N_2 Binding to an Iron-Sulfur-Carbon Site

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Supplementary Information

Supplementary Methods 2

Synthesis of LH_2 4

Synthesis of thiolate 4 8

Synthesis of iron complexes 10

Supplementary References 20

Supplementary Data 22

Magnetic Susceptibility Measurements 22

DFT Calculations 25

IR Spectra 29

UV-VIS Spectra 32

NMR Spectra 34

Mössbauer Spectra 36

EPR Spectra 38

Crystallographic Data 39

Supplementary Methods

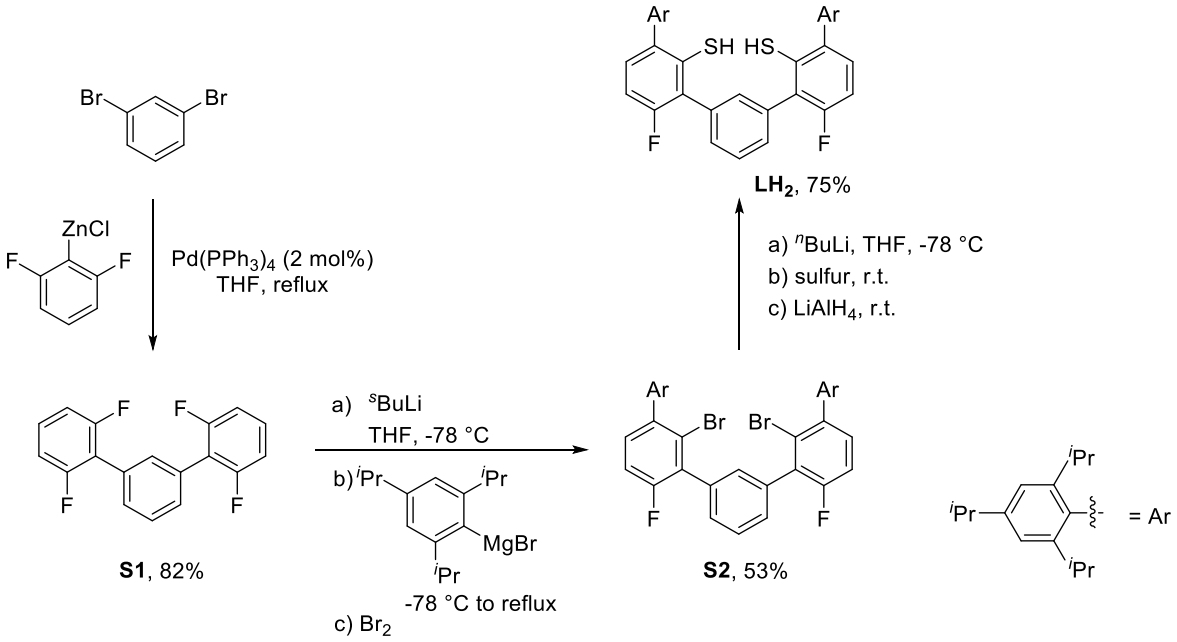
General Information. Unless otherwise stated, all manipulations were performed under a nitrogen atmosphere using Schlenk techniques or in an M. Braun glovebox maintained at or below 1 ppm of O_2 and H_2O. All new iron complexes were prepared and handled in the glovebox under N_2 atmosphere. Unless otherwise stated, all reagents were purchased from commercial suppliers and used without further purification. Perfluoropolyether oil Fomblin® Y with average molecular weight of 1800 g/mol was purchased from Sigma-Aldrich, degassed under vacuum overnight, and kept over 4 Å molecular sieves in a N_2-filled glovebox. Sulfur (99.999%) was purchased from Strem Chemicals. $Fe(N(SiMe_3)_2)_2$ was prepared according to the literature procedure[31], however in our hands distilled product was found to contain some of what is probably THF adduct $Fe(N(SiMe_3)_2)_2(THF)$[32], and the amount used in the reaction was adjusted to account for THF present (determined by ^1H NMR analysis of a solution in THF-d_8). Solid commercial potassium bis(trimethylsilyl)amide was triturated with hexane, dried, and crystallized from toluene at -40 °C prior to use. Glassware was dried at 150 °C overnight, and Celite was dried at 200 °C under vacuum. Pentane, hexane, and diethyl ether were purified by passage through activated alumina and Q5 columns from Glass Contour Co. THF was distilled from a potassium benzophenone ketyl solution under argon. Butane was vacuum transferred from potassium/benzophenone mixture which had been stirred at room temperature for several days. All solvents were stored over activated 4Å molecular sieves. Organic reactions were monitored by thin layer chromatography on silica gel pre-coated plastic sheets with fluorescent indicator (0.2 mm, Macherey-Nagel). Visualization was accomplished by irradiation with UV light at 254 nm. Column chromatography was performed on silica gel (Fisher Chemical, particle size 0.040-0.063 mm).

NMR data were recorded on Agilent DD2 400 MHz, Agilent DD2 500 MHz, or Agilent DD2 600 MHz spectrometers in deuterated solvents. Chemical shifts in ^1H NMR spectra were referenced

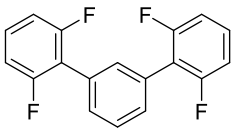
using residual solvent protons (THF-d_8 (1.73 ppm), C_6D_6 (7.16 ppm), $CDCl_3$ (7.26 ppm)), and reported in ppm (δ) relative to tetramethylsilane. Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, q = quartet, 7-et = heptet, m = multiplet, br = broad), coupling constants (Hz) and integration. Resonances in ^{13}C NMR and ^{19}F NMR spectra are referenced using absolute referencing, and reported in ppm (δ) relative to tetramethylsilane and CCl_3F, respectively. High resolution mass spectrometry (HRMS) measurements were performed on a Bruker Apex 9.4T Fourier Transform Ion Cyclotron Resonance Mass Spectrometer (Keck Biotechnology Resource Laboratory at Yale University) or a Waters 70-VSE (University of Illinois SCS Mass Spectrometry Laboratory). Elemental analyses were performed at the CENTC Elemental Analysis Facility at the University of Rochester. Microanalysis samples were weighed with a PerkinElmer Model AD-6 Autobalance and their compositions were determined with a PerkinElmer 2400 Series II Analyzer, and handled in a VAC Atmospheres glovebox under argon. IR data were recorded on a Bruker Alpha spectrometer equipped with a Platinum ATR attachment. The spectra often have an instrumental artifact around 2200 cm^{-1}, showing a "negative" peak that we have been unable to eliminate. Mössbauer data were recorded on a SEE Co. MS4 Mössbauer spectrometer with alternating constant acceleration integrated with a Janis SVT-400T He/N_2 cryostat for measurements at 80 K with a 0.07 T applied magnetic field. Isomer shifts were determined relative to α-Fe at 298 K. All Mössbauer spectra were fit to Lorentzian doublets using the program WMoss (SEE Co.). UV-vis spectra were recorded on a Cary 60 spectrophotometer using Schlenk-adapted quartz cuvettes with a 1 mm optical path length unless otherwise specified. Solution magnetic susceptibilities were determined by the Evans method[33]. X-band EPR spectra were recorded on a Bruker ELEXSYS E500 EPR spectrometer equipped with an SHQ resonator and an Oxford Instruments ESR-900 helium-flow cryostat. EPR spectra were simulated using the "pepper" function in

EasySpin version 4.5.5, with H-strain option to describe anisotropic broadening from unresolved hyperfine interactions[34].

Synthesis of LH_2



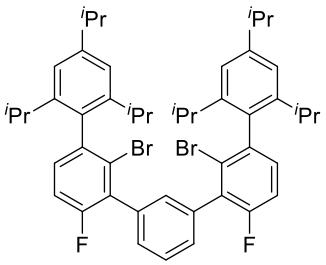
2,2'',6,6''-Tetrafluoro-1,1':3',1''-terphenyl (S1)



A 2.5 M solution of ^{n}BuLi in hexanes (12.8 mL, 32.0 mmol) at room temperature was added slowly to a solution of 1,3-difluorobenzene (3.65 g, 32.0 mmol) in THF (48 mL) at -78 °C under N_2 atmosphere. After stirring for 70 min at -78 °C, a 1.9 M solution of $ZnCl_2$ in 2-methyltetrahydrofuran (19.6 mL, 37.3 mmol) at room temperature was added slowly to the cold reaction mixture. The resulting mixture was stirred for 5 min at -78 °C, the cooling bath was then removed, and the mixture was allowed to warm to room temperature with stirring. 1,3-Dibromobenzene (2.52 g, 10.7 mmol) and $Pd(PPh)_4$ were added to the mixture at room temperature under N_2 atmosphere. The resulting mixture was heated to reflux (oil bath heating) for 24 h, then kept at room temperature for 2 days. The mixture was exposed to air, the solvent was removed under reduced pressure and the residue was separated between water (50 mL) and hexane (50 mL). The organic layer was collected, and

the aqueous layer was extracted with hexane (2 × 30 mL). The combined organic extracts were dried ($MgSO_4$), filtered, and the solvent was removed under reduced pressure. The residue was purified by column chromatography on silica gel using hexane as the eluent yielding the title compound as a colorless oil that crystalizes upon standing at room temperature (2.64 g, 82%).^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (s, 1H), 7.59 – 7.49 (m, 3H), 7.35 – 7.24 (m, 2H), 7.05 – 6.95 (m, 4H). $^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$) δ 160.1 (dd, J = 248.9, 7.0 Hz), 132.3 (quintet, J = 1.9 Hz), 130.1 (t, J = 2.0 Hz), 129.2, 129.0 (t, J = 10.4 Hz), 128.2, 118.1 (t, J = 18.5 Hz), 112.0 – 111.3 (m). ^{19}F NMR (376 MHz, $CDCl_3$) δ -114.37 – -114.48 (m). HRMS (ESI^+) (*m/z*): [M+Na] calcd for $C_{18}H_{10}F_4Na$, 325.0611; found, 325.0608.

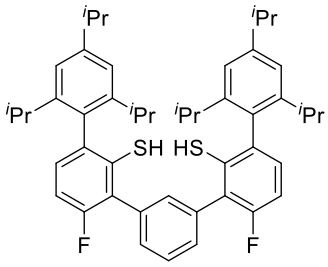
Dibromide S2



To Mg turnings (1.13 g, 46.4 mmol) activated with 1,2-dibromoethane (0.1 mL) in THF (5 mL) under N_2 atmosphere, 1-bromo-2,4,6-triisopropylbenzene (11.95 g, 42.2 mmol) and THF (35 mL) were added alternately. Heating was applied with a heat gun early in the reaction to initiate the reaction, and then the rate of addition was varied to maintain reflux. After complete addition, the mixture was heated to reflux (oil bath heating) for 20 h, and allowed to cool to room temperature briefly before it was added to the reaction mixture below. In a separate flask, a 1.4 M solution of ^{s}BuLi in cyclohexane (12.7 mL, 17.7 mmol) was added dropwise to a solution of 2,2'',6,6''-tetrafluoro-1,1':3',1''-terphenyl (**S1**, 2.55 g, 8.44 mmol) in THF (44 mL) at -78 °C under N_2 atmosphere. After being stirred for 20 min at -78 °C, to the reaction mixture the Grignard solution prepared above was added via syringe (first half dropwise). After complete addition the cooling bath was removed, and the mixture was allowed to warm to room temperature, and was then heated to reflux (oil bath heating) for 3.5 h.

This mixture was then cooled to -78 °C and Br_2 (7.42 g, 46.4 mmol) was added dropwise, and the mixture was stirred for 10 min at -78 °C. The cooling bath was then removed, and the mixture was allowed to warm to 0 °C. To the reaction mixture concentrated aqueous solutions of sodium thiosulfate (20 mL), water (20 mL), and hexane (110 mL) were then added, and the resulting mixture was stirred vigorously. The mixture was exposed to air, the organic layer was separated and aqueous layer was extracted with ethyl acetate (1 × 75 mL, 1 × 35 mL). The combined organic extracts were dried over $MgSO_4$, filtered, and the solution was concentrated under reduced pressure at 40 °C to a total weight of 63 g. The solution was then left at room temperature for 2 hours, during which time a colorless solid precipitated. The precipitate was filtered off, washed with ethyl acetate (3 × 6 mL), and dried under reduced pressure. To remove residual ethyl acetate, the solid was dissolved in THF (20 mL) with heating, concentrated and dried (repeated two more times). The title compound was obtained as a colorless solid (3.69 g, 53%). Although ^{1}H-NMR analysis indicates a presence of a minor impurity, the material was used for the next step without further purification. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.59 (t, *J* = 8.0 Hz, 1H), 7.47 (dd, *J* = 7.6, 1.6 Hz, 2H), 7.45 (br s, 1H), 7.18 (d, *J* = 7.2 Hz, 4H), 7.07 (s, 4H), 2.96 (7-et, *J* = 6.9 Hz, 2H), 2.51 (7-et, *J* = 6.9 Hz, 4H), 1.32 (d, *J* = 6.9 Hz, 12H), 1.19 (d, *J* = 7.2 Hz, 12H), 1.08 (d, *J* = 6.8 Hz, 12H). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 158.7 (d, *J* = 248.5 Hz), 148.6, 146.1, 138.3 (d, *J* = 3.9 Hz), 135.7, 135.1, 132.3, 131.1 (d, *J* = 8.3 Hz), 130.8 (d, *J* = 18.3 Hz), 129.8, 127.8, 127.2, 120.8, 114.2 (d, *J* = 22.8 Hz), 34.2, 30.8, 24.7, 24.0, 23.6. ^{19}F NMR (471 MHz, $CDCl_3$) δ -111.17, -111.54 (*syn* and *anti* rotamers). HRMS (FAB$^+$) (*m*/*z*): [M] calcd for $C_{48}H_{54}Br_2F_2$, 826.2561; found, 826.2550.

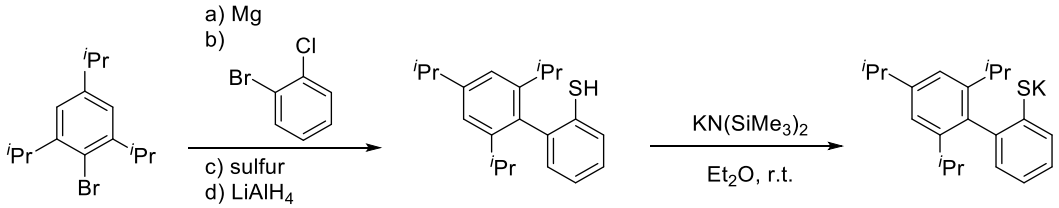
LH_2



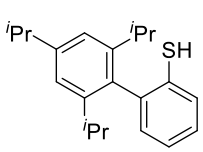
Dibromide **S2** (3.64 g, 4.39 mmol) was dissolved in THF (50 mL) with heating under N_2 atmosphere. The solution was then cooled to -78 °C and a 2.5 M solution of ^{n}BuLi in hexanes (4.39 mL, 11.0 mmol) was added dropwise. The mixture was stirred for 35 min at -78 °C, and then sulfur powder (1.06 g, 32.9 mmol) was added under positive pressure of N_2. The resulting mixture was stirred for 15 min at -78 °C. The cooling bath was then removed, and the mixture was allowed to warm to room temperature, then stirred at room temperature for 30 min. To the resulting reaction mixture $LiAlH_4$ (833 mg, 22.0 mmol) was added in portions over 15 minutes, keeping the reaction temperature close to room temperature with occasional brief cooling with dry ice/acetone cooling bath. After complete addition, the mixture was stirred at room temperature for further 140 min. The resulting mixture was treated with concentrated aqueous HCl in small portions until pH < 2, keeping the reaction temperature close to room temperature with occasional brief cooling with dry ice/acetone cooling bath (CAUTION: toxic H_2S gas evolving). To the resulting gray suspension, hexane (40 mL) and excess solid NaCl were added, and the resulting mixture was stirred vigorously for 5-10 minutes. The mixture was exposed to air, the organic solution was decanted, and the precipitate was washed with hexane (3 × 40 mL, mixture stirred vigorously each time before decanting). The combined organic solutions were dried over $MgSO_4$, filtered, and the solvent was removed under reduced pressure. The residue was crystallized by dissolving in boiling hexane (*ca*. 110 mL) and standing at room temperature for 1 day. The solid product was filtered off, washed with hexane (3 × 4 mL), and dried in vacuum, yielding the title compound as a white solid (1.96 g). An additional 0.47 g of the product was obtained by concentrating the mother liquor, and crystallizing the same way from hexane (*ca*. 25 mL). The total product isolated was 2.43 g (75%). Although ^{1}H NMR analysis indicates a presence of a minor impurity, the material

was used for preparation of iron complex without further purification. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.62 (t, *J* = 7.4 Hz, 1H), 7.53 – 7.46 (m, 3H), 7.10 (s, 4H), 7.08 – 7.03 (m, 2H), 6.97 (t, *J* = 8.6 Hz, 2H), 3.32 (s, 2H), 2.95 (7-et, *J* = 6.9 Hz, 2H), 2.55 (7-et, *J* = 6.9 Hz, 4H), 1.31 (d, *J* = 6.9 Hz, 12H), 1.20 (d, *J* = 6.9 Hz, 12H), 1.08 (d, *J* = 6.9 Hz, 12H). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 158.9 (d, *J* = 245.8 Hz), 149.1, 147.0, 136.4 (d, *J* = 2.7 Hz), 134.9, 134.4, 134.0 (d, *J* = 3.8 Hz), 131.9, 130.5 (d, *J* = 8.3 Hz), 130.1, 128.9, 126.8 (d, *J* = 18.7 Hz), 121.3, 111.4 (d, *J* = 23.0 Hz), 34.3, 30.6, 24.8, 24.0, 23.7. ^{19}F NMR (471 MHz, $CDCl_3$) δ -114.55. HRMS (FAB^{+}) (*m/z*): [M] calcd for $C_{48}H_{56}F_2S_2$, 734.3792; found, 734.3810.

Synthesis of thiolate 4



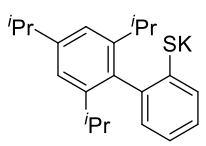
2',4',6'-Triisopropyl-[1,1'-biphenyl]-2-thiol (S3)



To magnesium turnings (1.22 g, 50.0 mmol) activated with 1,2-dibromoethane (0.1 mL) in hot THF (5 mL) under N_2 atmosphere, 1-bromo-2,4,6-triisopropylbenzene (5.67 g, 20.0 mmol) and THF (25 mL) were added alternately to maintain reflux. After complete addition the mixture was refluxed (oil bath heating) for 17 h. To the refluxing reaction mixture 1-bromo-2-chlorobenzene (3.83 g, 20.0 mmol) was added in portions (0.1 mL/2.5 min). After complete addition, the mixture was further refluxed for 6 h. Hot Grignard solution was then transferred (10 mL of THF used for washing the flask) quickly (to avoid precipitation upon cooling) to the

suspension of sulfur (1.92 g) in THF (10 mL) at -78 °C (cooling causes the resulting mixture to solidify). The cooling bath was removed and the mixture was allowed to freely warm to room temperature and then further stirred for 14 h at room temperature. To the resulting reaction mixture lithium aluminum hydride (1.52 g, 40.0 mmol) was added in portions over 30 minutes, keeping the reaction temperature close to room temperature with occasional brief cooling with dry ice/acetone cooling bath. After complete addition, the mixture was stirred at room temperature for further 5.5 h. The resulting mixture was treated with concentrated aqueous HCl (20 mL) added in small portions over 1.5 h, keeping the reaction temperature close to room temperature with occasional brief cooling with dry ice/acetone cooling bath (CAUTION: toxic H_2S gas evolving). To the resulting slurry hexane (50 mL) and solid NaCl (10 g) were added, and the resulting mixture stirred vigorously for few minutes. The mixture was exposed to air, the organic solution was then decanted from aqueous slurry, and slurry washed with hexane (3 × 10 mL, mixture stirred vigorously each time before decanting). Combined organic solutions were dried over $MgSO_4$, filtered, and the solvent was removed under reduced pressure. The residue was purified by column chromatography on silica gel using hexane as the eluent yielding the title compound as a colorless solid (3.97 g, 64%). ^{1}H NMR (400 MHz, C_6D_6) δ 7.25 (s, 2H), 7.11 – 7.07 (m, 1H), 7.07 – 7.04 (m, 1H), 6.94 – 6.83 (m, 2H), 3.07 (s, 1H), 2.86 (7-et, *J* = 7.0 Hz, 1H), 2.72 (7-et, *J* = 6.9 Hz, 2H), 1.30 (d, *J* = 6.9 Hz, 6H), 1.26 (d, *J* = 6.9 Hz, 6H), 1.10 (d, *J* = 6.9 Hz, 6H). ^{13}C{^{1}H} NMR (101 MHz, C_6D_6) δ 149.0, 147.0, 138.3, 135.1, 133.7, 130.7, 127.9, 127.6, 124.7, 121.2, 34.5, 30.6, 24.7, 24.0, 23.7. HRMS (ESI$^-$) (*m/z*): [M–H] calcd for $C_{21}H_{27}S$, 311.1839; found, 311.1832.

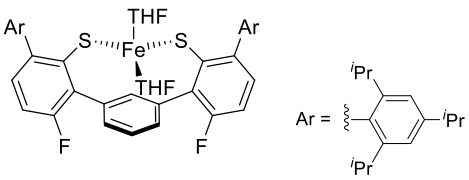
Potassium 2',4',6'-triisopropyl-[1,1'-biphenyl]-2-thiolate (4)



A solution of potassium bis(trimethylsilyl)amide (99.7 mg, 0.500 mmol) in diethyl ether (2 mL, additional 2 × 1 mL used for washing the vial) was added to a solution of 2',4',6'-triisopropyl-[1,1'-biphenyl]-2-thiol (156.3 mg, 0.500 mmol) in diethyl ether (1 mL) at room temperature in an N_2-filled glovebox. A colorless solid immediately precipitated. After 30 min the solid was filtered off, washed with diethyl ether (3 × 2 mL), and dried under vacuum yielding the title compound as a colorless solid (152 mg, 87%). ^{1}H NMR (400 MHz, THF-d_8) δ 7.36 – 7.27 (m, 1H), 7.02 (s, 2H), 6.67 (td, J = 7.4, 1.8 Hz, 1H), 6.60 (dd, J = 7.4, 1.8 Hz, 1H), 6.53 (td, J = 7.1, 1.4 Hz, 1H), 2.91 (7-et, J = 6.9 Hz, 1H), 2.76 (7-et, J = 6.9 Hz, 2H), 1.30 (dd, J = 6.9, 2.0 Hz, 6H), 1.19 (d, J = 6.9 Hz, 6H), 0.96 (d, J = 6.9 Hz, 6H). ^{13}C{^{1}H} NMR (101 MHz, THF-d_8) δ 157.1, 147.1, 145.8, 143.0, 140.7, 134.9, 128.4, 124.7, 119.5, 116.7, 34.2, 30.0, 24.0, 23.7, 23.6. Anal. Calcd for $C_{21}H_{27}KS$: C, 71.94; H, 7.76; N, 0.00. Found: C, 71.59; H, 7.88; N, -0.12.

Synthesis of iron complexes

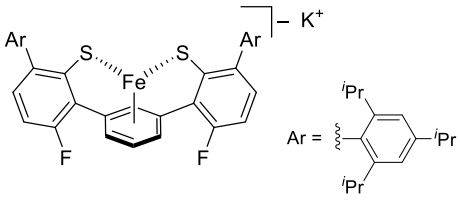
LFe(THF)$_2$ (1)



A solution of Fe(N(SiMe$_3$)$_2$)$_2$ (0.720 mmol) in THF (1 mL, additional 0.5 mL used for washing the vial) was added to a stirring solution of LH_2 (544 mg, 0.740 mmol) in THF (4.5 mL) at room temperature under N_2 atmosphere. The color of the solution immediately turned dark yellow, and yellow precipitate started forming after few minutes. After being stirred for 135 min at room temperature, the mixture was cooled to -40 °C for 5 hours. The yellow precipitate was filtered off cold,

washed with cold (-40 °C) THF (2 × 0.5 mL), dried under vacuum for 10 min, then crushed into a fine powder with a spatula, and dried for a further 30 min under vacuum. The title compound was obtained as a yellow powder, 568 mg, 82%. ^{1}H NMR (500 MHz, THF-d_8) δ 25.2 (br s, 2H), 23.2 (s, 2H), 4.7 (s, 2H), 4.3 (s, 2H), 3.6 (s, 8H, THF), 2.4 (br s, 2H), 1.8 (s, 8H, THF), 1.1 (s, 6H), 0.04 – -0.02 (m, 15H), -1.2 (br s, 6H), -1.4 (s, 6H), -3.8 (s, 6H), -7.3 (br s, 2H), -26.7 (s, 2H), -61.6 (br s, 1H). ^{19}F NMR (471 MHz, THF-d_8) δ -65.3 (s). IR (cm^{-1}): 2955 (s), 2929 (m), 2888 (m), 2864 (m), 1607 (w), 1597 (w), 1575 (m), 1561 (w), 1479 (w, sh), 1459 (s), 1448 (m, sh), 1429 (vw), 1397 (w), 1374 (m), 1359 (s), 1340 (w), 1318 (w), 1236 (m), 1215 (m), 1192 (vw), 1183 (w), 1169 (w), 1135 (w), 1099 (w), 1090 (vw), 1078 (w), 1069 (m), 1054 (w), 1031 (m), 1021 (m), 1010 (w), 996 (vw), 948 (vw), 912 (w), 894 (s), 873 (s), 864 (s, sh), 841 (m), 821 (w), 806 (s), 786 (m), 779 (w), 752 (m), 718 (m), 696 (vw), 677 (w), 651 (m), 578 (vw), 542 (m), 517 (vw), 504 (w), 474 (w), 429 (w), 417 (vw). Anal. Calcd for $C_{56}H_{70}F_2FeO_2S_2$: C, 72.08; H, 7.56; N, 0.00. Found: C, 71.82; H, 7.68; N, -0.02. μ_{eff} (THF-d_8, 25 °C) = 5.2(1) μ_B. UV-vis (THF, 21 °C; λ_{max}, nm (ε, mM^{-1}cm^{-1})): 348 (7.4), 389 (sh). Zero-field Mössbauer (80 K): δ = 0.89 mm/s, $|\Delta E_Q|$ = 3.77 mm/s. Single crystals for X-ray analysis were obtained by slow cooling of a hot solution of LFe(THF)$_2$ (33 mg) in THF (0.3 mL).

LFeK (2)

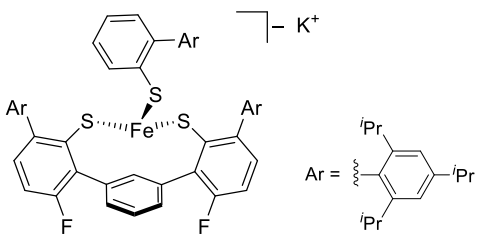


THF was briefly dried over activated alumina prior to use. All manipulations were performed in N_2 filled glovebox (<0.3 ppm O_2) in a cold well using dry ice/acetone cooling bath. The temperature in the cold well during the reaction was -70 °C. All equipment, glassware, solutions and solvents used in the procedure were cooled in the cold well before use. LFe(THF)$_2$ (**1**, 46.7 mg, 0.0500 mmol) was dissolved in THF (1.5 mL) with slight heating, and then

immediately cooled to -70 °C. To the stirred cold yellow solution, a cold suspension of KC_8 (7.1 mg, 0.053 mmol, 1.05 equiv) in THF (0.2 mL, additional 0.1 mL of cold THF used for washing the vial) was added. After being stirred for 45 min at -70 °C the brown-yellow mixture was diluted with cold hexane (2 mL), filtered cold (short plug of Celite in a pipette), and then further diluted with cold hexane (6 mL). The resulting brown-yellow solution was left in the freezer (-40 °C) for 2 days, during which time large brown-yellow crystals formed. The solution was quickly removed with a pipette from the crystals while cold, and the crystals were quickly washed with cold THF/hexane 1:5 (2 × 0.5 mL, precooled at -40 °C). The product was dried under vacuum, then crushed into a fine powder with a spatula, and dried for further several hours under vacuum. The title compound was obtained as a brown powder, 36 mg. The product contained residual THF (1.54 equiv) which was quantified by integration of ^{1}H NMR spectra of the diamagnetic region; sample weights used for analyses were corrected by multiplying with the factor 0.88. The corrected yield is 32 mg, 77%. ^{1}H NMR (500 MHz, THF-d_8) δ 7.1 (br s, 2H), 6.9 (br s, 2H), 4.7 (overlapped br s, 3H), 2.8 (overlapped s, 4H), 2.6-1.8 (overlapped br s, 12H), 1.2 (br s, 18H), 0.6 (br s, 6H). IR (cm^{-1}): 3050 (vw), 2955 (s), 2929 (m), 2864 (m), 1588 (w), 1559 (w), 1484 (w), 1458 (s), 1449 (s), 1427 (w, sh), 1373 (m), 1359 (m), 1346 (m, sh), 1317 (w), 1295 (w), 1268 (vw), 1237 (m), 1210 (s), 1184 (w), 1169 (w), 1136 (m), 1100 (w), 1049 (s), 1006 (w), 976 (vw), 945 (vw), 940 (vw), 896 (s), 875 (m), 847 (w), 840 (w), 827 (w), 797 (s, sh), 790 (s), 756 (w), 687 (vw), 667 (vw), 652 (w), 613 (vw), 573 (vw), 540 (w, sh), 533 (m), 495 (w, sh), 489 (w), 429 (w), 422 (vw), 408 (vw). Anal. Calcd for $C_{48}H_{54}F_2FeKS_2(C_4H_8O)_{1.54}$: C, 69.27; H, 7.12; N, 0.00. Found: C, 69.38; H, 7.09; N, -0.24. μ_{eff} (THF-d_8, 24 °C) = 2.1(1) μ_B. UV-vis (THF, 21 °C; λ_{max}, nm (ε, $mM^{-1}cm^{-1}$)): 745 (1.1), 464 (1.7, sh), 408 (3.4, sh), 378 (5.7), 306 (8.2, sh). Zero-field Mössbauer (80 K): δ = 0.59 mm/s, $|\Delta E_Q|$ = 0.53 mm/s. Single crystals for X-ray analysis were obtained as follows. A sample (0.5 mL) of the reaction mixture

after dilution with hexane at -70 °C was added to hexane (0.5 mL) at room temperature. After 16 h at room temperature brown-yellow needles formed.

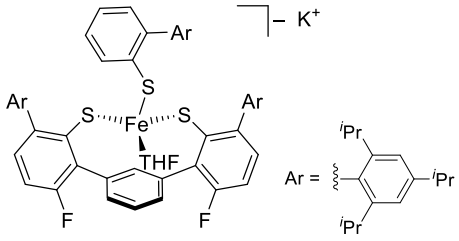
[LFeSC$_6$H$_4$Ar]K (5)



LFe(THF)$_2$ (**1**, 272 mg, 0.291 mmol) was weighed in a vial and most of the solid was transferred with a spatula to a vial containing potassium 2',4',6'-triisopropyl-[1,1'-biphenyl]-2-thiolate (**4**, 102 mg, 0.291 mmol). To the combined solids THF (1.5 mL) was added, and the remaining LFe(THF)$_2$ was added by washing the vial with THF (3 × 0.5 mL). The color of the solution immediately turned orange, and after a few minutes the solids completely dissolved. After stirring for 15 min at room temperature, the solution was concentrated under vacuum. The brownish-orange residue was dissolved in Et_2O (1 mL), and the resulting solution was filtered (short plug of Celite, additional 3 × 0.2 mL of Et_2O were used for washing the vial and the plug). A layer of pentane (2.5 mL) was carefully added above the solution, and the layer diffusion setup was left at room temperature for 1 day. The precipitate was washed with 1:1 Et_2O/pentane (2 × 0.5 mL), dried under vacuum, crushed into a fine powder with a spatula, and dried for further several hours under vacuum. The title compound was obtained as an orange powder, 312 mg. The product contained residual solvent: THF (0.74 equiv), Et_2O (0.34 equiv), and pentane (0.31 equiv), as determined by integration of ^{1}H NMR spectra of the diamagnetic region. The corrected yield is 287 mg, 87%. ^{1}H NMR (600 MHz, THF-d_8) δ 44.0 (s, 1H), 29.6 (br s, 1H), 28.8 (s, 2H), 22.2 (br s, 2H), 19.7 (br s, 2H), 14.6 (s, 2H), 7.5 – 7.3 (m, 18H), 7.0 (s, 1H), 6.5 (s, 6H), 5.4 (s, 2H), 3.9 (s, 6H), 2.6 (s, 2H), 0.5 (s, 2H), -1.3 (s, 6H), -1.5 (s, 6H), -1.5 (s, 6H), -3.9 (s, 6H), -8.1 (s, 2H), -22.6 (s, 1H), -23.7 (s, 2H), -43.8 (overlapped

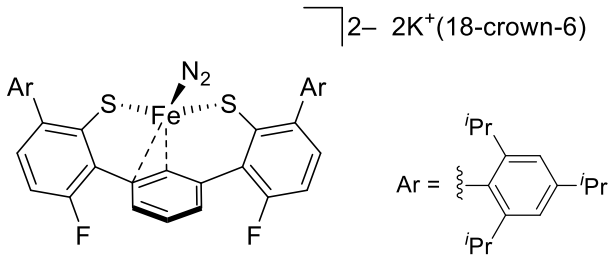
br s, 3H), -99.6 (s, 1H); (one of the 1H peaks could not be located, but might be a part of the 7.49 – 7.30 ppm multiplet). ^{19}F NMR (376 MHz, THF-d_8): δ -41.85 (br s). IR (cm^{-1}): 2955 (s), 2928 (m), 2906 (m, sh), 2865 (m), 1606 (w), 1595 (w), 1579 (w), 1569 (w), 562 (w), 1480 (vw), 1459 (s), 1447 (m, sh), 1425 (w), 1392 (vw), 1376 (m), 1359 (m), 1339 (vw), 1319 (w), 1307 (vw, sh), 1239 (m), 1211 (m), 1182 (w), 1168 (w), 1152 (vw), 1133 (w), 1121 (w), 1098 (w), 1068 (m), 1048 (m), 1035 (m), 1005 (w), 947 (vw), 937 (vw), 916 (vw), 903 (m, sh), 890 (s), 873 (s), 841 (m), 819 (vw), 804 (s), 787 (m), 761 (m), 750 (m), 738 (s), 713 (s), 668 (w), 651 (m), 594 (vw), 578 (vw), 563 (vw), 542 (m), 517 (w), 502 (m), 465 (w), 429 (w), 415 (w). Anal. Calcd for $C_{69}H_{81}F_2FeKS_3(C_4H_8O)_{0.74}(C_4H_{10}O)_{0.34}(C_5H_{12})_{0.31}$: C, 72.50; H, 7.65; N, 0.00. Found: C, 72.29; H, 7.66; N, -0.18. μ_{eff} (THF-d_8, 24 °C) = 5.3(1) μ_B. UV-vis (THF, 21°C; λ_{max}, nm (ε, mM^{-1}cm^{-1})): 343 (sh, 9.7), 400 (sh, 4.8). Zero-field Mössbauer (80 K): δ = 0.69 mm/s, $|\Delta E_Q|$ = 1.50 mm/s. Single crystals for X-ray analysis were obtained by slow evaporation of a solution of [LFeSC$_6$H$_4$Ar]K (30 mg, crude product after concentration of the reaction mixture) in Et$_2$O (0.2 mL) at room temperature.

