¹H NMR spectroscopy. After three days, the reaction mixture was concentrated under vacuum. The resulting residue was purified by flash chromatography (pentane/Et₂O), which furnished the desired product as a yellow solid (30 mg, 85%). ¹H NMR indicated a de >95%.

Crystals suitable for X-ray analysis were grown from a concentrated pentane/benzene solution at -30 °C.

^1H NMR (500 MHz, CD_2Cl_2): δ 7.67 (d, $^3J_{\text{HH}} = 8.0$ Hz, 1H), 7.32 (d, $^3J_{\text{HH}} = 8.5$ Hz, 1H), 7.21-7.17 (m, 2H), 7.10 (t, $^3J_{\text{HH}} = 7.3$ Hz, 1H), 5.67 (s, 1H), 5.46 (s, 1H), 4.48 (d, $^3J_{\text{HH}} = 5.5$ Hz, 1H), 3.77 (s, 3H), 3.58 (s, 3H), 2.53 (d, $^3J_{\text{HH}} = 5.5$ Hz, 1H), 1.35 (s, 9H), 1.34 (s, 3H), 1.08 (s, 3H), -0.13 (s, 9H).

^{13}C NMR (125 MHz, CD_2Cl_2): δ 215.2, 215.1, 177.5, 137.0, 129.9, 128.6, 121.6, 119.6, 119.5, 111.7, 109.8, 88.1, 82.6, 78.8, 57.8 (br), 55.4, 52.1, 49.6, 33.3, 30.4, 23.0, 19.3, 7.1.

^{11}B NMR (160 MHz, CD_2Cl_2): δ 22.2.

FTIR (thin film) 2947, 2886, 1974, 1914, 1735, 1651, 1549, 1470, 1434, 1411, 1385, 1366, 1256, 1239, 1134 cm^{-1} .

HRMS (ESI) calcd for $\text{C}_{27}\text{H}_{39}\text{BFeN}_2\text{NaO}_5\text{Si}$ ($\text{M}^+ + \text{Na}$) 589.1963, found 589.1935.

mp 147-148 $^\circ\text{C}$.

Table 1, entry 4. In a glove box, a vial was charged with a solution of (+)-**1** (30.0 mg, 0.0600 mmol) in CD_3CN (0.6 mL). Indole-3-carboxaldehyde (20.0 mg, 0.125 mmol) was added at room temperature, followed by the nucleophile (38.5 mg, 0.133 mmol). After 20 h, ^1H NMR spectroscopy showed that the reaction was complete (74% de). The desired product precipitated out of solution upon concentration under vacuum. The yellow precipitate was washed thoroughly with pentane and then with cold Et_2O to furnish the aldol adduct as yellow crystals (26 mg, 72%; de >95% according to ^1H NMR).

Crystals suitable for X-ray analysis were grown from a concentrated pentane/benzene/ CH_2Cl_2 solution at -30 $^\circ\text{C}$.

^1H NMR (500 MHz, CD_2Cl_2): δ 7.71 (d, $^3J_{\text{HH}} = 8.0$ Hz, 1H), 7.31 (d, $^3J_{\text{HH}} = 8.5$ Hz, 1H), 7.21 (td, $^3J_{\text{HH}} = 8.0$ Hz, 1.0 Hz, 1H), 7.14 (s, 1H), 7.10 (td, $^3J_{\text{HH}} = 8.0$ Hz, 1.0 Hz, 1H), 5.70 (dd, $^3J_{\text{HH}} = 9.5$ Hz, 4.0 Hz, 1H), 5.49 (s, 1H), 4.58 (d, $^3J_{\text{HH}} = 5.0$ Hz, 1H), 3.75 (s, 3H), 3.33 (dd, $^3J_{\text{HH}} = 15.0$ Hz, 9.5 Hz, 1H), 2.92 (dd, $^3J_{\text{HH}} = 15.0$ Hz, 4.0 Hz, 1H), 2.83 (d, $^3J_{\text{HH}} = 5.0$ Hz, 1H), 1.40 (s, 9H), 1.34 (s, 9H), 0.05 (s, 9H).

^{13}C NMR (125 MHz, CD_2Cl_2): δ 215.10, 215.06, 197.9, 138.0, 128.0, 126.5, 122.0, 120.0, 119.5, 115.1, 110.0, 88.2, 82.6, 71.3, 57.6 (br), 55.5, 53.6, 48.5, 33.2, 30.5, 30.0, 7.2.

^{11}B NMR (160 MHz, CD_2Cl_2): δ 21.9.

FTIR (thin film) 2962, 1976, 1914, 1683, 1557, 1408, 1392, 1366, 1239, 1209 cm^{-1} .

HRMS (ESI) calcd for $\text{C}_{28}\text{H}_{41}\text{BFeN}_2\text{NaO}_4\text{SSi}$ ($\text{M}^+ + \text{Na}$) 619.1981, found 619.1902.

mp 180-183 $^\circ\text{C}$ (decomposition).

V. Hydrolysis of the Boron Aldolate (e.g., eq 3)

Eight drops of a 1.0 M TBAF solution in THF were added to a solution of the boron aldolate (31.0 mg, 0.0570 mmol) in wet THF (1.5 mL, along with 2 drops of water). After 4 h of stirring, a mixture of Et₂O/water was added. The aqueous phase was extracted three times with Et₂O. The combined organic layers were dried over Na₂SO₄, filtered, and concentrated under reduced pressure. The resulting crude material was purified by flash chromatography (pentane/Et₂O=1:1) to furnish the desired product as a colorless oil (11.8 mg, 87%). The spectral data are identical to those reported in the literature.³

$[\alpha]_D^{20} = -22^\circ$ (c=1.0, CH₂Cl₂).

The enantiomeric excess was determined to be 96% by HPLC analysis (Daicel Chiralpak OD, hexane:*i*-PrOH = 95:5, 0.8 mL/min; (S) isomer (minor): 15.7 min, (R) isomer (major): 19.4 min). The assignment of absolute configuration was made by comparison with the reported HPLC retention times: (S) isomer: 15.5 min, (R) isomer: 19.1 min.³

Product of Table 1, entry 2. Eight drops of a 1.0 M TBAF solution in THF were added to a solution of the boron aldolate (28.0 mg, 0.0500 mmol) in wet THF (1.5 mL, along with 2 drops of water). After 4 h of stirring, a mixture of Et₂O/water was added. The aqueous phase was extracted three times with Et₂O. The combined organic layers were dried over Na₂SO₄, filtered, and concentrated under reduced pressure. The resulting crude material was purified by flash chromatography (pentane/Et₂O=1:1) to furnish the desired product as a white solid (12.5 mg, 99%).

¹H NMR (500 MHz, CD₂Cl₂): δ 7.13 (d, ³*J*_{HH} = 8.5 Hz, 2H), 6.67 (d, ³*J*_{HH} = 9.0 Hz, 2H), 4.77 (s, 1H), 3.68 (s, 3H), 2.93 (s, 6H), 2.78 (s, 1H), 1.11 (s, 3H), 1.06 (s, 3H).

¹³C NMR (125 MHz, CD₂Cl₂): δ 178.5, 150.8, 128.8, 128.4, 112.1, 79.0, 52.3, 48.4, 40.8, 23.2, 19.6.

FTIR (thin film) 3471, 2988, 2953, 2888, 2806, 1705, 1693, 1614, 1524, 1471, 1444, 1430,

1364, 1339, 1273, 1230, 1188, 1154, 1054 cm^{-1} .

HRMS (EI) calcd for $\text{C}_{14}\text{H}_{21}\text{NO}_3$ (M^+) 251.1516, found 251.1510.

$[\alpha]_{\text{D}}^{20} = -32^\circ$ ($c=1.0$, CH_2Cl_2).

mp 110-112 $^\circ\text{C}$.

The enantiomeric excess was determined to be 99% by HPLC analysis (Daicel Chiralpak OD, hexane:*i*-PrOH = 95:5, 1.0 mL/min; (S) isomer (minor): 14.9 min, (R) isomer (major): 17.4 min).

The assignment of absolute configuration was made by analogy to our assignments for entries 1, 3, and 4.

VI. X-ray Crystal Structures

A yellow pentane/benzene solution was prepared. Crystals suitable for X-ray structural analysis were obtained by solvent evaporation at $-30\text{ }^{\circ}\text{C}$.

A yellow needle of dimensions $0.29 \times 0.14 \times 0.1\text{ mm}^3$ was mounted under STP and transferred to a Bruker AXS/CCD three-circle diffractometer equipped with a cold stream of N_2 gas. An initial unit cell was determined with monochromated $\text{Mo K}\alpha$ radiation ($\lambda = 0.71073\text{ \AA}$). The cell thus determined was orthorhombic.

A hemisphere of data was then collected using ω scans of 0.30° and 30-s frames. The raw data frames were integrated using the Bruker program SAINT+ for NT version 6.01. The data that were collected (7849 total reflections, 4972 unique, $R_{\text{int}} = 0.0815$) had the following Miller index ranges: -7 to 4 in h , -15 to 18 in k , and -27 to 35 in l . No absorption correction was performed.

All aspects of the solution and refinement were handled by SHELXTL NT version 5.10. The structure was solved by direct methods in the chiral orthorhombic space group $P2_12_12_1$, $a = 6.760(4)\text{ \AA}$; $b = 16.787(11)\text{ \AA}$; $c = 32.061(16)\text{ \AA}$; $\alpha = 90^{\circ}$; $\beta = 90^{\circ}$; $\gamma = 90^{\circ}$, and refined using standard difference Fourier techniques. Final, full-matrix least-squares refinement (4972 data for 357 parameters) on F^2 yielded residuals of R_1 and wR_2 of 0.0849 and 0.2126 for data $I > 2\sigma(I)$, and 0.1307 and 0.2508 , respectively, for all data. During the final refinement all non-hydrogen atoms were treated anisotropically. Hydrogen atoms were included in calculated positions and refined isotropically on a riding model. No extinction coefficient was used in the refinement. Residual electron density amounted to a maximum of $1.955\text{ e/\AA}^{-3}$ and a minimum of $-0.819\text{ e/\AA}^{-3}$.

The absolute structure (Flack) parameter for the correct enantiomer is $-0.08(6)$. The structure was also inverted and refined in order to confirm the initial assignment of absolute stereochemistry.

Tables 1-6 provide the full crystallographic data for the X-ray structure.

Table 1. Crystal data and structure refinement for 03199SL0.

Identification code	03199sl0	
Empirical formula	C ₁₄ H ₂₆ B Fe N O _{3.50} Si	
Formula weight	359.11	
Temperature	193(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 6.760(4) Å	a = 90°.
	b = 16.787(11) Å	b = 90°.
	c = 32.061(16) Å	g = 90°.
Volume	3638(4) Å ³	
Z	8	
Density (calculated)	1.311 Mg/m ³	
Absorption coefficient	0.905 mm ⁻¹	
F(000)	1520	
Crystal size	0.29 x 0.14 x 0.1 mm ³	
Theta range for data collection	1.27 to 23.28°.	
Index ranges	-7<=h<=4, -15<=k<=18, -27<=l<=35	
Reflections collected	7849	
Independent reflections	4972 [R(int) = 0.0815]	
Completeness to theta = 23.28°	97.1 %	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	4972 / 0 / 400	
Goodness-of-fit on F ²	0.945	
Final R indices [I>2sigma(I)]	R1 = 0.0677, wR2 = 0.1419	
R indices (all data)	R1 = 0.1141, wR2 = 0.1691	
Absolute structure parameter	-0.08(4)	
Largest diff. peak and hole	0.411 and -0.676 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 03199SL0. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
Fe(1)	8262(2)	3461(1)	8314(1)	36(1)
Fe(2)	3822(2)	3710(1)	5937(1)	33(1)
Si(1)	7578(4)	4822(2)	8347(1)	41(1)
Si(2)	5205(4)	3175(2)	6540(1)	39(1)
O(3)	10900(12)	3984(5)	7648(2)	63(2)
N(1)	7633(12)	2231(5)	8230(3)	41(2)
O(5)	536(11)	4163(5)	6470(2)	61(2)
C(26)	2751(15)	4068(6)	4941(3)	42(3)
C(11)	9853(16)	3763(6)	7912(3)	39(3)
C(10)	9909(17)	3636(7)	8710(3)	49(3)
N(2)	3883(12)	4248(4)	5341(2)	32(2)
C(30)	1858(16)	3974(6)	6260(3)	36(3)
C(24)	6500(16)	4231(6)	5794(3)	46(3)
O(2)	11012(13)	3758(5)	8983(2)	73(2)
C(32)	6077(16)	3980(6)	6910(3)	50(3)
O(6)	2784(12)	2055(4)	5797(2)	58(2)
C(23)	5265(15)	4841(6)	5943(3)	45(3)
B(2)	3620(19)	4927(7)	5626(4)	43(3)
C(14)	9887(16)	5456(6)	8385(4)	56(3)
C(25)	5687(14)	3864(6)	5450(3)	38(3)
C(33)	3359(18)	2583(7)	6854(3)	57(3)
C(5)	6479(19)	2716(7)	7967(4)	57(3)
C(6)	8903(18)	1573(6)	8051(3)	48(3)
C(28)	3321(18)	3247(6)	4773(3)	58(3)
C(8)	7640(20)	794(7)	8049(4)	84(4)
C(13)	6196(19)	5210(6)	7882(4)	68(4)
C(12)	6014(19)	5086(7)	8794(3)	67(3)
C(3)	5655(18)	3093(6)	8631(5)	72(4)
C(27)	3250(20)	4695(7)	4625(3)	67(4)
C(31)	3257(15)	2719(7)	5853(3)	48(3)
C(4)	5309(18)	3200(8)	8185(5)	75(4)
C(34)	7309(16)	2477(6)	6426(3)	54(3)
C(7)	9440(30)	1766(8)	7608(4)	127(7)
B(1)	7000(20)	2378(8)	8648(5)	59(4)
C(29)	561(15)	4068(7)	5055(3)	62(3)
O(1)	7716(15)	1946(4)	8993(2)	81(3)
C(9)	10681(18)	1481(8)	8314(5)	100(5)
O(4)	2118(12)	5475(4)	5575(2)	54(2)
O(7)	8120(50)	7301(12)	4754(6)	283(14)
C(51)	7500(90)	6170(30)	5270(20)	510(40)
C(53)	7750(80)	7650(20)	5160(8)	340(30)
C(50)	7990(100)	6373(13)	4827(15)	480(50)

C(52)

7450(80)

6940(20)

5447(14)

370(40)

Table 3. Bond lengths [Å] and angles [°] for 03199SL0.