[LFeSC$_6$H$_4$Ar(THF)]K (5·THF)



[LFeSC$_6$H$_4$Ar(THF)]K (**5**·THF) is in equilibrium with [LFeSC$_6$H$_4$Ar]K (**5**) in THF solution (see Supplementary Data/ UV-Vis spectra). Single crystals of [LFeSC$_6$H$_4$Ar(THF)]K for X-ray analysis were obtained from a concentrated solution of **5** in THF at -40 °C.

[LFeN$_2$][K(18-crown-6)(THF)$_2$]$_2$ (3)



THF was briefly dried over activated alumina prior to use. All manipulations were performed in an N_2 filled glovebox (<0.2 ppm O_2) in a cold well using a dry ice/acetone cooling bath. The temperature in the cold well during the reaction was -70 °C. All equipment, glassware, solutions and solvents used in the procedure were cooled in the cold well before use. Volumes of solvents used for the reaction were measured with a syringe at room temperature.

***Procedure A*:** A cold suspension of KC_8 (28.5 mg, 0.211 mmol, 2.4 equiv) in THF (0.6 mL, additional 2 × 0.2 mL of cold THF used for washing the vial) was added to a stirred cold solution of [LFeSC$_6$H$_4$Ar]K (**5**, 100.3 mg, 0.0880 mmol) in THF (1 mL) at -70 °C. After the deep red-black mixture was stirred for 40 min at -70 °C, a solution of 18-crown-6 (93.0 mg, 0.352 mmol) in THF (0.6 mL) was added. (Cooling in the cold well causes precipitation of crown ether from the solution of 18-crown-6 in THF, so it was briefly warmed until it dissolved before adding.) The mixture was stirred for 1 min at -70 °C, and then filtered cold (short plug of Celite in a pipette, additional 0.4 mL of cold THF were used for washing the vial and the plug) to a cold 20 mL vial. The resulting dark red-black solution was left undisturbed in a freezer at -38 °C for 24 h, during which time dark crystals precipitated. A small glass frit filter was cooled at -70 °C in the cold well, and the vial was quickly removed from the freezer and filtered. The solution was pushed through the filter with cold nitrogen using a cooled syringe. Cold THF (2 × 0.5 mL) was used for washing the vial and the solid, and then solid was additionally washed with cold THF (0.5 mL) and cold butane (3 × 0.5 mL). (The filtrate was added to 2 M HCl in Et_2O (2 mL) at -70 °C, the mixture was concentrated, the residue was dissolved in toluene-d_8, and an internal standard

of Ph_3CH was added. Integration of ^1H NMR spectra showed that the amounts of the **S3** and LH_2 were 1.04 equiv. and 0.09 equiv., respectively, relative to the amount of **5** used in the reaction.) The solid was then dried by passing cold nitrogen (*ca*. 45 mL) through the filter using the cold syringe. The product was then transferred to a cold vial and samples for analyses were prepared at -70 °C. This yielded a dark brown solid, 224 mg (balanced cold and loosely capped), which contains >30% butane by ^1H NMR analysis (NMR sample prepared similarly as described in procedure B below).

IR spectra were recorded by transferring the cold sample to the ATR in the glove box rapidly. The sample for SQUID magnetometry was prepared at -70 °C by placing *ca*. 20-30 mg of the product in a short J. Young NMR tube using a small aluminum funnel. The sample was secured at the bottom of the tube by placing quartz wool above the sample. The tube was closed and taken cold outside the glovebox, immediately placed in liquid N_2, and sealed below the J. Young adapter. The amount of the sample used (16.2 mg) was determined after the measurement by quantification of the ligand as described in procedure B below. Details of the SQUID measurement are given below. The sample for Mössbauer analysis was transferred in the cold well to a cold plastic cup holder. IR (cm^{-1}): 2956 (m), 2923 (m, sh), 2895 (m, sh), 2863 (m), 1869 (s, ν_{NN}), 1605 (vw), 1579 (w), 1566 (w), 1548 (w), 1459 (m), 1440 (w), 1376 (w), 1350 (s), 1317 (w), 1297 (w), 1285 (w), 1248 (m), 1237 (w, sh), 1198 (w), 1183 (w), 1169(vw), 1130 (m), 1102 (s), 1070 (s), 1058(s, sh), 998 (w), 960 (s), 914 (w, sh), 899 (m, sh), 890 (s), 872 (m), 837 (s), 783 (m), 762 (w), 748 (w), 731 (w), 686 (vw), 650 (w), 539 (w, sh), 530 (w), 505 (w, sh), 485 (vw), 466 (vw), 419 (vw). ν_{NN} = 1869 cm^{-1}. This N-N stretching frequency is somewhat lower than observed in samples washed only with cold THF (procedure E, 1880 cm^{-1}). This is probably due to washing the product with butane, which could remove THF molecules present in the crystals (see X-ray crystallography data for **3** below). Zero-field Mössbauer (80 K): δ = 0.75 mm/s, $|\Delta E_Q|$ = 1.77 mm/s.

***Procedure B*:** A cold suspension of KC_8 (28.5 mg, 0.211 mmol, 2.4 equiv) in THF (0.4 mL, additional 2 × 0.2 mL of cold THF used for washing the vial) was added to a stirred cold solution of [$LFeSC_6H_4Ar$]K (**5**, 100.3 mg, 0.0880 mmol) in THF (0.8 mL) at -70 °C. After the deep red-black mixture was stirred for 40 min at -70 °C, a solution of 18-crown-6 (93.0 mg, 0.352 mmol) in THF (0.5 mL) was added. (Cooling in the cold well causes precipitation of crown ether from the solution of 18-crown-6 in THF, so it was briefly warmed until it dissolved before adding.) The mixture was stirred for 1 min at -70 °C, and then filtered cold (short plug of Celite in a pipette, additional 0.4 mL of cold THF were used for washing the vial and the plug) to a cold 20 mL vial. The resulting dark red-black solution was left undisturbed in a freezer at -38 °C for 23 h, during which time dark crystals precipitated. A small glass frit filter was cooled at -70 °C in the cold well, and the vial was quickly removed from the freezer and filtered. The solution was pushed through the filter with cold nitrogen using a cooled syringe. Cold THF (3 × 0.5 mL) and cold butane (3 × 0.5 mL) were used for washing the vial and the solid. The solid was then dried by passing cold nitrogen (*ca*. 45 mL) through the filter using the cold syringe. The product was then transferred to a cold vial, and further dried cold by applying vacuum in periods of 20 seconds (5 times). The product was obtained as a dark brown solid, 131 mg (balanced cold and loosely capped), which contained 6% butane by NMR, yield 82%. IR spectra were recorded immediately by using the cold sample, which showed an IR spectrum as above, with ν_{NN} = 1872 cm^{-1}. The sample for Mössbauer analysis was transferred in the cold well to a cold plastic cup holder. Zero-field Mössbauer (80 K): δ = 0.74 mm/s, $|\Delta E_Q|$ = 1.79 mm/s.

Relative quantification of ligand, crown ether and iron: A separate sample was transferred to a cold 1 mL vial capped with a septum, taken cold out of the glovebox and treated with a degassed 5:1 mixture of toluene-d_8 and acetic acid-d_4 (0.5 mL), which had been precooled at -40 °C. The initial yellow brown mixture turned to a colorless solution upon warming to room temperature. The solution was

immediately transferred to an NMR tube, and the vial was washed with an additional 0.3 mL of the solvent. Upon mixing with air in the NMR tube, the colorless solution turned light brown-pink and a brown-pink precipitate separates after few minutes. The NMR tube was left at RT overnight for precipitate to settle, and then was analyzed by ^{1}H NMR. An internal standard of Ph_3CH (18.3 mg) was added in toluene-d_8 (0.4 mL), the mixture was shaken, the precipitate was allowed to settle, and then the sample was analyzed by ^{1}H NMR. The relative concentrations of ligand and 18-crown-6 were determined by comparison of the integration of ^{1}H signals of the signals for the C*H* protons of ^{i}Pr groups in the ligand, the 18-crown-6, and added Ph_3CH. The solution from NMR tube was transferred to a 20 mL vial, and the tube was washed with acetone. The sample in the vial was concentrated under reduced pressure at 40 °C. The residues in the vial and the NMR tube were dissolved in a total of 6 mL of 3 M HCl(aq), the solutions combined and diluted to 50 mL with water. The amount of Fe was quantified by colorimetric assay using phenanthroline according to the literature[35]. The ratio of **L**/Fe/18-crown-6 was measured as 1:0.88:2.16.

***Procedure C ($^{14}N_2$/$^{15}N_2$ exchange)*: 3** was synthesized according to procedure A at 1/2 of the scale given above. Most of the reaction mixture after filtration was placed in a cold Schlenk tube. (The rest of the reaction mixture was left in a vial at -38 °C for 27 h, handled as described in procedure D below, and the crystals gave the same unit cell as described below.) After 25 h at -38 °C, the Schlenk tube was placed in the cold well at -70 °C, and the mother liquor was removed from the precipitate with a cold pipette, and the product was washed with cold THF (2 × 0.5 mL) and cold butane (2 × 0.5 mL). The product was briefly (30 sec) dried under vacuum at -70 °C until excess of butane solvent cannot be observed anymore, and a sample was immediately analyzed by IR spectroscopy, showing ν_{NN} = 1873 cm^{-1}. The rest of the product was kept at -70 °C, cold butane (0.1 mL) was added, and the Schlenk tube was exposed to vacuum at -70 °C until excess of butane solvent cannot be observed anymore (1-2 min),

refilled with $^{15}N_2$ gas (1 atm), and left in the cold well for 2 h. The sample was then quickly analyzed by IR, showing ν_{NN} bands at 1875, 1813 cm^{-1}.

***Procedure D (from LFeK)*:** A cold suspension of KC_8 (6.9 mg, 0.051 mmol, 1.0 equiv) in THF (0.2 mL) was added to a stirred cold solution of LFeK (42 mg, 0.051 mmol, crude product obtained by filtering and concentrating the reaction mixture as described above) in THF (0.3 mL) at -70 °C. The resulting deep red-black mixture was stirred for 25 min at -70 °C, then 1/3 of the mixture was filtered cold (short plug of Celite in a pipette), and kept in the cold well for several days after which a fine precipitate separated. To the mixture a cold solution of 18-crown-6 (5 mg, 0.02 mmol) in THF (0.05 mL) was added. The mixture was filtered cold (short plug of Celite in a pipette). The resulting dark red-black solution was left in the cold well for 1 day, and then kept in the freezer (-38 °C). After a few hours, dark crystals started to form. The crystals were taken into cold Fomblin Y oil in the cold well (-70 °C) and transported cold (-78 °C) in a closed jar. A suitable crystal was selected under microscope while keeping the sample under cold nitrogen stream (< -80 °C). A pin with the crystal was immediately placed on liquid N_2 cryo-tongs, transported on dry ice, and the crystal was placed on the goniometer under a cold N_2 stream.

***Procedure E (crystals washed only with THF)*: 3** was synthesized according to Procedure A at 1/2 of the scale given above, and crystals were washed only with cold THF. The sample was then quickly analyzed by IR, showing ν_{NN} band at 1880 cm^{-1}.

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Supplementary Data

Magnetic Susceptibility Measurements

Magnetic Susceptibility. Magnetic susceptibility data were measured from a solid sample of **3** in the temperature range 2 - 270 K by using a SQUID susceptometer with a field of 1.0 T (MPMS-7, Quantum Design, calibrated with standard palladium reference sample, error <2%). Variable-temperature magnetization measurements were done at 1 T, 4 T, and 7 T in the range 2-260 K with the magnetization equidistantly sampled on a 1/T temperature scale. The sample was contained in sealed borosilicate NMR tubes, and quartz wool was packed above the sample to constrain it. The SQUID response curves (raw data) were corrected for holder and solvent contributions by subtracting the corresponding response curves obtained from an identical NMR tube without sample. The experimental magnetization data obtained from independent simulation of the corrected SQUID response curves were corrected for underlying diamagnetism[36] by use of tabulated Pascal's constants[37,38], as well as for temperature-independent paramagnetism. Handling and simulation of the SQUID raw data as well as spin-Hamiltonian simulation of the susceptibility and magnetization data were done with our own package julX for exchange-coupled systems (available from E.B. by mail to ebill@gwdg.de). The simulations are based on the usual spin-Hamilton operator for monomeric compounds with zero-field splitting:

$$\hat{H}_S = D\,[\hat{S}_z^2 - \frac{1}{3}S(S+1) + \frac{E}{D}(\hat{S}_x^2 - \hat{S}_y^2)] + \mu_B \vec{B}\cdot g \cdot \hat{\vec{S}}$$

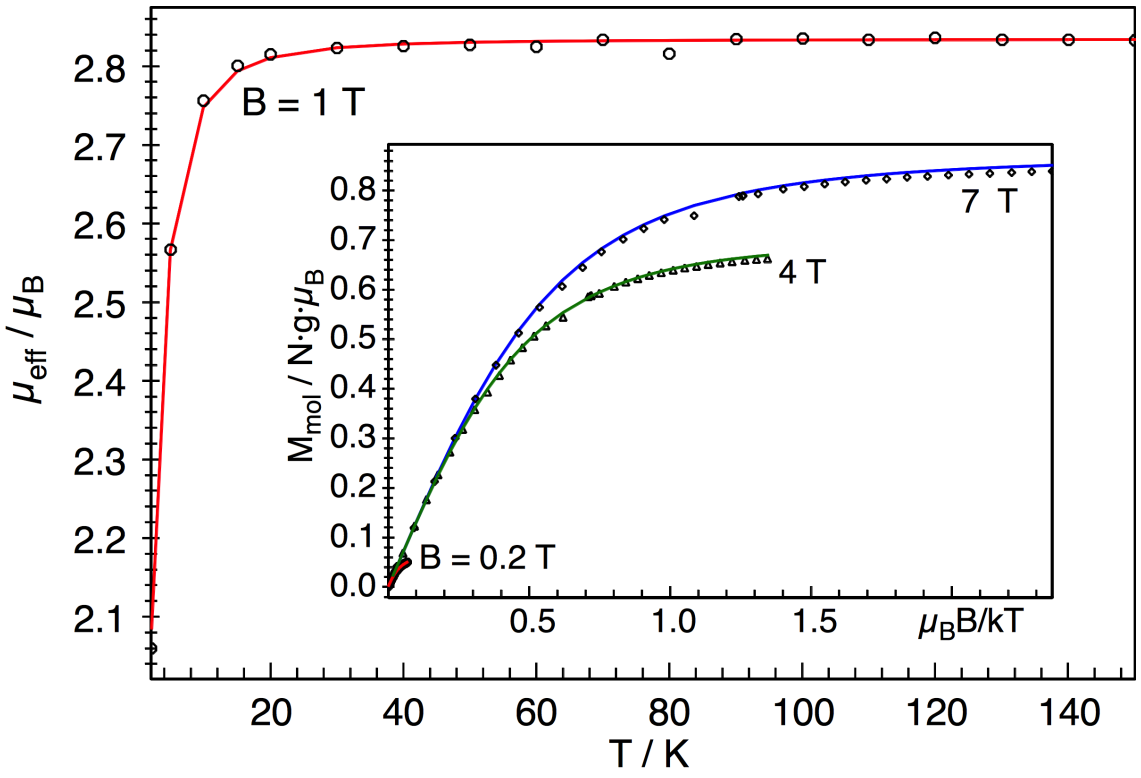
where g_{av} is the average electronic g value and D and E/D are the axial zero-field splitting and rhombicity parameters.

Diagonalization of the total Hamiltonian was performed with the routine ZHEEV from the LAPACK Library (available from E. B.), and magnetic moments were calculated from the eigenfunctions by using the Hellman-Feyman theorem:

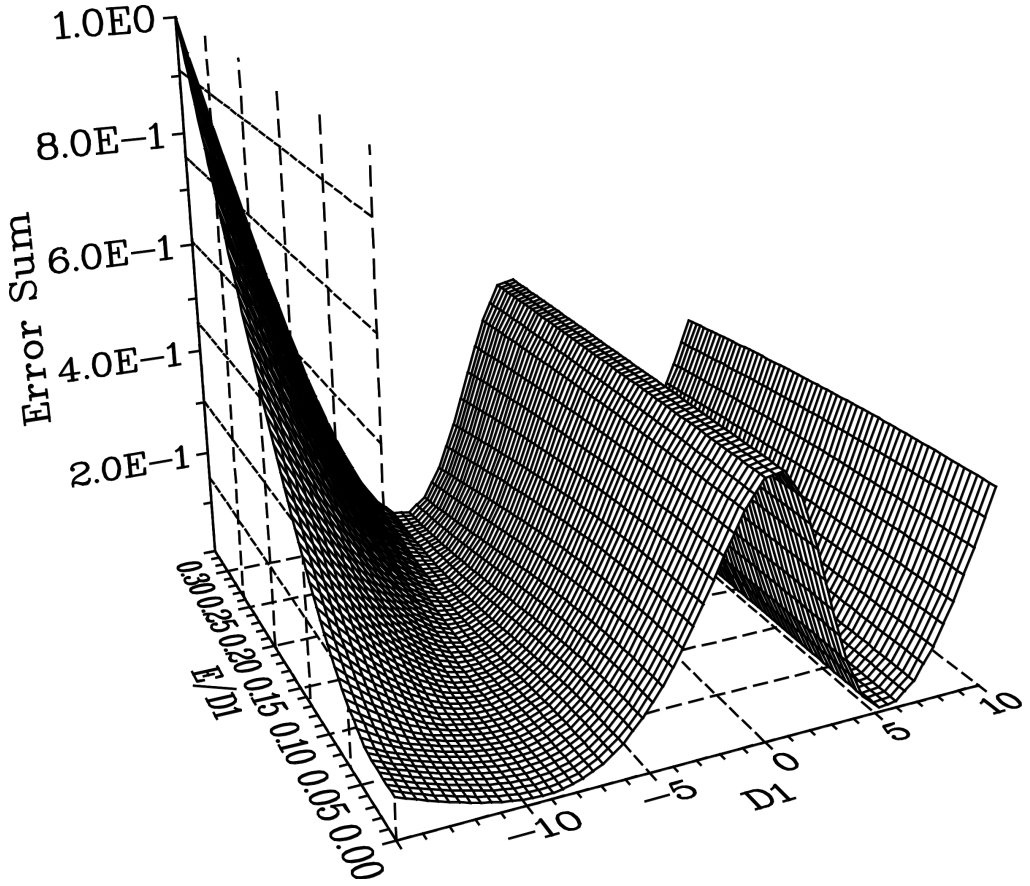
$$\vec{\mu}_i(\vec{B}) = -\langle \psi_i | d\hat{H} / d\vec{B} | \psi_i \rangle$$

The powder summations were done by using a 16-point Lebedev grid[39,40].

The following figure shows the susceptibility data, with lines representing simulations with $S = 1$, $\mathbf{g} = [2.004, 2.004, 2.004]$, $D = -7.37$ cm^{-1}, $E/D = 0.177$, TIP = 100 x 10^{-6} emu.



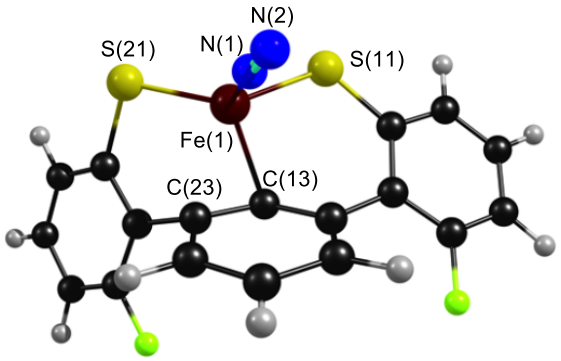
The following is an error scan for D and E/D, which shows that a fit to the data with D = +5.5 cm^{-1} would also be acceptable, but is not as good of a global fit as the one with negative D given above. Future studies will use variable-field Mössbauer spectroscopy to evaluate this compound's magnetic properties in more detail.

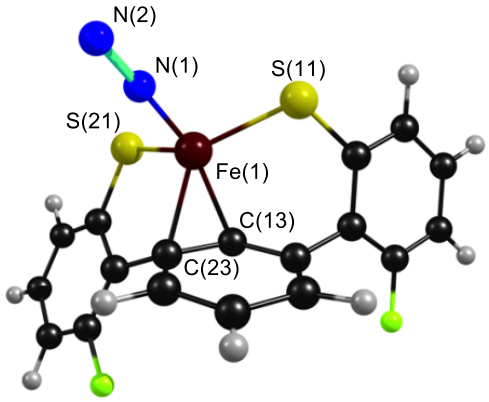


DFT Calculations

DFT calculations were performed with the ORCA program package, version 3.0.3[41], using the BP86 functional[42,43], atom-pairwise dispersion correction with the Becke-Johnson damping scheme (D3BJ)[44,45], the scalar relativistic zero-order regular approximation (ZORA)[46], and the scalar relativistically recontracted version of the def2-TZVP basis set[47,48]. The SCF calculations were tightly converged (TightSCF) with unrestricted spin (UKS). Numerical integrations during all DFT calculations were done on a dense grid (ORCA grid4). Initial geometry for calculations was taken from the crystal structure, with $-(^{i}Pr)_3C_6H_2$ groups being replaced by –H. The calculated structures were confirmed to be minima on the potential energy surface by the absence of imaginary frequencies after analytical frequency calculations on the optimized structures.

Calculated structures of truncated dianion of N_2 complex **3** with $S = 1$ and $S = 0$ spin states and comparison of selected geometrical parameters with the crystal structure. Thermodynamic parameters are relative values at 298 K.





	$S = 1$	$S = 0$
$\Delta G°$	0.0 kJ/mol	37.4 kJ/mol
$\Delta H°$	0.0 kJ/mol	31.3 kJ/mol
$\Delta S°$	0.0 J/mol•K)	-20.5 J/mol•K

	Crystal	Calculated for $S = 1$	Calculated for $S = 0$
Fe(1)-N(1)	1.790(5)	1.79	1.74
Fe(1)-C(13)	2.037(5)	2.03	2.04
Fe(1)-C(23)	2.239(5)	2.17	2.07
Fe(1)-S(21)	2.3201(16)	2.28	2.19
Fe(1)-S(11)	2.3549(16)	2.34	2.22
N(1)-N(2)	1.132(7)	1.15	1.15

Sample input used for calculations.

```
!UKS BP86 def2-TZVP D3BJ ZORA NORI TightSCF Grid4 NoFinalGrid SlowConv TightOpt
!Opt

*xyz -2 3
(atomic coordinates)
*
```

Atomic coordinates for optimized structure of truncated dianion of N_2 complex **3** with $S = 1$.

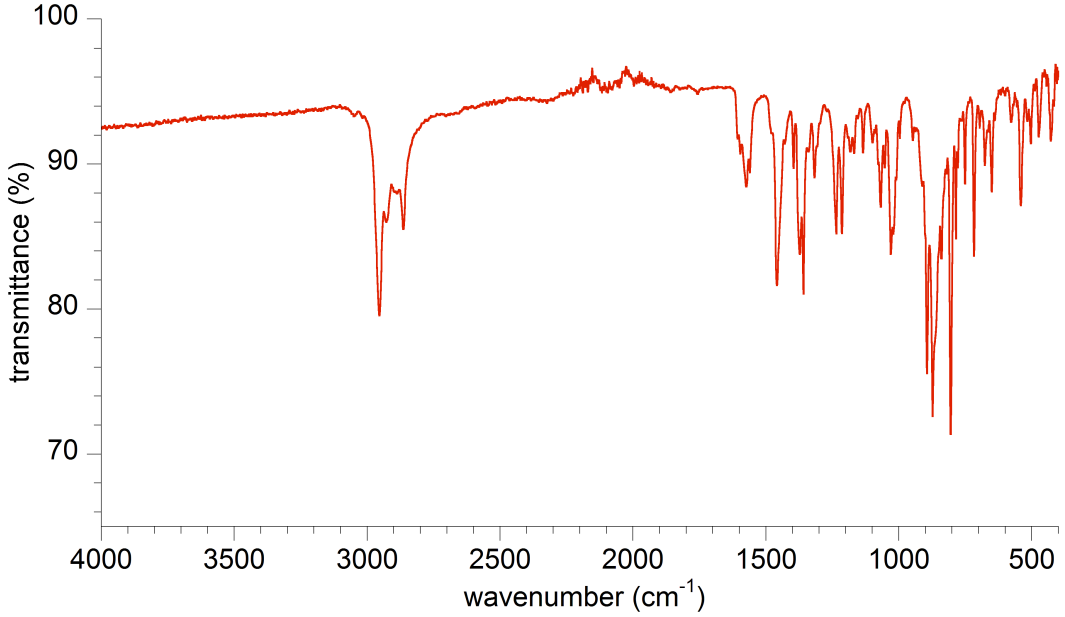
Fe	14.07647997292359	16.54407867035174	16.73237751421186
N	14.94969997166823	17.33393243471027	15.38350153890495
N	15.43115334898496	17.88736235377869	14.50117018287384
S	14.04298038237994	18.15856775854165	18.43053400672441
S	14.60067572626798	14.40055609302932	17.31883471406408
C	12.79104670162796	19.33883724249792	18.14254655898091
C	11.86559663649255	19.28271822364994	17.03333439712176
C	10.93708230302679	20.32437553276251	16.93460762496671
C	10.83836271061531	21.40103985567990	17.81421106209623
H	10.06901292405003	22.15822613940552	17.65991575563917
C	11.74631332565430	21.44231575639864	18.88306185585515
H	11.71074739150546	22.27208240617768	19.59572151057091
C	12.69245203515350	20.43646650523028	19.03817470877713
F	10.00715251091914	20.29988794614018	15.91448826090813
C	13.07059982010790	13.63270560255454	16.97106058680756
C	12.09434822391206	14.33241514032715	16.19409844861718
C	10.91629105893848	13.64283554574104	15.89717027251646
C	10.63088273548793	12.34110902524866	16.31319668831677
H	9.67515596510180	11.88592275511152	16.05030398565281
C	11.59625796932222	11.68144669543078	17.08988691044048
H	11.40590494311087	10.66167374700294	17.43895390491809
C	12.78916526707697	12.31812881682459	17.41733317944821
F	9.93442975687936	14.27438107401197	15.16799439309879
C	12.07279767733090	16.84416316349357	16.60724012992446
H	11.69213592069122	16.64250159621534	17.61226610649897
C	12.33725449138546	15.72763233498731	15.71792463689876
C	12.26781675091310	15.99127932589935	14.30395207487483
H	12.41438214694739	15.15208752418811	13.61878428479966
C	12.04499484883263	17.26060404601595	13.81111786869475
H	12.04485012982871	17.43070460958877	12.73104255778883
C	11.88469636848496	18.36333632427781	14.68931808131161
H	11.81657157413607	19.37606790042610	14.29093678386144
C	11.91166883375991	18.16812184698769	16.06644463909547
H	13.54612365385476	11.80687944451785	18.01642039673026
H	13.40628892262756	20.47592456279462	19.86390937800939

Atomic coordinates for optimized structure of truncated dianion of N_2 complex **3** with $S = 0$.

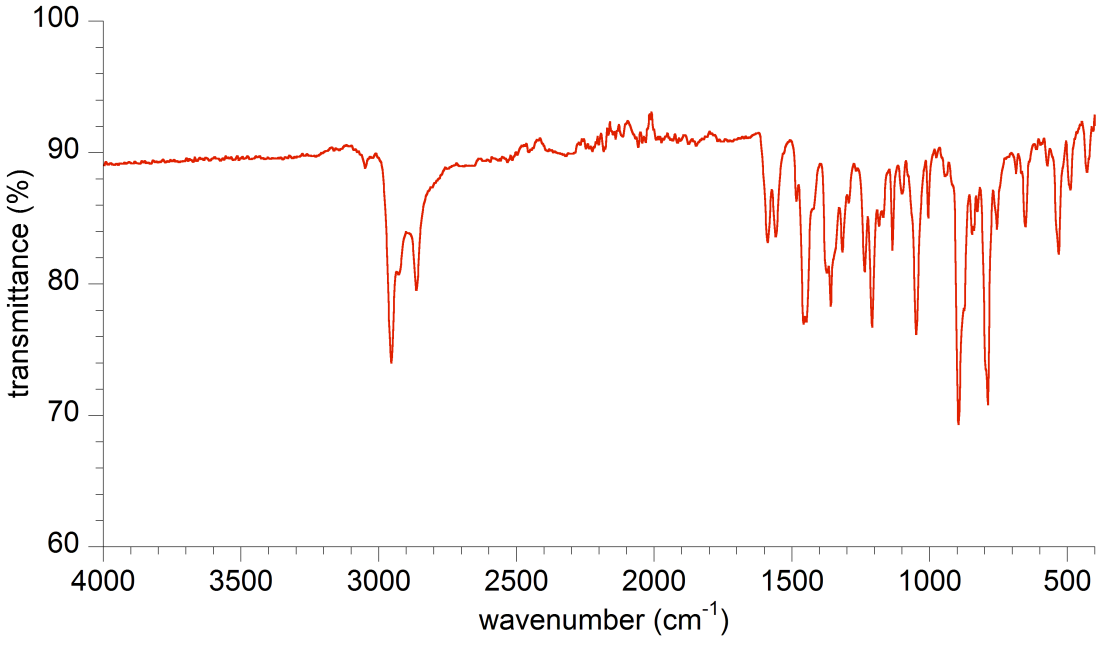
Fe	14.02697474097535	16.69612967928490	16.60490810856594
N	15.54194882751229	16.35998137739580	15.80932764232482
N	16.49570834229515	16.14685213441541	15.20381892399219
S	14.40236195793358	18.83730402434047	17.04739911358885
S	14.09568748138308	14.88760626031974	17.83547119042067
C	12.92973303370751	19.64937135951196	17.58681910906609
C	11.65713885264508	19.31609936432115	17.02272441062582
C	10.54812853819811	20.03850967993375	17.44129655469710
C	10.59796290337013	21.07304180896409	18.38199978400034
H	9.68376229260644	21.59640156339623	18.66451882251024
C	11.84735659583392	21.38435294085269	18.93295696970836
H	11.92452771087240	22.18604068761683	19.67403721328692
C	12.99148247505613	20.68749445289388	18.54472775397131
F	9.30954274822441	19.73945991732739	16.91387686028335
C	12.80568090511140	13.89832610104384	17.20166402657060
C	12.09623250611983	14.43789416110167	16.08717567564259
C	11.12375071062181	13.61802225338781	15.51638216434744
C	10.80703822552303	12.33334761380084	15.97097979676770
H	10.02584016985500	11.76145896222712	15.46815471507631
C	11.50006105985473	11.84221540884771	17.08837758188961
H	11.27428094648076	10.84041096645209	17.46820604212835
C	12.47956727017669	12.61888702744760	17.70308103957730
F	10.37611841446222	14.07833953918527	14.45161512066778
C	12.00133773275870	16.91953854385544	16.57495321935128
H	11.61850177251940	16.67479994244713	17.57247112438910
C	12.39310547613345	15.84179916615919	15.66213352687726
C	12.37454125844948	16.16541388820828	14.24666706271433
H	12.66333890184318	15.37870369011924	13.54459291533775
C	11.97358639668672	17.39150074756468	13.77641155538271
H	11.99392083769857	17.59279854937796	12.70111124400567
C	11.62123295067877	18.44678571699190	14.68022083870080
H	11.46932725160671	19.46300689949765	14.30941594522012
C	11.65619979813537	18.21359308652406	16.03706229024444
H	13.03945154174317	12.23317223329027	18.55929343778981
H	13.96594729992738	20.94170688689596	18.96798320927686

IR Spectra

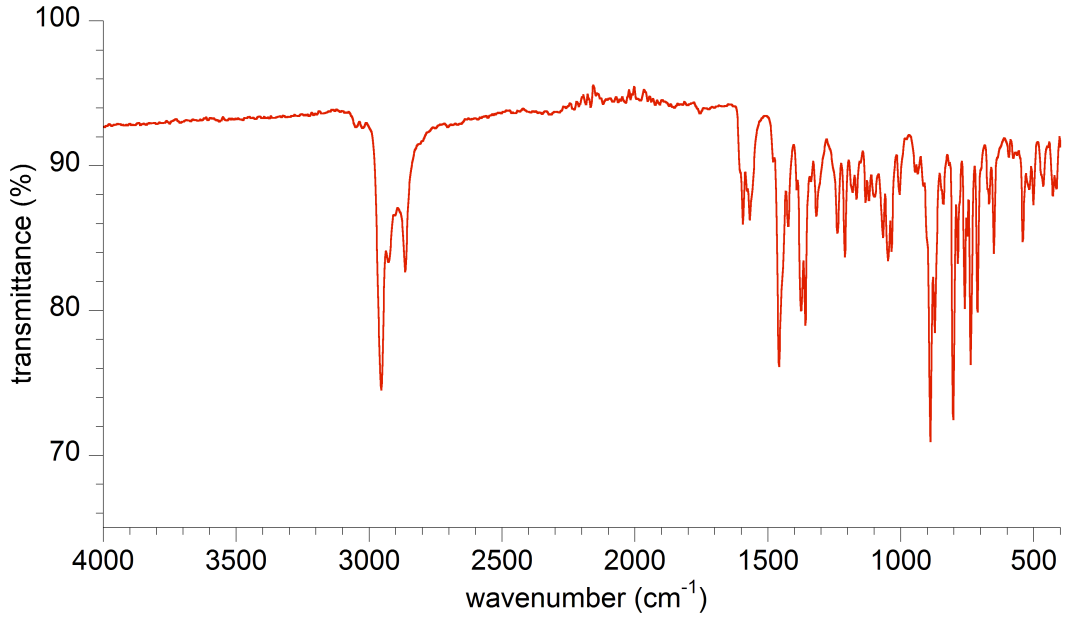
IR spectrum of $LFe(THF)_2$ (**1**).



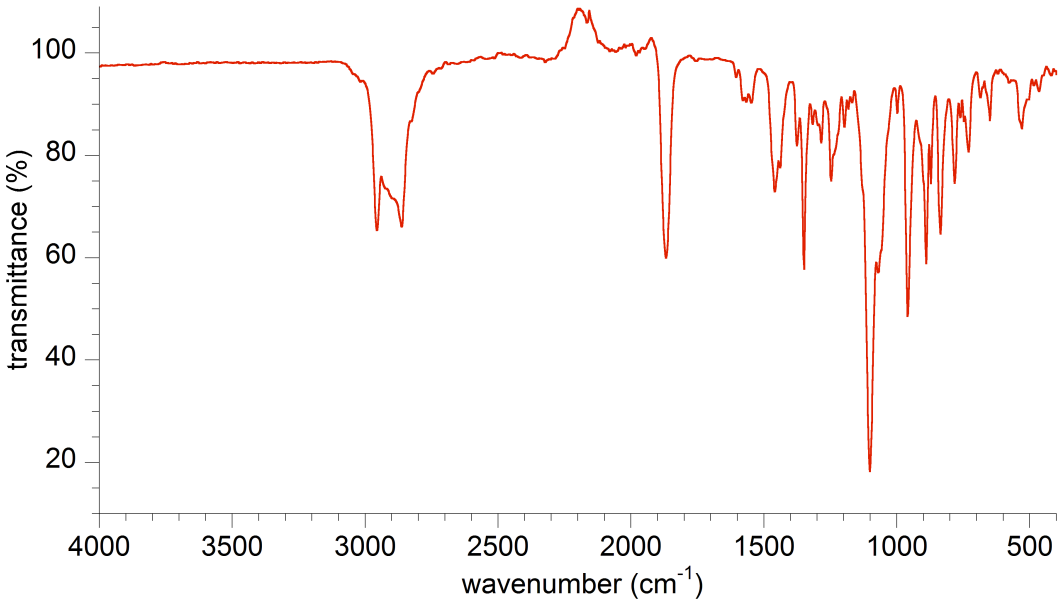
IR spectrum of LFeK (**2**).



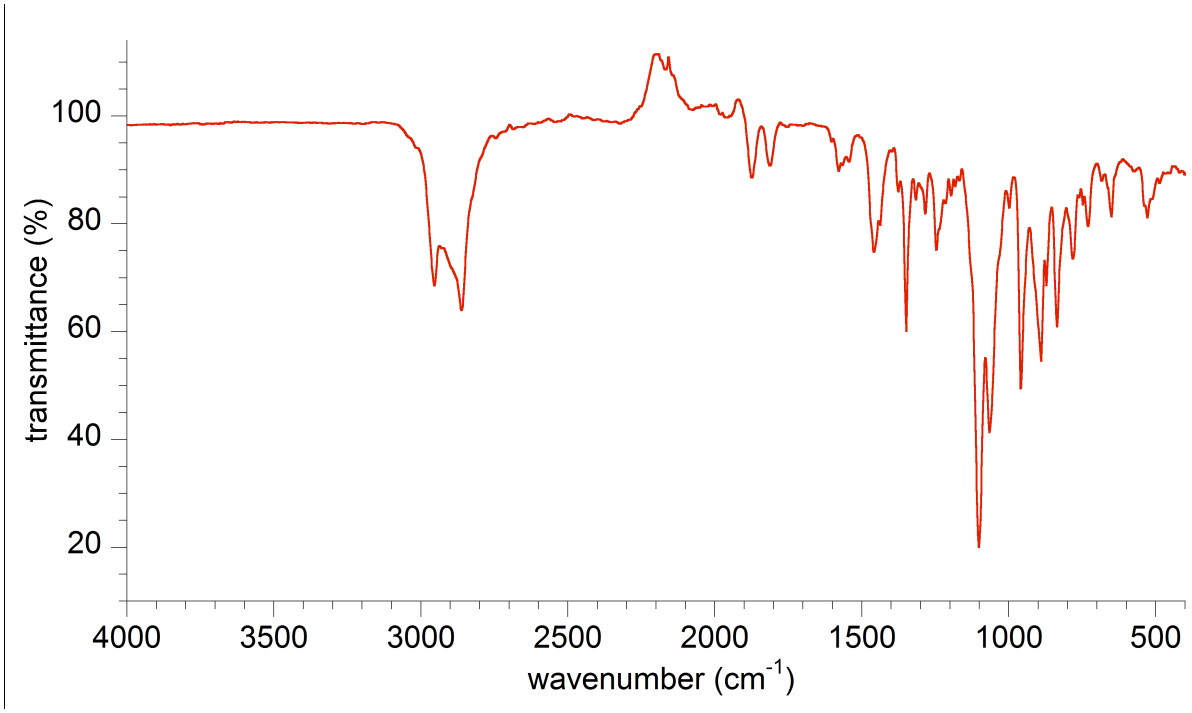
IR spectrum of [LFeSC$_6$H$_4$Ar]K (**5**).



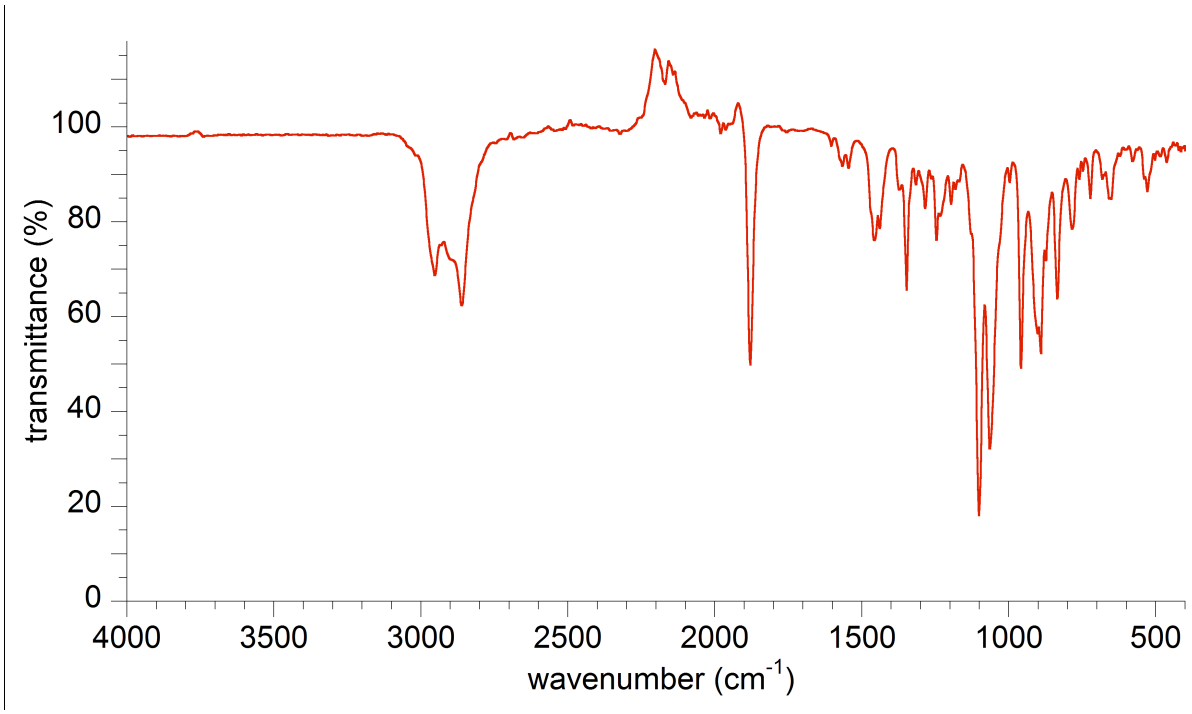
IR spectrum of [LFeN$_2$][K(18-crown-6)(THF)$_2$]$_2$ (**3**) (Procedure A).



IR spectrum of **3** after exchange of $^{14}N_2$ ligand with $^{15}N_2$ at -70 °C (Procedure C).

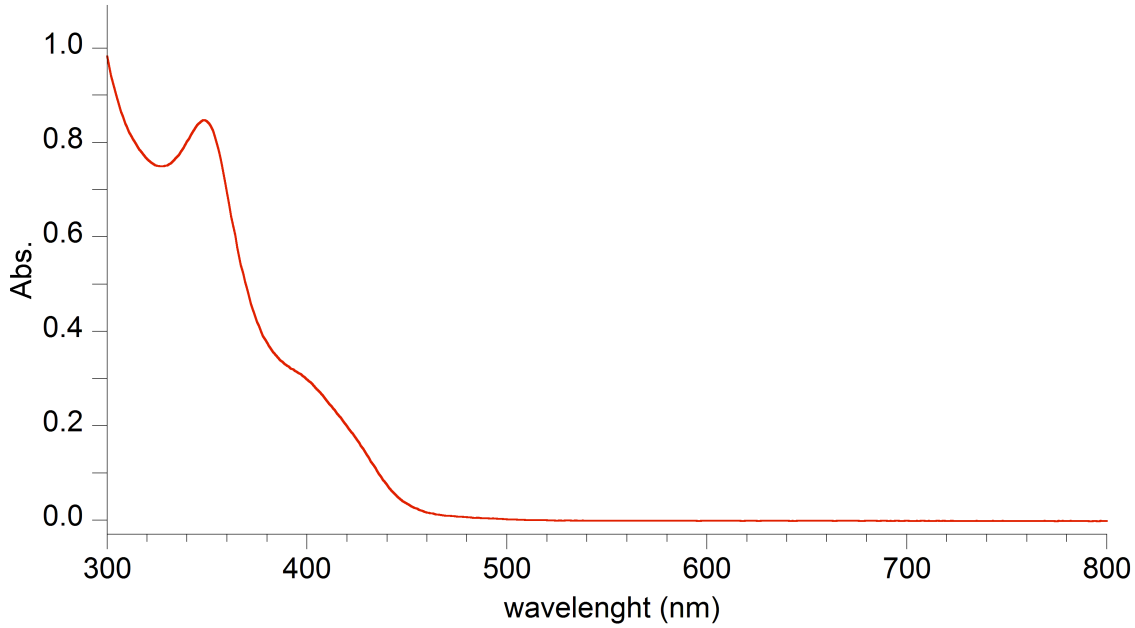


IR spectrum of $[LFeN_2][K(18\text{-crown-6})(THF)_2]_2$ (**3**) (Procedure E).

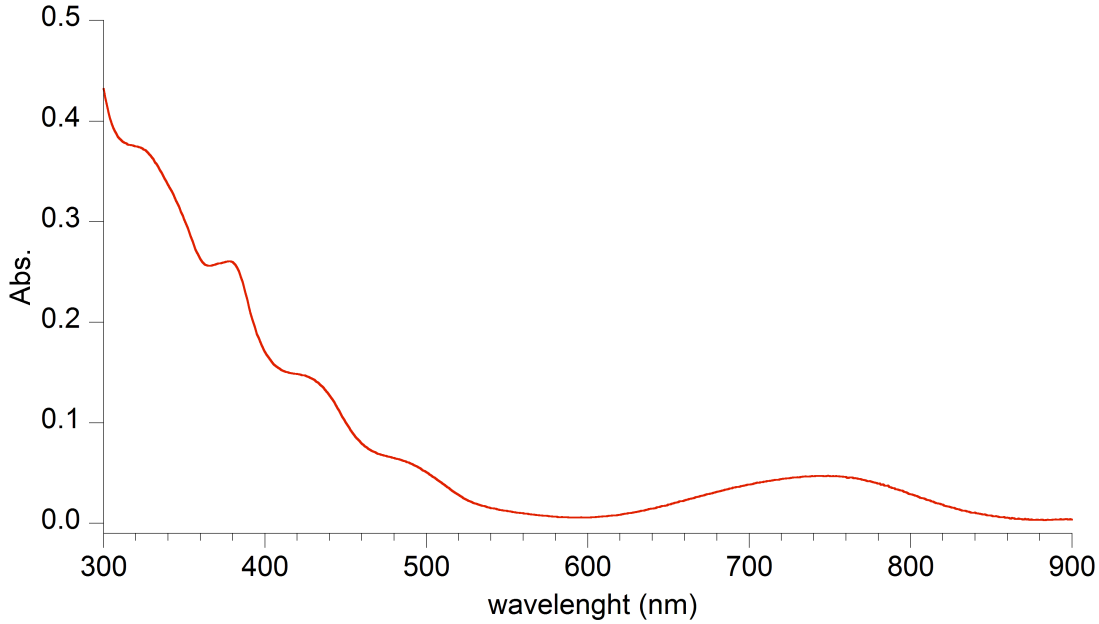


UV-VIS Spectra

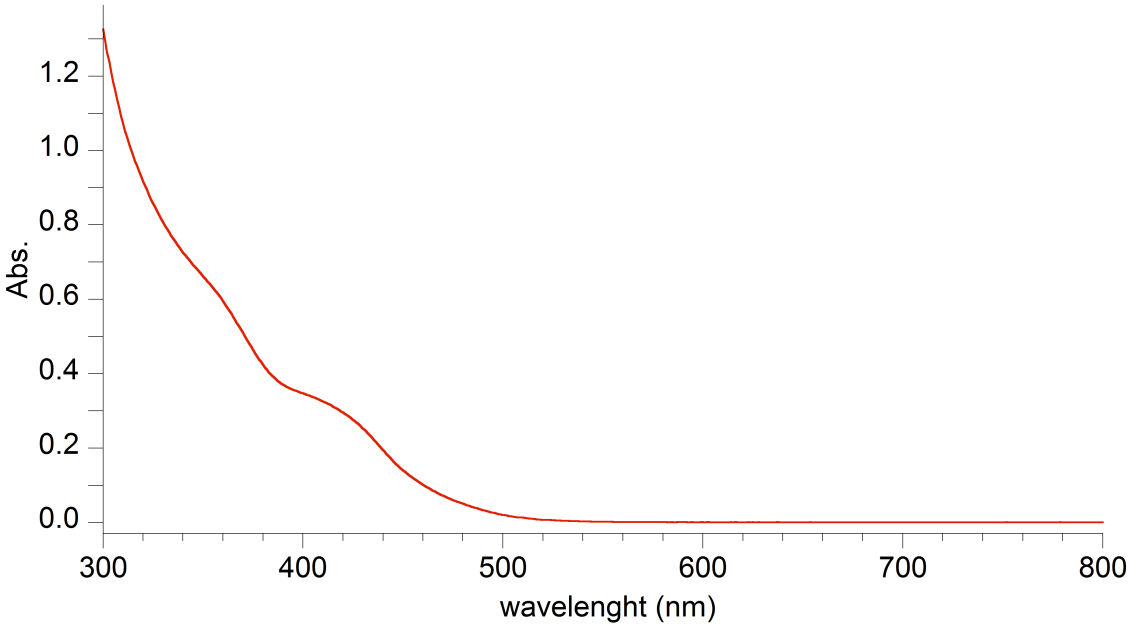
UV-VIS spectrum of $LFe(THF)_2$ (**1**) in THF, 1.15 mM, 21 °C, path length 0.1 cm.



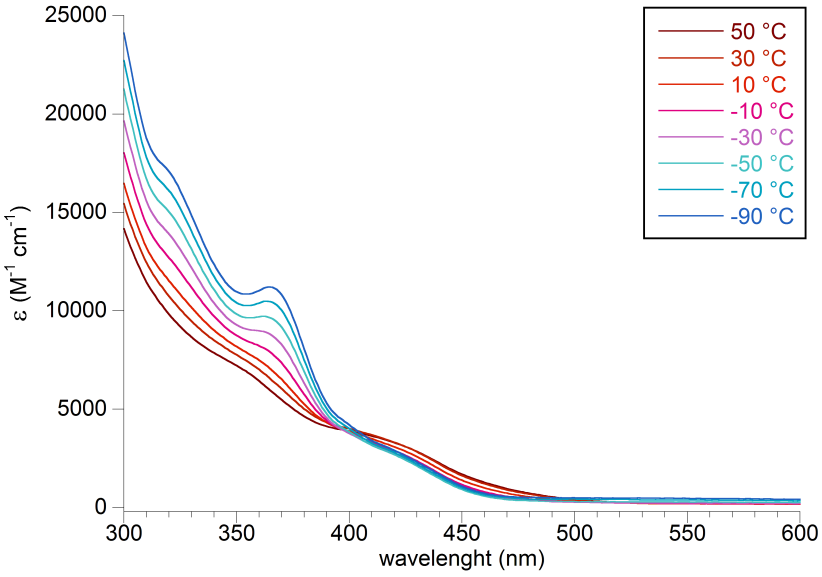
UV-VIS spectrum of LFeK (**2**) in THF, 0.48 mM, 21 °C, path length 0.1 cm.



UV-VIS spectrum of [LFeSC$_6$H$_4$Ar]K (**5**) in THF, 0.73 mM, 21 °C, path length 0.1 cm.

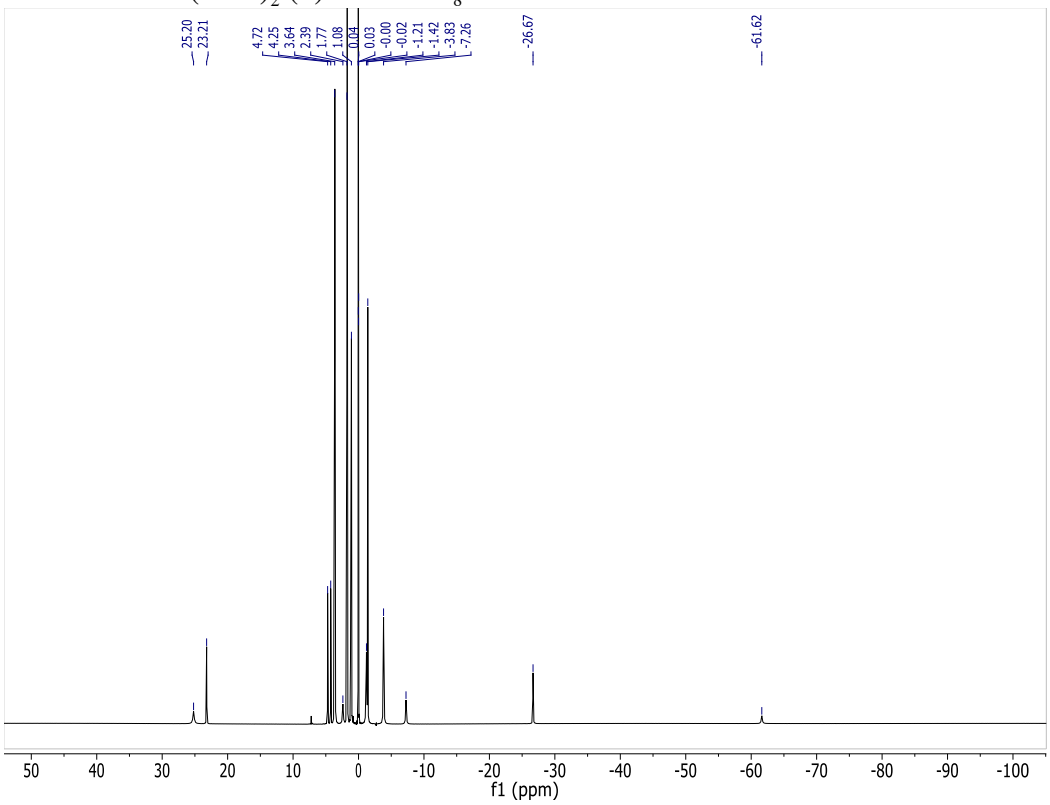


Temperature dependence of UV-VIS spectra of **5**/**5**·THF in THF. The concentration was corrected for cubic expansion coefficient of THF[49]. These data show the appearance of a new species at lower temperature, which we attribute to the crystallographically characterized compound **5**•THF.

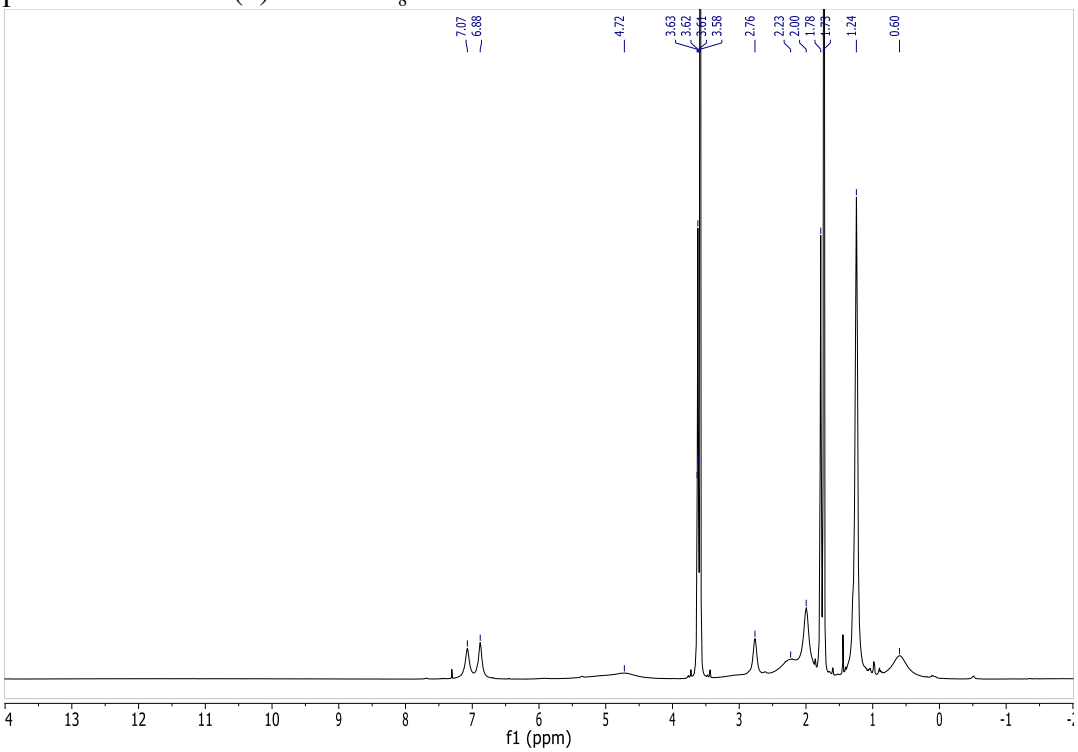


NMR Spectra

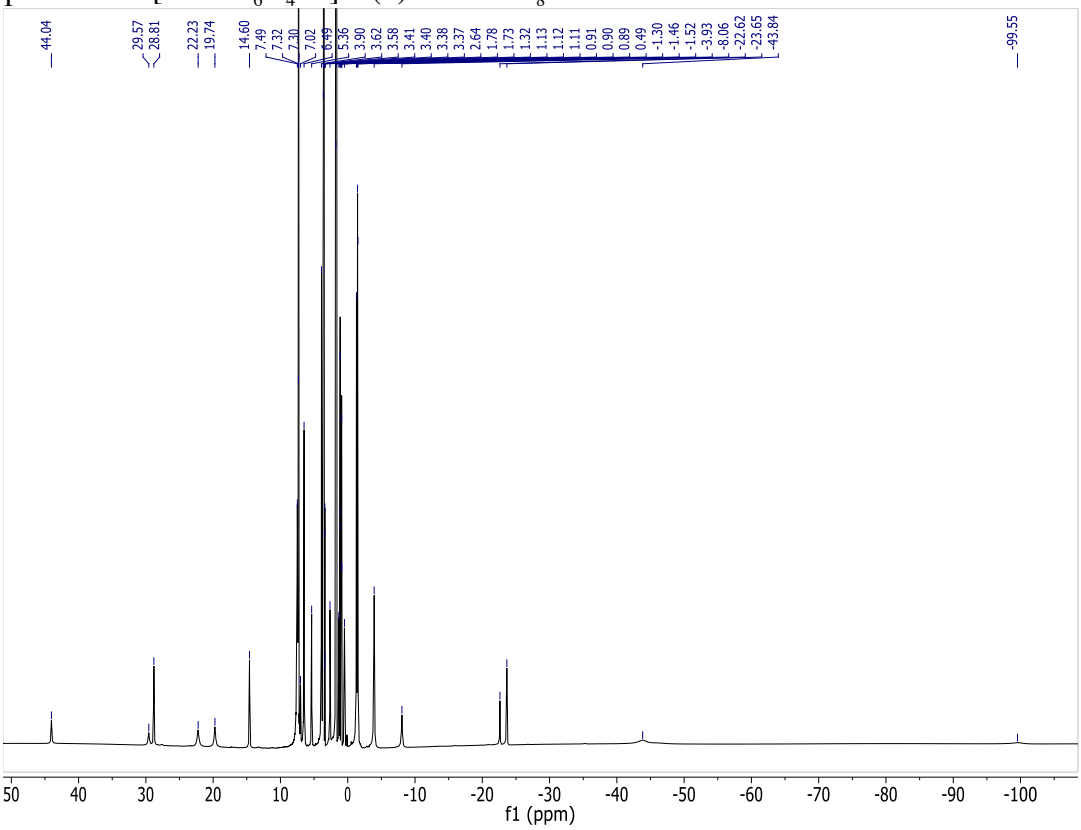
^{1}H NMR spectrum of LFe(THF)$_2$ (**1**) in THF-d_8.



^{1}H NMR spectrum of LFeK (**2**) in THF-d_8.

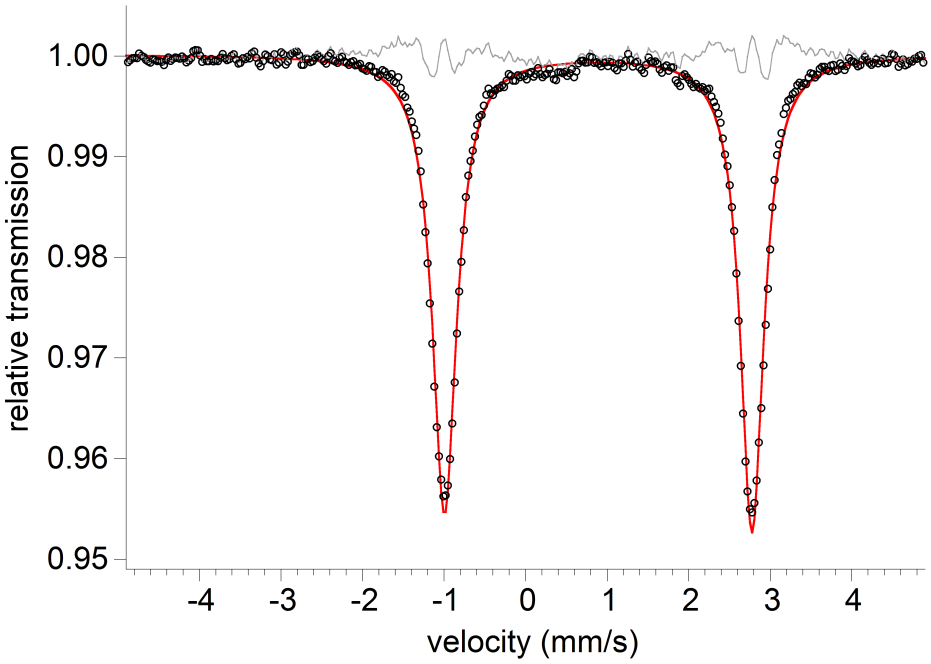


^{1}H NMR spectrum of [LFeSC$_6$H$_4$Ar]K (**5**) in THF-d_8.

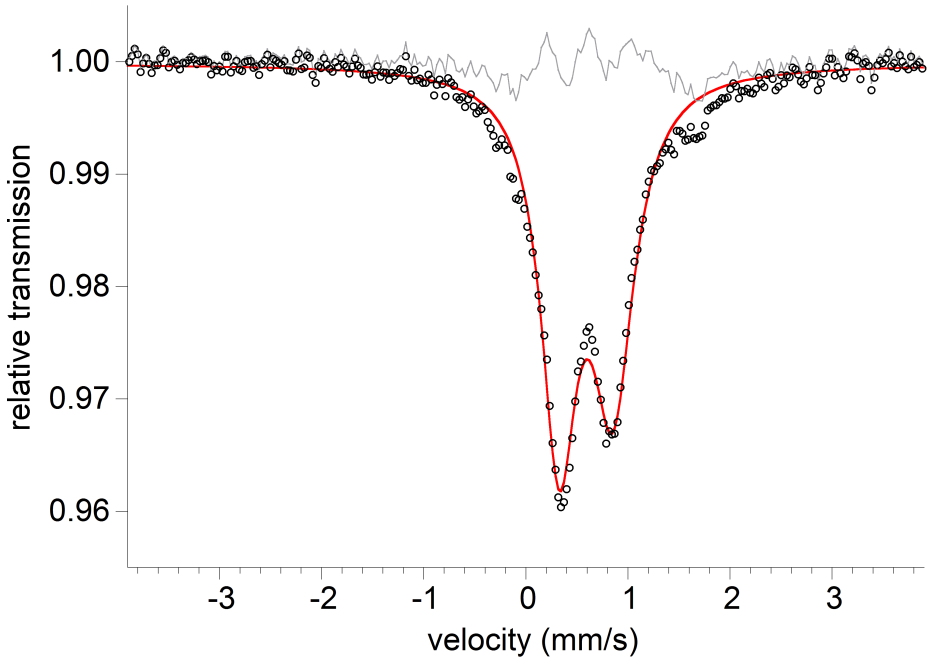


Mössbauer Spectra

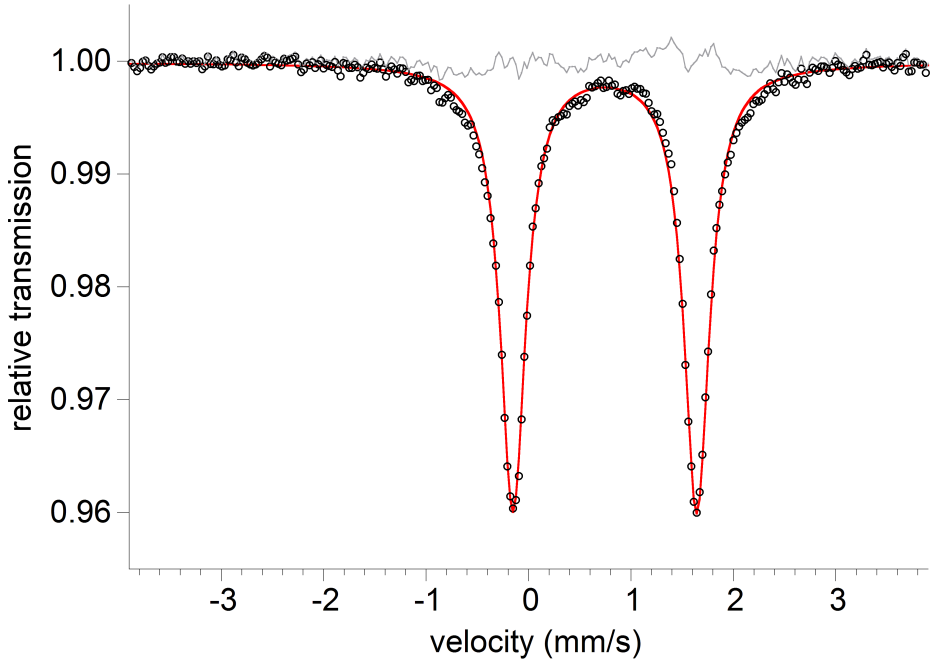
Zero-field Mössbauer spectrum of $LFe(THF)_2$ (**1**), recorded at 80 K. The black circles are the data, the red line is a simulation with $\delta = 0.89$ mm/s and $|\Delta E_Q| = 3.77$ mm/s, and gray line is the residual.