Fe(1)-C(10)	1.713(12)
Fe(1)-C(11)	1.754(12)
Fe(1)-C(5)	2.062(11)
Fe(1)-C(4)	2.085(11)
Fe(1)-N(1)	2.124(8)
Fe(1)-C(3)	2.127(11)
Fe(1)-B(1)	2.275(12)
Fe(1)-Si(1)	2.333(3)
Fe(2)-C(31)	1.728(13)
Fe(2)-C(30)	1.740(11)
Fe(2)-C(25)	2.024(10)
Fe(2)-C(24)	2.062(10)
Fe(2)-N(2)	2.113(7)
Fe(2)-C(23)	2.136(10)
Fe(2)-B(2)	2.277(12)
Fe(2)-Si(2)	2.328(3)
Si(1)-C(12)	1.834(11)
Si(1)-C(13)	1.875(11)
Si(1)-C(14)	1.893(10)
Si(2)-C(34)	1.879(10)
Si(2)-C(33)	1.886(11)
Si(2)-C(32)	1.892(10)
O(3)-C(11)	1.163(11)
N(1)-C(5)	1.406(13)
N(1)-B(1)	1.430(16)
N(1)-C(6)	1.513(13)
O(5)-C(30)	1.164(11)
C(26)-C(27)	1.500(14)
C(26)-N(2)	1.526(12)
C(26)-C(29)	1.525(15)
C(26)-C(28)	1.527(14)
C(10)-O(2)	1.168(11)
N(2)-C(25)	1.422(12)
N(2)-B(2)	1.471(14)
C(24)-C(25)	1.379(12)
C(24)-C(23)	1.405(14)
O(6)-C(31)	1.174(12)
C(23)-B(2)	1.513(16)
B(2)-O(4)	1.379(13)
C(5)-C(4)	1.332(16)
C(6)-C(9)	1.476(15)
C(6)-C(7)	1.502(14)
C(6)-C(8)	1.561(15)
C(3)-C(4)	1.461(17)
C(3)-B(1)	1.507(18)

B(1)-O(1)	1.408(16)
O(7)-C(53)	1.45(2)
O(7)-C(50)	1.58(3)
C(51)-C(50)	1.49(7)
C(51)-C(52)	1.42(7)
C(53)-C(52)	1.52(4)
C(10)-Fe(1)-C(11)	95.6(5)
C(10)-Fe(1)-C(5)	152.0(5)
C(11)-Fe(1)-C(5)	97.9(5)
C(10)-Fe(1)-C(4)	143.6(6)
C(11)-Fe(1)-C(4)	120.1(6)
C(5)-Fe(1)-C(4)	37.5(5)
C(10)-Fe(1)-N(1)	113.0(4)
C(11)-Fe(1)-N(1)	108.0(4)
C(5)-Fe(1)-N(1)	39.2(4)
C(4)-Fe(1)-N(1)	65.1(4)
C(10)-Fe(1)-C(3)	103.5(6)
C(11)-Fe(1)-C(3)	160.7(6)
C(5)-Fe(1)-C(3)	66.3(5)
C(4)-Fe(1)-C(3)	40.6(5)
N(1)-Fe(1)-C(3)	67.2(4)
C(10)-Fe(1)-B(1)	91.8(5)
C(11)-Fe(1)-B(1)	143.8(5)
C(5)-Fe(1)-B(1)	63.3(5)
C(4)-Fe(1)-B(1)	64.4(6)
N(1)-Fe(1)-B(1)	37.7(4)
C(3)-Fe(1)-B(1)	39.9(5)
C(10)-Fe(1)-Si(1)	85.8(4)
C(11)-Fe(1)-Si(1)	82.7(3)
C(5)-Fe(1)-Si(1)	120.2(4)
C(4)-Fe(1)-Si(1)	91.4(4)
N(1)-Fe(1)-Si(1)	156.5(2)
C(3)-Fe(1)-Si(1)	95.6(3)
B(1)-Fe(1)-Si(1)	133.3(4)
C(31)-Fe(2)-C(30)	99.8(5)
C(31)-Fe(2)-C(25)	98.0(4)
C(30)-Fe(2)-C(25)	154.4(4)
C(31)-Fe(2)-C(24)	124.6(5)
C(30)-Fe(2)-C(24)	133.9(4)
C(25)-Fe(2)-C(24)	39.4(4)
C(31)-Fe(2)-N(2)	105.9(4)
C(30)-Fe(2)-N(2)	116.3(4)
C(25)-Fe(2)-N(2)	40.1(3)
C(24)-Fe(2)-N(2)	66.5(4)
C(31)-Fe(2)-C(23)	163.4(5)
C(30)-Fe(2)-C(23)	96.7(4)

C(25)-Fe(2)-C(23)	66.9(4)
C(24)-Fe(2)-C(23)	39.1(4)
N(2)-Fe(2)-C(23)	67.5(3)
C(31)-Fe(2)-B(2)	141.4(5)
C(30)-Fe(2)-B(2)	89.2(5)
C(25)-Fe(2)-B(2)	65.5(4)
C(24)-Fe(2)-B(2)	64.9(4)
N(2)-Fe(2)-B(2)	38.9(4)
C(23)-Fe(2)-B(2)	39.9(4)
C(31)-Fe(2)-Si(2)	81.2(3)
C(30)-Fe(2)-Si(2)	84.9(3)
C(25)-Fe(2)-Si(2)	116.1(3)
C(24)-Fe(2)-Si(2)	89.7(3)
N(2)-Fe(2)-Si(2)	155.2(2)
C(23)-Fe(2)-Si(2)	98.8(3)
B(2)-Fe(2)-Si(2)	137.2(3)
C(12)-Si(1)-C(13)	104.4(6)
C(12)-Si(1)-C(14)	106.8(5)
C(13)-Si(1)-C(14)	105.5(5)
C(12)-Si(1)-Fe(1)	112.7(4)
C(13)-Si(1)-Fe(1)	113.7(4)
C(14)-Si(1)-Fe(1)	112.9(3)
C(34)-Si(2)-C(33)	106.0(5)
C(34)-Si(2)-C(32)	109.4(5)
C(33)-Si(2)-C(32)	104.4(5)
C(34)-Si(2)-Fe(2)	112.5(4)
C(33)-Si(2)-Fe(2)	112.4(4)
C(32)-Si(2)-Fe(2)	111.8(3)
C(5)-N(1)-B(1)	107.3(10)
C(5)-N(1)-C(6)	120.8(9)
B(1)-N(1)-C(6)	130.6(9)
C(5)-N(1)-Fe(1)	68.0(5)
B(1)-N(1)-Fe(1)	76.9(6)
C(6)-N(1)-Fe(1)	130.1(6)
C(27)-C(26)-N(2)	108.4(8)
C(27)-C(26)-C(29)	112.4(10)
N(2)-C(26)-C(29)	106.5(8)
C(27)-C(26)-C(28)	109.8(9)
N(2)-C(26)-C(28)	110.4(8)
C(29)-C(26)-C(28)	109.3(10)
O(3)-C(11)-Fe(1)	178.2(10)
O(2)-C(10)-Fe(1)	179.2(10)
C(25)-N(2)-B(2)	107.7(8)
C(25)-N(2)-C(26)	123.1(8)
B(2)-N(2)-C(26)	128.0(8)
C(25)-N(2)-Fe(2)	66.6(5)
B(2)-N(2)-Fe(2)	76.6(5)

C(26)-N(2)-Fe(2)	131.8(6)
O(5)-C(30)-Fe(2)	178.6(10)
C(25)-C(24)-C(23)	111.1(10)
C(25)-C(24)-Fe(2)	68.8(6)
C(23)-C(24)-Fe(2)	73.3(6)
C(24)-C(23)-B(2)	106.2(9)
C(24)-C(23)-Fe(2)	67.6(6)
B(2)-C(23)-Fe(2)	75.1(6)
O(4)-B(2)-N(2)	122.2(10)
O(4)-B(2)-C(23)	133.1(11)
N(2)-B(2)-C(23)	104.7(9)
O(4)-B(2)-Fe(2)	133.9(8)
N(2)-B(2)-Fe(2)	64.5(5)
C(23)-B(2)-Fe(2)	65.0(6)
C(24)-C(25)-N(2)	109.6(9)
C(24)-C(25)-Fe(2)	71.8(6)
N(2)-C(25)-Fe(2)	73.3(5)
C(4)-C(5)-N(1)	111.7(11)
C(4)-C(5)-Fe(1)	72.2(7)
N(1)-C(5)-Fe(1)	72.8(6)
C(9)-C(6)-N(1)	108.8(9)
C(9)-C(6)-C(7)	111.5(13)
N(1)-C(6)-C(7)	109.7(9)
C(9)-C(6)-C(8)	111.1(10)
N(1)-C(6)-C(8)	107.6(9)
C(7)-C(6)-C(8)	108.1(11)
C(4)-C(3)-B(1)	103.3(12)
C(4)-C(3)-Fe(1)	68.1(7)
B(1)-C(3)-Fe(1)	75.4(7)
O(6)-C(31)-Fe(2)	177.0(10)
C(5)-C(4)-C(3)	110.0(12)
C(5)-C(4)-Fe(1)	70.3(7)
C(3)-C(4)-Fe(1)	71.3(7)
O(1)-B(1)-N(1)	123.2(11)
O(1)-B(1)-C(3)	130.2(13)
N(1)-B(1)-C(3)	106.5(12)
O(1)-B(1)-Fe(1)	130.8(10)
N(1)-B(1)-Fe(1)	65.4(6)
C(3)-B(1)-Fe(1)	64.8(6)
C(53)-O(7)-C(50)	105(2)
C(50)-C(51)-C(52)	100(4)
O(7)-C(53)-C(52)	104(3)
C(51)-C(50)-O(7)	112(4)
C(51)-C(52)-C(53)	118(5)

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 03199SL0. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2 a^{*2}U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Fe(1)	36(1)	32(1)	41(1)	4(1)	2(1)	-2(1)
Fe(2)	29(1)	35(1)	35(1)	0(1)	-2(1)	-2(1)
Si(1)	47(2)	30(2)	47(2)	-3(2)	1(2)	1(1)
Si(2)	38(2)	40(2)	39(2)	1(2)	-8(1)	-1(1)
O(3)	69(6)	67(6)	54(5)	8(4)	17(5)	-15(5)
N(1)	45(5)	33(5)	46(6)	10(4)	4(5)	-12(4)
O(5)	36(4)	83(6)	64(5)	-25(5)	11(4)	3(4)
C(26)	38(6)	47(7)	41(7)	3(6)	2(5)	-1(5)
C(11)	45(6)	26(6)	45(7)	3(6)	-15(5)	8(5)
C(10)	54(7)	44(7)	49(7)	0(6)	-2(6)	7(6)
N(2)	34(5)	35(5)	27(4)	4(4)	1(4)	3(4)
C(30)	41(6)	50(7)	18(5)	-11(5)	-14(5)	-16(6)
C(24)	32(6)	56(7)	50(7)	9(6)	-2(5)	-15(6)
O(2)	87(6)	69(5)	61(5)	-12(5)	-20(5)	13(5)
C(32)	47(6)	66(7)	36(6)	8(5)	-7(6)	-8(6)
O(6)	77(6)	38(5)	59(5)	-4(4)	-15(4)	-19(4)
C(23)	52(7)	46(7)	38(6)	-6(6)	6(6)	-7(6)
B(2)	41(8)	38(8)	51(8)	15(7)	-5(7)	0(7)
C(14)	64(7)	24(6)	80(9)	0(6)	-7(7)	-10(5)
C(25)	35(6)	41(6)	38(6)	3(5)	-3(5)	-7(5)
C(33)	69(8)	74(8)	28(6)	18(6)	-10(6)	-7(7)
C(5)	61(9)	41(7)	70(8)	18(7)	-14(8)	-17(7)
C(6)	69(8)	27(6)	48(7)	-6(5)	15(6)	7(6)
C(28)	67(8)	64(8)	42(7)	-24(6)	-5(6)	7(7)
C(8)	105(12)	48(8)	97(10)	4(8)	2(9)	-10(8)
C(13)	74(9)	34(6)	95(9)	-1(7)	-13(8)	3(7)
C(12)	73(9)	55(7)	71(8)	-12(7)	8(7)	9(7)
C(3)	54(8)	34(7)	128(13)	13(8)	38(9)	-7(6)
C(27)	81(9)	65(8)	56(8)	18(7)	-21(7)	-12(8)
C(31)	33(6)	68(8)	42(7)	1(6)	-6(5)	-8(6)
C(4)	36(7)	51(9)	137(14)	21(9)	-29(8)	-23(6)
C(34)	51(7)	46(7)	64(8)	-3(6)	-10(6)	22(6)
C(7)	250(20)	66(9)	66(10)	0(8)	86(12)	38(12)
B(1)	64(10)	37(8)	76(11)	16(8)	24(9)	-16(7)
C(29)	38(7)	88(9)	59(8)	-16(7)	-7(6)	2(6)
O(1)	149(9)	41(5)	54(5)	6(4)	28(6)	-5(5)
C(9)	62(8)	92(10)	148(14)	-42(11)	-7(10)	24(8)
O(4)	73(6)	37(4)	51(5)	-12(4)	-3(4)	14(4)
O(7)	510(50)	181(17)	162(17)	-24(14)	-90(20)	-10(20)
C(51)	280(50)	560(100)	690(90)	70(80)	210(60)	-180(60)
C(53)	640(100)	270(40)	101(19)	-60(20)	-70(40)	0(50)
C(50)	790(130)	26(14)	640(80)	-30(30)	-240(80)	50(40)

C(52)	290(50)	420(60)	410(70)	340(60)	-10(50)	0(50)
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Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for 03199SL0.

	x	y	z	U(eq)
H(24)	7792	4078	5924	55
H(32A)	6666	3733	7158	75
H(32B)	4949	4310	6994	75
H(32C)	7066	4313	6771	75
H(23)	5504	5188	6191	55
H(14A)	9518	6020	8386	84
H(14B)	10746	5347	8145	84
H(14C)	10594	5328	8643	84
H(25)	6322	3424	5287	45
H(33A)	2639	2220	6669	85
H(33B)	2422	2947	6989	85
H(33C)	4056	2274	7068	85
H(5)	6497	2686	7656	68
H(28A)	4683	3263	4669	86
H(28B)	2425	3100	4545	86
H(28C)	3221	2853	4997	86
H(8A)	8451	348	7951	126
H(8B)	6502	863	7863	126
H(8C)	7168	684	8333	126
H(13A)	5114	5554	7976	102
H(13B)	5654	4761	7723	102
H(13C)	7099	5516	7705	102
H(12A)	5919	5667	8815	100
H(12B)	6598	4871	9050	100
H(12C)	4689	4860	8754	100
H(3)	4971	3364	8869	86
H(27A)	2807	5216	4726	101
H(27B)	2594	4573	4360	101
H(27C)	4689	4707	4582	101
H(4)	4338	3582	8061	90
H(34A)	7991	2343	6687	80
H(34B)	8241	2734	6235	80
H(34C)	6794	1989	6298	80
H(7A)	10495	2167	7605	190
H(7B)	8276	1976	7462	190
H(7C)	9901	1283	7467	190
H(29A)	285	3625	5245	93
H(29B)	-234	4009	4801	93
H(29C)	225	4572	5192	93
H(1A)	7180	2116	9212	98
H(9A)	11458	1026	8216	151

H(9B)	10280	1391	8604	151
H(9C)	11484	1966	8298	151
H(4A)	2184	5818	5765	64
H(51A)	8543	5832	5395	613
H(51B)	6210	5895	5290	613
H(53A)	6553	7993	5153	404
H(53B)	8891	7979	5252	404
H(50A)	6955	6149	4641	580
H(50B)	9264	6125	4751	580
H(52A)	8481	6962	5666	446
H(52B)	6156	7004	5587	446

Table 6. Torsion angles [°] for 03199SL0.