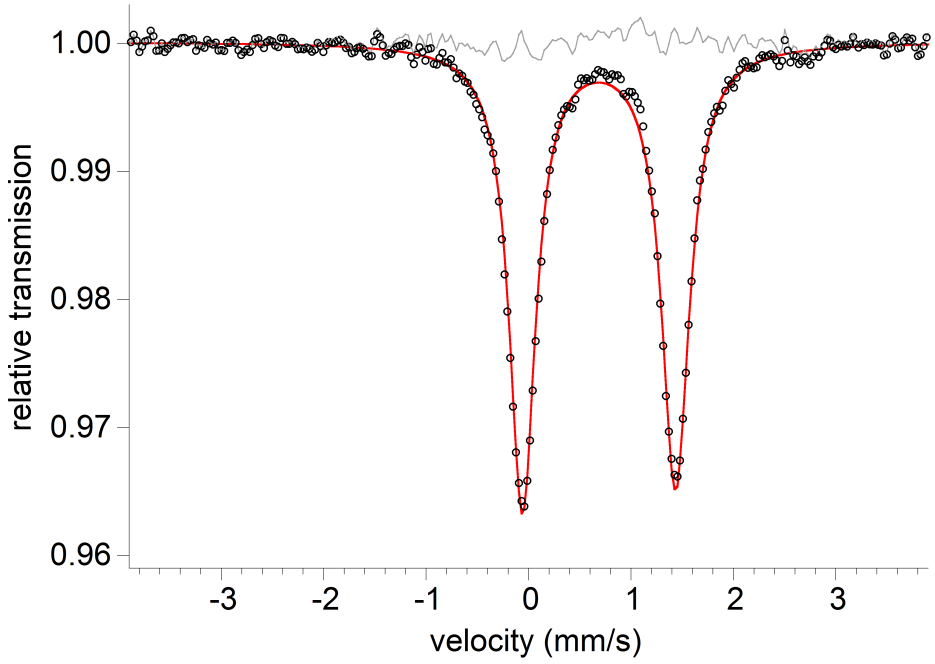
Zero-field Mössbauer spectrum of LFeK (**2**), recorded at 80 K. The black circles are the data, the red line is a simulation with $\delta = 0.59$ mm/s, $|\Delta E_Q| = 0.53$ mm/s, and gray line is the residual.



Zero-field Mössbauer spectrum of **3**, recorded at 80 K. The black circles are the data, the red line is a simulation with $\delta = 0.74$ mm/s, $|\Delta E_Q| = 1.79$ mm/s, and gray line is the residual.

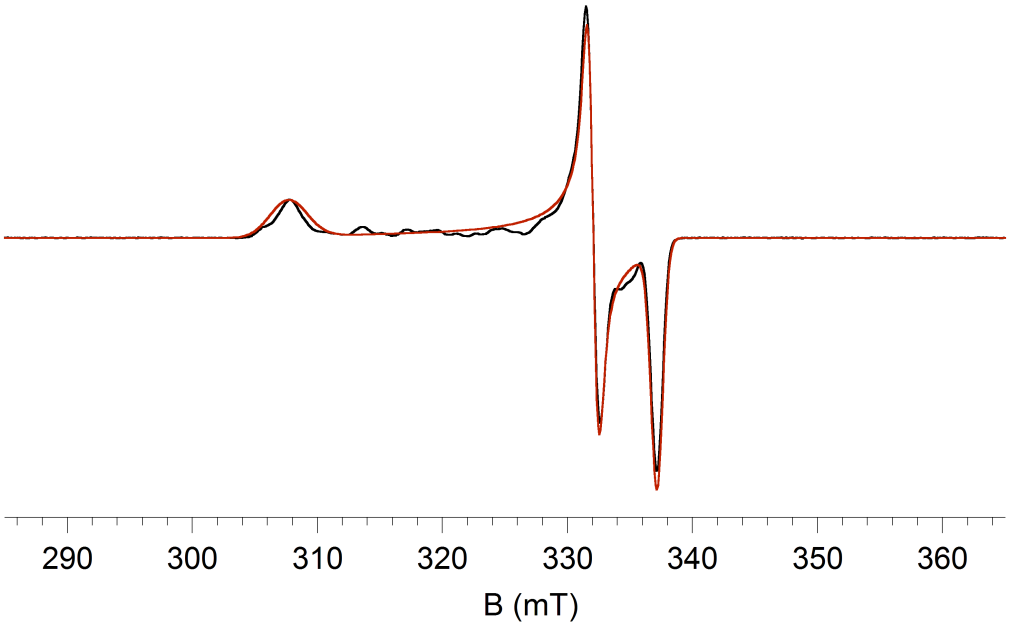


Zero-field Mössbauer spectrum of [LFeSC$_6$H$_4$Ar]K (**5**), recorded at 80 K. The black circles are the data, the red line is a simulation with $\delta = 0.69$ mm/s, $|\Delta E_Q| = 1.50$ mm/s, and gray line is the residual.



EPR Spectra

X-band EPR spectrum of LFeK (**2**) in frozen THF solution. Recorded at 9.4 ± 0.1 K. Acquisition parameters: frequency = 9.386 GHz, power = 0.01 mW, conversion time = 41 ms, modulation amplitude = 10 G, modulation frequency = 100 kHz, time constant = 10 ms, sweep time 42 s. The data are shown in black; in red is a simulation with **g** = [2.180, 2.020, 1.989] and H-Strain = [106, 25, 31] MHz.

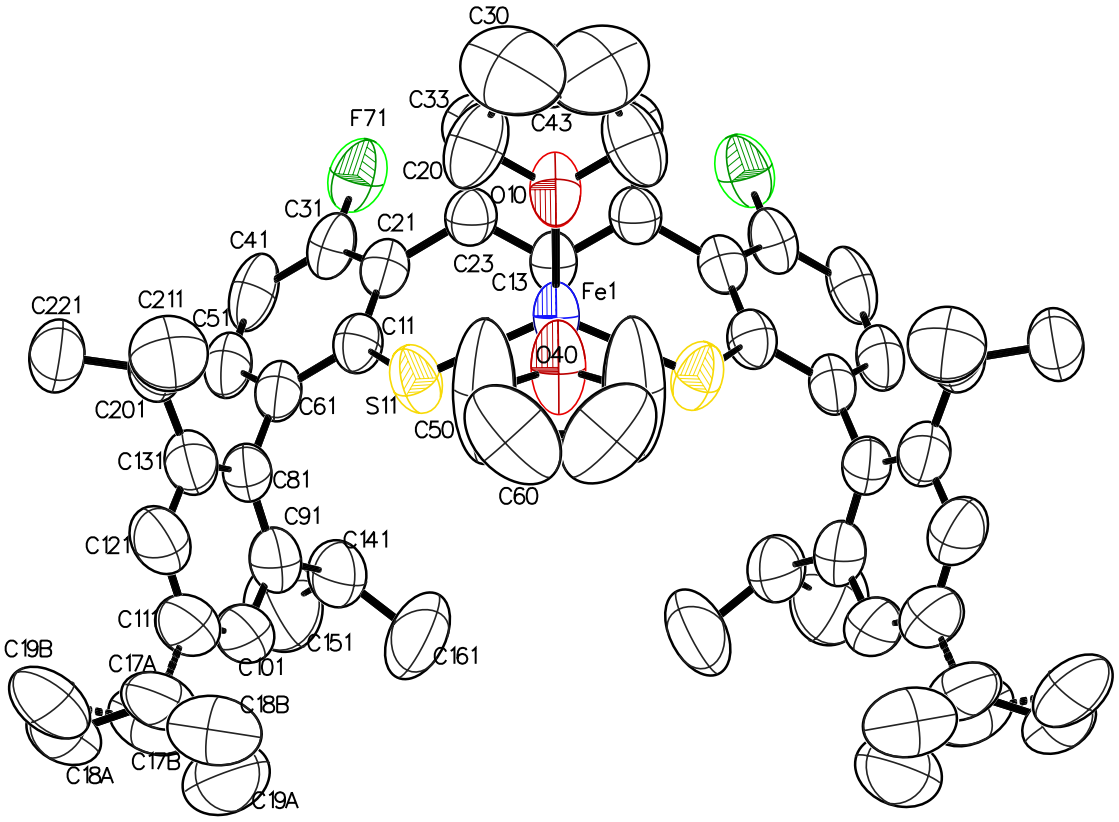


Crystallographic Data

Experimental and Refinement Details for LFe(THF)$_2$ (1)

Single crystals for X-ray analysis were obtained by slow cooling of a hot solution of LFe(THF)$_2$ (**1**) (33 mg) in THF (0.3 mL). Low-temperature diffraction data (ω-scans) were collected on a Rigaku MicroMax-007HF diffractometer coupled to a Saturn994+ CCD detector with Cu Kα (λ = 1.54178 Å). All structures were solved by direct methods and were refined against F^2 on all data by full-matrix least squares[50]. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included in the model at geometrically calculated positions and refined using a riding model. The isotropic displacement parameters of all hydrogen atoms were fixed to 1.2 times the U value of the atoms to which they are linked (1.5 times for methyl groups).

The crystal structure reported here contains solvent accessible voids in the unit cell. In spite of numerous attempts, no sensible solvent model could be established, and the solvent is assumed to be disordered within these voids. The crystals had been obtained from THF. The program SQUEEZE was used to compensate for the contribution of disordered solvents contained in voids within the crystal lattice from the diffraction intensities[51]. This procedure was applied to the data file and the submitted model is based on the solvent removed data. Based on the total electron density found in the voids (347.7 e/Å^3), it is likely that ~11 THF molecules are present in the unit cell. See "_platon_squeeze_details" in the .cif for more information. Reflections [-1 4 2], [-3 9 3] [2 1 0] and [-2 11 2] are omitted, due to the close proximity of these reflections to the beam-stop. One isopropyl moiety is disordered over two positions. The site occupancy factors of the two positions were freely refined and converged at the values of 0.55(2) and 0.45(2). The major position involves atoms {C17A, C18A, C19A}; the minor component contains {C17B, C18B, C19B}. A rigid bond restraint was applied to the major and minor disordered sites. The refinement became unstable without rigid bond restraints, which is likely related to the close proximity of the atoms in the disordered model.



The full numbering scheme of $LFe(THF)_2$ (**1**), which resides on a crystallographic mirror plane. The symmetry equivalents of the numbered atoms are generated by the operation x, ½-y, z. All atoms shown are depicted with 50% thermal contours. The hydrogen atoms have been removed for clarity.

Crystal data and structure refinement for $LFe(THF)_2$ (1).

Identification code	007-14182	
Empirical formula	$C_{56}H_{70}F_2FeO_2S_2$	
Formula weight	933.09	
Temperature	193(2) K	
Wavelength	1.54187 Å	
Crystal system	Monoclinic	
Space group	P 2_1/m	
Unit cell dimensions	a = 8.8407(2) Å	α = 90°.
	b = 23.7861(5) Å	β = 100.433(7)°.
	c = 17.0387(12) Å	γ = 90°.
Volume	3523.8(3) $Å^3$	
Z	2	
Density (calculated)	0.879 g/cm^3	
Absorption coefficient	2.533 mm^{-1}	
F(000)	996	
Crystal size	0.180 x 0.170 x 0.160 mm^3	
Crystal color and habit	Yellow needle	
Diffractometer	Rigaku Saturn 944+ CCD	
Θ range for data collection	2.637 to 65.088°.	
Index ranges	$-10 < \leq h \leq 9, -27 \leq k \leq 27, -20 \leq l \leq 20$	
Reflections collected	93006	
Independent reflections	6133 [R(int) = 0.2179]	
Observed reflections (I > 2σ(I))	3452	
Completeness to theta = 65.088°	99.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.687 and 0.435	
Solution method	SHELXT-2014/5 (Sheldrick, 2014)	
Refinement method	SHELXL-2014/7 (Sheldrick, 2014)	
Data / restraints / parameters	6133 / 49 / 329	
Goodness-of-fit on F^2	1.027	
Final R indices [I>2σ(I)]	R1 = 0.0775, wR2 = 0.2307	
R indices (all data)	R1 = 0.1138, wR2 = 0.2513	
Extinction coefficient	0.0035(6)	
Largest diff. peak and hole	0.346 and -0.290 e.$Å^{-3}$	

Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $LFe(THF)_2$ (1). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Fe(1)	5173(1)	2500	5749(1)	69(1)
S(11)	4898(1)	3371(1)	6285(1)	86(1)
C(11)	3166(5)	3719(2)	5942(2)	66(1)
C(21)	2067(5)	3544(2)	5267(2)	66(1)
C(31)	791(5)	3867(2)	5046(3)	71(1)
C(41)	485(6)	4349(2)	5436(3)	87(1)
C(51)	1561(6)	4518(2)	6091(3)	77(1)
C(61)	2869(5)	4213(2)	6342(3)	68(1)
F(71)	-276(3)	3698(1)	4412(2)	93(1)
C(81)	3967(6)	4415(2)	7071(3)	76(1)
C(91)	3745(7)	4247(2)	7833(3)	94(2)
C(101)	4711(8)	4447(2)	8492(3)	113(2)
C(111)	5911(9)	4801(3)	8431(3)	123(2)
C(121)	6146(7)	4968(2)	7687(3)	107(2)
C(131)	5176(6)	4768(2)	6996(3)	84(1)
C(141)	2457(8)	3858(2)	7939(3)	109(2)
C(151)	1090(10)	4190(3)	8194(5)	168(3)
C(161)	2952(10)	3367(3)	8497(5)	162(3)
C(17A)	7370(30)	4991(6)	9114(9)	151(7)
C(18A)	6990(50)	5580(8)	9386(15)	165(8)
C(19A)	7700(30)	4580(8)	9804(12)	174(8)
C(17B)	6740(20)	5042(8)	9282(9)	133(7)
C(18B)	8150(20)	4651(12)	9390(17)	156(8)
C(19B)	6970(60)	5666(9)	9110(20)	182(12)
C(201)	5439(6)	4986(2)	6186(3)	82(1)
C(211)	7060(7)	4908(3)	6071(4)	124(2)
C(221)	4897(8)	5590(2)	6047(4)	115(2)
C(13)	2230(6)	2500	5231(4)	62(1)
C(23)	2217(5)	3009(2)	4830(3)	66(1)
C(33)	2180(5)	3004(2)	4025(3)	79(1)
C(43)	2200(8)	2500	3607(4)	87(2)
O(10)	5793(5)	2500	4657(3)	89(1)
C(20)	6284(8)	2990(2)	4271(4)	128(2)
C(30)	7034(12)	2762(4)	3637(5)	224(5)
O(40)	7577(5)	2500	6242(4)	116(2)
C(50)	8533(8)	2963(3)	6460(8)	233(6)
C(60)	9910(8)	2796(3)	6865(5)	178(3)

Bond lengths [Å] and angles [°] for $LFe(THF)_2$ (1).

Fe(1)-O(10)	2.032(5)
Fe(1)-O(40)	2.139(5)
Fe(1)-S(11)	2.2937(11)
Fe(1)-S(11)#1	2.2937(11)

S(11)-C(11)	1.747(4)
C(11)-C(61)	1.407(5)
C(11)-C(21)	1.426(6)
C(21)-C(31)	1.360(5)
C(21)-C(23)	1.492(5)
C(31)-F(71)	1.359(5)
C(31)-C(41)	1.377(6)
C(41)-C(51)	1.389(6)
C(41)-H(41)	0.9500
C(51)-C(61)	1.367(6)
C(51)-H(51)	0.9500
C(61)-C(81)	1.509(6)
C(81)-C(131)	1.384(6)
C(81)-C(91)	1.406(6)
C(91)-C(101)	1.367(7)
C(91)-C(141)	1.503(7)
C(101)-C(111)	1.373(8)
C(101)-H(101)	0.9500
C(111)-C(121)	1.379(8)
C(111)-C(17B)	1.607(14)
C(111)-C(17A)	1.637(15)
C(121)-C(131)	1.409(7)
C(121)-H(121)	0.9500
C(131)-C(201)	1.529(7)
C(141)-C(161)	1.519(8)
C(141)-C(151)	1.570(10)
C(141)-H(141)	1.0000
C(151)-H(15A)	0.9800
C(151)-H(15B)	0.9800
C(151)-H(15C)	0.9800
C(161)-H(16A)	0.9800
C(161)-H(16B)	0.9800
C(161)-H(16C)	0.9800
C(17A)-C(19A)	1.516(16)
C(17A)-C(18A)	1.531(17)
C(17A)-H(17A)	1.0000
C(18A)-H(18A)	0.9800
C(18A)-H(18B)	0.9800
C(18A)-H(18C)	0.9800
C(19A)-H(19A)	0.9800
C(19A)-H(19B)	0.9800
C(19A)-H(19C)	0.9800
C(17B)-C(19B)	1.533(18)
C(17B)-C(18B)	1.536(16)
C(17B)-H(17B)	1.0000
C(18B)-H(18D)	0.9800
C(18B)-H(18E)	0.9800
C(18B)-H(18F)	0.9800
C(19B)-H(19D)	0.9800
C(19B)-H(19E)	0.9800
C(19B)-H(19F)	0.9800
C(201)-C(211)	1.493(8)
C(201)-C(221)	1.522(7)
C(201)-H(201)	1.0000
C(211)-H(21A)	0.9800
C(211)-H(21B)	0.9800

C(211)-H(21C)	0.9800
C(221)-H(22A)	0.9800
C(221)-H(22B)	0.9800
C(221)-H(22C)	0.9800
C(13)-C(23)#1	1.390(5)
C(13)-C(23)	1.390(5)
C(13)-H(13)	0.9500
C(23)-C(33)	1.366(6)
C(33)-C(43)	1.396(6)
C(33)-H(33)	0.9500
C(43)-C(33)#1	1.397(6)
C(43)-H(43)	0.9500
O(10)-C(20)#1	1.444(5)
O(10)-C(20)	1.444(5)
C(20)-C(30)	1.470(10)
C(20)-H(20A)	0.9900
C(20)-H(20B)	0.9900
C(30)-C(30)#1	1.247(19)
C(30)-H(30A)	0.9900
C(30)-H(30B)	0.9900
O(40)-C(50)#1	1.396(6)
O(40)-C(50)	1.396(6)
C(50)-C(60)	1.346(10)
C(50)-H(50A)	0.9900
C(50)-H(50B)	0.9900
C(60)-C(60)#1	1.406(16)
C(60)-H(60A)	0.9900
C(60)-H(60B)	0.9900

O(10)-Fe(1)-O(40)	86.9(2)
O(10)-Fe(1)-S(11)	115.45(4)
O(40)-Fe(1)-S(11)	90.74(8)
O(10)-Fe(1)-S(11)#1	115.45(4)
O(40)-Fe(1)-S(11)#1	90.75(8)
S(11)-Fe(1)-S(11)#1	129.08(8)
C(11)-S(11)-Fe(1)	116.42(15)
C(61)-C(11)-C(21)	118.4(4)
C(61)-C(11)-S(11)	117.6(3)
C(21)-C(11)-S(11)	124.0(3)
C(31)-C(21)-C(11)	117.9(4)
C(31)-C(21)-C(23)	119.2(4)
C(11)-C(21)-C(23)	122.8(3)
F(71)-C(31)-C(21)	118.4(4)
F(71)-C(31)-C(41)	117.4(4)
C(21)-C(31)-C(41)	124.2(4)
C(31)-C(41)-C(51)	117.6(4)
C(31)-C(41)-H(41)	121.2
C(51)-C(41)-H(41)	121.2
C(61)-C(51)-C(41)	121.1(4)
C(61)-C(51)-H(51)	119.5
C(41)-C(51)-H(51)	119.5
C(51)-C(61)-C(11)	120.8(4)
C(51)-C(61)-C(81)	118.1(4)
C(11)-C(61)-C(81)	121.1(4)
C(131)-C(81)-C(91)	119.9(4)
C(131)-C(81)-C(61)	120.6(4)

C(91)-C(81)-C(61)	119.5(4)
C(101)-C(91)-C(81)	119.2(5)
C(101)-C(91)-C(141)	119.3(5)
C(81)-C(91)-C(141)	121.5(5)
C(91)-C(101)-C(111)	121.9(5)
C(91)-C(101)-H(101)	119.1
C(111)-C(101)-H(101)	119.1
C(101)-C(111)-C(121)	119.5(5)
C(101)-C(111)-C(17B)	112.6(10)
C(121)-C(111)-C(17B)	127.3(10)
C(101)-C(111)-C(17A)	129.5(9)
C(121)-C(111)-C(17A)	110.1(10)
C(111)-C(121)-C(131)	120.1(5)
C(111)-C(121)-H(121)	120.0
C(131)-C(121)-H(121)	120.0
C(81)-C(131)-C(121)	119.4(5)
C(81)-C(131)-C(201)	122.4(4)
C(121)-C(131)-C(201)	118.1(5)
C(91)-C(141)-C(161)	114.2(6)
C(91)-C(141)-C(151)	111.1(5)
C(161)-C(141)-C(151)	111.3(6)
C(91)-C(141)-H(141)	106.6
C(161)-C(141)-H(141)	106.6
C(151)-C(141)-H(141)	106.6
C(141)-C(151)-H(15A)	109.5
C(141)-C(151)-H(15B)	109.5
H(15A)-C(151)-H(15B)	109.5
C(141)-C(151)-H(15C)	109.5
H(15A)-C(151)-H(15C)	109.5
H(15B)-C(151)-H(15C)	109.5
C(141)-C(161)-H(16A)	109.5
C(141)-C(161)-H(16B)	109.5
H(16A)-C(161)-H(16B)	109.5
C(141)-C(161)-H(16C)	109.5
H(16A)-C(161)-H(16C)	109.5
H(16B)-C(161)-H(16C)	109.5
C(19A)-C(17A)-C(18A)	112(2)
C(19A)-C(17A)-C(111)	112.8(14)
C(18A)-C(17A)-C(111)	106.3(19)
C(19A)-C(17A)-H(17A)	108.5
C(18A)-C(17A)-H(17A)	108.5
C(111)-C(17A)-H(17A)	108.5
C(17A)-C(18A)-H(18A)	109.5
C(17A)-C(18A)-H(18B)	109.5
H(18A)-C(18A)-H(18B)	109.5
C(17A)-C(18A)-H(18C)	109.5
H(18A)-C(18A)-H(18C)	109.5
H(18B)-C(18A)-H(18C)	109.5
C(17A)-C(19A)-H(19A)	109.5
C(17A)-C(19A)-H(19B)	109.5
H(19A)-C(19A)-H(19B)	109.5
C(17A)-C(19A)-H(19C)	109.5
H(19A)-C(19A)-H(19C)	109.5
H(19B)-C(19A)-H(19C)	109.5
C(19B)-C(17B)-C(18B)	118(3)
C(19B)-C(17B)-C(111)	103.4(18)

C(18B)-C(17B)-C(111)	96.9(13)
C(19B)-C(17B)-H(17B)	112.2
C(18B)-C(17B)-H(17B)	112.2
C(111)-C(17B)-H(17B)	112.2
C(17B)-C(18B)-H(18D)	109.5
C(17B)-C(18B)-H(18E)	109.5
H(18D)-C(18B)-H(18E)	109.5
C(17B)-C(18B)-H(18F)	109.5
H(18D)-C(18B)-H(18F)	109.5
H(18E)-C(18B)-H(18F)	109.5
C(17B)-C(19B)-H(19D)	109.5
C(17B)-C(19B)-H(19E)	109.5
H(19D)-C(19B)-H(19E)	109.5
C(17B)-C(19B)-H(19F)	109.5
H(19D)-C(19B)-H(19F)	109.5
H(19E)-C(19B)-H(19F)	109.5
C(211)-C(201)-C(221)	112.3(4)
C(211)-C(201)-C(131)	112.5(4)
C(221)-C(201)-C(131)	111.5(4)
C(211)-C(201)-H(201)	106.7
C(221)-C(201)-H(201)	106.7
C(131)-C(201)-H(201)	106.7
C(201)-C(211)-H(21A)	109.5
C(201)-C(211)-H(21B)	109.5
H(21A)-C(211)-H(21B)	109.5
C(201)-C(211)-H(21C)	109.5
H(21A)-C(211)-H(21C)	109.5
H(21B)-C(211)-H(21C)	109.5
C(201)-C(221)-H(22A)	109.5
C(201)-C(221)-H(22B)	109.5
H(22A)-C(221)-H(22B)	109.5
C(201)-C(221)-H(22C)	109.5
H(22A)-C(221)-H(22C)	109.5
H(22B)-C(221)-H(22C)	109.5
C(23)#1-C(13)-C(23)	121.3(5)
C(23)#1-C(13)-H(13)	119.3
C(23)-C(13)-H(13)	119.3
C(33)-C(23)-C(13)	118.8(4)
C(33)-C(23)-C(21)	121.4(3)
C(13)-C(23)-C(21)	119.4(4)
C(23)-C(33)-C(43)	121.3(4)
C(23)-C(33)-H(33)	119.3
C(43)-C(33)-H(33)	119.3
C(33)-C(43)-C(33)#1	118.3(6)
C(33)-C(43)-H(43)	120.8
C(33)#1-C(43)-H(43)	120.8
C(20)#1-O(10)-C(20)	107.8(6)
C(20)#1-O(10)-Fe(1)	124.8(3)
C(20)-O(10)-Fe(1)	124.8(3)
O(10)-C(20)-C(30)	104.4(6)
O(10)-C(20)-H(20A)	110.9
C(30)-C(20)-H(20A)	110.9
O(10)-C(20)-H(20B)	110.9
C(30)-C(20)-H(20B)	110.9
H(20A)-C(20)-H(20B)	108.9
C(30)#1-C(30)-C(20)	111.7(4)

C(30)#1-C(30)-H(30A)	109.3
C(20)-C(30)-H(30A)	109.3
C(30)#1-C(30)-H(30B)	109.3
C(20)-C(30)-H(30B)	109.3
H(30A)-C(30)-H(30B)	107.9
C(50)#1-O(40)-C(50)	104.1(7)
C(50)#1-O(40)-Fe(1)	127.9(3)
C(50)-O(40)-Fe(1)	127.9(3)
C(60)-C(50)-O(40)	110.6(6)
C(60)-C(50)-H(50A)	109.5
O(40)-C(50)-H(50A)	109.5
C(60)-C(50)-H(50B)	109.5
O(40)-C(50)-H(50B)	109.5
H(50A)-C(50)-H(50B)	108.1
C(50)-C(60)-C(60)#1	107.2(4)
C(50)-C(60)-H(60A)	110.3
C(60)#1-C(60)-H(60A)	110.3
C(50)-C(60)-H(60B)	110.3
C(60)#1-C(60)-H(60B)	110.3
H(60A)-C(60)-H(60B)	108.5

Symmetry transformations used to generate equivalent atoms:
#1 x,-y+1/2,z

Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $LFe(THF)_2$ (1). The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Fe(1)	54(1)	48(1)	104(1)	0	12(1)	0
S(11)	75(1)	65(1)	108(1)	-18(1)	-8(1)	15(1)
C(11)	64(3)	56(2)	81(3)	5(2)	20(2)	8(2)
C(21)	67(3)	54(2)	79(3)	8(2)	21(2)	3(2)
C(31)	58(3)	55(2)	98(3)	17(2)	8(2)	4(2)
C(41)	72(3)	59(3)	138(4)	30(3)	40(3)	21(2)
C(51)	85(3)	52(2)	100(3)	7(2)	36(3)	9(2)
C(61)	77(3)	49(2)	85(3)	6(2)	29(2)	5(2)
F(71)	70(2)	81(2)	123(2)	21(1)	-1(2)	7(1)
C(81)	100(4)	54(2)	78(3)	-2(2)	26(3)	2(2)
C(91)	123(4)	61(3)	98(4)	-6(2)	23(3)	-10(3)
C(101)	177(6)	83(3)	79(3)	-9(3)	24(4)	-33(4)
C(111)	180(6)	98(4)	86(4)	-15(3)	14(4)	-35(4)
C(121)	129(5)	85(3)	106(4)	-21(3)	22(4)	-20(3)
C(131)	95(3)	64(3)	96(4)	-8(2)	25(3)	0(2)
C(141)	148(5)	80(3)	105(4)	-6(3)	37(4)	-35(3)
C(151)	184(8)	144(6)	200(7)	-9(5)	101(7)	-40(6)
C(161)	210(8)	99(4)	170(7)	50(4)	15(6)	-30(5)
C(17A)	239(15)	131(9)	77(8)	-27(5)	16(9)	-52(9)
C(18A)	270(20)	129(10)	90(13)	-31(7)	28(13)	-53(9)
C(19A)	209(18)	178(12)	120(11)	28(9)	-10(11)	-59(11)
C(17B)	135(11)	161(12)	108(10)	-43(8)	36(8)	-39(8)

C(18B)	155(12)	203(16)	111(14)	-16(11)	23(10)	-12(11)
C(19B)	250(20)	152(11)	120(20)	-53(9)	-14(17)	-63(10)
C(201)	92(3)	65(3)	96(3)	-6(2)	30(3)	-12(2)
C(211)	110(5)	140(5)	132(5)	-1(4)	47(4)	0(4)
C(221)	162(6)	70(3)	126(4)	8(3)	56(4)	2(3)
C(13)	51(3)	49(3)	84(4)	0	5(3)	0
C(23)	61(3)	61(2)	75(3)	3(2)	8(2)	6(2)
C(33)	75(3)	75(3)	86(3)	10(2)	13(2)	6(2)
C(43)	93(5)	74(4)	89(5)	0	6(4)	0
O(10)	87(3)	59(2)	131(4)	0	46(3)	0
C(20)	122(5)	99(4)	172(6)	40(4)	48(4)	-25(3)
C(30)	241(9)	266(13)	194(7)	-38(7)	116(7)	-129(8)
O(40)	65(3)	68(3)	204(5)	0	-5(3)	0
C(50)	76(4)	91(4)	491(16)	10(6)	-55(7)	-29(3)
C(60)	93(4)	211(8)	226(8)	-78(6)	19(5)	-24(4)

Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $LFe(THF)_2$ (1).

	x	y	z	U(eq)
H(41)	-430	4558	5263	104
H(51)	1385	4851	6368	92
H(101)	4547	4338	9006	136
H(121)	6964	5218	7641	128
H(141)	2052	3692	7403	131
H(15A)	1421	4346	8730	252
H(15B)	219	3936	8195	252
H(15C)	778	4497	7816	252
H(16A)	3802	3167	8323	243
H(16B)	2083	3110	8487	243
H(16C)	3290	3508	9041	243
H(17A)	8304	5017	8862	181
H(18A)	6929	5843	8938	247
H(18B)	7798	5703	9825	247
H(18C)	6001	5571	9568	247
H(19A)	6822	4573	10085	261
H(19B)	8623	4698	10174	261
H(19C)	7853	4204	9600	261
H(17B)	6106	4985	9705	159
H(18D)	7805	4259	9394	234
H(18E)	8826	4737	9897	234
H(18F)	8704	4707	8949	234
H(19D)	7463	5703	8644	272
H(19E)	7635	5838	9576	272
H(19F)	5976	5857	9015	272
H(201)	4780	4752	5770	99
H(21A)	7747	5137	6460	186
H(21B)	7151	5024	5529	186

H(21C)	7346	4511	6146	186
H(22A)	3812	5617	6098	173
H(22B)	5013	5708	5510	173
H(22C)	5515	5835	6443	173
H(13)	2249	2500	5790	74
H(33)	2139	3350	3744	95
H(43)	2228	2500	3052	104
H(20A)	7015	3218	4653	154
H(20B)	5392	3228	4044	154
H(30A)	6490	2900	3113	269
H(30B)	8108	2900	3714	269
H(50A)	8676	3170	5975	279
H(50B)	8044	3220	6796	279
H(60A)	10071	2940	7419	213
H(60B)	10746	2940	6604	213

Torsion angles [°] for $LFe(THF)_2$ (1).

Fe(1)-S(11)-C(11)-C(61)	170.7(3)
Fe(1)-S(11)-C(11)-C(21)	-11.6(4)
C(61)-C(11)-C(21)-C(31)	0.2(6)
S(11)-C(11)-C(21)-C(31)	-177.5(3)
C(61)-C(11)-C(21)-C(23)	-176.1(4)
S(11)-C(11)-C(21)-C(23)	6.2(6)
C(11)-C(21)-C(31)-F(71)	-178.9(3)
C(23)-C(21)-C(31)-F(71)	-2.4(6)
C(11)-C(21)-C(31)-C(41)	-0.6(6)
C(23)-C(21)-C(31)-C(41)	175.8(4)
F(71)-C(31)-C(41)-C(51)	179.1(4)
C(21)-C(31)-C(41)-C(51)	0.8(7)
C(31)-C(41)-C(51)-C(61)	-0.6(6)
C(41)-C(51)-C(61)-C(11)	0.3(6)
C(41)-C(51)-C(61)-C(81)	-178.5(4)
C(21)-C(11)-C(61)-C(51)	-0.1(6)
S(11)-C(11)-C(61)-C(51)	177.8(3)
C(21)-C(11)-C(61)-C(81)	178.7(4)
S(11)-C(11)-C(61)-C(81)	-3.5(5)
C(51)-C(61)-C(81)-C(131)	-92.5(5)
C(11)-C(61)-C(81)-C(131)	88.7(5)
C(51)-C(61)-C(81)-C(91)	86.8(5)
C(11)-C(61)-C(81)-C(91)	-91.9(5)
C(131)-C(81)-C(91)-C(101)	1.6(7)
C(61)-C(81)-C(91)-C(101)	-177.7(5)
C(131)-C(81)-C(91)-C(141)	-179.2(5)
C(61)-C(81)-C(91)-C(141)	1.4(7)
C(81)-C(91)-C(101)-C(111)	-1.1(9)
C(141)-C(91)-C(101)-C(111)	179.7(6)
C(91)-C(101)-C(111)-C(121)	0.9(10)
C(91)-C(101)-C(111)-C(17B)	172.5(8)
C(91)-C(101)-C(111)-C(17A)	-167.2(12)
C(101)-C(111)-C(121)-C(131)	-1.1(9)

C(17B)-C(111)-C(121)-C(131)	-171.4(9)
C(17A)-C(111)-C(121)-C(131)	169.1(9)
C(91)-C(81)-C(131)-C(121)	-1.8(7)
C(61)-C(81)-C(131)-C(121)	177.5(4)
C(91)-C(81)-C(131)-C(201)	-177.4(4)
C(61)-C(81)-C(131)-C(201)	1.9(6)
C(111)-C(121)-C(131)-C(81)	1.6(8)
C(111)-C(121)-C(131)-C(201)	177.3(5)
C(101)-C(91)-C(141)-C(161)	-49.8(8)
C(81)-C(91)-C(141)-C(161)	131.0(6)
C(101)-C(91)-C(141)-C(151)	77.1(7)
C(81)-C(91)-C(141)-C(151)	-102.1(6)
C(101)-C(111)-C(17A)-C(19A)	22(3)
C(121)-C(111)-C(17A)-C(19A)	-147(2)
C(101)-C(111)-C(17A)-C(18A)	-101.3(18)
C(121)-C(111)-C(17A)-C(18A)	90(2)
C(101)-C(111)-C(17B)-C(19B)	-136(3)
C(121)-C(111)-C(17B)-C(19B)	34(3)
C(101)-C(111)-C(17B)-C(18B)	102.1(18)
C(121)-C(111)-C(17B)-C(18B)	-87.0(17)
C(81)-C(131)-C(201)-C(211)	-130.6(5)
C(121)-C(131)-C(201)-C(211)	53.8(6)
C(81)-C(131)-C(201)-C(221)	102.2(5)
C(121)-C(131)-C(201)-C(221)	-73.4(6)
C(23)#1-C(13)-C(23)-C(33)	0.4(8)
C(23)#1-C(13)-C(23)-C(21)	173.6(3)
C(31)-C(21)-C(23)-C(33)	58.0(6)
C(11)-C(21)-C(23)-C(33)	-125.7(4)
C(31)-C(21)-C(23)-C(13)	-115.0(5)
C(11)-C(21)-C(23)-C(13)	61.3(6)
C(13)-C(23)-C(33)-C(43)	-1.9(7)
C(21)-C(23)-C(33)-C(43)	-175.0(5)
C(23)-C(33)-C(43)-C(33)#1	3.3(9)
C(20)#1-O(10)-C(20)-C(30)	1.5(9)
Fe(1)-O(10)-C(20)-C(30)	163.5(5)
O(10)-C(20)-C(30)-C(30)#1	-0.9(6)
C(50)#1-O(40)-C(50)-C(60)	-6.9(16)
Fe(1)-O(40)-C(50)-C(60)	170.1(6)
O(40)-C(50)-C(60)-C(60)#1	4.4(11)

Symmetry transformations used to generate equivalent atoms:
#1 x,-y+1/2,z

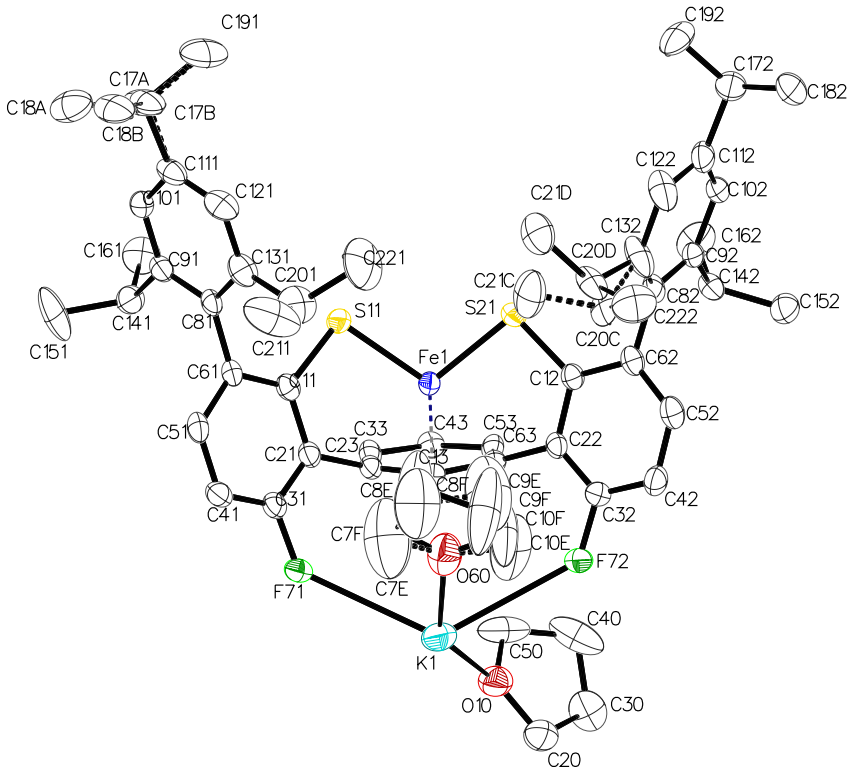
Experimental and Refinement Details for LFeK (2)

Single crystals for X-ray analysis were obtained as follows. A sample (0.5 mL) of the reaction mixture after dilution with hexane at -70 °C was added to hexane (0.5 mL) at room temperature. After 16 h at room temperature brown-yellow needles formed. Low-temperature diffraction data (ω-scans) were collected on a Rigaku MicroMax-007HF diffractometer coupled to a Saturn994+ CCD detector with Cu Kα (λ = 1.54178 Å). The structure was solved by direct methods using SHELXT and was refined against F^2 on all data by full-matrix least squares with SHELXL[50]. All non-hydrogen atoms were refined anisotropically. Unless otherwise noted, hydrogen atoms were included in the model at geometrically calculated positions and refined using a riding model. The isotropic displacement parameters of all hydrogen atoms were fixed to 1.2 times the U value of the atoms to which they are linked (1.5 times for methyl groups).

There are three sites in the difference map were signs of obvious disorder existed. One of the terminal isopropyl groups was modeled over two positions with atoms {C17A, C18A, C19A} and {C17B, C18B, C19B}. The site occupancies were freely refined and converged at 0.35(2) and 0.65(2) for the "A" and "B" sites, respectively. An identical approach was used for a second terminal isopropyl group. The two positions in this model contained atoms {C20C, C21C} and {C20D, C21D}. The site occupancies were freely refined and converged at 0.42(1) and 0.58(2) for the "C" and "D" sites, respectively. Finally, the THF molecule coordinated to the potassium has two orientations for each of its carbon atoms. The atoms involved are {C7E, C8E, C9E, C10E} and {C7F, C8F, C9F, C10F}. The site occupancies were freely refined and converged at 0.42(1) and 0.58(2) for the "C" and "D" sites, respectively.

The hydrogen atoms of the disordered model were placed and fixed in their geometrically expected positions and refined with an atomic displacement parameters riding on their parent carbon atoms. The positions and occupancies reflect their respective disordered model.

In all three disordered areas of the model, the two positions modeled are chemically identical and expected to have similar bond distances and atomic displacement parameters. Consequently, similarity restraints were used to refine the models to convergence.



The full numbering scheme of LFeK (**2**). All atoms shown are depicted with 50% thermal contours. Hydrogen atoms have been removed for clarity.

Crystal data and structure refinement for LFeK (2).

Identification code	007-15046	
Empirical formula	$C_{56}H_{70}F_2FeKO_2S_2$	
Formula weight	972.19	
Temperature	93(2) K	
Wavelength	1.54187 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	a = 9.0455(6) Å	α = 69.061(3)°.
	b = 15.7673(11) Å	β = 82.861(3)°.
	c = 19.5139(13) Å	γ = 84.192(3)°.
Volume	2574.3(3) $Å^3$	
Z	2	
Density (calculated)	1.254 g/cm^3	
Absorption coefficient	4.197 mm^{-1}	
F(000)	1034	
Crystal size	0.140 x 0.050 x 0.040 mm^3	
Crystal color and habit	Yellow plate	
Diffractometer	Rigaku Saturn 944+ CCD	
Θ range for data collection	2.435 to 68.173°.	
Index ranges	$-10 \le h \le 10, -18 \le k \le 18, -23 \le l \le 23$	
Reflections collected	74227	
Independent reflections	9114 [R(int) = 0.2786]	
Observed reflections (I > 2σ(I))	6183	
Completeness to θ = 67.687°	97.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.850 and 0.554	
Solution method	SHELXT-2014/5 (Sheldrick, 2014)	
Refinement method	SHELXL-2014/7 (Sheldrick, 2014)	
Data / restraints / parameters	9114 / 128 / 664	
Goodness-of-fit on F^2	0.977	
Final R indices [I>2σ(I)]	R1 = 0.0651, wR2 = 0.1607	
R indices (all data)	R1 = 0.0887, wR2 = 0.1697	
Largest diff. peak and hole	0.874 and -0.852 $e.Å^{-3}$	

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

	x	y	z	U(eq)
Fe(1)	4033(1)	8195(1)	6156(1)	22(1)
S(11)	4872(1)	8840(1)	6896(1)	31(1)
S(21)	5307(1)	6812(1)	6563(1)	28(1)
C(11)	3150(3)	9338(2)	7165(2)	26(1)
C(21)	1882(3)	9326(2)	6813(2)	25(1)
C(31)	509(3)	9613(2)	7086(2)	27(1)
C(41)	317(4)	9940(2)	7654(2)	30(1)
C(51)	1583(4)	9967(2)	7981(2)	29(1)
C(61)	3004(3)	9659(2)	7754(2)	24(1)
F(71)	-727(2)	9547(1)	6762(1)	34(1)
C(81)	4286(3)	9605(2)	8185(2)	25(1)
C(91)	5162(3)	10343(2)	8026(2)	27(1)
C(101)	6289(4)	10276(2)	8469(2)	32(1)
C(111)	6588(4)	9485(2)	9060(2)	35(1)
C(121)	5728(4)	8760(2)	9203(2)	38(1)
C(131)	4574(4)	8796(2)	8779(2)	38(1)
C(141)	4950(4)	11199(2)	7364(3)	39(1)
C(151)	4435(7)	12018(3)	7603(4)	77(2)
C(161)	6356(5)	11391(3)	6837(3)	49(1)
C(17A)	7820(30)	9513(15)	9521(14)	48(6)
C(18A)	7334(15)	10108(15)	10020(11)	60(5)
C(17B)	7793(14)	9433(9)	9555(8)	49(4)
C(18B)	7037(8)	9337(8)	10344(5)	62(3)
C(191)	8812(5)	8595(4)	9703(4)	72(2)
C(201)	3647(5)	7984(3)	8976(3)	60(2)
C(211)	2788(6)	7795(4)	9737(4)	87(2)
C(221)	4610(7)	7138(3)	8951(5)	94(3)
C(12)	3944(3)	6108(2)	6520(2)	24(1)
C(22)	2582(3)	6529(2)	6242(2)	24(1)
C(32)	1451(3)	5989(2)	6282(2)	30(1)
C(42)	1565(4)	5057(2)	6555(2)	32(1)
C(52)	2934(4)	4653(2)	6798(2)	34(1)
C(62)	4116(4)	5151(2)	6789(2)	27(1)
F(72)	108(2)	6420(1)	6046(2)	38(1)
C(82)	5543(4)	4646(2)	7091(2)	29(1)
C(92)	6685(3)	4453(2)	6610(2)	27(1)
C(102)	7952(4)	3917(2)	6898(2)	32(1)
C(112)	8140(5)	3606(2)	7627(3)	42(1)
C(122)	7011(6)	3819(3)	8100(3)	55(1)
C(132)	5687(5)	4325(2)	7841(3)	49(1)
C(142)	6587(4)	4782(2)	5787(2)	29(1)
C(152)	6297(4)	4012(2)	5532(3)	40(1)
C(162)	7968(5)	5262(3)	5338(3)	52(1)
C(172)	9551(5)	3031(3)	7911(3)	54(1)
C(182)	9261(5)	2044(3)	8222(4)	62(2)
C(192)	10210(6)	3341(3)	8451(3)	61(2)
C(20C)	4164(15)	4475(7)	8307(7)	48(3)
C(21C)	4284(15)	5275(8)	8542(9)	66(4)
C(20D)	4628(10)	4546(6)	8437(5)	46(2)
C(21D)	5346(10)	4873(5)	8950(5)	55(3)

C(222)	3788(6)	3679(4)	8925(4)	74(2)
C(13)	1768(3)	8001(2)	6414(2)	23(1)
C(23)	2055(3)	8937(2)	6221(2)	24(1)
C(33)	2880(4)	9398(2)	5539(2)	27(1)
C(43)	3467(4)	8937(2)	5051(2)	27(1)
C(53)	3256(3)	8004(2)	5266(2)	26(1)
C(63)	2423(3)	7530(2)	5947(2)	23(1)
K(1)	-1928(1)	8006(1)	6401(1)	50(1)
O(10)	-1834(3)	8262(2)	4960(2)	47(1)
C(20)	-2732(4)	7991(3)	4525(3)	46(1)
C(30)	-1701(5)	7778(3)	3928(3)	57(1)
C(40)	-192(5)	7720(4)	4186(3)	74(2)
C(50)	-376(4)	8388(3)	4584(3)	64(2)
O(60)	-1052(4)	7022(2)	7719(2)	59(1)
C(7E)	-1170(60)	7340(20)	8331(14)	149(16)
C(8E)	-860(60)	6514(19)	8979(17)	120(10)
C(9E)	-330(60)	5860(30)	8590(30)	157(14)
C(10E)	-1000(30)	6055(9)	7889(18)	104(10)
C(7F)	-872(13)	7340(8)	8300(6)	42(4)
C(8F)	-430(50)	6563(10)	8940(13)	134(12)
C(9F)	-890(40)	5750(9)	8825(10)	151(11)
C(10F)	-790(30)	6058(6)	8009(9)	96(7)

Bond lengths [Å] and angles [°] for LFeK (2).

Fe(1)-C(63)	2.035(3)
Fe(1)-C(23)	2.052(3)
Fe(1)-C(13)	2.075(3)
Fe(1)-C(53)	2.078(4)
Fe(1)-C(33)	2.101(3)
Fe(1)-C(43)	2.151(4)
Fe(1)-S(11)	2.2762(11)
Fe(1)-S(21)	2.2791(7)
Fe(1)-K(1)#1	3.7120(9)
S(11)-C(11)	1.778(3)
S(11)-K(1)#1	3.2374(11)
S(21)-C(12)	1.768(4)
S(21)-K(1)#1	3.1996(12)
C(11)-C(61)	1.401(5)
C(11)-C(21)	1.413(5)
C(21)-C(31)	1.388(5)
C(21)-C(23)	1.476(5)
C(31)-C(41)	1.365(6)
C(31)-F(71)	1.381(4)
C(41)-C(51)	1.390(5)
C(41)-H(41)	0.9500
C(51)-C(61)	1.404(5)
C(51)-H(51)	0.9500
C(61)-C(81)	1.494(5)
F(71)-K(1)	3.086(2)
C(81)-C(91)	1.395(5)

C(81)-C(131)	1.410(5)
C(91)-C(101)	1.388(5)
C(91)-C(141)	1.512(5)
C(101)-C(111)	1.394(5)
C(101)-H(101)	0.9500
C(111)-C(121)	1.374(6)
C(111)-C(17B)	1.522(9)
C(111)-C(17A)	1.527(15)
C(121)-C(131)	1.395(6)
C(121)-H(121)	0.9500
C(131)-C(201)	1.509(6)
C(141)-C(161)	1.516(6)
C(141)-C(151)	1.535(6)
C(141)-H(141)	1.0000
C(151)-H(15A)	0.9800
C(151)-H(15B)	0.9800
C(151)-H(15C)	0.9800
C(161)-H(16A)	0.9800
C(161)-H(16B)	0.9800
C(161)-H(16C)	0.9800
C(17A)-C(191)	1.575(15)
C(17A)-C(18A)	1.576(14)
C(17A)-H(17A)	1.0000
C(18A)-H(18A)	0.9800
C(18A)-H(18B)	0.9800
C(18A)-H(18C)	0.9800
C(17B)-C(191)	1.491(11)
C(17B)-C(18B)	1.566(14)
C(17B)-H(17B)	1.0000
C(18B)-H(18D)	0.9800
C(18B)-H(18E)	0.9800
C(18B)-H(18F)	0.9800
C(191)-H(19A)	0.9800
C(191)-H(19B)	0.9800
C(191)-H(19C)	0.9800
C(191)-H(19D)	0.9800
C(191)-H(19E)	0.9800
C(191)-H(19F)	0.9800
C(201)-C(221)	1.530(7)
C(201)-C(211)	1.531(9)
C(201)-H(201)	1.0000
C(211)-H(21A)	0.9800
C(211)-H(21B)	0.9800
C(211)-H(21C)	0.9800
C(221)-H(22A)	0.9800
C(221)-H(22B)	0.9800
C(221)-H(22C)	0.9800
C(12)-C(62)	1.408(4)
C(12)-C(22)	1.412(4)
C(22)-C(32)	1.375(5)
C(22)-C(63)	1.472(4)
C(32)-C(42)	1.371(5)
C(32)-F(72)	1.377(3)
C(42)-C(52)	1.391(5)
C(42)-H(42)	0.9500
C(52)-C(62)	1.384(5)

C(52)-H(52)	0.9500
C(62)-C(82)	1.514(4)
F(72)-K(1)	3.181(2)
C(82)-C(132)	1.386(6)
C(82)-C(92)	1.392(6)
C(92)-C(102)	1.404(4)
C(92)-C(142)	1.512(6)
C(102)-C(112)	1.355(6)
C(102)-H(102)	0.9500
C(112)-C(122)	1.388(7)
C(112)-C(172)	1.530(5)
C(122)-C(132)	1.412(6)
C(122)-H(122)	0.9500
C(132)-C(20D)	1.529(9)
C(132)-C(20C)	1.599(12)
C(142)-C(152)	1.522(6)
C(142)-C(162)	1.532(6)
C(142)-H(142)	1.0000
C(152)-H(15D)	0.9800
C(152)-H(15E)	0.9800
C(152)-H(15F)	0.9800
C(162)-H(16D)	0.9800
C(162)-H(16E)	0.9800
C(162)-H(16F)	0.9800
C(172)-C(182)	1.491(6)
C(172)-C(192)	1.512(7)
C(172)-H(172)	1.0000
C(182)-H(18G)	0.9800
C(182)-H(18H)	0.9800
C(182)-H(18I)	0.9800
C(192)-H(19G)	0.9800
C(192)-H(19H)	0.9800
C(192)-H(19I)	0.9800
C(20C)-C(222)	1.431(12)
C(20C)-C(21C)	1.505(13)
C(20C)-H(20C)	1.0000
C(21C)-H(21D)	0.9800
C(21C)-H(21E)	0.9800
C(21C)-H(21F)	0.9800
C(20D)-C(21D)	1.512(11)
C(20D)-C(222)	1.567(10)
C(20D)-H(20D)	1.0000
C(21D)-H(21G)	0.9800
C(21D)-H(21H)	0.9800
C(21D)-H(21I)	0.9800
C(222)-H(22G)	0.9800
C(222)-H(22H)	0.9800
C(222)-H(22I)	0.9800
C(222)-H(22D)	0.9800
C(222)-H(22E)	0.9800
C(222)-H(22F)	0.9800
C(13)-C(63)	1.411(5)
C(13)-C(23)	1.428(4)
C(13)-K(1)	3.346(3)
C(13)-H(13)	0.9500
C(23)-C(33)	1.423(5)

C(33)-C(43)	1.417(5)
C(33)-H(33)	0.9500
C(43)-C(53)	1.404(5)
C(43)-H(43)	0.9500
C(53)-C(63)	1.432(5)
C(53)-H(53)	0.9500
K(1)-O(60)	2.656(4)
K(1)-O(10)	2.686(4)
K(1)-S(21)#2	3.1996(12)
K(1)-S(11)#2	3.2374(11)
O(10)-C(50)	1.423(6)
O(10)-C(20)	1.437(6)
C(20)-C(30)	1.511(7)
C(20)-H(20A)	0.9900
C(20)-H(20B)	0.9900
C(30)-C(40)	1.496(8)
C(30)-H(30A)	0.9900
C(30)-H(30B)	0.9900
C(40)-C(50)	1.502(9)
C(40)-H(40A)	0.9900
C(40)-H(40B)	0.9900
C(50)-H(50A)	0.9900
C(50)-H(50B)	0.9900
O(60)-C(10F)	1.426(9)
O(60)-C(7F)	1.426(9)
O(60)-C(10E)	1.437(14)
O(60)-C(7E)	1.440(15)
C(7E)-C(8E)	1.486(16)
C(7E)-H(7EA)	0.9900
C(7E)-H(7EB)	0.9900
C(8E)-C(9E)	1.499(17)
C(8E)-H(8EA)	0.9900
C(8E)-H(8EB)	0.9900
C(9E)-C(10E)	1.485(18)
C(9E)-H(9EA)	0.9900
C(9E)-H(9EB)	0.9900
C(10E)-H(10A)	0.9900
C(10E)-H(10B)	0.9900
C(7F)-C(8F)	1.467(13)
C(7F)-H(7FA)	0.9900
C(7F)-H(7FB)	0.9900
C(8F)-C(9F)	1.487(16)
C(8F)-H(8FA)	0.9900
C(8F)-H(8FB)	0.9900
C(9F)-C(10F)	1.483(14)
C(9F)-H(9FA)	0.9900
C(9F)-H(9FB)	0.9900
C(10F)-H(10C)	0.9900
C(10F)-H(10D)	0.9900

C(63)-Fe(1)-C(23)	73.38(13)
C(63)-Fe(1)-C(13)	40.15(14)
C(23)-Fe(1)-C(13)	40.49(12)
C(63)-Fe(1)-C(53)	40.73(14)
C(23)-Fe(1)-C(53)	86.07(14)
C(13)-Fe(1)-C(53)	72.82(14)

C(63)-Fe(1)-C(33)	86.05(12)
C(23)-Fe(1)-C(33)	40.07(14)
C(13)-Fe(1)-C(33)	72.59(12)
C(53)-Fe(1)-C(33)	70.88(13)
C(63)-Fe(1)-C(43)	72.32(13)
C(23)-Fe(1)-C(43)	72.03(13)
C(13)-Fe(1)-C(43)	85.61(13)
C(53)-Fe(1)-C(43)	38.72(13)
C(33)-Fe(1)-C(43)	38.92(14)
C(63)-Fe(1)-S(11)	149.17(11)
C(23)-Fe(1)-S(11)	86.79(11)
C(13)-Fe(1)-S(11)	110.68(11)
C(53)-Fe(1)-S(11)	162.90(9)
C(33)-Fe(1)-S(11)	93.83(11)
C(43)-Fe(1)-S(11)	124.18(10)
C(63)-Fe(1)-S(21)	86.28(8)
C(23)-Fe(1)-S(21)	146.61(10)
C(13)-Fe(1)-S(21)	108.34(8)
C(53)-Fe(1)-S(21)	95.63(8)
C(33)-Fe(1)-S(21)	165.81(12)
C(43)-Fe(1)-S(21)	127.02(10)
S(11)-Fe(1)-S(21)	98.87(4)
C(63)-Fe(1)-K(1)#1	141.99(8)
C(23)-Fe(1)-K(1)#1	144.47(10)
C(13)-Fe(1)-K(1)#1	159.29(10)
C(53)-Fe(1)-K(1)#1	122.07(9)
C(33)-Fe(1)-K(1)#1	124.09(10)
C(43)-Fe(1)-K(1)#1	115.05(9)
S(11)-Fe(1)-K(1)#1	59.88(3)
S(21)-Fe(1)-K(1)#1	58.92(3)
C(11)-S(11)-Fe(1)	99.05(13)
C(11)-S(11)-K(1)#1	177.72(12)
Fe(1)-S(11)-K(1)#1	82.66(3)
C(12)-S(21)-Fe(1)	99.89(9)
C(12)-S(21)-K(1)#1	169.99(13)
Fe(1)-S(21)-K(1)#1	83.49(3)
C(61)-C(11)-C(21)	120.1(3)
C(61)-C(11)-S(11)	121.5(3)
C(21)-C(11)-S(11)	118.2(3)
C(31)-C(21)-C(11)	117.8(4)
C(31)-C(21)-C(23)	123.1(3)
C(11)-C(21)-C(23)	118.9(3)
C(41)-C(31)-F(71)	119.0(3)
C(41)-C(31)-C(21)	124.1(3)
F(71)-C(31)-C(21)	116.9(3)
C(31)-C(41)-C(51)	117.2(3)
C(31)-C(41)-H(41)	121.4
C(51)-C(41)-H(41)	121.4
C(41)-C(51)-C(61)	122.2(4)
C(41)-C(51)-H(51)	118.9
C(61)-C(51)-H(51)	118.9
C(11)-C(61)-C(51)	118.6(3)
C(11)-C(61)-C(81)	121.7(3)
C(51)-C(61)-C(81)	119.4(4)
C(31)-F(71)-K(1)	133.94(15)
C(91)-C(81)-C(131)	119.9(3)

C(91)-C(81)-C(61)	121.4(3)
C(131)-C(81)-C(61)	118.6(3)
C(101)-C(91)-C(81)	119.2(3)
C(101)-C(91)-C(141)	119.4(3)
C(81)-C(91)-C(141)	121.3(3)
C(91)-C(101)-C(111)	121.8(4)
C(91)-C(101)-H(101)	119.1
C(111)-C(101)-H(101)	119.1
C(121)-C(111)-C(101)	118.2(4)
C(121)-C(111)-C(17B)	120.6(7)
C(101)-C(111)-C(17B)	121.1(7)
C(121)-C(111)-C(17A)	125.2(11)
C(101)-C(111)-C(17A)	116.5(11)
C(111)-C(121)-C(131)	122.2(3)
C(111)-C(121)-H(121)	118.9
C(131)-C(121)-H(121)	118.9
C(121)-C(131)-C(81)	118.7(4)
C(121)-C(131)-C(201)	119.5(3)
C(81)-C(131)-C(201)	121.8(4)
C(91)-C(141)-C(161)	111.6(3)
C(91)-C(141)-C(151)	111.1(4)
C(161)-C(141)-C(151)	110.6(4)
C(91)-C(141)-H(141)	107.8
C(161)-C(141)-H(141)	107.8
C(151)-C(141)-H(141)	107.8
C(141)-C(151)-H(15A)	109.5
C(141)-C(151)-H(15B)	109.5
H(15A)-C(151)-H(15B)	109.5
C(141)-C(151)-H(15C)	109.5
H(15A)-C(151)-H(15C)	109.5
H(15B)-C(151)-H(15C)	109.5
C(141)-C(161)-H(16A)	109.5
C(141)-C(161)-H(16B)	109.5
H(16A)-C(161)-H(16B)	109.5
C(141)-C(161)-H(16C)	109.5
H(16A)-C(161)-H(16C)	109.5
H(16B)-C(161)-H(16C)	109.5
C(111)-C(17A)-C(191)	109.1(10)
C(111)-C(17A)-C(18A)	113.0(12)
C(191)-C(17A)-C(18A)	128.6(14)
C(111)-C(17A)-H(17A)	100.1
C(191)-C(17A)-H(17A)	100.1
C(18A)-C(17A)-H(17A)	100.1
C(17A)-C(18A)-H(18A)	109.5
C(17A)-C(18A)-H(18B)	109.5
H(18A)-C(18A)-H(18B)	109.5
C(17A)-C(18A)-H(18C)	109.5
H(18A)-C(18A)-H(18C)	109.5
H(18B)-C(18A)-H(18C)	109.5
C(191)-C(17B)-C(111)	114.0(7)
C(191)-C(17B)-C(18B)	102.4(9)
C(111)-C(17B)-C(18B)	108.9(9)
C(191)-C(17B)-H(17B)	110.4
C(111)-C(17B)-H(17B)	110.4
C(18B)-C(17B)-H(17B)	110.4
C(17B)-C(18B)-H(18D)	109.5

C(17B)-C(18B)-H(18E)	109.5
H(18D)-C(18B)-H(18E)	109.5
C(17B)-C(18B)-H(18F)	109.5
H(18D)-C(18B)-H(18F)	109.5
H(18E)-C(18B)-H(18F)	109.5
C(17A)-C(191)-H(19A)	109.5
C(17A)-C(191)-H(19B)	109.5
H(19A)-C(191)-H(19B)	109.5
C(17A)-C(191)-H(19C)	109.5
H(19A)-C(191)-H(19C)	109.5
H(19B)-C(191)-H(19C)	109.5
C(17B)-C(191)-H(19D)	109.5
C(17B)-C(191)-H(19E)	109.5
H(19D)-C(191)-H(19E)	109.5
C(17B)-C(191)-H(19F)	109.5
H(19D)-C(191)-H(19F)	109.5
H(19E)-C(191)-H(19F)	109.5
C(131)-C(201)-C(221)	111.5(4)
C(131)-C(201)-C(211)	110.8(5)
C(221)-C(201)-C(211)	110.2(4)
C(131)-C(201)-H(201)	108.1
C(221)-C(201)-H(201)	108.1
C(211)-C(201)-H(201)	108.1
C(201)-C(211)-H(21A)	109.5
C(201)-C(211)-H(21B)	109.5
H(21A)-C(211)-H(21B)	109.5
C(201)-C(211)-H(21C)	109.5
H(21A)-C(211)-H(21C)	109.5
H(21B)-C(211)-H(21C)	109.5
C(201)-C(221)-H(22A)	109.5
C(201)-C(221)-H(22B)	109.5
H(22A)-C(221)-H(22B)	109.5
C(201)-C(221)-H(22C)	109.5
H(22A)-C(221)-H(22C)	109.5
H(22B)-C(221)-H(22C)	109.5
C(62)-C(12)-C(22)	118.7(3)
C(62)-C(12)-S(21)	123.2(2)
C(22)-C(12)-S(21)	118.0(2)
C(32)-C(22)-C(12)	118.6(3)
C(32)-C(22)-C(63)	123.0(3)
C(12)-C(22)-C(63)	118.3(3)
C(42)-C(32)-C(22)	124.3(3)
C(42)-C(32)-F(72)	118.3(3)
C(22)-C(32)-F(72)	117.3(3)
C(32)-C(42)-C(52)	116.2(3)
C(32)-C(42)-H(42)	121.9
C(52)-C(42)-H(42)	121.9
C(62)-C(52)-C(42)	122.9(3)
C(62)-C(52)-H(52)	118.6
C(42)-C(52)-H(52)	118.6
C(52)-C(62)-C(12)	119.2(3)
C(52)-C(62)-C(82)	118.7(3)
C(12)-C(62)-C(82)	122.0(3)
C(32)-F(72)-K(1)	132.2(2)
C(132)-C(82)-C(92)	119.8(3)
C(132)-C(82)-C(62)	120.9(4)