C(10)-Fe(1)-Si(1)-C(12)	-76.3(6)
C(11)-Fe(1)-Si(1)-C(12)	-172.5(6)
C(5)-Fe(1)-Si(1)-C(12)	92.6(6)
C(4)-Fe(1)-Si(1)-C(12)	67.3(7)
N(1)-Fe(1)-Si(1)-C(12)	68.3(8)
C(3)-Fe(1)-Si(1)-C(12)	26.8(7)
B(1)-Fe(1)-Si(1)-C(12)	12.1(7)
C(10)-Fe(1)-Si(1)-C(13)	165.0(6)
C(11)-Fe(1)-Si(1)-C(13)	68.8(6)
C(5)-Fe(1)-Si(1)-C(13)	-26.1(6)
C(4)-Fe(1)-Si(1)-C(13)	-51.4(7)
N(1)-Fe(1)-Si(1)-C(13)	-50.3(8)
C(3)-Fe(1)-Si(1)-C(13)	-91.8(7)
B(1)-Fe(1)-Si(1)-C(13)	-106.5(7)
C(10)-Fe(1)-Si(1)-C(14)	44.9(5)
C(11)-Fe(1)-Si(1)-C(14)	-51.3(5)
C(5)-Fe(1)-Si(1)-C(14)	-146.2(6)
C(4)-Fe(1)-Si(1)-C(14)	-171.5(6)
N(1)-Fe(1)-Si(1)-C(14)	-170.5(7)
C(3)-Fe(1)-Si(1)-C(14)	148.0(6)
B(1)-Fe(1)-Si(1)-C(14)	133.3(7)
C(31)-Fe(2)-Si(2)-C(34)	63.6(5)
C(30)-Fe(2)-Si(2)-C(34)	164.4(5)
C(25)-Fe(2)-Si(2)-C(34)	-31.1(5)
C(24)-Fe(2)-Si(2)-C(34)	-61.5(5)
N(2)-Fe(2)-Si(2)-C(34)	-45.5(7)
C(23)-Fe(2)-Si(2)-C(34)	-99.6(5)
B(2)-Fe(2)-Si(2)-C(34)	-112.4(6)
C(31)-Fe(2)-Si(2)-C(33)	-55.9(5)
C(30)-Fe(2)-Si(2)-C(33)	44.8(5)
C(25)-Fe(2)-Si(2)-C(33)	-150.6(5)
C(24)-Fe(2)-Si(2)-C(33)	179.0(5)
N(2)-Fe(2)-Si(2)-C(33)	-165.1(6)
C(23)-Fe(2)-Si(2)-C(33)	140.9(5)
B(2)-Fe(2)-Si(2)-C(33)	128.1(6)
C(31)-Fe(2)-Si(2)-C(32)	-172.9(5)
C(30)-Fe(2)-Si(2)-C(32)	-72.1(5)
C(25)-Fe(2)-Si(2)-C(32)	92.4(5)
C(24)-Fe(2)-Si(2)-C(32)	62.0(5)
N(2)-Fe(2)-Si(2)-C(32)	78.0(7)
C(23)-Fe(2)-Si(2)-C(32)	23.9(5)
B(2)-Fe(2)-Si(2)-C(32)	11.1(6)
C(10)-Fe(1)-N(1)-C(5)	175.4(7)
C(11)-Fe(1)-N(1)-C(5)	-80.2(8)
C(4)-Fe(1)-N(1)-C(5)	35.3(7)

C(3)-Fe(1)-N(1)-C(5)	79.9(8)
B(1)-Fe(1)-N(1)-C(5)	115.0(10)
Si(1)-Fe(1)-N(1)-C(5)	34.2(10)
C(10)-Fe(1)-N(1)-B(1)	60.4(8)
C(11)-Fe(1)-N(1)-B(1)	164.8(8)
C(5)-Fe(1)-N(1)-B(1)	-115.0(10)
C(4)-Fe(1)-N(1)-B(1)	-79.7(9)
C(3)-Fe(1)-N(1)-B(1)	-35.2(8)
Si(1)-Fe(1)-N(1)-B(1)	-80.8(9)
C(10)-Fe(1)-N(1)-C(6)	-72.2(9)
C(11)-Fe(1)-N(1)-C(6)	32.2(9)
C(5)-Fe(1)-N(1)-C(6)	112.4(11)
C(4)-Fe(1)-N(1)-C(6)	147.7(10)
C(3)-Fe(1)-N(1)-C(6)	-167.7(10)
B(1)-Fe(1)-N(1)-C(6)	-132.6(12)
Si(1)-Fe(1)-N(1)-C(6)	146.6(7)
C(10)-Fe(1)-C(11)-O(3)	-75(28)
C(5)-Fe(1)-C(11)-O(3)	130(28)
C(4)-Fe(1)-C(11)-O(3)	98(28)
N(1)-Fe(1)-C(11)-O(3)	169(100)
C(3)-Fe(1)-C(11)-O(3)	96(28)
B(1)-Fe(1)-C(11)-O(3)	-176(100)
Si(1)-Fe(1)-C(11)-O(3)	10(28)
C(11)-Fe(1)-C(10)-O(2)	147(84)
C(5)-Fe(1)-C(10)-O(2)	-95(84)
C(4)-Fe(1)-C(10)-O(2)	-22(84)
N(1)-Fe(1)-C(10)-O(2)	-101(84)
C(3)-Fe(1)-C(10)-O(2)	-30(84)
B(1)-Fe(1)-C(10)-O(2)	-69(84)
Si(1)-Fe(1)-C(10)-O(2)	64(84)
C(27)-C(26)-N(2)-C(25)	-98.5(11)
C(29)-C(26)-N(2)-C(25)	140.3(9)
C(28)-C(26)-N(2)-C(25)	21.8(12)
C(27)-C(26)-N(2)-B(2)	67.0(13)
C(29)-C(26)-N(2)-B(2)	-54.2(13)
C(28)-C(26)-N(2)-B(2)	-172.7(9)
C(27)-C(26)-N(2)-Fe(2)	174.7(7)
C(29)-C(26)-N(2)-Fe(2)	53.5(12)
C(28)-C(26)-N(2)-Fe(2)	-65.1(11)
C(31)-Fe(2)-N(2)-C(25)	-83.5(6)
C(30)-Fe(2)-N(2)-C(25)	166.7(6)
C(24)-Fe(2)-N(2)-C(25)	37.8(6)
C(23)-Fe(2)-N(2)-C(25)	80.4(6)
B(2)-Fe(2)-N(2)-C(25)	116.3(8)
Si(2)-Fe(2)-N(2)-C(25)	20.4(8)
C(31)-Fe(2)-N(2)-B(2)	160.2(7)
C(30)-Fe(2)-N(2)-B(2)	50.4(7)

C(25)-Fe(2)-N(2)-B(2)	-116.3(8)
C(24)-Fe(2)-N(2)-B(2)	-78.5(7)
C(23)-Fe(2)-N(2)-B(2)	-36.0(6)
Si(2)-Fe(2)-N(2)-B(2)	-96.0(7)
C(31)-Fe(2)-N(2)-C(26)	30.7(9)
C(30)-Fe(2)-N(2)-C(26)	-79.0(9)
C(25)-Fe(2)-N(2)-C(26)	114.2(10)
C(24)-Fe(2)-N(2)-C(26)	152.0(9)
C(23)-Fe(2)-N(2)-C(26)	-165.4(9)
B(2)-Fe(2)-N(2)-C(26)	-129.4(11)
Si(2)-Fe(2)-N(2)-C(26)	134.6(7)
C(31)-Fe(2)-C(30)-O(5)	-127(38)
C(25)-Fe(2)-C(30)-O(5)	6(39)
C(24)-Fe(2)-C(30)-O(5)	68(38)
N(2)-Fe(2)-C(30)-O(5)	-14(38)
C(23)-Fe(2)-C(30)-O(5)	55(38)
B(2)-Fe(2)-C(30)-O(5)	15(38)
Si(2)-Fe(2)-C(30)-O(5)	153(38)
C(31)-Fe(2)-C(24)-C(25)	55.2(8)
C(30)-Fe(2)-C(24)-C(25)	-143.1(7)
N(2)-Fe(2)-C(24)-C(25)	-38.4(6)
C(23)-Fe(2)-C(24)-C(25)	-121.3(9)
B(2)-Fe(2)-C(24)-C(25)	-81.3(7)
Si(2)-Fe(2)-C(24)-C(25)	134.3(6)
C(31)-Fe(2)-C(24)-C(23)	176.5(6)
C(30)-Fe(2)-C(24)-C(23)	-21.8(9)
C(25)-Fe(2)-C(24)-C(23)	121.3(9)
N(2)-Fe(2)-C(24)-C(23)	82.9(6)
B(2)-Fe(2)-C(24)-C(23)	40.0(6)
Si(2)-Fe(2)-C(24)-C(23)	-104.4(6)
C(25)-C(24)-C(23)-B(2)	-7.2(12)
Fe(2)-C(24)-C(23)-B(2)	-65.8(7)
C(25)-C(24)-C(23)-Fe(2)	58.6(7)
C(31)-Fe(2)-C(23)-C(24)	-10.2(18)
C(30)-Fe(2)-C(23)-C(24)	164.4(6)
C(25)-Fe(2)-C(23)-C(24)	-36.2(6)
N(2)-Fe(2)-C(23)-C(24)	-79.9(6)
B(2)-Fe(2)-C(23)-C(24)	-115.0(9)
Si(2)-Fe(2)-C(23)-C(24)	78.6(6)
C(31)-Fe(2)-C(23)-B(2)	104.8(16)
C(30)-Fe(2)-C(23)-B(2)	-80.6(7)
C(25)-Fe(2)-C(23)-B(2)	78.8(7)
C(24)-Fe(2)-C(23)-B(2)	115.0(9)
N(2)-Fe(2)-C(23)-B(2)	35.1(6)
Si(2)-Fe(2)-C(23)-B(2)	-166.5(6)
C(25)-N(2)-B(2)-O(4)	172.9(9)
C(26)-N(2)-B(2)-O(4)	5.6(16)

Fe(2)-N(2)-B(2)-O(4)	-127.4(10)
C(25)-N(2)-B(2)-C(23)	-7.2(10)
C(26)-N(2)-B(2)-C(23)	-174.5(8)
Fe(2)-N(2)-B(2)-C(23)	52.4(7)
C(25)-N(2)-B(2)-Fe(2)	-59.7(6)
C(26)-N(2)-B(2)-Fe(2)	133.1(9)
C(24)-C(23)-B(2)-O(4)	-171.4(12)
Fe(2)-C(23)-B(2)-O(4)	127.7(13)
C(24)-C(23)-B(2)-N(2)	8.7(11)
Fe(2)-C(23)-B(2)-N(2)	-52.1(7)
C(24)-C(23)-B(2)-Fe(2)	60.8(7)
C(31)-Fe(2)-B(2)-O(4)	79.5(14)
C(30)-Fe(2)-B(2)-O(4)	-25.2(12)
C(25)-Fe(2)-B(2)-O(4)	150.5(13)
C(24)-Fe(2)-B(2)-O(4)	-165.8(14)
N(2)-Fe(2)-B(2)-O(4)	111.1(14)
C(23)-Fe(2)-B(2)-O(4)	-126.7(15)
Si(2)-Fe(2)-B(2)-O(4)	-106.8(11)
C(31)-Fe(2)-B(2)-N(2)	-31.6(10)
C(30)-Fe(2)-B(2)-N(2)	-136.3(6)
C(25)-Fe(2)-B(2)-N(2)	39.4(5)
C(24)-Fe(2)-B(2)-N(2)	83.1(6)
C(23)-Fe(2)-B(2)-N(2)	122.2(9)
Si(2)-Fe(2)-B(2)-N(2)	142.1(4)
C(31)-Fe(2)-B(2)-C(23)	-153.8(7)
C(30)-Fe(2)-B(2)-C(23)	101.5(7)
C(25)-Fe(2)-B(2)-C(23)	-82.8(7)
C(24)-Fe(2)-B(2)-C(23)	-39.1(6)
N(2)-Fe(2)-B(2)-C(23)	-122.2(9)
Si(2)-Fe(2)-B(2)-C(23)	19.9(9)
C(23)-C(24)-C(25)-N(2)	2.7(11)
Fe(2)-C(24)-C(25)-N(2)	64.0(6)
C(23)-C(24)-C(25)-Fe(2)	-61.3(7)
B(2)-N(2)-C(25)-C(24)	3.2(10)
C(26)-N(2)-C(25)-C(24)	171.2(8)
Fe(2)-N(2)-C(25)-C(24)	-63.0(7)
B(2)-N(2)-C(25)-Fe(2)	66.2(6)
C(26)-N(2)-C(25)-Fe(2)	-125.8(8)
C(31)-Fe(2)-C(25)-C(24)	-136.9(7)
C(30)-Fe(2)-C(25)-C(24)	89.5(10)
N(2)-Fe(2)-C(25)-C(24)	117.8(8)
C(23)-Fe(2)-C(25)-C(24)	35.8(6)
B(2)-Fe(2)-C(25)-C(24)	79.6(7)
Si(2)-Fe(2)-C(25)-C(24)	-52.8(7)
C(31)-Fe(2)-C(25)-N(2)	105.2(6)
C(30)-Fe(2)-C(25)-N(2)	-28.4(11)
C(24)-Fe(2)-C(25)-N(2)	-117.8(8)