C(92)-C(82)-C(62)	119.2(4)
C(82)-C(92)-C(102)	119.1(4)
C(82)-C(92)-C(142)	122.1(3)
C(102)-C(92)-C(142)	118.8(3)
C(112)-C(102)-C(92)	122.6(4)
C(112)-C(102)-H(102)	118.7
C(92)-C(102)-H(102)	118.7
C(102)-C(112)-C(122)	117.9(3)
C(102)-C(112)-C(172)	120.4(4)
C(122)-C(112)-C(172)	121.7(5)
C(112)-C(122)-C(132)	121.7(4)
C(112)-C(122)-H(122)	119.1
C(132)-C(122)-H(122)	119.1
C(82)-C(132)-C(122)	118.9(4)
C(82)-C(132)-C(20D)	126.9(4)
C(122)-C(132)-C(20D)	113.9(5)
C(82)-C(132)-C(20C)	112.0(6)
C(122)-C(132)-C(20C)	128.5(6)
C(92)-C(142)-C(152)	111.7(3)
C(92)-C(142)-C(162)	113.2(3)
C(152)-C(142)-C(162)	109.7(4)
C(92)-C(142)-H(142)	107.3
C(152)-C(142)-H(142)	107.3
C(162)-C(142)-H(142)	107.3
C(142)-C(152)-H(15D)	109.5
C(142)-C(152)-H(15E)	109.5
H(15D)-C(152)-H(15E)	109.5
C(142)-C(152)-H(15F)	109.5
H(15D)-C(152)-H(15F)	109.5
H(15E)-C(152)-H(15F)	109.5
C(142)-C(162)-H(16D)	109.5
C(142)-C(162)-H(16E)	109.5
H(16D)-C(162)-H(16E)	109.5
C(142)-C(162)-H(16F)	109.5
H(16D)-C(162)-H(16F)	109.5
H(16E)-C(162)-H(16F)	109.5
C(182)-C(172)-C(192)	112.3(4)
C(182)-C(172)-C(112)	110.8(4)
C(192)-C(172)-C(112)	112.2(4)
C(182)-C(172)-H(172)	107.1
C(192)-C(172)-H(172)	107.1
C(112)-C(172)-H(172)	107.1
C(172)-C(182)-H(18G)	109.5
C(172)-C(182)-H(18H)	109.5
H(18G)-C(182)-H(18H)	109.5
C(172)-C(182)-H(18I)	109.5
H(18G)-C(182)-H(18I)	109.5
H(18H)-C(182)-H(18I)	109.5
C(172)-C(192)-H(19G)	109.5
C(172)-C(192)-H(19H)	109.5
H(19G)-C(192)-H(19H)	109.5
C(172)-C(192)-H(19I)	109.5
H(19G)-C(192)-H(19I)	109.5
H(19H)-C(192)-H(19I)	109.5
C(222)-C(20C)-C(21C)	111.5(10)
C(222)-C(20C)-C(132)	112.7(8)

C(21C)-C(20C)-C(132)	108.8(9)
C(222)-C(20C)-H(20C)	107.9
C(21C)-C(20C)-H(20C)	107.9
C(132)-C(20C)-H(20C)	107.9
C(20C)-C(21C)-H(21D)	109.5
C(20C)-C(21C)-H(21E)	109.5
H(21D)-C(21C)-H(21E)	109.5
C(20C)-C(21C)-H(21F)	109.5
H(21D)-C(21C)-H(21F)	109.5
H(21E)-C(21C)-H(21F)	109.5
C(21D)-C(20D)-C(132)	115.8(7)
C(21D)-C(20D)-C(222)	107.3(7)
C(132)-C(20D)-C(222)	109.3(6)
C(21D)-C(20D)-H(20D)	108.0
C(132)-C(20D)-H(20D)	108.0
C(222)-C(20D)-H(20D)	108.0
C(20D)-C(21D)-H(21G)	109.5
C(20D)-C(21D)-H(21H)	109.5
H(21G)-C(21D)-H(21H)	109.5
C(20D)-C(21D)-H(21I)	109.5
H(21G)-C(21D)-H(21I)	109.5
H(21H)-C(21D)-H(21I)	109.5
C(20C)-C(222)-H(22G)	109.5
C(20C)-C(222)-H(22H)	109.5
H(22G)-C(222)-H(22H)	109.5
C(20C)-C(222)-H(22I)	109.5
H(22G)-C(222)-H(22I)	109.5
H(22H)-C(222)-H(22I)	109.5
C(20D)-C(222)-H(22D)	109.5
C(20D)-C(222)-H(22E)	109.5
H(22D)-C(222)-H(22E)	109.5
C(20D)-C(222)-H(22F)	109.5
H(22D)-C(222)-H(22F)	109.5
H(22E)-C(222)-H(22F)	109.5
C(63)-C(13)-C(23)	118.7(3)
C(63)-C(13)-Fe(1)	68.43(18)
C(23)-C(13)-Fe(1)	68.91(17)
C(63)-C(13)-K(1)	106.4(2)
C(23)-C(13)-K(1)	104.59(16)
Fe(1)-C(13)-K(1)	166.09(16)
C(63)-C(13)-H(13)	120.7
C(23)-C(13)-H(13)	120.7
Fe(1)-C(13)-H(13)	135.5
K(1)-C(13)-H(13)	58.4
C(33)-C(23)-C(13)	120.2(3)
C(33)-C(23)-C(21)	119.3(3)
C(13)-C(23)-C(21)	118.1(3)
C(33)-C(23)-Fe(1)	71.80(16)
C(13)-C(23)-Fe(1)	70.59(15)
C(21)-C(23)-Fe(1)	114.7(2)
C(43)-C(33)-C(23)	121.0(3)
C(43)-C(33)-Fe(1)	72.47(16)
C(23)-C(33)-Fe(1)	68.13(16)
C(43)-C(33)-H(33)	119.5
C(23)-C(33)-H(33)	119.5
Fe(1)-C(33)-H(33)	133.2

C(53)-C(43)-C(33)	118.4(3)
C(53)-C(43)-Fe(1)	67.8(2)
C(33)-C(43)-Fe(1)	68.6(2)
C(53)-C(43)-H(43)	120.8
C(33)-C(43)-H(43)	120.8
Fe(1)-C(43)-H(43)	136.4
C(43)-C(53)-C(63)	121.3(3)
C(43)-C(53)-Fe(1)	73.4(2)
C(63)-C(53)-Fe(1)	68.0(2)
C(43)-C(53)-H(53)	119.3
C(63)-C(53)-H(53)	119.3
Fe(1)-C(53)-H(53)	132.3
C(13)-C(63)-C(53)	120.2(3)
C(13)-C(63)-C(22)	119.2(3)
C(53)-C(63)-C(22)	118.7(3)
C(13)-C(63)-Fe(1)	71.42(19)
C(53)-C(63)-Fe(1)	71.3(2)
C(22)-C(63)-Fe(1)	116.3(2)
O(60)-K(1)-O(10)	148.62(9)
O(60)-K(1)-F(71)	81.69(9)
O(10)-K(1)-F(71)	115.40(8)
O(60)-K(1)-F(72)	78.55(9)
O(10)-K(1)-F(72)	70.08(7)
F(71)-K(1)-F(72)	124.42(5)
O(60)-K(1)-S(21)#2	94.57(8)
O(10)-K(1)-S(21)#2	84.42(7)
F(71)-K(1)-S(21)#2	146.86(5)
F(72)-K(1)-S(21)#2	86.40(4)
O(60)-K(1)-S(11)#2	99.67(8)
O(10)-K(1)-S(11)#2	108.10(6)
F(71)-K(1)-S(11)#2	83.04(4)
F(72)-K(1)-S(11)#2	151.26(5)
S(21)#2-K(1)-S(11)#2	65.04(3)
O(60)-K(1)-C(13)	68.56(10)
O(10)-K(1)-C(13)	95.16(9)
F(71)-K(1)-C(13)	62.51(6)
F(72)-K(1)-C(13)	61.91(7)
S(21)#2-K(1)-C(13)	145.95(6)
S(11)#2-K(1)-C(13)	144.46(7)
C(50)-O(10)-C(20)	107.6(4)
C(50)-O(10)-K(1)	113.7(3)
C(20)-O(10)-K(1)	134.2(3)
O(10)-C(20)-C(30)	107.7(3)
O(10)-C(20)-H(20A)	110.2
C(30)-C(20)-H(20A)	110.2
O(10)-C(20)-H(20B)	110.2
C(30)-C(20)-H(20B)	110.2
H(20A)-C(20)-H(20B)	108.5
C(40)-C(30)-C(20)	102.8(5)
C(40)-C(30)-H(30A)	111.2
C(20)-C(30)-H(30A)	111.2
C(40)-C(30)-H(30B)	111.2
C(20)-C(30)-H(30B)	111.2
H(30A)-C(30)-H(30B)	109.1
C(30)-C(40)-C(50)	102.9(4)
C(30)-C(40)-H(40A)	111.2

C(50)-C(40)-H(40A)	111.2
C(30)-C(40)-H(40B)	111.2
C(50)-C(40)-H(40B)	111.2
H(40A)-C(40)-H(40B)	109.1
O(10)-C(50)-C(40)	104.2(4)
O(10)-C(50)-K(1)	44.5(2)
C(40)-C(50)-K(1)	127.0(3)
O(10)-C(50)-H(50A)	110.9
C(40)-C(50)-H(50A)	110.9
K(1)-C(50)-H(50A)	67.0
O(10)-C(50)-H(50B)	110.9
C(40)-C(50)-H(50B)	110.9
K(1)-C(50)-H(50B)	119.7
H(50A)-C(50)-H(50B)	108.9
C(10F)-O(60)-C(7F)	106.1(10)
C(10E)-O(60)-C(7E)	117.1(19)
C(10F)-O(60)-K(1)	126.8(8)
C(7F)-O(60)-K(1)	126.9(5)
C(10E)-O(60)-K(1)	114.6(15)
C(7E)-O(60)-K(1)	124.2(14)
O(60)-C(7E)-C(8E)	105(2)
O(60)-C(7E)-H(7EA)	110.8
C(8E)-C(7E)-H(7EA)	110.8
O(60)-C(7E)-H(7EB)	110.8
C(8E)-C(7E)-H(7EB)	110.8
H(7EA)-C(7E)-H(7EB)	108.8
C(7E)-C(8E)-C(9E)	99(2)
C(7E)-C(8E)-H(8EA)	111.9
C(9E)-C(8E)-H(8EA)	111.9
C(7E)-C(8E)-H(8EB)	111.9
C(9E)-C(8E)-H(8EB)	111.9
H(8EA)-C(8E)-H(8EB)	109.6
C(10E)-C(9E)-C(8E)	114(3)
C(10E)-C(9E)-H(9EA)	108.8
C(8E)-C(9E)-H(9EA)	108.8
C(10E)-C(9E)-H(9EB)	108.8
C(8E)-C(9E)-H(9EB)	108.8
H(9EA)-C(9E)-H(9EB)	107.7
O(60)-C(10E)-C(9E)	93(3)
O(60)-C(10E)-K(1)	43.6(11)
C(9E)-C(10E)-K(1)	136.3(19)
O(60)-C(10E)-H(10A)	113.1
C(9E)-C(10E)-H(10A)	113.1
K(1)-C(10E)-H(10A)	86.8
O(60)-C(10E)-H(10B)	113.1
C(9E)-C(10E)-H(10B)	113.1
K(1)-C(10E)-H(10B)	93.3
H(10A)-C(10E)-H(10B)	110.5
O(60)-C(7F)-C(8F)	108.8(10)
O(60)-C(7F)-H(7FA)	109.9
C(8F)-C(7F)-H(7FA)	109.9
O(60)-C(7F)-H(7FB)	109.9
C(8F)-C(7F)-H(7FB)	109.9
H(7FA)-C(7F)-H(7FB)	108.3
C(7F)-C(8F)-C(9F)	105.2(15)
C(7F)-C(8F)-H(8FA)	110.7

C(9F)-C(8F)-H(8FA)	110.7
C(7F)-C(8F)-H(8FB)	110.7
C(9F)-C(8F)-H(8FB)	110.7
H(8FA)-C(8F)-H(8FB)	108.8
C(10F)-C(9F)-C(8F)	101.3(17)
C(10F)-C(9F)-H(9FA)	111.5
C(8F)-C(9F)-H(9FA)	111.5
C(10F)-C(9F)-H(9FB)	111.5
C(8F)-C(9F)-H(9FB)	111.5
H(9FA)-C(9F)-H(9FB)	109.3
O(60)-C(10F)-C(9F)	109.3(11)
O(60)-C(10F)-H(10C)	109.8
C(9F)-C(10F)-H(10C)	109.8
O(60)-C(10F)-H(10D)	109.8
C(9F)-C(10F)-H(10D)	109.8
H(10C)-C(10F)-H(10D)	108.3

Symmetry transformations used to generate equivalent atoms:
#1 x+1,y,z #2 x-1,y,z

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

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Fe(1)	24(1)	21(1)	24(1)	-10(1)	-5(1)	1(1)
S(11)	25(1)	39(1)	38(1)	-26(1)	-6(1)	2(1)
S(21)	25(1)	22(1)	36(1)	-9(1)	-7(1)	2(1)
C(11)	27(1)	20(1)	27(2)	-5(1)	0(2)	-1(1)
C(21)	30(2)	21(1)	26(2)	-9(1)	-6(2)	3(1)
C(31)	32(2)	22(1)	26(2)	-8(1)	-7(2)	4(1)
C(41)	28(2)	29(2)	33(2)	-11(2)	-6(2)	6(1)
C(51)	41(2)	23(1)	26(2)	-12(1)	-4(2)	4(1)
C(61)	28(1)	20(1)	26(2)	-10(1)	-2(2)	2(1)
F(71)	27(1)	38(1)	40(1)	-18(1)	-11(1)	7(1)
C(81)	32(2)	24(1)	23(2)	-13(1)	-6(2)	7(1)
C(91)	29(2)	25(2)	28(2)	-10(2)	-4(2)	5(1)
C(101)	32(2)	34(2)	39(2)	-22(2)	-9(2)	6(1)
C(111)	35(2)	47(2)	26(2)	-18(2)	-9(2)	17(2)
C(121)	42(2)	38(2)	24(2)	-1(2)	-6(2)	8(2)
C(131)	46(2)	27(2)	32(2)	-3(2)	-3(2)	4(2)
C(141)	43(2)	24(2)	48(3)	-6(2)	-18(2)	-1(1)
C(151)	102(4)	21(2)	88(5)	-6(2)	16(4)	16(2)
C(161)	64(2)	47(2)	28(2)	-1(2)	-8(2)	-3(2)
C(17A)	36(9)	79(9)	28(10)	-20(8)	-13(8)	12(7)
C(18A)	42(7)	102(12)	50(10)	-42(9)	-4(6)	-8(7)
C(17B)	41(5)	75(6)	43(6)	-35(5)	-24(5)	25(4)
C(18B)	51(4)	106(8)	47(5)	-48(5)	-26(4)	27(4)
C(191)	56(2)	83(3)	73(4)	-16(3)	-37(3)	15(2)
C(201)	66(3)	32(2)	65(4)	11(2)	-16(3)	-8(2)
C(211)	53(2)	66(3)	89(5)	31(3)	5(3)	-1(2)

C(221)	108(4)	31(2)	125(7)	-4(3)	-9(4)	-9(2)
C(12)	27(1)	20(1)	25(2)	-6(1)	-1(2)	-2(1)
C(22)	30(2)	22(1)	22(2)	-11(1)	-4(2)	3(1)
C(32)	26(2)	31(2)	34(2)	-15(2)	-8(2)	3(1)
C(42)	35(2)	26(2)	39(2)	-15(2)	-1(2)	-7(1)
C(52)	41(2)	22(1)	36(2)	-9(2)	1(2)	-1(1)
C(62)	33(2)	22(1)	22(2)	-7(1)	2(2)	1(1)
F(72)	28(1)	31(1)	57(2)	-16(1)	-14(1)	1(1)
C(82)	37(2)	17(1)	33(2)	-7(1)	-7(2)	3(1)
C(92)	30(2)	18(1)	34(2)	-9(1)	-10(2)	1(1)
C(102)	34(2)	24(2)	41(3)	-14(2)	-14(2)	6(1)
C(112)	59(2)	24(2)	50(3)	-17(2)	-26(2)	9(2)
C(122)	98(3)	37(2)	30(2)	-14(2)	-29(3)	27(2)
C(132)	82(3)	30(2)	28(2)	-6(2)	-10(2)	24(2)
C(142)	30(2)	26(2)	30(2)	-10(2)	-4(2)	5(1)
C(152)	47(2)	37(2)	40(3)	-16(2)	-14(2)	2(2)
C(162)	54(2)	62(2)	41(3)	-16(2)	7(2)	-22(2)
C(172)	64(2)	39(2)	65(4)	-20(2)	-42(3)	16(2)
C(182)	66(3)	38(2)	89(5)	-26(2)	-41(3)	20(2)
C(192)	87(3)	34(2)	64(4)	-4(2)	-52(3)	-7(2)
C(20C)	77(7)	48(5)	28(5)	-24(4)	-23(5)	11(5)
C(21C)	80(8)	68(6)	61(9)	-42(6)	19(7)	-19(5)
C(20D)	68(5)	46(4)	22(4)	-13(3)	-21(4)	30(3)
C(21D)	68(5)	56(4)	41(5)	-23(4)	3(4)	4(4)
C(222)	57(3)	82(3)	83(4)	-29(3)	-7(3)	-10(2)
C(13)	21(1)	22(1)	26(2)	-10(1)	-6(1)	1(1)
C(23)	26(1)	22(1)	24(2)	-9(1)	-7(2)	3(1)
C(33)	35(2)	20(1)	26(2)	-8(1)	-7(2)	3(1)
C(43)	33(2)	26(2)	20(2)	-5(1)	-6(2)	1(1)
C(53)	32(2)	25(1)	24(2)	-12(1)	-5(2)	-1(1)
C(63)	25(1)	22(1)	22(2)	-8(1)	-6(2)	1(1)
K(1)	34(1)	63(1)	61(1)	-32(1)	-10(1)	-1(1)
O(10)	43(1)	41(1)	55(2)	-10(1)	-14(2)	-2(1)
C(20)	37(2)	52(2)	51(3)	-21(2)	-2(2)	-2(2)
C(30)	58(2)	52(2)	53(3)	-13(2)	11(3)	-7(2)
C(40)	53(2)	90(4)	46(3)	6(3)	5(2)	28(3)
C(50)	34(2)	71(3)	60(4)	16(3)	-17(2)	-13(2)
O(60)	66(2)	52(2)	62(3)	-25(2)	6(2)	-12(1)
C(7E)	260(40)	95(14)	85(18)	-33(12)	20(20)	-12(17)
C(8E)	190(20)	80(13)	83(14)	-24(9)	25(14)	-30(12)
C(9E)	240(30)	111(16)	130(19)	-63(13)	0(20)	12(18)
C(10E)	141(17)	72(14)	93(15)	-29(10)	58(14)	-65(12)
C(7F)	49(6)	42(5)	44(6)	-26(4)	15(4)	-21(3)
C(8F)	280(30)	49(7)	85(11)	-26(6)	-74(15)	4(8)
C(9F)	370(30)	42(6)	44(8)	-7(5)	-33(10)	-44(9)
C(10F)	210(20)	38(7)	45(7)	-22(5)	-27(9)	8(8)

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

	x	y	z	U(eq)
H(41)	-642	10140	7818	36
H(51)	1483	10202	8371	35
H(101)	6872	10783	8366	39
H(121)	5925	8217	9603	45
H(141)	4147	11102	7096	47
H(15A)	3481	11903	7908	116
H(15B)	4312	12563	7165	116
H(15C)	5185	12111	7887	116
H(16A)	7127	11562	7066	74
H(16B)	6137	11890	6382	74
H(16C)	6713	10845	6722	74
H(17A)	8498	9929	9130	57
H(18A)	6882	10696	9723	91
H(18B)	8213	10206	10223	91
H(18C)	6606	9791	10424	91
H(17B)	8380	9988	9348	59
H(18D)	6461	9904	10326	94
H(18E)	7808	9212	10684	94
H(18F)	6369	8835	10514	94
H(19A)	9602	8610	9999	109
H(19B)	8192	8085	9980	109
H(19C)	9262	8520	9243	109
H(19D)	9555	8608	10024	109
H(19E)	8231	8058	9946	109
H(19F)	9320	8569	9236	109
H(201)	2904	8128	8605	73
H(21A)	3495	7679	10107	130
H(21B)	2205	7260	9857	130
H(21C)	2115	8323	9734	130
H(22A)	5177	7273	8467	142
H(22B)	3967	6639	9038	142
H(22C)	5303	6961	9334	142
H(42)	755	4706	6576	39
H(52)	3064	4008	6977	40
H(102)	8709	3766	6570	38
H(122)	7131	3620	8612	66
H(142)	5714	5235	5676	35
H(15D)	7070	3519	5688	60
H(15E)	6318	4239	4993	60
H(15F)	5316	3783	5750	60
H(16D)	8197	5725	5530	78
H(16E)	7772	5553	4820	78
H(16F)	8819	4815	5377	78
H(172)	10309	3118	7477	64
H(18G)	8416	1946	8602	93
H(18H)	10150	1693	8439	93
H(18I)	9026	1846	7828	93
H(19G)	10468	3976	8209	91
H(19H)	11111	2957	8617	91

H(19I)	9479	3291	8876	91
H(20C)	3344	4631	7975	57
H(21D)	5232	5212	8755	99
H(21E)	3454	5297	8910	99
H(21F)	4243	5838	8112	99
H(20D)	3869	5029	8188	55
H(21G)	6028	4388	9234	82
H(21H)	4570	5036	9287	82
H(21I)	5905	5408	8660	82
H(22G)	3720	3172	8754	110
H(22H)	4562	3523	9268	110
H(22I)	2826	3797	9177	110
H(22D)	3308	3448	8609	110
H(22E)	4504	3209	9201	110
H(22F)	3028	3836	9272	110
H(13)	1148	7702	6847	27
H(33)	3041	10025	5410	32
H(43)	3990	9251	4590	33
H(53)	3674	7681	4952	31
H(20A)	-3477	8488	4302	55
H(20B)	-3269	7448	4838	55
H(30A)	-1920	7194	3892	68
H(30B)	-1784	8267	3444	68
H(40A)	586	7898	3765	89
H(40B)	73	7099	4522	89
H(50A)	387	8256	4937	76
H(50B)	-295	9019	4232	76
H(7EA)	-2180	7617	8403	179
H(7EB)	-428	7796	8249	179
H(8EA)	-1769	6322	9318	144
H(8EB)	-73	6603	9254	144
H(9EA)	767	5864	8487	188
H(9EB)	-570	5236	8924	188
H(10A)	-343	5851	7526	125
H(10B)	-2004	5817	7961	125
H(7FA)	-1821	7640	8435	51
H(7FB)	-98	7791	8137	51
H(8FA)	-935	6619	9403	160
H(8FB)	666	6524	8963	160
H(9FA)	-208	5210	9032	181
H(9FB)	-1925	5607	9046	181
H(10C)	216	5882	7817	115
H(10D)	-1536	5763	7854	115

Torsion angles [°] for LFeK (2).

Fe(1)-S(11)-C(11)-C(61)	166.0(2)
Fe(1)-S(11)-C(11)-C(21)	-8.1(3)
C(61)-C(11)-C(21)-C(31)	-2.0(5)
S(11)-C(11)-C(21)-C(31)	172.2(2)
C(61)-C(11)-C(21)-C(23)	-176.7(3)
S(11)-C(11)-C(21)-C(23)	-2.4(4)
C(11)-C(21)-C(31)-C(41)	2.8(5)
C(23)-C(21)-C(31)-C(41)	177.2(3)
C(11)-C(21)-C(31)-F(71)	-176.4(3)
C(23)-C(21)-C(31)-F(71)	-2.0(4)
F(71)-C(31)-C(41)-C(51)	177.9(3)
C(21)-C(31)-C(41)-C(51)	-1.2(5)
C(31)-C(41)-C(51)-C(61)	-1.1(5)
C(21)-C(11)-C(61)-C(51)	-0.2(5)
S(11)-C(11)-C(61)-C(51)	-174.2(2)
C(21)-C(11)-C(61)-C(81)	174.3(3)
S(11)-C(11)-C(61)-C(81)	0.3(4)
C(41)-C(51)-C(61)-C(11)	1.8(5)
C(41)-C(51)-C(61)-C(81)	-172.8(3)
C(41)-C(31)-F(71)-K(1)	-128.9(3)
C(21)-C(31)-F(71)-K(1)	50.3(4)
C(11)-C(61)-C(81)-C(91)	96.4(4)
C(51)-C(61)-C(81)-C(91)	-89.1(4)
C(11)-C(61)-C(81)-C(131)	-85.6(4)
C(51)-C(61)-C(81)-C(131)	88.8(4)
C(131)-C(81)-C(91)-C(101)	-1.5(5)
C(61)-C(81)-C(91)-C(101)	176.4(3)
C(131)-C(81)-C(91)-C(141)	176.0(4)
C(61)-C(81)-C(91)-C(141)	-6.1(5)
C(81)-C(91)-C(101)-C(111)	1.2(6)
C(141)-C(91)-C(101)-C(111)	-176.3(4)
C(91)-C(101)-C(111)-C(121)	-0.4(6)
C(91)-C(101)-C(111)-C(17B)	-178.0(6)
C(91)-C(101)-C(111)-C(17A)	-177.7(10)
C(101)-C(111)-C(121)-C(131)	-0.2(6)
C(17B)-C(111)-C(121)-C(131)	177.4(6)
C(17A)-C(111)-C(121)-C(131)	176.8(10)
C(111)-C(121)-C(131)-C(81)	-0.1(6)
C(111)-C(121)-C(131)-C(201)	-178.6(4)
C(91)-C(81)-C(131)-C(121)	0.9(6)
C(61)-C(81)-C(131)-C(121)	-177.0(3)
C(91)-C(81)-C(131)-C(201)	179.4(4)
C(61)-C(81)-C(131)-C(201)	1.4(6)
C(101)-C(91)-C(141)-C(161)	57.6(5)
C(81)-C(91)-C(141)-C(161)	-119.9(4)
C(101)-C(91)-C(141)-C(151)	-66.3(5)
C(81)-C(91)-C(141)-C(151)	116.2(4)
C(121)-C(111)-C(17A)-C(191)	45(2)
C(101)-C(111)-C(17A)-C(191)	-137.7(13)
C(121)-C(111)-C(17A)-C(18A)	-104.6(17)
C(101)-C(111)-C(17A)-C(18A)	72(2)
C(121)-C(111)-C(17B)-C(191)	49.4(13)
C(101)-C(111)-C(17B)-C(191)	-133.1(9)
C(121)-C(111)-C(17B)-C(18B)	-64.2(9)

C(101)-C(111)-C(17B)-C(18B)	113.3(9)
C(121)-C(131)-C(201)-C(221)	-59.6(7)
C(81)-C(131)-C(201)-C(221)	122.0(5)
C(121)-C(131)-C(201)-C(211)	63.5(5)
C(81)-C(131)-C(201)-C(211)	-115.0(5)
Fe(1)-S(21)-C(12)-C(62)	-173.3(3)
K(1)#1-S(21)-C(12)-C(62)	77.7(7)
Fe(1)-S(21)-C(12)-C(22)	2.6(3)
K(1)#1-S(21)-C(12)-C(22)	-106.4(5)
C(62)-C(12)-C(22)-C(32)	3.4(6)
S(21)-C(12)-C(22)-C(32)	-172.8(3)
C(62)-C(12)-C(22)-C(63)	-178.7(3)
S(21)-C(12)-C(22)-C(63)	5.1(5)
C(12)-C(22)-C(32)-C(42)	-2.1(6)
C(63)-C(22)-C(32)-C(42)	-179.9(4)
C(12)-C(22)-C(32)-F(72)	176.4(3)
C(63)-C(22)-C(32)-F(72)	-1.4(6)
C(22)-C(32)-C(42)-C(52)	-0.4(7)
F(72)-C(32)-C(42)-C(52)	-178.9(4)
C(32)-C(42)-C(52)-C(62)	1.7(7)
C(42)-C(52)-C(62)-C(12)	-0.4(6)
C(42)-C(52)-C(62)-C(82)	177.9(4)
C(22)-C(12)-C(62)-C(52)	-2.2(6)
S(21)-C(12)-C(62)-C(52)	173.8(3)
C(22)-C(12)-C(62)-C(82)	179.5(4)
S(21)-C(12)-C(62)-C(82)	-4.5(6)
C(42)-C(32)-F(72)-K(1)	129.6(3)
C(22)-C(32)-F(72)-K(1)	-49.1(5)
C(52)-C(62)-C(82)-C(132)	-82.4(5)
C(12)-C(62)-C(82)-C(132)	95.9(5)
C(52)-C(62)-C(82)-C(92)	93.5(4)
C(12)-C(62)-C(82)-C(92)	-88.2(5)
C(132)-C(82)-C(92)-C(102)	1.4(5)
C(62)-C(82)-C(92)-C(102)	-174.6(3)
C(132)-C(82)-C(92)-C(142)	179.8(4)
C(62)-C(82)-C(92)-C(142)	3.9(5)
C(82)-C(92)-C(102)-C(112)	-2.6(5)
C(142)-C(92)-C(102)-C(112)	178.9(3)
C(92)-C(102)-C(112)-C(122)	1.2(6)
C(92)-C(102)-C(112)-C(172)	-179.5(3)
C(102)-C(112)-C(122)-C(132)	1.4(7)
C(172)-C(112)-C(122)-C(132)	-177.9(4)
C(92)-C(82)-C(132)-C(122)	1.1(6)
C(62)-C(82)-C(132)-C(122)	177.0(4)
C(92)-C(82)-C(132)-C(20D)	173.5(6)
C(62)-C(82)-C(132)-C(20D)	-10.6(8)
C(92)-C(82)-C(132)-C(20C)	-170.5(5)
C(62)-C(82)-C(132)-C(20C)	5.4(7)
C(112)-C(122)-C(132)-C(82)	-2.5(7)
C(112)-C(122)-C(132)-C(20D)	-176.0(5)
C(112)-C(122)-C(132)-C(20C)	167.4(7)
C(82)-C(92)-C(142)-C(152)	-105.9(4)
C(102)-C(92)-C(142)-C(152)	72.5(4)
C(82)-C(92)-C(142)-C(162)	129.6(4)
C(102)-C(92)-C(142)-C(162)	-52.0(4)
C(102)-C(112)-C(172)-C(182)	-99.6(6)

C(122)-C(112)-C(172)-C(182)	79.7(6)
C(102)-C(112)-C(172)-C(192)	134.1(5)
C(122)-C(112)-C(172)-C(192)	-46.6(6)
C(82)-C(132)-C(20C)-C(222)	132.8(8)
C(122)-C(132)-C(20C)-C(222)	-37.8(13)
C(82)-C(132)-C(20C)-C(21C)	-103.0(10)
C(122)-C(132)-C(20C)-C(21C)	86.5(11)
C(82)-C(132)-C(20D)-C(21D)	-128.4(7)
C(122)-C(132)-C(20D)-C(21D)	44.4(8)
C(82)-C(132)-C(20D)-C(222)	110.2(7)
C(122)-C(132)-C(20D)-C(222)	-77.0(8)
C(63)-C(13)-C(23)-C(33)	5.3(4)
Fe(1)-C(13)-C(23)-C(33)	54.0(2)
K(1)-C(13)-C(23)-C(33)	-113.1(3)
C(63)-C(13)-C(23)-C(21)	-157.0(3)
Fe(1)-C(13)-C(23)-C(21)	-108.3(3)
K(1)-C(13)-C(23)-C(21)	84.6(3)
C(63)-C(13)-C(23)-Fe(1)	-48.7(2)
K(1)-C(13)-C(23)-Fe(1)	-167.07(17)
C(31)-C(21)-C(23)-C(33)	117.1(3)
C(11)-C(21)-C(23)-C(33)	-68.5(4)
C(31)-C(21)-C(23)-C(13)	-80.4(4)
C(11)-C(21)-C(23)-C(13)	94.0(4)
C(31)-C(21)-C(23)-Fe(1)	-160.7(3)
C(11)-C(21)-C(23)-Fe(1)	13.7(4)
C(13)-C(23)-C(33)-C(43)	-1.8(4)
C(21)-C(23)-C(33)-C(43)	160.3(3)
Fe(1)-C(23)-C(33)-C(43)	51.7(3)
C(13)-C(23)-C(33)-Fe(1)	-53.5(2)
C(21)-C(23)-C(33)-Fe(1)	108.7(3)
C(23)-C(33)-C(43)-C(53)	-2.0(5)
Fe(1)-C(33)-C(43)-C(53)	47.8(3)
C(23)-C(33)-C(43)-Fe(1)	-49.8(3)
C(33)-C(43)-C(53)-C(63)	2.3(5)
Fe(1)-C(43)-C(53)-C(63)	50.4(3)
C(33)-C(43)-C(53)-Fe(1)	-48.1(3)
C(23)-C(13)-C(63)-C(53)	-5.0(4)
Fe(1)-C(13)-C(63)-C(53)	-54.0(3)
K(1)-C(13)-C(63)-C(53)	112.4(3)
C(23)-C(13)-C(63)-C(22)	159.3(3)
Fe(1)-C(13)-C(63)-C(22)	110.4(3)
K(1)-C(13)-C(63)-C(22)	-83.3(3)
C(23)-C(13)-C(63)-Fe(1)	48.9(2)
K(1)-C(13)-C(63)-Fe(1)	166.33(14)
C(43)-C(53)-C(63)-C(13)	1.3(5)
Fe(1)-C(53)-C(63)-C(13)	54.1(3)
C(43)-C(53)-C(63)-C(22)	-163.2(3)
Fe(1)-C(53)-C(63)-C(22)	-110.4(3)
C(43)-C(53)-C(63)-Fe(1)	-52.8(3)
C(32)-C(22)-C(63)-C(13)	83.7(5)
C(12)-C(22)-C(63)-C(13)	-94.1(4)
C(32)-C(22)-C(63)-C(53)	-111.7(4)
C(12)-C(22)-C(63)-C(53)	70.5(5)
C(32)-C(22)-C(63)-Fe(1)	166.2(3)
C(12)-C(22)-C(63)-Fe(1)	-11.6(5)
C(50)-O(10)-C(20)-C(30)	10.6(4)