C(23)-Fe(2)-C(25)-N(2)	-82.0(5)
B(2)-Fe(2)-C(25)-N(2)	-38.2(5)
Si(2)-Fe(2)-C(25)-N(2)	-170.6(4)
B(1)-N(1)-C(5)-C(4)	5.4(12)
C(6)-N(1)-C(5)-C(4)	173.2(9)
Fe(1)-N(1)-C(5)-C(4)	-62.1(8)
B(1)-N(1)-C(5)-Fe(1)	67.5(7)
C(6)-N(1)-C(5)-Fe(1)	-124.7(8)
C(10)-Fe(1)-C(5)-C(4)	111.3(13)
C(11)-Fe(1)-C(5)-C(4)	-130.7(9)
N(1)-Fe(1)-C(5)-C(4)	120.4(11)
C(3)-Fe(1)-C(5)-C(4)	37.8(8)
B(1)-Fe(1)-C(5)-C(4)	82.0(9)
Si(1)-Fe(1)-C(5)-C(4)	-44.6(9)
C(10)-Fe(1)-C(5)-N(1)	-9.0(15)
C(11)-Fe(1)-C(5)-N(1)	108.9(7)
C(4)-Fe(1)-C(5)-N(1)	-120.4(11)
C(3)-Fe(1)-C(5)-N(1)	-82.5(6)
B(1)-Fe(1)-C(5)-N(1)	-38.4(6)
Si(1)-Fe(1)-C(5)-N(1)	-165.0(5)
C(5)-N(1)-C(6)-C(9)	147.9(10)
B(1)-N(1)-C(6)-C(9)	-47.5(15)
Fe(1)-N(1)-C(6)-C(9)	61.8(12)
C(5)-N(1)-C(6)-C(7)	25.7(15)
B(1)-N(1)-C(6)-C(7)	-169.7(13)
Fe(1)-N(1)-C(6)-C(7)	-60.4(14)
C(5)-N(1)-C(6)-C(8)	-91.6(11)
B(1)-N(1)-C(6)-C(8)	73.0(14)
Fe(1)-N(1)-C(6)-C(8)	-177.7(7)
C(10)-Fe(1)-C(3)-C(4)	172.6(8)
C(11)-Fe(1)-C(3)-C(4)	1.7(17)
C(5)-Fe(1)-C(3)-C(4)	-35.0(7)
N(1)-Fe(1)-C(3)-C(4)	-77.8(8)
B(1)-Fe(1)-C(3)-C(4)	-111.2(11)
Si(1)-Fe(1)-C(3)-C(4)	85.5(7)
C(10)-Fe(1)-C(3)-B(1)	-76.2(10)
C(11)-Fe(1)-C(3)-B(1)	112.8(15)
C(5)-Fe(1)-C(3)-B(1)	76.2(8)
C(4)-Fe(1)-C(3)-B(1)	111.2(11)
N(1)-Fe(1)-C(3)-B(1)	33.4(8)
Si(1)-Fe(1)-C(3)-B(1)	-163.3(8)
C(30)-Fe(2)-C(31)-O(6)	32(18)
C(25)-Fe(2)-C(31)-O(6)	-129(17)
C(24)-Fe(2)-C(31)-O(6)	-161(17)
N(2)-Fe(2)-C(31)-O(6)	-89(18)
C(23)-Fe(2)-C(31)-O(6)	-153(17)
B(2)-Fe(2)-C(31)-O(6)	-69(18)

Si(2)-Fe(2)-C(31)-O(6)	116(18)
N(1)-C(5)-C(4)-C(3)	2.0(14)
Fe(1)-C(5)-C(4)-C(3)	-60.4(8)
N(1)-C(5)-C(4)-Fe(1)	62.5(8)
B(1)-C(3)-C(4)-C(5)	-8.1(13)
Fe(1)-C(3)-C(4)-C(5)	59.9(9)
B(1)-C(3)-C(4)-Fe(1)	-68.0(8)
C(10)-Fe(1)-C(4)-C(5)	-132.6(10)
C(11)-Fe(1)-C(4)-C(5)	60.3(9)
N(1)-Fe(1)-C(4)-C(5)	-36.9(7)
C(3)-Fe(1)-C(4)-C(5)	-120.4(11)
B(1)-Fe(1)-C(4)-C(5)	-78.8(8)
Si(1)-Fe(1)-C(4)-C(5)	142.6(8)
C(10)-Fe(1)-C(4)-C(3)	-12.2(13)
C(11)-Fe(1)-C(4)-C(3)	-179.4(7)
C(5)-Fe(1)-C(4)-C(3)	120.4(11)
N(1)-Fe(1)-C(4)-C(3)	83.4(7)
B(1)-Fe(1)-C(4)-C(3)	41.5(7)
Si(1)-Fe(1)-C(4)-C(3)	-97.0(7)
C(5)-N(1)-B(1)-O(1)	174.3(11)
C(6)-N(1)-B(1)-O(1)	8.1(19)
Fe(1)-N(1)-B(1)-O(1)	-124.0(12)
C(5)-N(1)-B(1)-C(3)	-10.2(12)
C(6)-N(1)-B(1)-C(3)	-176.4(10)
Fe(1)-N(1)-B(1)-C(3)	51.4(8)
C(5)-N(1)-B(1)-Fe(1)	-61.6(6)
C(6)-N(1)-B(1)-Fe(1)	132.2(11)
C(4)-C(3)-B(1)-O(1)	-174.0(13)
Fe(1)-C(3)-B(1)-O(1)	123.2(14)
C(4)-C(3)-B(1)-N(1)	11.0(13)
Fe(1)-C(3)-B(1)-N(1)	-51.8(8)
C(4)-C(3)-B(1)-Fe(1)	62.8(7)
C(10)-Fe(1)-B(1)-O(1)	-13.3(12)
C(11)-Fe(1)-B(1)-O(1)	88.6(15)
C(5)-Fe(1)-B(1)-O(1)	153.4(14)
C(4)-Fe(1)-B(1)-O(1)	-164.7(15)
N(1)-Fe(1)-B(1)-O(1)	113.6(15)
C(3)-Fe(1)-B(1)-O(1)	-122.4(17)
Si(1)-Fe(1)-B(1)-O(1)	-99.2(12)
C(10)-Fe(1)-B(1)-N(1)	-126.8(7)
C(11)-Fe(1)-B(1)-N(1)	-24.9(12)
C(5)-Fe(1)-B(1)-N(1)	39.9(7)
C(4)-Fe(1)-B(1)-N(1)	81.8(8)
C(3)-Fe(1)-B(1)-N(1)	124.1(12)
Si(1)-Fe(1)-B(1)-N(1)	147.3(5)
C(10)-Fe(1)-B(1)-C(3)	109.1(9)
C(11)-Fe(1)-B(1)-C(3)	-149.0(9)

C(5)-Fe(1)-B(1)-C(3)	-84.2(9)
C(4)-Fe(1)-B(1)-C(3)	-42.3(8)
N(1)-Fe(1)-B(1)-C(3)	-124.1(12)
Si(1)-Fe(1)-B(1)-C(3)	23.2(11)
C(50)-O(7)-C(53)-C(52)	1(5)
C(52)-C(51)-C(50)-O(7)	-2(8)
C(53)-O(7)-C(50)-C(51)	1(7)
C(50)-C(51)-C(52)-C(53)	3(8)
O(7)-C(53)-C(52)-C(51)	-3(7)

A yellow pentane/benzene solution was prepared. Crystals suitable for X-ray structural analysis were obtained by solvent evaporation at $-30\text{ }^{\circ}\text{C}$.

A yellow needle of dimensions $0.4 \times 0.21 \times 0.19\text{ mm}^3$ was mounted under STP and transferred to a Bruker AXS/CCD three-circle diffractometer equipped with a cold stream of N_2 gas. An initial unit cell was determined with monochromated $\text{Mo K}\alpha$ radiation ($\lambda = 0.71073\text{ \AA}$). The cell thus determined was triclinic.

A hemisphere of data was then collected using ω scans of 0.30° and 30-s frames. The raw data frames were integrated using the Bruker program SAINT+ for NT version 6.01. The data that were collected (6475 total reflections, 4531 unique, $R_{\text{int}} = 0.0303$) had the following Miller index ranges: -11 to 11 in h , -6 to 12 in k , and -15 to 15 in l . A SADABS absorption correction was performed, with $T_{\text{min}} = 0.700093$ and $T_{\text{max}} = 0.926385$.

All aspects of the solution and refinement were handled by SHELXTL NT version 5.10. The structure was solved by direct methods in the triclinic space group $P-1$, $a = 10.5502(9)\text{ \AA}$; $b = 11.3979(9)\text{ \AA}$; $c = 14.2293(12)\text{ \AA}$; $\alpha = 96.9350(10)^{\circ}$; $\beta = 92.9950(10)^{\circ}$; $\gamma = 107.6400(10)^{\circ}$, and refined using standard difference Fourier techniques. Final, full-matrix least-squares refinement (4531 data for 345 parameters) on F^2 yielded residuals of R_1 and wR_2 of 0.0676 and 0.1767 for data $I > 2\sigma(I)$, and 0.0728 and 0.1802 , respectively, for all data. During the final refinement all non-hydrogen atoms were treated anisotropically. Hydrogen atoms were included in calculated positions and refined isotropically on a riding model. No extinction coefficient was used in the refinement. Residual electron density amounted to a maximum of $0.704\text{ e/\AA}^{-3}$ and a minimum of $-0.760\text{ e/\AA}^{-3}$.

Tables 1-6 provide the full crystallographic data for the X-ray structure.

Table 1. Crystal data and structure refinement for 02145SLS.

Identification code	02145sls	
Empirical formula	C ₂₇ H ₃₉ B Fe N ₂ O ₅ Si	
Formula weight	566.35	
Temperature	193(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.5502(9) Å	a = 96.9350(10)°.
	b = 11.3979(9) Å	b = 92.9950(10)°.
	c = 14.2293(12) Å	g = 107.6400(10)°.
Volume	1611.5(2) Å ³	
Z	2	
Density (calculated)	1.167 Mg/m ³	
Absorption coefficient	0.539 mm ⁻¹	
F(000)	600	
Crystal size	0.4 x 0.21 x 0.19 mm ³	
Theta range for data collection	2.38 to 23.26°.	
Index ranges	-11<=h<=11, -6<=k<=12, -15<=l<=15	
Reflections collected	6475	
Independent reflections	4531 [R(int) = 0.0303]	
Completeness to theta = 23.26°	97.8 %	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	4531 / 0 / 345	
Goodness-of-fit on F ²	1.145	
Final R indices [I>2sigma(I)]	R1 = 0.0676, wR2 = 0.1767	
R indices (all data)	R1 = 0.0728, wR2 = 0.1802	
Extinction coefficient	0.0011(12)	
Largest diff. peak and hole	0.704 and -0.760 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 02145SLS. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
Fe(1)	4121(1)	934(1)	2169(1)	26(1)
Si(1)	4036(1)	-750(1)	2964(1)	35(1)
O(1)	5823(4)	-18(3)	946(3)	53(1)
O(2)	1724(4)	-854(4)	1151(3)	60(1)
O(3)	6593(3)	3640(3)	1904(2)	29(1)
O(4)	7872(5)	6701(4)	1522(3)	65(1)
O(5)	7930(4)	6372(3)	3023(3)	47(1)
N(1)	4135(4)	2777(3)	2024(3)	27(1)
N(2)	8899(4)	1126(4)	1763(3)	39(1)
B(1)	5544(5)	2973(4)	2361(4)	28(1)
C(5)	3335(5)	2260(4)	2725(3)	31(1)
C(4)	4119(5)	2026(4)	3455(3)	34(1)
C(3)	5451(5)	2325(4)	3234(3)	29(1)
C(6)	3606(4)	3237(4)	1185(3)	32(1)
C(7)	4005(6)	4646(5)	1423(4)	50(1)
C(8)	2098(5)	2697(5)	1004(4)	47(1)
C(9)	4243(5)	2869(5)	317(4)	45(1)
C(10)	5180(5)	387(4)	1438(4)	36(1)
C(11)	2675(5)	-115(5)	1563(4)	39(1)
C(12)	2576(6)	-1153(5)	3683(4)	50(1)
C(13)	3897(6)	-2224(5)	2147(4)	51(1)
C(14)	5583(6)	-441(5)	3790(4)	51(1)
C(15)	7923(4)	3963(4)	2374(3)	31(1)
C(16)	8443(4)	2881(4)	2304(3)	31(1)
C(17)	9075(5)	2495(4)	3080(4)	35(1)
C(18)	9433(5)	2954(5)	4047(4)	44(1)
C(19)	10042(6)	2333(6)	4597(4)	54(2)
C(20)	10316(6)	1269(6)	4217(5)	56(2)
C(21)	9972(5)	769(5)	3272(4)	48(1)
C(22)	9347(5)	1397(5)	2716(4)	37(1)
C(23)	8372(5)	2020(4)	1537(3)	35(1)
C(24)	8857(6)	-7(5)	1132(4)	53(2)
C(25)	8773(5)	5098(4)	1947(4)	36(1)
C(26)	10180(5)	5558(5)	2474(5)	58(2)
C(27)	8822(7)	4784(6)	881(5)	61(2)
C(28)	8142(5)	6138(5)	2112(4)	40(1)
C(29)	7344(6)	7354(6)	3253(5)	59(2)

Table 3. Bond lengths [Å] and angles [°] for 02145SLS.

Fe(1)-C(11)	1.734(5)
Fe(1)-C(10)	1.762(5)
Fe(1)-C(5)	2.034(4)
Fe(1)-C(4)	2.087(5)
Fe(1)-N(1)	2.131(3)
Fe(1)-C(3)	2.152(4)
Fe(1)-Si(1)	2.3244(14)
Fe(1)-B(1)	2.328(5)
Si(1)-C(12)	1.865(6)
Si(1)-C(14)	1.876(6)
Si(1)-C(13)	1.886(5)
O(1)-C(10)	1.151(6)
O(2)-C(11)	1.170(6)
O(3)-B(1)	1.383(6)
O(3)-C(15)	1.442(5)
O(4)-C(28)	1.189(6)
O(5)-C(28)	1.337(7)
O(5)-C(29)	1.447(6)
N(1)-C(5)	1.408(6)
N(1)-B(1)	1.480(6)
N(1)-C(6)	1.507(6)
N(2)-C(23)	1.361(6)
N(2)-C(22)	1.379(7)
N(2)-C(24)	1.469(7)
B(1)-C(3)	1.513(7)
C(5)-C(4)	1.394(7)
C(4)-C(3)	1.404(7)
C(6)-C(9)	1.512(7)
C(6)-C(8)	1.517(7)
C(6)-C(7)	1.521(7)
C(15)-C(16)	1.489(7)
C(15)-C(25)	1.546(6)
C(16)-C(23)	1.359(7)
C(16)-C(17)	1.441(7)
C(17)-C(18)	1.400(7)
C(17)-C(22)	1.411(7)
C(18)-C(19)	1.373(8)
C(19)-C(20)	1.384(9)
C(20)-C(21)	1.379(9)
C(21)-C(22)	1.394(7)
C(25)-C(27)	1.523(8)
C(25)-C(28)	1.527(7)
C(25)-C(26)	1.536(7)
C(11)-Fe(1)-C(10)	93.6(2)

C(11)-Fe(1)-C(5)	98.7(2)
C(10)-Fe(1)-C(5)	153.3(2)
C(11)-Fe(1)-C(4)	122.6(2)
C(10)-Fe(1)-C(4)	142.5(2)
C(5)-Fe(1)-C(4)	39.53(19)
C(11)-Fe(1)-N(1)	109.08(19)
C(10)-Fe(1)-N(1)	113.99(19)
C(5)-Fe(1)-N(1)	39.44(16)
C(4)-Fe(1)-N(1)	66.12(17)
C(11)-Fe(1)-C(3)	161.3(2)
C(10)-Fe(1)-C(3)	104.76(19)
C(5)-Fe(1)-C(3)	66.16(18)
C(4)-Fe(1)-C(3)	38.64(18)
N(1)-Fe(1)-C(3)	66.79(16)
C(11)-Fe(1)-Si(1)	81.66(17)
C(10)-Fe(1)-Si(1)	85.41(16)
C(5)-Fe(1)-Si(1)	119.69(14)
C(4)-Fe(1)-Si(1)	90.27(14)
N(1)-Fe(1)-Si(1)	156.33(11)
C(3)-Fe(1)-Si(1)	96.11(13)
C(11)-Fe(1)-B(1)	145.2(2)
C(10)-Fe(1)-B(1)	92.5(2)
C(5)-Fe(1)-B(1)	64.23(18)
C(4)-Fe(1)-B(1)	63.99(18)
N(1)-Fe(1)-B(1)	38.44(16)
C(3)-Fe(1)-B(1)	39.23(18)
Si(1)-Fe(1)-B(1)	132.97(14)
C(12)-Si(1)-C(14)	107.5(3)
C(12)-Si(1)-C(13)	105.5(3)
C(14)-Si(1)-C(13)	105.7(3)
C(12)-Si(1)-Fe(1)	112.55(19)
C(14)-Si(1)-Fe(1)	111.54(19)
C(13)-Si(1)-Fe(1)	113.61(19)
B(1)-O(3)-C(15)	117.7(3)
C(28)-O(5)-C(29)	116.0(4)
C(5)-N(1)-B(1)	107.7(4)
C(5)-N(1)-C(6)	123.4(4)
B(1)-N(1)-C(6)	128.1(4)
C(5)-N(1)-Fe(1)	66.6(2)
B(1)-N(1)-Fe(1)	78.0(2)
C(6)-N(1)-Fe(1)	128.6(3)
C(23)-N(2)-C(22)	108.1(4)
C(23)-N(2)-C(24)	125.9(4)
C(22)-N(2)-C(24)	125.6(4)
O(3)-B(1)-N(1)	121.9(4)
O(3)-B(1)-C(3)	134.1(4)
N(1)-B(1)-C(3)	103.9(4)

O(3)-B(1)-Fe(1)	136.1(3)
N(1)-B(1)-Fe(1)	63.5(2)
C(3)-B(1)-Fe(1)	64.1(2)
C(4)-C(5)-N(1)	110.4(4)
C(4)-C(5)-Fe(1)	72.3(3)
N(1)-C(5)-Fe(1)	74.0(2)
C(5)-C(4)-C(3)	109.7(4)
C(5)-C(4)-Fe(1)	68.2(3)
C(3)-C(4)-Fe(1)	73.2(3)
C(4)-C(3)-B(1)	107.2(4)
C(4)-C(3)-Fe(1)	68.1(3)
B(1)-C(3)-Fe(1)	76.7(3)
N(1)-C(6)-C(9)	108.5(4)
N(1)-C(6)-C(8)	111.6(4)
C(9)-C(6)-C(8)	109.5(4)
N(1)-C(6)-C(7)	106.6(4)
C(9)-C(6)-C(7)	110.7(4)
C(8)-C(6)-C(7)	109.9(4)
O(1)-C(10)-Fe(1)	176.9(4)
O(2)-C(11)-Fe(1)	177.6(4)
O(3)-C(15)-C(16)	112.0(4)
O(3)-C(15)-C(25)	105.9(4)
C(16)-C(15)-C(25)	115.1(4)
C(23)-C(16)-C(17)	105.4(4)
C(23)-C(16)-C(15)	128.9(4)
C(17)-C(16)-C(15)	125.7(4)
C(18)-C(17)-C(22)	118.1(5)
C(18)-C(17)-C(16)	134.7(5)
C(22)-C(17)-C(16)	107.2(4)
C(19)-C(18)-C(17)	119.1(5)
C(18)-C(19)-C(20)	121.5(6)
C(21)-C(20)-C(19)	121.8(5)
C(20)-C(21)-C(22)	116.6(5)
N(2)-C(22)-C(21)	129.6(5)
N(2)-C(22)-C(17)	107.5(4)
C(21)-C(22)-C(17)	122.9(5)
C(16)-C(23)-N(2)	111.8(4)
C(27)-C(25)-C(28)	108.3(4)
C(27)-C(25)-C(26)	111.3(5)
C(28)-C(25)-C(26)	108.2(4)
C(27)-C(25)-C(15)	111.5(4)
C(28)-C(25)-C(15)	108.6(4)
C(26)-C(25)-C(15)	108.7(4)
O(4)-C(28)-O(5)	122.4(5)
O(4)-C(28)-C(25)	125.8(5)
O(5)-C(28)-C(25)	111.8(4)

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 02145SLS. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2 a^{*2}U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Fe(1)	26(1)	20(1)	31(1)	3(1)	1(1)	6(1)
Si(1)	41(1)	25(1)	42(1)	9(1)	6(1)	12(1)
O(1)	47(2)	41(2)	64(3)	-15(2)	17(2)	11(2)
O(2)	41(2)	39(2)	88(3)	-4(2)	-21(2)	4(2)
O(3)	24(2)	27(2)	33(2)	7(1)	-1(1)	4(1)
O(4)	78(3)	60(3)	66(3)	26(2)	2(2)	30(2)
O(5)	53(2)	39(2)	53(2)	6(2)	1(2)	23(2)
N(1)	28(2)	17(2)	36(2)	5(2)	2(2)	8(2)
N(2)	34(2)	32(2)	52(3)	3(2)	5(2)	14(2)
B(1)	25(3)	18(2)	36(3)	-4(2)	-1(2)	3(2)
C(5)	28(2)	21(2)	40(3)	0(2)	10(2)	4(2)
C(4)	39(3)	23(2)	35(3)	-2(2)	10(2)	5(2)
C(3)	32(2)	21(2)	30(2)	-1(2)	-2(2)	3(2)
C(6)	29(2)	24(2)	40(3)	9(2)	-7(2)	5(2)
C(7)	58(4)	32(3)	62(4)	12(3)	-6(3)	17(3)
C(8)	37(3)	41(3)	65(4)	14(3)	-8(3)	14(2)
C(9)	47(3)	56(3)	36(3)	7(2)	-2(2)	20(3)
C(10)	34(3)	26(3)	41(3)	2(2)	-3(2)	1(2)
C(11)	44(3)	31(3)	46(3)	5(2)	4(2)	19(3)
C(12)	58(4)	39(3)	57(3)	13(3)	14(3)	15(3)
C(13)	67(4)	29(3)	61(4)	9(3)	9(3)	22(3)
C(14)	59(4)	47(3)	51(3)	11(3)	-4(3)	22(3)
C(15)	25(2)	31(3)	33(2)	7(2)	0(2)	5(2)
C(16)	24(2)	32(3)	36(3)	8(2)	0(2)	7(2)
C(17)	26(2)	32(3)	43(3)	9(2)	7(2)	2(2)
C(18)	38(3)	47(3)	45(3)	9(2)	1(2)	9(2)
C(19)	47(3)	72(4)	45(3)	25(3)	0(3)	15(3)
C(20)	41(3)	64(4)	71(4)	36(3)	7(3)	17(3)
C(21)	32(3)	40(3)	75(4)	25(3)	7(3)	11(2)
C(22)	27(2)	35(3)	48(3)	6(2)	4(2)	8(2)
C(23)	31(3)	34(3)	39(3)	7(2)	-2(2)	10(2)
C(24)	46(3)	44(3)	71(4)	-2(3)	4(3)	22(3)
C(25)	28(2)	30(3)	46(3)	11(2)	6(2)	2(2)
C(26)	32(3)	36(3)	99(5)	14(3)	2(3)	0(2)
C(27)	71(4)	54(4)	68(4)	27(3)	36(3)	20(3)
C(28)	25(3)	35(3)	55(3)	12(3)	-3(2)	1(2)
C(29)	61(4)	46(3)	76(4)	3(3)	1(3)	31(3)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for 02145SLS.

	x	y	z	U(eq)
H(5)	2358	2148	2728	37
H(4)	3785	1700	4047	40
H(3)	6216	2226	3628	35
H(7A)	3580	4867	1985	75
H(7B)	3714	4991	884	75
H(7C)	4978	4988	1555	75
H(8A)	1840	1787	933	71
H(8B)	1797	2952	421	71
H(8C)	1684	3003	1542	71
H(9A)	5217	3177	448	68
H(9B)	3974	3230	-221	68
H(9C)	3949	1960	162	68
H(12A)	2598	-1851	4017	75
H(12B)	1747	-1389	3262	75
H(12C)	2616	-431	4147	75
H(13A)	3849	-2898	2525	76
H(13B)	4682	-2093	1786	76
H(13C)	3088	-2448	1707	76
H(14A)	5670	282	4268	77
H(14B)	6367	-272	3427	77
H(14C)	5520	-1170	4108	77
H(15)	7881	4238	3063	37
H(18)	9256	3685	4318	53
H(19)	10282	2640	5253	65
H(20)	10752	872	4617	67
H(21)	10152	34	3014	57
H(23)	8000	2039	919	42
H(24A)	8238	-732	1349	79
H(24B)	9752	-97	1143	79
H(24C)	8552	51	482	79
H(26A)	10689	6345	2273	87
H(26B)	10637	4936	2324	87
H(26C)	10113	5686	3161	87
H(27A)	7911	4417	573	92
H(27B)	9319	4188	766	92
H(27C)	9269	5544	620	92
H(29A)	7918	8130	3073	88
H(29B)	7259	7469	3938	88
H(29C)	6458	7128	2905	88

Table 6. Torsion angles [°] for 02145SLS.

C(11)-Fe(1)-Si(1)-C(12)	-66.5(3)
C(10)-Fe(1)-Si(1)-C(12)	-160.9(3)
C(5)-Fe(1)-Si(1)-C(12)	28.7(3)
C(4)-Fe(1)-Si(1)-C(12)	56.5(3)
N(1)-Fe(1)-Si(1)-C(12)	52.7(3)
C(3)-Fe(1)-Si(1)-C(12)	94.7(2)
B(1)-Fe(1)-Si(1)-C(12)	110.0(3)
C(11)-Fe(1)-Si(1)-C(14)	172.6(3)
C(10)-Fe(1)-Si(1)-C(14)	78.2(3)
C(5)-Fe(1)-Si(1)-C(14)	-92.2(3)
C(4)-Fe(1)-Si(1)-C(14)	-64.5(2)
N(1)-Fe(1)-Si(1)-C(14)	-68.2(3)
C(3)-Fe(1)-Si(1)-C(14)	-26.2(2)
B(1)-Fe(1)-Si(1)-C(14)	-11.0(3)
C(11)-Fe(1)-Si(1)-C(13)	53.3(3)
C(10)-Fe(1)-Si(1)-C(13)	-41.1(3)
C(5)-Fe(1)-Si(1)-C(13)	148.5(3)
C(4)-Fe(1)-Si(1)-C(13)	176.2(3)
N(1)-Fe(1)-Si(1)-C(13)	172.5(3)
C(3)-Fe(1)-Si(1)-C(13)	-145.5(2)
B(1)-Fe(1)-Si(1)-C(13)	-130.3(3)
C(11)-Fe(1)-N(1)-C(5)	80.2(3)
C(10)-Fe(1)-N(1)-C(5)	-176.6(3)
C(4)-Fe(1)-N(1)-C(5)	-37.9(3)
C(3)-Fe(1)-N(1)-C(5)	-80.2(3)
Si(1)-Fe(1)-N(1)-C(5)	-33.8(4)
B(1)-Fe(1)-N(1)-C(5)	-115.5(4)
C(11)-Fe(1)-N(1)-B(1)	-164.2(3)
C(10)-Fe(1)-N(1)-B(1)	-61.1(3)
C(5)-Fe(1)-N(1)-B(1)	115.5(4)
C(4)-Fe(1)-N(1)-B(1)	77.7(3)
C(3)-Fe(1)-N(1)-B(1)	35.4(3)
Si(1)-Fe(1)-N(1)-B(1)	81.8(4)
C(11)-Fe(1)-N(1)-C(6)	-34.7(4)
C(10)-Fe(1)-N(1)-C(6)	68.5(4)
C(5)-Fe(1)-N(1)-C(6)	-114.9(4)
C(4)-Fe(1)-N(1)-C(6)	-152.7(4)
C(3)-Fe(1)-N(1)-C(6)	165.0(4)
Si(1)-Fe(1)-N(1)-C(6)	-148.7(3)
B(1)-Fe(1)-N(1)-C(6)	129.6(5)
C(15)-O(3)-B(1)-N(1)	169.6(4)
C(15)-O(3)-B(1)-C(3)	-9.2(7)
C(15)-O(3)-B(1)-Fe(1)	-106.7(5)
C(5)-N(1)-B(1)-O(3)	-170.0(4)
C(6)-N(1)-B(1)-O(3)	-0.5(7)