K(1)-O(10)-C(20)-C(30)	-143.3(3)
O(10)-C(20)-C(30)-C(40)	13.9(5)
C(20)-C(30)-C(40)-C(50)	-31.6(5)
C(20)-O(10)-C(50)-C(40)	-30.9(4)
K(1)-O(10)-C(50)-C(40)	129.0(3)
C(20)-O(10)-C(50)-K(1)	-159.9(3)
C(30)-C(40)-C(50)-O(10)	39.1(5)
C(30)-C(40)-C(50)-K(1)	82.1(4)
C(10E)-O(60)-C(7E)-C(8E)	12(5)
K(1)-O(60)-C(7E)-C(8E)	168(2)
O(60)-C(7E)-C(8E)-C(9E)	10(4)
C(7E)-C(8E)-C(9E)-C(10E)	-30(5)
C(7E)-O(60)-C(10E)-C(9E)	-28(4)
K(1)-O(60)-C(10E)-C(9E)	174(2)
C(7E)-O(60)-C(10E)-K(1)	158(3)
C(8E)-C(9E)-C(10E)-O(60)	34(5)
C(8E)-C(9E)-C(10E)-K(1)	40(7)
C(10F)-O(60)-C(7F)-C(8F)	3(2)
K(1)-O(60)-C(7F)-C(8F)	177.8(18)
O(60)-C(7F)-C(8F)-C(9F)	-21(3)
C(7F)-C(8F)-C(9F)-C(10F)	29(4)
C(7F)-O(60)-C(10F)-C(9F)	17(3)
K(1)-O(60)-C(10F)-C(9F)	-158.3(19)
C(8F)-C(9F)-C(10F)-O(60)	-29(4)

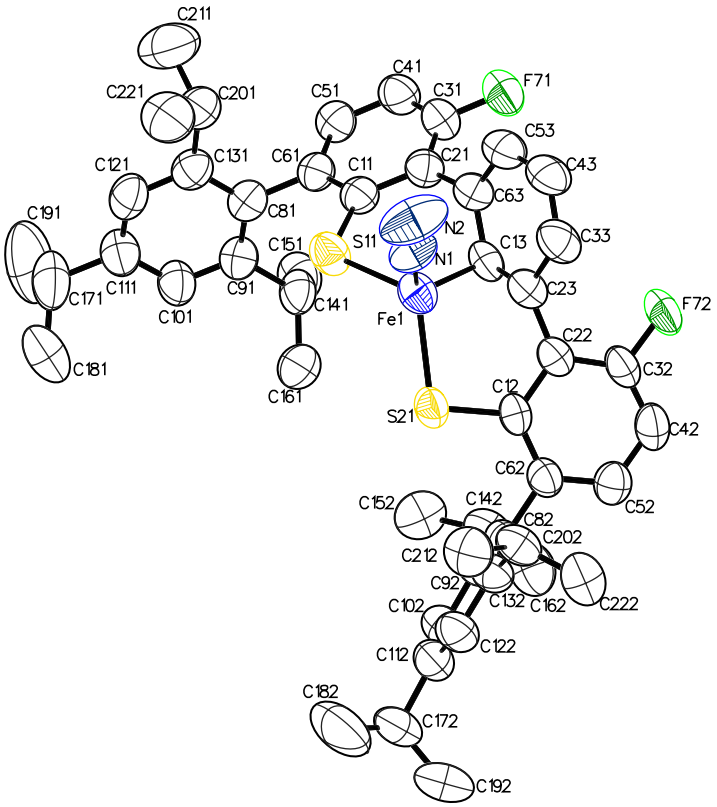
Symmetry transformations used to generate equivalent atoms:
#1 x+1,y,z #2 x-1,y,z

Experimental and Refinement Details for [LFeN$_2$][K(18-crown-6)(THF)$_2$]$_2$ (3)

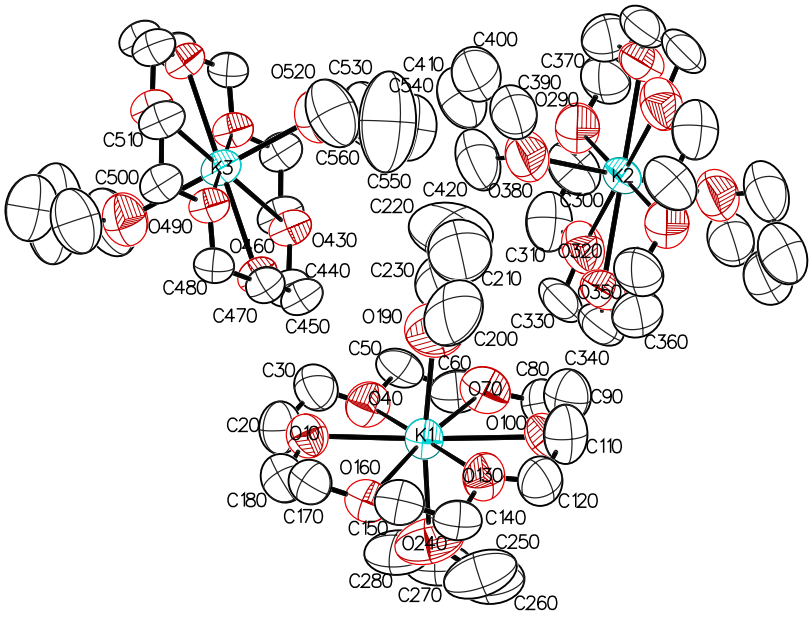
Single crystals for X-ray analysis were obtained from the reaction mixture in THF at -38 °C. Crystals were taken into cold Fomblin Y oil in the cold well (-70 °C) and transported cold (-78 °C) in a closed jar. Suitable crystal was selected under microscope while keeping the sample under cold nitrogen stream (< -80 °C). The pin with the crystal was immediately placed in the cold (liquid N_2) cryo-tongs, transported on dry ice, and the crystal was placed on the goniometer under cold nitrogen stream. Low-temperature diffraction data (ω-scans) were collected on a Rigaku R-AXIS RAPID diffractometer coupled to an R-AXIS RAPID imaging plate detector with Mo Kα radiation (λ = 0.71073 Å). All structures were solved by direct methods using SHELXS and were refined against F^2 on all data by full-matrix least squares with SHELXL[50]. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included in the model at geometrically calculated positions and refined using a riding model. The isotropic displacement parameters of all hydrogen atoms were fixed to 1.2 times the U value of the atoms to which they are linked (1.5 times for methyl groups).

The THF molecules that were modeled and included in this report are likely disordered. Rigid bond restraints were used to aid their refinement. Without these restrains, the models became unstable. A more traditional approach was tried, using multiple orientations of the solvents did not produce a stable refinement, which is likely related to the inherently weak data.

The program SQUEEZE was used to compensate for the contribution of disordered solvents contained in voids within the crystal lattice from the diffraction intensities[51]. This procedure was applied to the data file and the submitted model is based on the solvent removed data. Based on the total electron density found in the voids (375.8 e/Å), it is likely that ~9 THF molecules are present in the unit cell.



The full numbering scheme of the anionic portion of $[LFeN_2][K(18\text{-crown-6})(THF)_2]_2$ (**3**). All atoms shown are depicted with 50% thermal contours. The hydrogen atoms have been removed for clarity.



The full numbering scheme of the cationic portion of $[LFeN_2][K(18\text{-crown-6})(THF)_2]_2$ (**3**). All atoms shown are depicted with 50% thermal contours. The hydrogen atoms have been removed for clarity. K2 resides on an inversion center, and the symmetry equivalents of the numbered atoms are generated by the operation 2-x, 1-y, 1-z. K3 resides on an inversion center, and the symmetry equivalents of the numbered atoms are generated by the operation 1-x, 2-y, 1-z.

Crystal data and structure refinement for $[LFeN_2][K(18\text{-crown-6})(THF)_2]_2$ (3).

Identification code	spider-14110	
Empirical formula	$C_{88}H_{134}F_2FeK_2N_2O_{16}S_2$	
Formula weight	1712.13	
Temperature	173(2) K	
Wavelength	0.71075 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	a = 13.6187(13) Å	α = 76.340(5)°.
	b = 21.0216(19) Å	β = 85.562(6)°.
	c = 24.295(2) Å	γ = 71.430(5)°.
Volume	6406.6(11) $Å^3$	
Z	2	
Density (calculated)	0.888 g/cm^3	
Absorption coefficient	0.263 mm^{-1}	
F(000)	1836	
Crystal size	0.220 x 0.180 x 0.090 mm^3	
Crystal color and habit	Red block	
Diffractometer	Rigaku R-AXIS RAPID imaging plate	
Θ range for data collection	2.980 to 25.351°.	
Index ranges	$-16 \le h \le 16$, $-25 \le k \le 25$, $-29 \le l \le 29$	
Reflections collected	184743	
Independent reflections	23441 [R(int) = 0.1374]	
Observed reflections (I > 2σ(I))	11283	
Completeness to θ = 25.242°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.000 and 0.475	
Solution method	SHELXT-2014/5 (Sheldrick, 2014)	
Refinement method	SHELXL-2014/7 (Sheldrick, 2014)	
Data / restraints / parameters	23441 / 120 / 1033	
Goodness-of-fit on F^2	0.976	
Final R indices [I>2σ(I)]	R1 = 0.0973, wR2 = 0.2661	
R indices (all data)	R1 = 0.1684, wR2 = 0.3192	
Largest diff. peak and hole	0.549 and -0.503 $e.Å^{-3}$	

Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $[LFeN_2][K(18\text{-crown-6})(THF)_2]_2$ (3). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Fe(1)	6218(1)	6427(1)	7067(1)	67(1)
N(1)	6830(4)	6778(2)	6443(2)	78(1)
N(2)	7121(6)	7039(3)	6030(3)	131(3)
S(11)	5923(1)	7174(1)	7691(1)	76(1)
S(21)	6904(1)	5270(1)	7494(1)	66(1)
C(11)	4621(4)	7688(2)	7657(2)	62(1)
C(21)	3939(4)	7715(3)	7233(2)	64(1)
C(31)	2966(4)	8171(3)	7223(2)	74(1)
C(41)	2607(4)	8598(3)	7589(2)	75(1)
C(51)	3275(4)	8564(3)	8005(2)	68(1)
C(61)	4269(4)	8109(2)	8048(2)	59(1)
F(71)	2274(3)	8207(2)	6830(2)	94(1)
C(81)	4947(4)	8078(3)	8522(2)	62(1)
C(91)	5006(4)	7587(3)	9029(2)	67(1)
C(101)	5589(4)	7572(3)	9466(2)	76(2)
C(111)	6112(5)	8044(3)	9440(2)	79(2)
C(121)	6064(4)	8524(3)	8940(3)	79(2)
C(131)	5472(4)	8554(3)	8475(2)	70(1)
C(141)	4394(4)	7078(3)	9107(2)	75(2)
C(151)	3446(5)	7286(3)	9478(3)	91(2)
C(161)	5056(5)	6338(3)	9336(3)	90(2)
C(171)	6742(6)	8026(4)	9937(3)	110(2)
C(181)	7413(8)	7324(5)	10206(4)	152(4)
C(191)	6003(9)	8344(7)	10380(5)	196(5)
C(201)	5454(5)	9088(3)	7930(3)	84(2)
C(211)	4877(7)	9826(4)	8013(4)	137(3)
C(221)	6540(6)	9050(4)	7697(3)	113(2)
C(12)	6074(3)	4921(3)	7251(2)	56(1)
C(22)	5283(3)	5344(3)	6859(2)	60(1)
C(32)	4686(4)	5017(3)	6667(2)	68(1)
C(42)	4777(4)	4337(3)	6837(2)	75(2)
C(52)	5549(4)	3926(3)	7226(2)	68(1)
C(62)	6187(4)	4213(3)	7436(2)	61(1)
F(72)	3895(2)	5410(2)	6296(1)	89(1)
C(82)	6997(4)	3753(3)	7866(2)	64(1)
C(92)	6745(4)	3638(3)	8440(2)	73(1)
C(102)	7470(5)	3179(3)	8836(2)	78(2)
C(112)	8432(5)	2830(3)	8677(3)	80(2)
C(122)	8689(4)	2970(3)	8104(3)	79(2)
C(132)	7989(4)	3413(3)	7696(2)	69(1)
C(142)	5676(4)	4004(3)	8646(2)	80(2)
C(152)	5756(5)	4421(3)	9076(3)	97(2)
C(162)	5072(5)	3515(4)	8884(3)	98(2)
C(172)	9217(5)	2310(3)	9105(3)	97(2)
C(182)	10136(8)	2458(6)	9137(5)	204(6)
C(192)	9357(9)	1598(4)	9069(5)	183(5)
C(202)	8298(4)	3537(3)	7074(2)	77(2)
C(212)	9385(5)	3603(4)	6986(3)	96(2)

C(222)	8215(5)	2966(4)	6818(3)	97(2)
C(13)	4677(4)	6552(3)	7033(2)	62(1)
C(23)	5100(4)	6094(3)	6661(2)	66(1)
C(33)	4989(5)	6406(3)	6062(2)	81(2)
C(43)	4544(5)	7089(3)	5865(2)	88(2)
C(53)	4171(5)	7538(3)	6248(3)	88(2)
C(63)	4251(4)	7272(3)	6819(2)	69(1)
K(1)	10591(1)	5904(1)	8302(1)	79(1)
O(10)	11050(4)	4596(2)	8118(2)	106(1)
C(20)	12097(6)	4188(4)	8165(4)	124(3)
C(30)	12731(7)	4655(4)	7937(4)	127(3)
O(40)	12680(4)	5142(3)	8207(2)	110(1)
C(50)	13321(5)	5552(4)	8009(3)	100(2)
C(60)	13108(6)	6096(5)	8327(4)	122(3)
O(70)	12117(4)	6547(3)	8193(2)	120(2)
C(80)	11869(7)	7146(5)	8392(4)	120(3)
C(90)	10845(8)	7595(5)	8188(5)	139(3)
O(100)	10098(5)	7305(3)	8439(2)	118(2)
C(110)	9091(7)	7662(5)	8272(5)	140(3)
C(120)	8404(7)	7284(5)	8583(4)	138(3)
O(130)	8618(4)	6668(3)	8462(2)	116(2)
C(140)	7960(5)	6291(4)	8741(3)	100(2)
C(150)	8090(5)	5726(4)	8464(3)	107(2)
O(160)	9083(3)	5245(2)	8560(2)	99(1)
C(170)	9255(6)	4686(4)	8280(3)	102(2)
C(180)	10341(7)	4255(4)	8378(4)	117(2)
O(190)	10459(10)	6510(5)	7181(4)	211(4)
C(200)	9487(15)	6933(9)	6871(7)	248(6)
C(210)	9828(18)	7219(10)	6310(8)	263(7)
C(220)	10905(19)	7056(12)	6272(7)	317(11)
C(230)	11299(14)	6663(7)	6839(5)	206(5)
O(240)	10974(6)	5460(5)	9432(3)	182(3)
C(250)	10644(10)	5906(8)	9817(5)	201(5)
C(260)	11661(10)	5848(8)	10076(5)	186(4)
C(270)	12442(10)	5234(7)	9949(4)	175(4)
C(280)	11902(11)	4929(7)	9652(5)	189(4)
K(2)	5000	10000	5000	81(1)
O(290)	7145(4)	9415(3)	4800(3)	128(2)
C(300)	7727(8)	9117(5)	5309(5)	143(3)
C(310)	7203(8)	8693(5)	5718(5)	146(4)
O(320)	6260(6)	9082(3)	5883(3)	134(2)
C(330)	5746(9)	8686(4)	6290(4)	135(3)
C(340)	4701(10)	9166(5)	6439(4)	137(3)
O(350)	4116(6)	9421(3)	5978(2)	133(2)
C(360)	3105(8)	9837(6)	6114(5)	150(4)
C(370)	7520(9)	9876(6)	4424(6)	164(4)
C(390)	4018(10)	9258(5)	3954(5)	160(3)
C(400)	4738(12)	8918(6)	3615(6)	190(5)
C(410)	5545(11)	8541(6)	3974(7)	185(4)
C(420)	5168(11)	8497(5)	4577(5)	187(4)
O(380)	4384(7)	9156(3)	4498(3)	168(3)
K(3)	10000	5000	5000	73(1)
O(430)	10738(3)	5370(2)	5888(2)	76(1)
C(440)	10251(4)	5158(4)	6418(2)	85(2)
C(450)	9114(4)	5433(3)	6334(2)	78(2)
C(470)	7728(4)	5294(3)	5891(2)	74(1)

C(480)	7511(4)	4861(3)	5550(2)	73(1)
O(490)	7924(3)	5011(2)	4996(2)	72(1)
C(500)	7725(4)	4622(4)	4639(3)	83(2)
C(510)	8162(4)	4842(4)	4064(3)	88(2)
O(520)	9327(5)	6356(3)	4542(3)	143(2)
C(530)	9703(10)	6833(6)	4690(6)	182(4)
C(540)	8774(12)	7389(7)	4749(7)	206(5)
C(550)	8004(14)	7279(10)	4509(11)	317(13)
C(560)	8366(11)	6671(6)	4373(7)	194(5)
O(460)	8832(2)	5091(2)	5966(2)	71(1)

Bond lengths [Å] and angles [°] for [LFeN$_2$][K(18-crown-6)(THF)$_2$]$_2$ (3).

Fe(1)-N(1)	1.790(5)
Fe(1)-C(13)	2.037(5)
Fe(1)-C(23)	2.239(5)
Fe(1)-S(21)	2.3201(16)
Fe(1)-S(11)	2.3549(16)
N(1)-N(2)	1.132(7)
S(11)-C(11)	1.754(5)
S(21)-C(12)	1.733(4)
C(11)-C(61)	1.405(7)
C(11)-C(21)	1.421(7)
C(21)-C(31)	1.364(7)
C(21)-C(63)	1.476(7)
C(31)-F(71)	1.365(6)
C(31)-C(41)	1.367(8)
C(41)-C(51)	1.385(7)
C(41)-H(41)	0.9500
C(51)-C(61)	1.381(7)
C(51)-H(51)	0.9500
C(61)-C(81)	1.506(7)
C(81)-C(131)	1.384(7)
C(81)-C(91)	1.397(7)
C(91)-C(101)	1.363(7)
C(91)-C(141)	1.524(7)
C(101)-C(111)	1.382(8)
C(101)-H(101)	0.9500
C(111)-C(121)	1.374(8)
C(111)-C(171)	1.522(9)
C(121)-C(131)	1.417(8)
C(121)-H(121)	0.9500
C(131)-C(201)	1.516(8)
C(141)-C(161)	1.522(8)
C(141)-C(151)	1.523(8)
C(141)-H(141)	1.0000
C(151)-H(15A)	0.9800
C(151)-H(15B)	0.9800
C(151)-H(15C)	0.9800
C(161)-H(16A)	0.9800

C(161)-H(16B)	0.9800
C(161)-H(16C)	0.9800
C(171)-C(181)	1.489(11)
C(171)-C(191)	1.536(13)
C(171)-H(171)	1.0000
C(181)-H(18A)	0.9800
C(181)-H(18B)	0.9800
C(181)-H(18C)	0.9800
C(191)-H(19A)	0.9800
C(191)-H(19B)	0.9800
C(191)-H(19C)	0.9800
C(201)-C(221)	1.527(9)
C(201)-C(211)	1.552(10)
C(201)-H(201)	1.0000
C(211)-H(21A)	0.9800
C(211)-H(21B)	0.9800
C(211)-H(21C)	0.9800
C(221)-H(22A)	0.9800
C(221)-H(22B)	0.9800
C(221)-H(22C)	0.9800
C(12)-C(62)	1.411(7)
C(12)-C(22)	1.416(6)
C(22)-C(32)	1.385(7)
C(22)-C(23)	1.480(7)
C(32)-C(42)	1.360(8)
C(32)-F(72)	1.373(6)
C(42)-C(52)	1.390(7)
C(42)-H(42)	0.9500
C(52)-C(62)	1.388(7)
C(52)-H(52)	0.9500
C(62)-C(82)	1.505(7)
C(82)-C(92)	1.393(7)
C(82)-C(132)	1.394(7)
C(92)-C(102)	1.389(8)
C(92)-C(142)	1.522(8)
C(102)-C(112)	1.360(8)
C(102)-H(102)	0.9500
C(112)-C(122)	1.393(8)
C(112)-C(172)	1.519(8)
C(122)-C(132)	1.380(7)
C(122)-H(122)	0.9500
C(132)-C(202)	1.520(8)
C(142)-C(162)	1.502(9)
C(142)-C(152)	1.543(9)
C(142)-H(142)	1.0000
C(152)-H(15D)	0.9800
C(152)-H(15E)	0.9800
C(152)-H(15F)	0.9800
C(162)-H(16D)	0.9800
C(162)-H(16E)	0.9800
C(162)-H(16F)	0.9800
C(172)-C(182)	1.393(11)
C(172)-C(192)	1.472(11)
C(172)-H(172)	1.0000
C(182)-H(18D)	0.9800
C(182)-H(18E)	0.9800

C(182)-H(18F)	0.9800
C(192)-H(19D)	0.9800
C(192)-H(19E)	0.9800
C(192)-H(19F)	0.9800
C(202)-C(222)	1.513(8)
C(202)-C(212)	1.523(8)
C(202)-H(202)	1.0000
C(212)-H(21D)	0.9800
C(212)-H(21E)	0.9800
C(212)-H(21F)	0.9800
C(222)-H(22D)	0.9800
C(222)-H(22E)	0.9800
C(222)-H(22F)	0.9800
C(13)-C(63)	1.420(7)
C(13)-C(23)	1.432(7)
C(13)-H(13)	0.9500
C(23)-C(33)	1.446(7)
C(33)-C(43)	1.351(8)
C(33)-H(33)	0.9500
C(43)-C(53)	1.431(9)
C(43)-H(43)	0.9500
C(53)-C(63)	1.366(8)
C(53)-H(53)	0.9500
K(1)-O(130)	2.708(5)
K(1)-O(190)	2.715(9)
K(1)-O(240)	2.717(7)
K(1)-O(10)	2.756(5)
K(1)-O(160)	2.780(4)
K(1)-O(70)	2.784(5)
K(1)-O(40)	2.808(5)
K(1)-O(100)	2.899(5)
O(10)-C(180)	1.406(9)
O(10)-C(20)	1.407(8)
C(20)-C(30)	1.492(11)
C(20)-H(20A)	0.9900
C(20)-H(20B)	0.9900
C(30)-O(40)	1.321(9)
C(30)-H(30A)	0.9900
C(30)-H(30B)	0.9900
O(40)-C(50)	1.399(8)
C(50)-C(60)	1.468(10)
C(50)-H(50A)	0.9900
C(50)-H(50B)	0.9900
C(60)-O(70)	1.391(9)
C(60)-H(60A)	0.9900
C(60)-H(60B)	0.9900
O(70)-C(80)	1.388(9)
C(80)-C(90)	1.459(12)
C(80)-H(80A)	0.9900
C(80)-H(80B)	0.9900
C(90)-O(100)	1.380(10)
C(90)-H(90A)	0.9900
C(90)-H(90B)	0.9900
O(100)-C(110)	1.377(9)
C(110)-C(120)	1.468(11)
C(110)-H(11A)	0.9900

C(110)-H(11B)	0.9900
C(120)-O(130)	1.333(9)
C(120)-H(12A)	0.9900
C(120)-H(12B)	0.9900
O(130)-C(140)	1.413(8)
C(140)-C(150)	1.456(10)
C(140)-H(14A)	0.9900
C(140)-H(14B)	0.9900
C(150)-O(160)	1.403(8)
C(150)-H(15G)	0.9900
C(150)-H(15H)	0.9900
O(160)-C(170)	1.440(8)
C(170)-C(180)	1.472(10)
C(170)-H(17A)	0.9900
C(170)-H(17B)	0.9900
C(180)-H(18G)	0.9900
C(180)-H(18H)	0.9900
O(190)-C(230)	1.436(16)
O(190)-C(200)	1.482(17)
C(200)-C(210)	1.46(2)
C(200)-H(20C)	0.9900
C(200)-H(20D)	0.9900
C(210)-C(220)	1.40(3)
C(210)-H(21G)	0.9900
C(210)-H(21H)	0.9900
C(220)-C(230)	1.471(18)
C(220)-H(22G)	0.9900
C(220)-H(22H)	0.9900
C(230)-H(23A)	0.9900
C(230)-H(23B)	0.9900
O(240)-C(250)	1.427(14)
O(240)-C(280)	1.433(14)
C(250)-C(260)	1.523(15)
C(250)-H(25A)	0.9900
C(250)-H(25B)	0.9900
C(260)-C(270)	1.467(16)
C(260)-H(26A)	0.9900
C(260)-H(26B)	0.9900
C(270)-C(280)	1.441(15)
C(270)-H(27A)	0.9900
C(270)-H(27B)	0.9900
C(280)-H(28A)	0.9900
C(280)-H(28B)	0.9900
K(2)-O(380)#1	2.732(7)
K(2)-O(380)	2.732(7)
K(2)-O(350)	2.774(5)
K(2)-O(350)#1	2.774(6)
K(2)-O(320)	2.788(6)
K(2)-O(320)#1	2.788(6)
K(2)-O(290)#1	2.839(5)
K(2)-O(290)	2.839(5)
O(290)-C(370)	1.364(10)
O(290)-C(300)	1.420(10)
C(300)-C(310)	1.473(13)
C(300)-H(30C)	0.9900
C(300)-H(30D)	0.9900

C(310)-O(320)	1.372(11)
C(310)-H(31A)	0.9900
C(310)-H(31B)	0.9900
O(320)-C(330)	1.428(10)
C(330)-C(340)	1.533(13)
C(330)-H(33A)	0.9900
C(330)-H(33B)	0.9900
C(340)-O(350)	1.327(10)
C(340)-H(34A)	0.9900
C(340)-H(34B)	0.9900
O(350)-C(360)	1.439(11)
C(360)-C(370)#1	1.506(15)
C(360)-H(36A)	0.9900
C(360)-H(36B)	0.9900
C(370)-C(360)#1	1.506(15)
C(370)-H(37A)	0.9900
C(370)-H(37B)	0.9900
C(390)-C(400)	1.362(15)
C(390)-O(380)	1.394(11)
C(390)-H(39A)	0.9900
C(390)-H(39B)	0.9900
C(400)-C(410)	1.365(16)
C(400)-H(40A)	0.9900
C(400)-H(40B)	0.9900
C(410)-C(420)	1.505(17)
C(410)-H(41A)	0.9900
C(410)-H(41B)	0.9900
C(420)-O(380)	1.435(13)
C(420)-H(42A)	0.9900
C(420)-H(42B)	0.9900
K(3)-O(520)#2	2.684(6)
K(3)-O(520)	2.684(6)
K(3)-O(460)	2.741(3)
K(3)-O(460)#2	2.741(3)
K(3)-O(430)#2	2.811(3)
K(3)-O(430)	2.811(3)
K(3)-O(490)#2	2.822(3)
K(3)-O(490)	2.822(3)
O(430)-C(510)#2	1.426(6)
O(430)-C(440)	1.443(7)
C(440)-C(450)	1.482(7)
C(440)-H(44A)	0.9900
C(440)-H(44B)	0.9900
C(450)-O(460)	1.413(6)
C(450)-H(45A)	0.9900
C(450)-H(45B)	0.9900
C(470)-O(460)	1.440(6)
C(470)-C(480)	1.473(7)
C(470)-H(47A)	0.9900
C(470)-H(47B)	0.9900
C(480)-O(490)	1.423(6)
C(480)-H(48A)	0.9900
C(480)-H(48B)	0.9900
O(490)-C(500)	1.415(6)
C(500)-C(510)	1.503(8)
C(500)-H(50C)	0.9900

C(500)-H(50D)	0.9900
C(510)-O(430)#2	1.426(6)
C(510)-H(51A)	0.9900
C(510)-H(51B)	0.9900
O(520)-C(560)	1.312(12)
O(520)-C(530)	1.386(12)
C(530)-C(540)	1.448(16)
C(530)-H(53A)	0.9900
C(530)-H(53B)	0.9900
C(540)-C(550)	1.345(18)
C(540)-H(54A)	0.9900
C(540)-H(54B)	0.9900
C(550)-C(560)	1.325(18)
C(550)-H(55A)	0.9900
C(550)-H(55B)	0.9900
C(560)-H(56A)	0.9900
C(560)-H(56B)	0.9900

N(1)-Fe(1)-C(13)	118.3(2)
N(1)-Fe(1)-C(23)	99.2(2)
C(13)-Fe(1)-C(23)	38.77(19)
N(1)-Fe(1)-S(21)	118.88(15)
C(13)-Fe(1)-S(21)	102.71(15)
C(23)-Fe(1)-S(21)	85.25(14)
N(1)-Fe(1)-S(11)	108.09(15)
C(13)-Fe(1)-S(11)	91.57(14)
C(23)-Fe(1)-S(11)	130.34(13)
S(21)-Fe(1)-S(11)	114.30(6)
N(2)-N(1)-Fe(1)	173.1(6)
C(11)-S(11)-Fe(1)	110.05(18)
C(12)-S(21)-Fe(1)	101.46(17)
C(61)-C(11)-C(21)	119.7(5)
C(61)-C(11)-S(11)	118.3(4)
C(21)-C(11)-S(11)	122.0(4)
C(31)-C(21)-C(11)	116.9(5)
C(31)-C(21)-C(63)	120.7(5)
C(11)-C(21)-C(63)	122.4(5)
C(21)-C(31)-F(71)	119.2(5)
C(21)-C(31)-C(41)	124.8(5)
F(71)-C(31)-C(41)	116.0(5)
C(31)-C(41)-C(51)	117.9(5)
C(31)-C(41)-H(41)	121.1
C(51)-C(41)-H(41)	121.1
C(61)-C(51)-C(41)	120.9(5)
C(61)-C(51)-H(51)	119.5
C(41)-C(51)-H(51)	119.5
C(51)-C(61)-C(11)	119.8(5)
C(51)-C(61)-C(81)	118.5(4)
C(11)-C(61)-C(81)	121.7(4)
C(131)-C(81)-C(91)	119.0(5)
C(131)-C(81)-C(61)	120.9(5)
C(91)-C(81)-C(61)	119.9(4)
C(101)-C(91)-C(81)	120.2(5)
C(101)-C(91)-C(141)	119.3(5)
C(81)-C(91)-C(141)	120.5(5)
C(91)-C(101)-C(111)	122.6(5)

C(91)-C(101)-H(101)	118.7
C(111)-C(101)-H(101)	118.7
C(121)-C(111)-C(101)	117.4(5)
C(121)-C(111)-C(171)	120.9(6)
C(101)-C(111)-C(171)	121.7(6)
C(111)-C(121)-C(131)	121.6(5)
C(111)-C(121)-H(121)	119.2
C(131)-C(121)-H(121)	119.2
C(81)-C(131)-C(121)	119.1(5)
C(81)-C(131)-C(201)	121.3(5)
C(121)-C(131)-C(201)	119.6(5)
C(161)-C(141)-C(151)	111.4(5)
C(161)-C(141)-C(91)	112.6(5)
C(151)-C(141)-C(91)	110.7(5)
C(161)-C(141)-H(141)	107.3
C(151)-C(141)-H(141)	107.3
C(91)-C(141)-H(141)	107.3
C(141)-C(151)-H(15A)	109.5
C(141)-C(151)-H(15B)	109.5
H(15A)-C(151)-H(15B)	109.5
C(141)-C(151)-H(15C)	109.5
H(15A)-C(151)-H(15C)	109.5
H(15B)-C(151)-H(15C)	109.5
C(141)-C(161)-H(16A)	109.5
C(141)-C(161)-H(16B)	109.5
H(16A)-C(161)-H(16B)	109.5
C(141)-C(161)-H(16C)	109.5
H(16A)-C(161)-H(16C)	109.5
H(16B)-C(161)-H(16C)	109.5
C(181)-C(171)-C(111)	113.9(6)
C(181)-C(171)-C(191)	110.0(8)
C(111)-C(171)-C(191)	109.0(7)
C(181)-C(171)-H(171)	107.9
C(111)-C(171)-H(171)	107.9
C(191)-C(171)-H(171)	107.9
C(171)-C(181)-H(18A)	109.5
C(171)-C(181)-H(18B)	109.5
H(18A)-C(181)-H(18B)	109.5
C(171)-C(181)-H(18C)	109.5
H(18A)-C(181)-H(18C)	109.5
H(18B)-C(181)-H(18C)	109.5
C(171)-C(191)-H(19A)	109.5
C(171)-C(191)-H(19B)	109.5
H(19A)-C(191)-H(19B)	109.5
C(171)-C(191)-H(19C)	109.5
H(19A)-C(191)-H(19C)	109.5
H(19B)-C(191)-H(19C)	109.5
C(131)-C(201)-C(221)	112.3(5)
C(131)-C(201)-C(211)	111.2(6)
C(221)-C(201)-C(211)	109.8(6)
C(131)-C(201)-H(201)	107.8
C(221)-C(201)-H(201)	107.8
C(211)-C(201)-H(201)	107.8
C(201)-C(211)-H(21A)	109.5
C(201)-C(211)-H(21B)	109.5
H(21A)-C(211)-H(21B)	109.5