Fe(1)-N(1)-B(1)-O(3)	129.6(4)
C(5)-N(1)-B(1)-C(3)	9.1(4)
C(6)-N(1)-B(1)-C(3)	178.7(4)
Fe(1)-N(1)-B(1)-C(3)	-51.2(3)
C(5)-N(1)-B(1)-Fe(1)	60.4(3)
C(6)-N(1)-B(1)-Fe(1)	-130.1(4)
C(11)-Fe(1)-B(1)-O(3)	-82.8(6)
C(10)-Fe(1)-B(1)-O(3)	17.2(5)
C(5)-Fe(1)-B(1)-O(3)	-149.1(5)
C(4)-Fe(1)-B(1)-O(3)	166.7(6)
N(1)-Fe(1)-B(1)-O(3)	-109.6(6)
C(3)-Fe(1)-B(1)-O(3)	127.7(6)
Si(1)-Fe(1)-B(1)-O(3)	103.3(5)
C(11)-Fe(1)-B(1)-N(1)	26.7(5)
C(10)-Fe(1)-B(1)-N(1)	126.8(3)
C(5)-Fe(1)-B(1)-N(1)	-39.5(2)
C(4)-Fe(1)-B(1)-N(1)	-83.7(3)
C(3)-Fe(1)-B(1)-N(1)	-122.7(4)
Si(1)-Fe(1)-B(1)-N(1)	-147.12(19)
C(11)-Fe(1)-B(1)-C(3)	149.5(4)
C(10)-Fe(1)-B(1)-C(3)	-110.5(3)
C(5)-Fe(1)-B(1)-C(3)	83.2(3)
C(4)-Fe(1)-B(1)-C(3)	39.0(3)
N(1)-Fe(1)-B(1)-C(3)	122.7(4)
Si(1)-Fe(1)-B(1)-C(3)	-24.4(3)
B(1)-N(1)-C(5)-C(4)	-4.3(5)
C(6)-N(1)-C(5)-C(4)	-174.5(4)
Fe(1)-N(1)-C(5)-C(4)	63.6(3)
B(1)-N(1)-C(5)-Fe(1)	-67.9(3)
C(6)-N(1)-C(5)-Fe(1)	121.9(4)
C(11)-Fe(1)-C(5)-C(4)	132.2(3)
C(10)-Fe(1)-C(5)-C(4)	-111.3(5)
N(1)-Fe(1)-C(5)-C(4)	-118.2(4)
C(3)-Fe(1)-C(5)-C(4)	-36.3(3)
Si(1)-Fe(1)-C(5)-C(4)	47.0(3)
B(1)-Fe(1)-C(5)-C(4)	-79.6(3)
C(11)-Fe(1)-C(5)-N(1)	-109.6(3)
C(10)-Fe(1)-C(5)-N(1)	6.9(6)
C(4)-Fe(1)-C(5)-N(1)	118.2(4)
C(3)-Fe(1)-C(5)-N(1)	81.9(3)
Si(1)-Fe(1)-C(5)-N(1)	165.12(19)
B(1)-Fe(1)-C(5)-N(1)	38.5(2)
N(1)-C(5)-C(4)-C(3)	-2.9(5)
Fe(1)-C(5)-C(4)-C(3)	61.8(3)
N(1)-C(5)-C(4)-Fe(1)	-64.7(3)
C(11)-Fe(1)-C(4)-C(5)	-60.3(3)
C(10)-Fe(1)-C(4)-C(5)	136.6(4)

N(1)-Fe(1)-C(4)-C(5)	37.8(3)
C(3)-Fe(1)-C(4)-C(5)	119.9(4)
Si(1)-Fe(1)-C(4)-C(5)	-140.6(3)
B(1)-Fe(1)-C(4)-C(5)	80.3(3)
C(11)-Fe(1)-C(4)-C(3)	179.7(3)
C(10)-Fe(1)-C(4)-C(3)	16.7(5)
C(5)-Fe(1)-C(4)-C(3)	-119.9(4)
N(1)-Fe(1)-C(4)-C(3)	-82.2(3)
Si(1)-Fe(1)-C(4)-C(3)	99.5(3)
B(1)-Fe(1)-C(4)-C(3)	-39.6(3)
C(5)-C(4)-C(3)-B(1)	8.7(5)
Fe(1)-C(4)-C(3)-B(1)	67.4(3)
C(5)-C(4)-C(3)-Fe(1)	-58.7(3)
O(3)-B(1)-C(3)-C(4)	168.1(5)
N(1)-B(1)-C(3)-C(4)	-10.8(5)
Fe(1)-B(1)-C(3)-C(4)	-61.7(3)
O(3)-B(1)-C(3)-Fe(1)	-130.1(5)
N(1)-B(1)-C(3)-Fe(1)	50.9(3)
C(11)-Fe(1)-C(3)-C(4)	-0.7(7)
C(10)-Fe(1)-C(3)-C(4)	-169.6(3)
C(5)-Fe(1)-C(3)-C(4)	37.1(3)
N(1)-Fe(1)-C(3)-C(4)	80.3(3)
Si(1)-Fe(1)-C(3)-C(4)	-82.7(3)
B(1)-Fe(1)-C(3)-C(4)	114.9(4)
C(11)-Fe(1)-C(3)-B(1)	-115.6(6)
C(10)-Fe(1)-C(3)-B(1)	75.5(3)
C(5)-Fe(1)-C(3)-B(1)	-77.9(3)
C(4)-Fe(1)-C(3)-B(1)	-114.9(4)
N(1)-Fe(1)-C(3)-B(1)	-34.7(3)
Si(1)-Fe(1)-C(3)-B(1)	162.3(2)
C(5)-N(1)-C(6)-C(9)	-140.1(4)
B(1)-N(1)-C(6)-C(9)	51.9(6)
Fe(1)-N(1)-C(6)-C(9)	-54.9(5)
C(5)-N(1)-C(6)-C(8)	-19.3(6)
B(1)-N(1)-C(6)-C(8)	172.7(4)
Fe(1)-N(1)-C(6)-C(8)	65.9(5)
C(5)-N(1)-C(6)-C(7)	100.6(5)
B(1)-N(1)-C(6)-C(7)	-67.4(6)
Fe(1)-N(1)-C(6)-C(7)	-174.1(3)
C(11)-Fe(1)-C(10)-O(1)	-15(9)
C(5)-Fe(1)-C(10)-O(1)	-132(8)
C(4)-Fe(1)-C(10)-O(1)	151(8)
N(1)-Fe(1)-C(10)-O(1)	-128(9)
C(3)-Fe(1)-C(10)-O(1)	162(9)
Si(1)-Fe(1)-C(10)-O(1)	66(9)
B(1)-Fe(1)-C(10)-O(1)	-161(9)
C(10)-Fe(1)-C(11)-O(2)	38(12)

C(5)-Fe(1)-C(11)-O(2)	-166(12)
C(4)-Fe(1)-C(11)-O(2)	-132(12)
N(1)-Fe(1)-C(11)-O(2)	155(12)
C(3)-Fe(1)-C(11)-O(2)	-131(11)
Si(1)-Fe(1)-C(11)-O(2)	-47(12)
B(1)-Fe(1)-C(11)-O(2)	138(12)
B(1)-O(3)-C(15)-C(16)	76.3(5)
B(1)-O(3)-C(15)-C(25)	-157.5(4)
O(3)-C(15)-C(16)-C(23)	43.8(6)
C(25)-C(15)-C(16)-C(23)	-77.3(6)
O(3)-C(15)-C(16)-C(17)	-132.3(4)
C(25)-C(15)-C(16)-C(17)	106.6(5)
C(23)-C(16)-C(17)-C(18)	-179.4(5)
C(15)-C(16)-C(17)-C(18)	-2.6(8)
C(23)-C(16)-C(17)-C(22)	-0.1(5)
C(15)-C(16)-C(17)-C(22)	176.8(4)
C(22)-C(17)-C(18)-C(19)	0.8(7)
C(16)-C(17)-C(18)-C(19)	-179.9(5)
C(17)-C(18)-C(19)-C(20)	0.3(8)
C(18)-C(19)-C(20)-C(21)	-1.0(9)
C(19)-C(20)-C(21)-C(22)	0.6(8)
C(23)-N(2)-C(22)-C(21)	-179.2(5)
C(24)-N(2)-C(22)-C(21)	7.3(8)
C(23)-N(2)-C(22)-C(17)	0.2(5)
C(24)-N(2)-C(22)-C(17)	-173.3(4)
C(20)-C(21)-C(22)-N(2)	179.8(5)
C(20)-C(21)-C(22)-C(17)	0.4(7)
C(18)-C(17)-C(22)-N(2)	179.4(4)
C(16)-C(17)-C(22)-N(2)	-0.1(5)
C(18)-C(17)-C(22)-C(21)	-1.2(7)
C(16)-C(17)-C(22)-C(21)	179.4(4)
C(17)-C(16)-C(23)-N(2)	0.2(5)
C(15)-C(16)-C(23)-N(2)	-176.5(4)
C(22)-N(2)-C(23)-C(16)	-0.3(6)
C(24)-N(2)-C(23)-C(16)	173.2(5)
O(3)-C(15)-C(25)-C(27)	-61.3(5)
C(16)-C(15)-C(25)-C(27)	63.0(6)
O(3)-C(15)-C(25)-C(28)	58.0(5)
C(16)-C(15)-C(25)-C(28)	-177.7(4)
O(3)-C(15)-C(25)-C(26)	175.5(4)
C(16)-C(15)-C(25)-C(26)	-60.1(6)
C(29)-O(5)-C(28)-O(4)	0.2(7)
C(29)-O(5)-C(28)-C(25)	179.5(4)
C(27)-C(25)-C(28)-O(4)	-7.6(7)
C(26)-C(25)-C(28)-O(4)	113.2(6)
C(15)-C(25)-C(28)-O(4)	-128.9(5)
C(27)-C(25)-C(28)-O(5)	173.2(4)

C(26)-C(25)-C(28)-O(5)	-66.0(5)
C(15)-C(25)-C(28)-O(5)	51.9(5)

A yellow pentane/benzene/ CH_2Cl_2 solution was prepared. Crystals suitable for X-ray structural analysis were obtained by solvent evaporation at -30°C .

A yellow block of dimensions $0.25 \times 0.2 \times 0.19 \text{ mm}^3$ was mounted under STP and transferred to a Bruker AXS/CCD three-circle diffractometer equipped with a cold stream of N_2 gas. An initial unit cell was determined with monochromated $\text{Mo K}\alpha$ radiation ($\lambda = 0.71073 \text{ \AA}$). The cell thus determined was monoclinic.

A hemisphere of data was then collected using ω scans of 0.30° and 30-s frames. The raw data frames were integrated using the Bruker program SAINT+ for NT version 6.01. The data that were collected (14741 total reflections, 4616 unique, $R_{\text{int}} = 0.1062$) had the following Miller index ranges: -11 to 11 in h , -27 to 27 in k , and -10 to 13 in l . No absorption correction was performed.

All aspects of the solution and refinement were handled by SHELXTL NT version 5.10. The structure was solved by direct methods in the chiral monoclinic space group $P2(1)/c$, $a = 10.4994(11) \text{ \AA}$; $b = 24.850(3) \text{ \AA}$; $c = 12.3176(14) \text{ \AA}$; $\alpha = 90^\circ$; $\beta = 92.295^\circ$; $\gamma = 90^\circ$, and refined using standard difference Fourier techniques. Final, full-matrix least-squares refinement (4616 data for 353 parameters) on F^2 yielded residuals of R_1 and wR_2 of 0.0439 and 0.1007 for data $I > 2\sigma(I)$, and 0.0737 and 0.1121 , respectively, for all data. During the final refinement all non-hydrogen atoms were treated anisotropically. Hydrogen atoms were included in calculated positions and refined isotropically on a riding model. No extinction coefficient was used in the refinement. Residual electron density amounted to a maximum of $0.443 \text{ e/\AA}^{-3}$ and a minimum of $-0.477 \text{ e/\AA}^{-3}$.

Tables 1-6 provide the full crystallographic data for the X-ray structure.

Table 1. Crystal data and structure refinement for 03211slm.

Identification code	03211slm	
Empirical formula	C ₂₈ H ₄₁ B Fe N ₂ O ₄ S Si	
Formula weight	596.44	
Temperature	193(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 10.4994(11) Å	a = 90°.
	b = 24.850(3) Å	b = 92.295(2)°.
	c = 12.3176(14) Å	g = 90°.
Volume	3211.2(6) Å ³	
Z	4	
Density (calculated)	1.234 Mg/m ³	
Absorption coefficient	0.605 mm ⁻¹	
F(000)	1264	
Crystal size	0.25 x 0.2 x 0.19 mm ³	
Theta range for data collection	1.64 to 23.28°.	
Index ranges	-11<=h<=11, -27<=k<=27, -10<=l<=13	
Reflections collected	14741	
Independent reflections	4616 [R(int) = 0.1062]	
Completeness to theta = 23.28°	99.7 %	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	4616 / 0 / 353	
Goodness-of-fit on F ²	0.924	
Final R indices [I>2sigma(I)]	R1 = 0.0439, wR2 = 0.1007	
R indices (all data)	R1 = 0.0737, wR2 = 0.1121	
Largest diff. peak and hole	0.443 and -0.477 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 03211slm. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Fe(1)	3858(1)	6649(1)	8178(1)	28(1)
S(1)	9834(1)	5931(1)	10939(1)	39(1)
Si(1)	1845(1)	6488(1)	7387(1)	43(1)
N(1)	5114(2)	6795(1)	9535(2)	31(1)
N(2)	5643(3)	4565(1)	7016(2)	37(1)
O(1)	6527(2)	6013(1)	9257(2)	31(1)
O(2)	3493(2)	7698(1)	7189(2)	53(1)
O(3)	4783(2)	6113(1)	6265(2)	48(1)
O(4)	7600(2)	5554(1)	11539(2)	44(1)
B(1)	5317(3)	6221(2)	9343(3)	30(1)
C(3)	3971(3)	5984(2)	9291(3)	36(1)
C(4)	3159(3)	6393(2)	9644(3)	40(1)
C(5)	3812(3)	6874(2)	9752(3)	38(1)
C(6)	6113(3)	7226(2)	9729(3)	39(1)
C(7)	6785(4)	7096(2)	10812(3)	65(1)
C(8)	7033(3)	7198(2)	8810(3)	55(1)
C(9)	5522(4)	7783(2)	9772(4)	64(1)
C(10)	4445(3)	6323(2)	7037(3)	33(1)
C(11)	3634(3)	7277(2)	7595(3)	36(1)
C(12)	1391(4)	5767(2)	7535(4)	69(1)
C(13)	1723(4)	6641(2)	5892(4)	73(2)
C(14)	572(3)	6910(2)	8017(4)	69(1)
C(15)	6711(3)	5434(1)	9296(3)	30(1)
C(16)	8099(3)	5365(2)	9699(3)	35(1)
C(17)	8346(3)	5598(1)	10814(3)	31(1)
C(18)	10130(3)	6090(2)	12391(3)	37(1)
C(19)	10163(3)	5575(2)	13056(3)	48(1)
C(20)	11457(3)	6348(2)	12422(3)	61(1)
C(21)	9150(3)	6484(2)	12791(3)	54(1)
C(22)	5029(4)	4079(2)	6589(3)	52(1)
C(23)	5659(3)	4725(1)	8077(3)	36(1)
C(24)	6424(3)	5171(1)	8237(3)	29(1)
C(25)	6916(3)	5295(1)	7196(3)	31(1)
C(26)	7724(3)	5697(2)	6814(3)	42(1)
C(27)	8011(4)	5690(2)	5724(3)	54(1)
C(28)	7520(4)	5306(2)	5020(3)	60(1)
C(29)	6715(3)	4904(2)	5363(3)	48(1)
C(30)	6424(3)	4909(2)	6458(3)	34(1)

Table 3. Bond lengths [Å] and angles [°] for 03211slm.

Fe(1)-C(11)	1.731(4)
Fe(1)-C(10)	1.755(4)
Fe(1)-C(5)	2.021(3)
Fe(1)-C(4)	2.077(3)
Fe(1)-N(1)	2.119(3)
Fe(1)-C(3)	2.147(3)
Fe(1)-B(1)	2.314(4)
Fe(1)-Si(1)	2.3264(11)
S(1)-C(17)	1.768(3)
S(1)-C(18)	1.846(4)
Si(1)-C(12)	1.865(4)
Si(1)-C(13)	1.879(4)
Si(1)-C(14)	1.890(4)
N(1)-C(5)	1.417(4)
N(1)-B(1)	1.462(5)
N(1)-C(6)	1.511(4)
N(2)-C(23)	1.366(4)
N(2)-C(30)	1.385(4)
N(2)-C(22)	1.458(4)
O(1)-B(1)	1.380(4)
O(1)-C(15)	1.451(4)
O(2)-C(11)	1.166(4)
O(3)-C(10)	1.153(4)
O(4)-C(17)	1.217(4)
B(1)-C(3)	1.530(5)
C(3)-C(4)	1.407(5)
C(4)-C(5)	1.382(5)
C(6)-C(7)	1.519(5)
C(6)-C(8)	1.519(5)
C(6)-C(9)	1.518(5)
C(15)-C(24)	1.479(5)
C(15)-C(16)	1.531(4)
C(16)-C(17)	1.504(5)
C(18)-C(19)	1.517(5)
C(18)-C(21)	1.518(5)
C(18)-C(20)	1.533(5)
C(23)-C(24)	1.377(5)
C(24)-C(25)	1.436(4)
C(25)-C(26)	1.404(5)
C(25)-C(30)	1.405(5)
C(26)-C(27)	1.388(5)
C(27)-C(28)	1.377(6)
C(28)-C(29)	1.385(5)
C(29)-C(30)	1.395(5)

C(11)-Fe(1)-C(10)	97.48(16)
C(11)-Fe(1)-C(5)	98.04(16)
C(10)-Fe(1)-C(5)	156.77(14)
C(11)-Fe(1)-C(4)	126.16(15)
C(10)-Fe(1)-C(4)	134.69(16)
C(5)-Fe(1)-C(4)	39.39(14)
C(11)-Fe(1)-N(1)	104.00(14)
C(10)-Fe(1)-N(1)	118.93(13)
C(5)-Fe(1)-N(1)	39.94(11)
C(4)-Fe(1)-N(1)	66.21(13)
C(11)-Fe(1)-C(3)	164.18(15)
C(10)-Fe(1)-C(3)	98.30(15)
C(5)-Fe(1)-C(3)	66.62(15)
C(4)-Fe(1)-C(3)	38.87(13)
N(1)-Fe(1)-C(3)	67.14(13)
C(11)-Fe(1)-B(1)	138.28(16)
C(10)-Fe(1)-B(1)	92.29(14)
C(5)-Fe(1)-B(1)	64.71(14)
C(4)-Fe(1)-B(1)	64.44(13)
N(1)-Fe(1)-B(1)	38.20(13)
C(3)-Fe(1)-B(1)	39.89(13)
C(11)-Fe(1)-Si(1)	82.84(12)
C(10)-Fe(1)-Si(1)	85.86(11)
C(5)-Fe(1)-Si(1)	113.16(10)
C(4)-Fe(1)-Si(1)	87.99(10)
N(1)-Fe(1)-Si(1)	152.40(8)
C(3)-Fe(1)-Si(1)	99.30(10)
B(1)-Fe(1)-Si(1)	138.47(11)
C(17)-S(1)-C(18)	107.36(16)
C(12)-Si(1)-C(13)	106.4(2)
C(12)-Si(1)-C(14)	107.7(2)
C(13)-Si(1)-C(14)	105.6(2)
C(12)-Si(1)-Fe(1)	110.82(14)
C(13)-Si(1)-Fe(1)	113.61(14)
C(14)-Si(1)-Fe(1)	112.23(16)
C(5)-N(1)-B(1)	108.3(3)
C(5)-N(1)-C(6)	122.8(3)
B(1)-N(1)-C(6)	127.7(3)
C(5)-N(1)-Fe(1)	66.32(18)
B(1)-N(1)-Fe(1)	78.16(19)
C(6)-N(1)-Fe(1)	130.7(2)
C(23)-N(2)-C(30)	108.1(3)
C(23)-N(2)-C(22)	125.1(3)
C(30)-N(2)-C(22)	126.5(3)
B(1)-O(1)-C(15)	119.5(3)
O(1)-B(1)-N(1)	121.3(3)
O(1)-B(1)-C(3)	134.7(3)

N(1)-B(1)-C(3)	104.0(3)
O(1)-B(1)-Fe(1)	135.5(2)
N(1)-B(1)-Fe(1)	63.64(18)
C(3)-B(1)-Fe(1)	64.15(18)
C(4)-C(3)-B(1)	106.2(3)
C(4)-C(3)-Fe(1)	67.9(2)
B(1)-C(3)-Fe(1)	76.0(2)
C(5)-C(4)-C(3)	110.5(3)
C(5)-C(4)-Fe(1)	68.1(2)
C(3)-C(4)-Fe(1)	73.26(19)
C(4)-C(5)-N(1)	109.9(3)
C(4)-C(5)-Fe(1)	72.5(2)
N(1)-C(5)-Fe(1)	73.74(18)
N(1)-C(6)-C(7)	106.5(3)
N(1)-C(6)-C(8)	108.0(3)
C(7)-C(6)-C(8)	111.0(3)
N(1)-C(6)-C(9)	111.7(3)
C(7)-C(6)-C(9)	109.8(3)
C(8)-C(6)-C(9)	109.9(3)
O(3)-C(10)-Fe(1)	177.2(3)
O(2)-C(11)-Fe(1)	179.0(3)
O(1)-C(15)-C(24)	112.8(3)
O(1)-C(15)-C(16)	104.3(3)
C(24)-C(15)-C(16)	113.2(3)
C(17)-C(16)-C(15)	112.3(3)
O(4)-C(17)-C(16)	122.9(3)
O(4)-C(17)-S(1)	124.8(3)
C(16)-C(17)-S(1)	112.3(2)
C(19)-C(18)-C(21)	111.8(3)
C(19)-C(18)-C(20)	109.7(3)
C(21)-C(18)-C(20)	110.4(3)
C(19)-C(18)-S(1)	110.0(3)
C(21)-C(18)-S(1)	111.2(3)
C(20)-C(18)-S(1)	103.3(2)
N(2)-C(23)-C(24)	110.8(3)
C(23)-C(24)-C(25)	105.9(3)
C(23)-C(24)-C(15)	125.4(3)
C(25)-C(24)-C(15)	128.6(3)
C(26)-C(25)-C(30)	118.7(3)
C(26)-C(25)-C(24)	134.1(3)
C(30)-C(25)-C(24)	107.1(3)
C(27)-C(26)-C(25)	118.2(4)
C(28)-C(27)-C(26)	121.8(4)
C(29)-C(28)-C(27)	121.7(4)
C(28)-C(29)-C(30)	116.6(4)
N(2)-C(30)-C(29)	129.1(3)
N(2)-C(30)-C(25)	108.0(3)

C(29)-C(30)-C(25)

122.9(3)

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 03211slm. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2 a^{*2}U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Fe(1)	25(1)	34(1)	27(1)	3(1)	7(1)	4(1)
S(1)	31(1)	52(1)	35(1)	-4(1)	7(1)	-6(1)
Si(1)	27(1)	50(1)	52(1)	7(1)	0(1)	0(1)
N(1)	28(2)	35(2)	29(2)	-2(1)	4(1)	8(1)
N(2)	38(2)	37(2)	36(2)	-9(2)	-1(1)	-7(2)
O(1)	27(1)	29(1)	35(1)	-3(1)	1(1)	3(1)
O(2)	64(2)	43(2)	52(2)	14(2)	11(1)	15(1)
O(3)	55(2)	54(2)	35(2)	-9(1)	5(1)	11(1)
O(4)	32(1)	64(2)	36(2)	-3(1)	5(1)	-6(1)
B(1)	32(2)	38(3)	19(2)	3(2)	3(2)	3(2)
C(3)	33(2)	40(2)	36(2)	16(2)	8(2)	4(2)
C(4)	32(2)	53(3)	34(2)	11(2)	10(2)	8(2)
C(5)	38(2)	52(3)	26(2)	1(2)	10(2)	19(2)
C(6)	43(2)	33(2)	41(2)	-6(2)	-2(2)	2(2)
C(7)	71(3)	64(3)	58(3)	-14(2)	-19(2)	2(2)
C(8)	48(2)	46(3)	71(3)	-3(2)	13(2)	-12(2)
C(9)	70(3)	35(2)	86(3)	-13(2)	-4(3)	6(2)
C(10)	27(2)	39(2)	34(2)	6(2)	1(2)	1(2)
C(11)	32(2)	46(3)	30(2)	1(2)	8(2)	7(2)
C(12)	41(2)	58(3)	106(4)	-3(3)	-11(2)	-7(2)
C(13)	47(2)	113(4)	58(3)	5(3)	-16(2)	1(3)
C(14)	35(2)	80(3)	93(4)	16(3)	14(2)	17(2)
C(15)	27(2)	31(2)	31(2)	0(2)	4(2)	4(2)
C(16)	32(2)	35(2)	37(2)	-7(2)	1(2)	7(2)
C(17)	29(2)	29(2)	36(2)	-1(2)	-1(2)	6(2)
C(18)	28(2)	45(2)	37(2)	-3(2)	2(2)	-5(2)
C(19)	42(2)	55(3)	46(3)	1(2)	-1(2)	1(2)
C(20)	49(2)	81(3)	52(3)	-4(3)	-3(2)	-28(2)
C(21)	54(2)	58(3)	48(3)	-18(2)	-2(2)	16(2)
C(22)	50(2)	48(3)	58(3)	-14(2)	-3(2)	-10(2)
C(23)	38(2)	37(2)	32(2)	1(2)	3(2)	2(2)
C(24)	26(2)	31(2)	30(2)	-1(2)	3(2)	4(2)
C(25)	21(2)	38(2)	35(2)	-1(2)	3(2)	2(2)
C(26)	30(2)	52(3)	43(2)	-1(2)	2(2)	-3(2)
C(27)	40(2)	77(3)	47(3)	3(2)	14(2)	-14(2)
C(28)	48(2)	96(4)	36(3)	-3(3)	16(2)	-9(2)
C(29)	39(2)	67(3)	38(2)	-15(2)	2(2)	4(2)
C(30)	26(2)	41(2)	34(2)	-4(2)	3(2)	2(2)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for 03211slm.

	x	y	z	U(eq)
H(3)	3733	5602	9130	44
H(4)	2235	6343	9788	48
H(5)	3439	7218	10015	46
H(7A)	6157	7078	11378	97
H(7B)	7410	7378	10995	97
H(7C)	7222	6749	10761	97
H(8A)	7395	6835	8775	82
H(8B)	7721	7460	8941	82
H(8C)	6578	7282	8120	82
H(9A)	4982	7843	9116	96
H(9B)	6199	8054	9813	96
H(9C)	5005	7811	10415	96
H(12A)	581	5700	7133	103
H(12B)	1296	5684	8305	103
H(12C)	2056	5538	7244	103
H(13A)	2386	6443	5521	110
H(13B)	1838	7028	5780	110
H(13C)	882	6532	5596	110
H(14A)	-251	6842	7638	104
H(14B)	790	7292	7955	104
H(14C)	516	6814	8786	104
H(15)	6142	5279	9848	36
H(16A)	8312	4977	9714	42
H(16B)	8663	5543	9183	42
H(19A)	10331	5663	13824	72
H(19B)	10841	5340	12805	72
H(19C)	9341	5391	12969	72
H(20A)	11718	6432	13175	91
H(20B)	11431	6679	11991	91
H(20C)	12069	6097	12120	91
H(21A)	8301	6320	12733	80
H(21B)	9159	6812	12347	80
H(21C)	9357	6576	13552	80
H(22A)	5657	3788	6567	78
H(22B)	4677	4149	5853	78
H(22C)	4341	3974	7060	78
H(23)	5204	4552	8630	43
H(26)	8064	5967	7289	50
H(27)	8563	5958	5457	65
H(28)	7739	5316	4280	72
H(29)	6378	4638	4878	58

Table 6. Torsion angles [°] for 03211slm.

C(11)-Fe(1)-Si(1)-C(12)	173.2(2)
C(10)-Fe(1)-Si(1)-C(12)	75.1(2)
C(5)-Fe(1)-Si(1)-C(12)	-91.1(2)
C(4)-Fe(1)-Si(1)-C(12)	-60.0(2)
N(1)-Fe(1)-Si(1)-C(12)	-80.2(3)
C(3)-Fe(1)-Si(1)-C(12)	-22.6(2)
B(1)-Fe(1)-Si(1)-C(12)	-13.7(2)
C(11)-Fe(1)-Si(1)-C(13)	53.4(2)
C(10)-Fe(1)-Si(1)-C(13)	-44.7(2)
C(5)-Fe(1)-Si(1)-C(13)	149.1(2)
C(4)-Fe(1)-Si(1)-C(13)	-179.7(2)
N(1)-Fe(1)-Si(1)-C(13)	160.0(2)
C(3)-Fe(1)-Si(1)-C(13)	-142.4(2)
B(1)-Fe(1)-Si(1)-C(13)	-133.4(2)
C(11)-Fe(1)-Si(1)-C(14)	-66.3(2)
C(10)-Fe(1)-Si(1)-C(14)	-164.4(2)
C(5)-Fe(1)-Si(1)-C(14)	29.4(2)
C(4)-Fe(1)-Si(1)-C(14)	60.53(19)
N(1)-Fe(1)-Si(1)-C(14)	40.3(2)
C(3)-Fe(1)-Si(1)-C(14)	97.86(19)
B(1)-Fe(1)-Si(1)-C(14)	106.8(2)
C(11)-Fe(1)-N(1)-C(5)	85.8(2)
C(10)-Fe(1)-N(1)-C(5)	-167.3(2)
C(4)-Fe(1)-N(1)-C(5)	-37.9(2)
C(3)-Fe(1)-N(1)-C(5)	-80.4(2)
B(1)-Fe(1)-N(1)-C(5)	-116.2(3)
Si(1)-Fe(1)-N(1)-C(5)	-15.7(3)
C(11)-Fe(1)-N(1)-B(1)	-158.0(2)
C(10)-Fe(1)-N(1)-B(1)	-51.1(2)
C(5)-Fe(1)-N(1)-B(1)	116.2(3)
C(4)-Fe(1)-N(1)-B(1)	78.3(2)
C(3)-Fe(1)-N(1)-B(1)	35.85(19)
Si(1)-Fe(1)-N(1)-B(1)	100.5(2)
C(11)-Fe(1)-N(1)-C(6)	-27.9(3)
C(10)-Fe(1)-N(1)-C(6)	79.0(3)
C(5)-Fe(1)-N(1)-C(6)	-113.7(4)
C(4)-Fe(1)-N(1)-C(6)	-151.6(3)
C(3)-Fe(1)-N(1)-C(6)	165.9(3)
B(1)-Fe(1)-N(1)-C(6)	130.1(3)
Si(1)-Fe(1)-N(1)-C(6)	-129.4(2)
C(15)-O(1)-B(1)-N(1)	167.1(3)
C(15)-O(1)-B(1)-C(3)	-12.3(5)
C(15)-O(1)-B(1)-Fe(1)	-109.9(4)
C(5)-N(1)-B(1)-O(1)	-171.0(3)
C(6)-N(1)-B(1)-O(1)	-3.7(5)

Fe(1)-N(1)-B(1)-O(1)	129.1(3)
C(5)-N(1)-B(1)-C(3)	8.6(4)
C(6)-N(1)-B(1)-C(3)	175.8(3)
Fe(1)-N(1)-B(1)-C(3)	-51.3(2)
C(5)-N(1)-B(1)-Fe(1)	59.9(2)
C(6)-N(1)-B(1)-Fe(1)	-132.9(3)
C(11)-Fe(1)-B(1)-O(1)	-75.7(4)
C(10)-Fe(1)-B(1)-O(1)	28.2(4)
C(5)-Fe(1)-B(1)-O(1)	-148.4(4)
C(4)-Fe(1)-B(1)-O(1)	167.8(4)
N(1)-Fe(1)-B(1)-O(1)	-108.8(4)
C(3)-Fe(1)-B(1)-O(1)	128.4(5)
Si(1)-Fe(1)-B(1)-O(1)	114.6(3)
C(11)-Fe(1)-B(1)-N(1)	33.1(3)
C(10)-Fe(1)-B(1)-N(1)	137.1(2)
C(5)-Fe(1)-B(1)-N(1)	-39.56(19)
C(4)-Fe(1)-B(1)-N(1)	-83.4(2)
C(3)-Fe(1)-B(1)-N(1)	-122.7(3)
Si(1)-Fe(1)-B(1)-N(1)	-136.61(16)
C(11)-Fe(1)-B(1)-C(3)	155.8(2)
C(10)-Fe(1)-B(1)-C(3)	-100.2(2)
C(5)-Fe(1)-B(1)-C(3)	83.2(2)
C(4)-Fe(1)-B(1)-C(3)	39.3(2)
N(1)-Fe(1)-B(1)-C(3)	122.7(3)
Si(1)-Fe(1)-B(1)-C(3)	-13.9(3)
O(1)-B(1)-C(3)-C(4)	169.0(4)
N(1)-B(1)-C(3)-C(4)	-10.5(4)
Fe(1)-B(1)-C(3)-C(4)	-61.5(2)
O(1)-B(1)-C(3)-Fe(1)	-129.5(4)
N(1)-B(1)-C(3)-Fe(1)	51.0(2)
C(11)-Fe(1)-C(3)-C(4)	21.6(6)
C(10)-Fe(1)-C(3)-C(4)	-162.1(2)
C(5)-Fe(1)-C(3)-C(4)	36.4(2)
N(1)-Fe(1)-C(3)-C(4)	80.0(2)
B(1)-Fe(1)-C(3)-C(4)	114.3(3)
Si(1)-Fe(1)-C(3)-C(4)	-74.9(2)
C(11)-Fe(1)-C(3)-B(1)	-92.7(5)
C(10)-Fe(1)-C(3)-B(1)	83.6(2)
C(5)-Fe(1)-C(3)-B(1)	-78.0(2)
C(4)-Fe(1)-C(3)-B(1)	-114.3(3)
N(1)-Fe(1)-C(3)-B(1)	-34.38(19)
Si(1)-Fe(1)-C(3)-B(1)	170.72(18)
B(1)-C(3)-C(4)-C(5)	8.8(4)
Fe(1)-C(3)-C(4)-C(5)	-58.2(3)
B(1)-C(3)-C(4)-Fe(1)	67.0(2)
C(11)-Fe(1)-C(4)-C(5)	-51.9(3)
C(10)-Fe(1)-C(4)-C(5)	146.3(2)

N(1)-Fe(1)-C(4)-C(5)	38.41(19)
C(3)-Fe(1)-C(4)-C(5)	121.0(3)
B(1)-Fe(1)-C(4)-C(5)	80.6(2)
Si(1)-Fe(1)-C(4)-C(5)	-131.51(19)
C(11)-Fe(1)-C(4)-C(3)	-172.8(2)
C(10)-Fe(1)-C(4)-C(3)	25.4(3)
C(5)-Fe(1)-C(4)-C(3)	-121.0(3)
N(1)-Fe(1)-C(4)-C(3)	-82.5(2)
B(1)-Fe(1)-C(4)-C(3)	-40.4(2)
Si(1)-Fe(1)-C(4)-C(3)	107.5(2)
C(3)-C(4)-C(5)-N(1)	-3.5(4)
Fe(1)-C(4)-C(5)-N(1)	-64.7(2)
C(3)-C(4)-C(5)-Fe(1)	61.2(3)
B(1)-N(1)-C(5)-C(4)	-3.7(4)
C(6)-N(1)-C(5)-C(4)	-171.7(3)
Fe(1)-N(1)-C(5)-C(4)	63.9(2)
B(1)-N(1)-C(5)-Fe(1)	-67.6(2)
C(6)-N(1)-C(5)-Fe(1)	124.4(3)
C(11)-Fe(1)-C(5)-C(4)	140.1(2)
C(10)-Fe(1)-C(5)-C(4)	-88.4(4)
N(1)-Fe(1)-C(5)-C(4)	-117.7(3)
C(3)-Fe(1)-C(5)-C(4)	-35.89(19)
B(1)-Fe(1)-C(5)-C(4)	-79.8(2)
Si(1)-Fe(1)-C(5)-C(4)	54.5(2)
C(11)-Fe(1)-C(5)-N(1)	-102.2(2)
C(10)-Fe(1)-C(5)-N(1)	29.3(5)
C(4)-Fe(1)-C(5)-N(1)	117.7(3)
C(3)-Fe(1)-C(5)-N(1)	81.8(2)
B(1)-Fe(1)-C(5)-N(1)	37.85(19)
Si(1)-Fe(1)-C(5)-N(1)	172.15(15)
C(5)-N(1)-C(6)-C(7)	99.1(4)
B(1)-N(1)-C(6)-C(7)	-66.4(4)
Fe(1)-N(1)-C(6)-C(7)	-175.3(2)
C(5)-N(1)-C(6)-C(8)	-141.6(3)
B(1)-N(1)-C(6)-C(8)	52.8(4)
Fe(1)-N(1)-C(6)-C(8)	-56.0(4)
C(5)-N(1)-C(6)-C(9)	-20.7(5)
B(1)-N(1)-C(6)-C(9)	173.7(3)
Fe(1)-N(1)-C(6)-C(9)	64.9(4)
C(11)-Fe(1)-C(10)-O(3)	-63(7)
C(5)-Fe(1)-C(10)-O(3)	166(6)
C(4)-Fe(1)-C(10)-O(3)	103(7)
N(1)-Fe(1)-C(10)-O(3)	-173(100)
C(3)-Fe(1)-C(10)-O(3)	118(7)
B(1)-Fe(1)-C(10)-O(3)	158(7)
Si(1)-Fe(1)-C(10)-O(3)	20(7)
C(10)-Fe(1)-C(11)-O(2)	-7(20)

C(5)-Fe(1)-C(11)-O(2)	156(20)
C(4)-Fe(1)-C(11)-O(2)	-174(100)
N(1)-Fe(1)-C(11)-O(2)	116(20)
C(3)-Fe(1)-C(11)-O(2)	169(100)
B(1)-Fe(1)-C(11)-O(2)	95(20)
Si(1)-Fe(1)-C(11)-O(2)	-92(20)
B(1)-O(1)-C(15)-C(24)	81.9(3)
B(1)-O(1)-C(15)-C(16)	-154.9(3)
O(1)-C(15)-C(16)-C(17)	61.5(4)
C(24)-C(15)-C(16)-C(17)	-175.6(3)
C(15)-C(16)-C(17)-O(4)	40.5(5)
C(15)-C(16)-C(17)-S(1)	-140.2(3)
C(18)-S(1)-C(17)-O(4)	9.0(4)
C(18)-S(1)-C(17)-C(16)	-170.3(2)
C(17)-S(1)-C(18)-C(19)	60.1(3)
C(17)-S(1)-C(18)-C(21)	-64.4(3)
C(17)-S(1)-C(18)-C(20)	177.2(3)
C(30)-N(2)-C(23)-C(24)	0.5(4)
C(22)-N(2)-C(23)-C(24)	173.9(3)
N(2)-C(23)-C(24)-C(25)	0.0(4)
N(2)-C(23)-C(24)-C(15)	-176.8(3)
O(1)-C(15)-C(24)-C(23)	-130.8(3)
C(16)-C(15)-C(24)-C(23)	111.1(4)
O(1)-C(15)-C(24)-C(25)	53.1(4)
C(16)-C(15)-C(24)-C(25)	-65.0(4)
C(23)-C(24)-C(25)-C(26)	179.2(4)
C(15)-C(24)-C(25)-C(26)	-4.1(6)
C(23)-C(24)-C(25)-C(30)	-0.6(4)
C(15)-C(24)-C(25)-C(30)	176.1(3)
C(30)-C(25)-C(26)-C(27)	-0.8(5)
C(24)-C(25)-C(26)-C(27)	179.5(4)
C(25)-C(26)-C(27)-C(28)	0.5(6)
C(26)-C(27)-C(28)-C(29)	-0.2(6)
C(27)-C(28)-C(29)-C(30)	0.2(6)
C(23)-N(2)-C(30)-C(29)	179.4(4)
C(22)-N(2)-C(30)-C(29)	6.2(6)
C(23)-N(2)-C(30)-C(25)	-0.9(4)
C(22)-N(2)-C(30)-C(25)	-174.1(3)
C(28)-C(29)-C(30)-N(2)	179.2(3)
C(28)-C(29)-C(30)-C(25)	-0.5(5)
C(26)-C(25)-C(30)-N(2)	-178.9(3)
C(24)-C(25)-C(30)-N(2)	0.9(4)
C(26)-C(25)-C(30)-C(29)	0.8(5)
C(24)-C(25)-C(30)-C(29)	-179.4(3)

VII. Mechanistic Studies

Sample procedure for examining the order of the reaction in each reaction component (for the general procedure, see Section 4: entry 4 of Table 1). The Mukaiyama aldol reactions were monitored by ^1H NMR at 20 °C. Iron complex ($\pm$)-**1** (21.0 mg, 0.0440 mmol), indole-3-carboxaldehyde (14.0 mg, 0.880 mmol), and hexamethylbenzene (internal standard; 4.5 mg, 0.028 mmol) were dissolved in CD_3CN (1.23 mL), thereby generating a solution that was 0.0358 M in ($\pm$)-**1** and 0.0715 M in indole-3-carboxaldehyde ("Solution A"). Solution A (0.35 mL) was added to each of three J. Young NMR tubes, followed by the nucleophile [4.0 μL (0.013 mmol), 8.5 μL (0.028 mmol), 17.0 μL (0.0560 mmol)]. The time of mixing was taken as t_0 . The conversion of reactants to products at 20 °C was determined by integrating the resonances corresponding to the trimethylsilyl group of ($\pm$)-**1** versus the internal standard. The data are graphed below.

Variation in the concentration of nucleophile

Variation in the concentration of aldehyde

Variation in the concentration of (±)-1

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