C(201)-C(211)-H(21C)	109.5
H(21A)-C(211)-H(21C)	109.5
H(21B)-C(211)-H(21C)	109.5
C(201)-C(221)-H(22A)	109.5
C(201)-C(221)-H(22B)	109.5
H(22A)-C(221)-H(22B)	109.5
C(201)-C(221)-H(22C)	109.5
H(22A)-C(221)-H(22C)	109.5
H(22B)-C(221)-H(22C)	109.5
C(62)-C(12)-C(22)	119.5(4)
C(62)-C(12)-S(21)	120.3(3)
C(22)-C(12)-S(21)	120.1(4)
C(32)-C(22)-C(12)	116.3(5)
C(32)-C(22)-C(23)	121.4(4)
C(12)-C(22)-C(23)	122.3(4)
C(42)-C(32)-F(72)	116.2(4)
C(42)-C(32)-C(22)	125.4(5)
F(72)-C(32)-C(22)	118.3(5)
C(32)-C(42)-C(52)	117.9(5)
C(32)-C(42)-H(42)	121.1
C(52)-C(42)-H(42)	121.1
C(62)-C(52)-C(42)	120.3(5)
C(62)-C(52)-H(52)	119.9
C(42)-C(52)-H(52)	119.9
C(52)-C(62)-C(12)	120.6(4)
C(52)-C(62)-C(82)	118.6(5)
C(12)-C(62)-C(82)	120.8(4)
C(92)-C(82)-C(132)	119.2(5)
C(92)-C(82)-C(62)	119.9(5)
C(132)-C(82)-C(62)	120.8(5)
C(102)-C(92)-C(82)	120.1(5)
C(102)-C(92)-C(142)	118.9(5)
C(82)-C(92)-C(142)	121.0(5)
C(112)-C(102)-C(92)	121.5(5)
C(112)-C(102)-H(102)	119.2
C(92)-C(102)-H(102)	119.2
C(102)-C(112)-C(122)	117.8(5)
C(102)-C(112)-C(172)	121.8(6)
C(122)-C(112)-C(172)	120.4(6)
C(132)-C(122)-C(112)	122.7(5)
C(132)-C(122)-H(122)	118.7
C(112)-C(122)-H(122)	118.7
C(122)-C(132)-C(82)	118.6(5)
C(122)-C(132)-C(202)	120.7(5)
C(82)-C(132)-C(202)	120.7(5)
C(162)-C(142)-C(92)	112.0(5)
C(162)-C(142)-C(152)	111.4(5)
C(92)-C(142)-C(152)	110.9(5)
C(162)-C(142)-H(142)	107.4
C(92)-C(142)-H(142)	107.4
C(152)-C(142)-H(142)	107.4
C(142)-C(152)-H(15D)	109.5
C(142)-C(152)-H(15E)	109.5
H(15D)-C(152)-H(15E)	109.5
C(142)-C(152)-H(15F)	109.5
H(15D)-C(152)-H(15F)	109.5

H(15E)-C(152)-H(15F)	109.5
C(142)-C(162)-H(16D)	109.5
C(142)-C(162)-H(16E)	109.5
H(16D)-C(162)-H(16E)	109.5
C(142)-C(162)-H(16F)	109.5
H(16D)-C(162)-H(16F)	109.5
H(16E)-C(162)-H(16F)	109.5
C(182)-C(172)-C(192)	114.6(9)
C(182)-C(172)-C(112)	115.6(7)
C(192)-C(172)-C(112)	111.9(6)
C(182)-C(172)-H(172)	104.4
C(192)-C(172)-H(172)	104.4
C(112)-C(172)-H(172)	104.4
C(172)-C(182)-H(18D)	109.5
C(172)-C(182)-H(18E)	109.5
H(18D)-C(182)-H(18E)	109.5
C(172)-C(182)-H(18F)	109.5
H(18D)-C(182)-H(18F)	109.5
H(18E)-C(182)-H(18F)	109.5
C(172)-C(192)-H(19D)	109.5
C(172)-C(192)-H(19E)	109.5
H(19D)-C(192)-H(19E)	109.5
C(172)-C(192)-H(19F)	109.5
H(19D)-C(192)-H(19F)	109.5
H(19E)-C(192)-H(19F)	109.5
C(222)-C(202)-C(132)	110.2(5)
C(222)-C(202)-C(212)	110.2(5)
C(132)-C(202)-C(212)	112.4(5)
C(222)-C(202)-H(202)	108.0
C(132)-C(202)-H(202)	108.0
C(212)-C(202)-H(202)	108.0
C(202)-C(212)-H(21D)	109.5
C(202)-C(212)-H(21E)	109.5
H(21D)-C(212)-H(21E)	109.5
C(202)-C(212)-H(21F)	109.5
H(21D)-C(212)-H(21F)	109.5
H(21E)-C(212)-H(21F)	109.5
C(202)-C(222)-H(22D)	109.5
C(202)-C(222)-H(22E)	109.5
H(22D)-C(222)-H(22E)	109.5
C(202)-C(222)-H(22F)	109.5
H(22D)-C(222)-H(22F)	109.5
H(22E)-C(222)-H(22F)	109.5
C(63)-C(13)-C(23)	121.1(4)
C(63)-C(13)-Fe(1)	102.4(3)
C(23)-C(13)-Fe(1)	78.3(3)
C(63)-C(13)-H(13)	119.4
C(23)-C(13)-H(13)	119.4
Fe(1)-C(13)-H(13)	89.3
C(13)-C(23)-C(33)	115.8(5)
C(13)-C(23)-C(22)	121.0(4)
C(33)-C(23)-C(22)	119.6(5)
C(13)-C(23)-Fe(1)	63.0(3)
C(33)-C(23)-Fe(1)	111.7(4)
C(22)-C(23)-Fe(1)	110.7(3)
C(43)-C(33)-C(23)	122.1(5)

C(43)-C(33)-H(33)	119.0
C(23)-C(33)-H(33)	119.0
C(33)-C(43)-C(53)	120.7(5)
C(33)-C(43)-H(43)	119.6
C(53)-C(43)-H(43)	119.6
C(63)-C(53)-C(43)	119.7(5)
C(63)-C(53)-H(53)	120.1
C(43)-C(53)-H(53)	120.1
C(53)-C(63)-C(13)	120.3(5)
C(53)-C(63)-C(21)	122.1(5)
C(13)-C(63)-C(21)	117.6(4)
O(130)-K(1)-O(190)	90.5(3)
O(130)-K(1)-O(240)	92.9(2)
O(190)-K(1)-O(240)	168.2(3)
O(130)-K(1)-O(10)	121.59(16)
O(190)-K(1)-O(10)	93.7(2)
O(240)-K(1)-O(10)	94.2(2)
O(130)-K(1)-O(160)	61.53(16)
O(190)-K(1)-O(160)	108.1(3)
O(240)-K(1)-O(160)	83.39(19)
O(10)-K(1)-O(160)	61.92(15)
O(130)-K(1)-O(70)	117.36(18)
O(190)-K(1)-O(70)	78.9(3)
O(240)-K(1)-O(70)	89.5(2)
O(10)-K(1)-O(70)	120.61(17)
O(160)-K(1)-O(70)	172.65(16)
O(130)-K(1)-O(40)	175.62(18)
O(190)-K(1)-O(40)	92.4(3)
O(240)-K(1)-O(40)	83.7(2)
O(10)-K(1)-O(40)	61.55(16)
O(160)-K(1)-O(40)	120.52(16)
O(70)-K(1)-O(40)	60.05(17)
O(130)-K(1)-O(100)	58.46(16)
O(190)-K(1)-O(100)	83.6(2)
O(240)-K(1)-O(100)	88.4(2)
O(10)-K(1)-O(100)	177.32(16)
O(160)-K(1)-O(100)	118.78(16)
O(70)-K(1)-O(100)	59.05(17)
O(40)-K(1)-O(100)	118.58(17)
C(180)-O(10)-C(20)	115.1(6)
C(180)-O(10)-K(1)	113.1(4)
C(20)-O(10)-K(1)	116.9(4)
O(10)-C(20)-C(30)	107.2(7)
O(10)-C(20)-K(1)	42.8(3)
C(30)-C(20)-K(1)	72.1(4)
O(10)-C(20)-H(20A)	110.3
C(30)-C(20)-H(20A)	110.3
K(1)-C(20)-H(20A)	146.9
O(10)-C(20)-H(20B)	110.3
C(30)-C(20)-H(20B)	110.3
K(1)-C(20)-H(20B)	100.7
H(20A)-C(20)-H(20B)	108.5
O(40)-C(30)-C(20)	117.4(8)
O(40)-C(30)-K(1)	50.2(4)
C(20)-C(30)-K(1)	83.7(5)
O(40)-C(30)-H(30A)	107.9

C(20)-C(30)-H(30A)	107.9
K(1)-C(30)-H(30A)	157.8
O(40)-C(30)-H(30B)	107.9
C(20)-C(30)-H(30B)	107.9
K(1)-C(30)-H(30B)	86.0
H(30A)-C(30)-H(30B)	107.2
C(30)-O(40)-C(50)	116.9(6)
C(30)-O(40)-K(1)	108.6(5)
C(50)-O(40)-K(1)	113.4(4)
O(40)-C(50)-C(60)	109.6(6)
O(40)-C(50)-K(1)	45.7(3)
C(60)-C(50)-K(1)	77.6(4)
O(40)-C(50)-H(50A)	109.8
C(60)-C(50)-H(50A)	109.8
K(1)-C(50)-H(50A)	91.9
O(40)-C(50)-H(50B)	109.8
C(60)-C(50)-H(50B)	109.8
K(1)-C(50)-H(50B)	153.7
H(50A)-C(50)-H(50B)	108.2
O(70)-C(60)-C(50)	108.8(7)
O(70)-C(60)-K(1)	45.2(4)
C(50)-C(60)-K(1)	78.9(4)
O(70)-C(60)-H(60A)	109.9
C(50)-C(60)-H(60A)	109.9
K(1)-C(60)-H(60A)	90.1
O(70)-C(60)-H(60B)	109.9
C(50)-C(60)-H(60B)	109.9
K(1)-C(60)-H(60B)	154.2
H(60A)-C(60)-H(60B)	108.3
C(80)-O(70)-C(60)	115.1(7)
C(80)-O(70)-K(1)	116.5(5)
C(60)-O(70)-K(1)	114.0(5)
O(70)-C(80)-C(90)	109.6(7)
O(70)-C(80)-K(1)	43.5(3)
C(90)-C(80)-K(1)	78.5(5)
O(70)-C(80)-H(80A)	109.7
C(90)-C(80)-H(80A)	109.7
K(1)-C(80)-H(80A)	151.3
O(70)-C(80)-H(80B)	109.7
C(90)-C(80)-H(80B)	109.7
K(1)-C(80)-H(80B)	93.7
H(80A)-C(80)-H(80B)	108.2
O(100)-C(90)-C(80)	109.9(8)
O(100)-C(90)-K(1)	48.4(4)
C(80)-C(90)-K(1)	78.3(5)
O(100)-C(90)-H(90A)	109.7
C(80)-C(90)-H(90A)	109.7
K(1)-C(90)-H(90A)	157.2
O(100)-C(90)-H(90B)	109.7
C(80)-C(90)-H(90B)	109.7
K(1)-C(90)-H(90B)	87.9
H(90A)-C(90)-H(90B)	108.2
C(110)-O(100)-C(90)	116.5(7)
C(110)-O(100)-K(1)	109.2(5)
C(90)-O(100)-K(1)	110.8(5)
O(100)-C(110)-C(120)	109.2(8)

O(100)-C(110)-K(1)	49.6(4)
C(120)-C(110)-K(1)	77.9(5)
O(100)-C(110)-H(11A)	109.8
C(120)-C(110)-H(11A)	109.8
K(1)-C(110)-H(11A)	86.2
O(100)-C(110)-H(11B)	109.8
C(120)-C(110)-H(11B)	109.8
K(1)-C(110)-H(11B)	158.9
H(11A)-C(110)-H(11B)	108.3
O(130)-C(120)-C(110)	111.2(7)
O(130)-C(120)-K(1)	40.1(4)
C(110)-C(120)-K(1)	78.5(5)
O(130)-C(120)-H(12A)	109.4
C(110)-C(120)-H(12A)	109.4
K(1)-C(120)-H(12A)	100.6
O(130)-C(120)-H(12B)	109.4
C(110)-C(120)-H(12B)	109.4
K(1)-C(120)-H(12B)	145.0
H(12A)-C(120)-H(12B)	108.0
C(120)-O(130)-C(140)	113.3(6)
C(120)-O(130)-K(1)	121.4(5)
C(140)-O(130)-K(1)	115.3(4)
O(130)-C(140)-C(150)	107.3(6)
O(130)-C(140)-K(1)	43.6(3)
C(150)-C(140)-K(1)	77.2(4)
O(130)-C(140)-H(14A)	110.2
C(150)-C(140)-H(14A)	110.2
K(1)-C(140)-H(14A)	152.2
O(130)-C(140)-H(14B)	110.2
C(150)-C(140)-H(14B)	110.2
K(1)-C(140)-H(14B)	92.7
H(14A)-C(140)-H(14B)	108.5
O(160)-C(150)-C(140)	111.3(5)
O(160)-C(150)-K(1)	47.6(3)
C(140)-C(150)-K(1)	79.0(4)
O(160)-C(150)-H(15G)	109.4
C(140)-C(150)-H(15G)	109.4
K(1)-C(150)-H(15G)	156.0
O(160)-C(150)-H(15H)	109.4
C(140)-C(150)-H(15H)	109.4
K(1)-C(150)-H(15H)	89.3
H(15G)-C(150)-H(15H)	108.0
C(150)-O(160)-C(170)	113.2(5)
C(150)-O(160)-K(1)	110.5(4)
C(170)-O(160)-K(1)	112.8(4)
O(160)-C(170)-C(180)	107.5(5)
O(160)-C(170)-K(1)	45.5(3)
C(180)-C(170)-K(1)	76.5(4)
O(160)-C(170)-H(17A)	110.2
C(180)-C(170)-H(17A)	110.2
K(1)-C(170)-H(17A)	91.3
O(160)-C(170)-H(17B)	110.2
C(180)-C(170)-H(17B)	110.2
K(1)-C(170)-H(17B)	154.1
H(17A)-C(170)-H(17B)	108.5
O(10)-C(180)-C(170)	113.0(7)

O(10)-C(180)-K(1)	45.6(3)
C(170)-C(180)-K(1)	79.7(4)
O(10)-C(180)-H(18G)	109.0
C(170)-C(180)-H(18G)	109.0
K(1)-C(180)-H(18G)	92.9
O(10)-C(180)-H(18H)	109.0
C(170)-C(180)-H(18H)	109.0
K(1)-C(180)-H(18H)	152.6
H(18G)-C(180)-H(18H)	107.8
C(230)-O(190)-C(200)	107.2(12)
C(230)-O(190)-K(1)	124.8(8)
C(200)-O(190)-K(1)	125.3(11)
C(210)-C(200)-O(190)	104.5(16)
C(210)-C(200)-K(1)	140.1(13)
O(190)-C(200)-K(1)	36.0(7)
C(210)-C(200)-H(20C)	110.8
O(190)-C(200)-H(20C)	110.8
K(1)-C(200)-H(20C)	94.9
C(210)-C(200)-H(20D)	110.8
O(190)-C(200)-H(20D)	110.8
K(1)-C(200)-H(20D)	87.4
H(20C)-C(200)-H(20D)	108.9
C(220)-C(210)-C(200)	112.2(16)
C(220)-C(210)-H(21G)	109.2
C(200)-C(210)-H(21G)	109.2
C(220)-C(210)-H(21H)	109.2
C(200)-C(210)-H(21H)	109.2
H(21G)-C(210)-H(21H)	107.9
C(210)-C(220)-C(230)	105.7(19)
C(210)-C(220)-H(22G)	110.6
C(230)-C(220)-H(22G)	110.6
C(210)-C(220)-H(22H)	110.6
C(230)-C(220)-H(22H)	110.6
H(22G)-C(220)-H(22H)	108.7
O(190)-C(230)-C(220)	109.0(15)
O(190)-C(230)-K(1)	36.8(5)
C(220)-C(230)-K(1)	145.5(14)
O(190)-C(230)-H(23A)	109.9
C(220)-C(230)-H(23A)	109.9
K(1)-C(230)-H(23A)	92.3
O(190)-C(230)-H(23B)	109.9
C(220)-C(230)-H(23B)	109.9
K(1)-C(230)-H(23B)	86.4
H(23A)-C(230)-H(23B)	108.3
C(250)-O(240)-C(280)	108.1(8)
C(250)-O(240)-K(1)	122.7(8)
C(280)-O(240)-K(1)	121.8(7)
O(240)-C(250)-C(260)	102.5(10)
O(240)-C(250)-K(1)	38.3(5)
C(260)-C(250)-K(1)	118.7(7)
O(240)-C(250)-H(25A)	111.3
C(260)-C(250)-H(25A)	111.3
K(1)-C(250)-H(25A)	125.0
O(240)-C(250)-H(25B)	111.3
C(260)-C(250)-H(25B)	111.3
K(1)-C(250)-H(25B)	73.0

H(25A)-C(250)-H(25B)	109.2
C(270)-C(260)-C(250)	107.3(12)
C(270)-C(260)-H(26A)	110.3
C(250)-C(260)-H(26A)	110.3
C(270)-C(260)-H(26B)	110.3
C(250)-C(260)-H(26B)	110.3
H(26A)-C(260)-H(26B)	108.5
C(280)-C(270)-C(260)	105.8(11)
C(280)-C(270)-H(27A)	110.6
C(260)-C(270)-H(27A)	110.6
C(280)-C(270)-H(27B)	110.6
C(260)-C(270)-H(27B)	110.6
H(27A)-C(270)-H(27B)	108.7
O(240)-C(280)-C(270)	106.5(12)
O(240)-C(280)-K(1)	38.8(4)
C(270)-C(280)-K(1)	120.4(9)
O(240)-C(280)-H(28A)	110.4
C(270)-C(280)-H(28A)	110.4
K(1)-C(280)-H(28A)	71.6
O(240)-C(280)-H(28B)	110.4
C(270)-C(280)-H(28B)	110.4
K(1)-C(280)-H(28B)	125.5
H(28A)-C(280)-H(28B)	108.6
O(380)#1-K(2)-O(380)	180.0
O(380)#1-K(2)-O(350)	94.5(2)
O(380)-K(2)-O(350)	85.5(2)
O(380)#1-K(2)-O(350)#1	85.5(2)
O(380)-K(2)-O(350)#1	94.5(2)
O(350)-K(2)-O(350)#1	180.0
O(380)#1-K(2)-O(320)	76.85(18)
O(380)-K(2)-O(320)	103.15(18)
O(350)-K(2)-O(320)	60.0(2)
O(350)#1-K(2)-O(320)	120.0(2)
O(380)#1-K(2)-O(320)#1	103.15(18)
O(380)-K(2)-O(320)#1	76.85(19)
O(350)-K(2)-O(320)#1	120.0(2)
O(350)#1-K(2)-O(320)#1	60.0(2)
O(320)-K(2)-O(320)#1	180.0(3)
O(380)#1-K(2)-O(290)#1	95.1(2)
O(380)-K(2)-O(290)#1	84.9(2)
O(350)-K(2)-O(290)#1	61.1(2)
O(350)#1-K(2)-O(290)#1	118.9(2)
O(320)-K(2)-O(290)#1	119.5(2)
O(320)#1-K(2)-O(290)#1	60.5(2)
O(380)#1-K(2)-O(290)	84.9(2)
O(380)-K(2)-O(290)	95.1(2)
O(350)-K(2)-O(290)	118.9(2)
O(350)#1-K(2)-O(290)	61.1(2)
O(320)-K(2)-O(290)	60.5(2)
O(320)#1-K(2)-O(290)	119.5(2)
O(290)#1-K(2)-O(290)	180.0
C(370)-O(290)-C(300)	113.7(9)
C(370)-O(290)-K(2)	110.7(6)
C(300)-O(290)-K(2)	112.6(6)
O(290)-C(300)-C(310)	110.3(8)
O(290)-C(300)-K(2)	46.2(4)

C(310)-C(300)-K(2)	76.7(5)
O(290)-C(300)-H(30C)	109.6
C(310)-C(300)-H(30C)	109.6
K(2)-C(300)-H(30C)	93.1
O(290)-C(300)-H(30D)	109.6
C(310)-C(300)-H(30D)	109.6
K(2)-C(300)-H(30D)	153.4
H(30C)-C(300)-H(30D)	108.1
O(320)-C(310)-C(300)	111.8(9)
O(320)-C(310)-K(2)	44.7(4)
C(300)-C(310)-K(2)	79.8(5)
O(320)-C(310)-H(31A)	109.3
C(300)-C(310)-H(31A)	109.3
K(2)-C(310)-H(31A)	92.6
O(320)-C(310)-H(31B)	109.3
C(300)-C(310)-H(31B)	109.3
K(2)-C(310)-H(31B)	152.3
H(31A)-C(310)-H(31B)	107.9
C(310)-O(320)-C(330)	113.0(8)
C(310)-O(320)-K(2)	115.0(6)
C(330)-O(320)-K(2)	114.4(5)
O(320)-C(330)-C(340)	108.7(7)
O(320)-C(330)-K(2)	44.6(4)
C(340)-C(330)-K(2)	76.2(5)
O(320)-C(330)-H(33A)	109.9
C(340)-C(330)-H(33A)	109.9
K(2)-C(330)-H(33A)	151.9
O(320)-C(330)-H(33B)	109.9
C(340)-C(330)-H(33B)	109.9
K(2)-C(330)-H(33B)	94.2
H(33A)-C(330)-H(33B)	108.3
O(350)-C(340)-C(330)	108.6(9)
O(350)-C(340)-K(2)	43.7(4)
C(330)-C(340)-K(2)	79.2(5)
O(350)-C(340)-H(34A)	110.0
C(330)-C(340)-H(34A)	110.0
K(2)-C(340)-H(34A)	152.6
O(350)-C(340)-H(34B)	110.0
C(330)-C(340)-H(34B)	110.0
K(2)-C(340)-H(34B)	91.4
H(34A)-C(340)-H(34B)	108.3
C(340)-O(350)-C(360)	109.8(9)
C(340)-O(350)-K(2)	117.0(6)
C(360)-O(350)-K(2)	115.1(6)
O(350)-C(360)-C(370)#1	107.7(9)
O(350)-C(360)-K(2)	43.9(4)
C(370)#1-C(360)-K(2)	75.4(6)
O(350)-C(360)-H(36A)	110.2
C(370)#1-C(360)-H(36A)	110.2
K(2)-C(360)-H(36A)	95.1
O(350)-C(360)-H(36B)	110.2
C(370)#1-C(360)-H(36B)	110.2
K(2)-C(360)-H(36B)	151.1
H(36A)-C(360)-H(36B)	108.5
O(290)-C(370)-C(360)#1	111.7(10)
O(290)-C(370)-K(2)	48.3(4)

C(360)#1-C(370)-K(2)	80.4(6)
O(290)-C(370)-H(37A)	109.3
C(360)#1-C(370)-H(37A)	109.3
K(2)-C(370)-H(37A)	157.1
O(290)-C(370)-H(37B)	109.3
C(360)#1-C(370)-H(37B)	109.3
K(2)-C(370)-H(37B)	87.1
H(37A)-C(370)-H(37B)	107.9
C(400)-C(390)-O(380)	113.0(12)
C(400)-C(390)-K(2)	116.9(9)
O(380)-C(390)-K(2)	32.9(4)
C(400)-C(390)-H(39A)	109.0
O(380)-C(390)-H(39A)	109.0
K(2)-C(390)-H(39A)	129.1
C(400)-C(390)-H(39B)	109.0
O(380)-C(390)-H(39B)	109.0
K(2)-C(390)-H(39B)	77.4
H(39A)-C(390)-H(39B)	107.8
C(390)-C(400)-C(410)	103.4(13)
C(390)-C(400)-H(40A)	111.1
C(410)-C(400)-H(40A)	111.1
C(390)-C(400)-H(40B)	111.1
C(410)-C(400)-H(40B)	111.1
H(40A)-C(400)-H(40B)	109.1
C(400)-C(410)-C(420)	109.4(13)
C(400)-C(410)-K(2)	95.1(9)
C(420)-C(410)-K(2)	50.2(6)
C(400)-C(410)-H(41A)	109.8
C(420)-C(410)-H(41A)	109.8
K(2)-C(410)-H(41A)	70.4
C(400)-C(410)-H(41B)	109.8
C(420)-C(410)-H(41B)	109.8
K(2)-C(410)-H(41B)	153.2
H(41A)-C(410)-H(41B)	108.2
O(380)-C(420)-C(410)	98.3(9)
O(380)-C(420)-K(2)	47.8(5)
C(410)-C(420)-K(2)	110.4(7)
O(380)-C(420)-H(42A)	112.1
C(410)-C(420)-H(42A)	112.1
K(2)-C(420)-H(42A)	135.3
O(380)-C(420)-H(42B)	112.1
C(410)-C(420)-H(42B)	112.1
K(2)-C(420)-H(42B)	64.8
H(42A)-C(420)-H(42B)	109.7
C(390)-O(380)-C(420)	103.4(8)
C(390)-O(380)-K(2)	131.1(6)
C(420)-O(380)-K(2)	109.4(6)
O(520)#2-K(3)-O(520)	180.0
O(520)#2-K(3)-O(460)	85.27(16)
O(520)-K(3)-O(460)	94.74(16)
O(520)#2-K(3)-O(460)#2	94.73(16)
O(520)-K(3)-O(460)#2	85.26(16)
O(460)-K(3)-O(460)#2	180.0
O(520)#2-K(3)-O(430)#2	85.53(18)
O(520)-K(3)-O(430)#2	94.47(18)
O(460)-K(3)-O(430)#2	118.93(10)

O(460)#2-K(3)-O(430)#2	61.07(10)
O(520)#2-K(3)-O(430)	94.47(18)
O(520)-K(3)-O(430)	85.53(18)
O(460)-K(3)-O(430)	61.07(10)
O(460)#2-K(3)-O(430)	118.94(10)
O(430)#2-K(3)-O(430)	180.00(8)
O(520)#2-K(3)-O(490)#2	87.54(17)
O(520)-K(3)-O(490)#2	92.46(17)
O(460)-K(3)-O(490)#2	119.38(10)
O(460)#2-K(3)-O(490)#2	60.62(10)
O(430)#2-K(3)-O(490)#2	120.32(10)
O(430)-K(3)-O(490)#2	59.68(10)
O(520)#2-K(3)-O(490)	92.47(17)
O(520)-K(3)-O(490)	87.54(17)
O(460)-K(3)-O(490)	60.62(10)
O(460)#2-K(3)-O(490)	119.37(10)
O(430)#2-K(3)-O(490)	59.67(10)
O(430)-K(3)-O(490)	120.33(10)
O(490)#2-K(3)-O(490)	180.00(16)
C(510)#2-O(430)-C(440)	112.0(4)
C(510)#2-O(430)-K(3)	114.9(3)
C(440)-O(430)-K(3)	111.0(3)
O(430)-C(440)-C(450)	107.9(5)
O(430)-C(440)-K(3)	47.0(2)
C(450)-C(440)-K(3)	78.0(3)
O(430)-C(440)-H(44A)	110.1
C(450)-C(440)-H(44A)	110.1
K(3)-C(440)-H(44A)	156.4
O(430)-C(440)-H(44B)	110.1
C(450)-C(440)-H(44B)	110.1
K(3)-C(440)-H(44B)	88.2
H(44A)-C(440)-H(44B)	108.4
O(460)-C(450)-C(440)	108.6(4)
O(460)-C(450)-K(3)	43.5(2)
C(440)-C(450)-K(3)	78.2(3)
O(460)-C(450)-H(45A)	110.0
C(440)-C(450)-H(45A)	110.0
K(3)-C(450)-H(45A)	151.7
O(460)-C(450)-H(45B)	110.0
C(440)-C(450)-H(45B)	110.0
K(3)-C(450)-H(45B)	93.1
H(45A)-C(450)-H(45B)	108.3
O(460)-C(470)-C(480)	108.0(4)
O(460)-C(470)-K(3)	43.1(2)
C(480)-C(470)-K(3)	78.7(3)
O(460)-C(470)-H(47A)	110.1
C(480)-C(470)-H(47A)	110.1
K(3)-C(470)-H(47A)	92.2
O(460)-C(470)-H(47B)	110.1
C(480)-C(470)-H(47B)	110.1
K(3)-C(470)-H(47B)	152.0
H(47A)-C(470)-H(47B)	108.4
O(490)-C(480)-C(470)	109.3(4)
O(490)-C(480)-K(3)	45.9(2)
C(470)-C(480)-K(3)	77.8(3)
O(490)-C(480)-H(48A)	109.8

C(470)-C(480)-H(48A)	109.8
K(3)-C(480)-H(48A)	91.0
O(490)-C(480)-H(48B)	109.8
C(470)-C(480)-H(48B)	109.8
K(3)-C(480)-H(48B)	154.3
H(48A)-C(480)-H(48B)	108.3
C(500)-O(490)-C(480)	112.5(4)
C(500)-O(490)-K(3)	114.8(3)
C(480)-O(490)-K(3)	112.9(3)
O(490)-C(500)-C(510)	107.6(5)
O(490)-C(500)-K(3)	44.6(2)
C(510)-C(500)-K(3)	78.1(3)
O(490)-C(500)-H(50C)	110.2
C(510)-C(500)-H(50C)	110.2
K(3)-C(500)-H(50C)	153.7
O(490)-C(500)-H(50D)	110.2
C(510)-C(500)-H(50D)	110.2
K(3)-C(500)-H(50D)	90.7
H(50C)-C(500)-H(50D)	108.5
O(430)#2-C(510)-C(500)	108.0(5)
O(430)#2-C(510)-K(3)	44.3(2)
C(500)-C(510)-K(3)	78.1(3)
O(430)#2-C(510)-H(51A)	110.1
C(500)-C(510)-H(51A)	110.1
K(3)-C(510)-H(51A)	153.2
O(430)#2-C(510)-H(51B)	110.1
C(500)-C(510)-H(51B)	110.1
K(3)-C(510)-H(51B)	91.4
H(51A)-C(510)-H(51B)	108.4
C(560)-O(520)-C(530)	107.8(9)
C(560)-O(520)-K(3)	121.7(7)
C(530)-O(520)-K(3)	123.8(7)
O(520)-C(530)-C(540)	103.5(10)
O(520)-C(530)-K(3)	37.8(5)
C(540)-C(530)-K(3)	127.4(9)
O(520)-C(530)-H(53A)	111.1
C(540)-C(530)-H(53A)	111.1
K(3)-C(530)-H(53A)	116.0
O(520)-C(530)-H(53B)	111.1
C(540)-C(530)-H(53B)	111.1
K(3)-C(530)-H(53B)	74.6
H(53A)-C(530)-H(53B)	109.0
C(550)-C(540)-C(530)	106.3(14)
C(550)-C(540)-H(54A)	110.5
C(530)-C(540)-H(54A)	110.5
C(550)-C(540)-H(54B)	110.5
C(530)-C(540)-H(54B)	110.5
H(54A)-C(540)-H(54B)	108.7
C(560)-C(550)-C(540)	108.4(15)
C(560)-C(550)-H(55A)	110.0
C(540)-C(550)-H(55A)	110.0
C(560)-C(550)-H(55B)	110.0
C(540)-C(550)-H(55B)	110.0
H(55A)-C(550)-H(55B)	108.4
O(520)-C(560)-C(550)	111.2(13)
O(520)-C(560)-K(3)	40.0(5)

C(550)-C(560)-K(3)	136.9(13)
O(520)-C(560)-H(56A)	109.4
C(550)-C(560)-H(56A)	109.4
K(3)-C(560)-H(56A)	71.3
O(520)-C(560)-H(56B)	109.4
C(550)-C(560)-H(56B)	109.4
K(3)-C(560)-H(56B)	111.0
H(56A)-C(560)-H(56B)	108.0
C(450)-O(460)-C(470)	112.4(4)
C(450)-O(460)-K(3)	115.8(3)
C(470)-O(460)-K(3)	115.8(3)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+2,-z+1 #2 -x+2,-y+1,-z+1

Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $[LFeN_2][K(18\text{-crown-6})(THF)_2]_2$ (3). The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Fe(1)	58(1)	81(1)	62(1)	-13(1)	-1(1)	-21(1)
N(1)	85(3)	66(3)	85(3)	-14(2)	24(3)	-32(2)
N(2)	169(6)	89(4)	127(5)	-15(4)	66(5)	-50(4)
S(11)	60(1)	87(1)	76(1)	-25(1)	-7(1)	-11(1)
S(21)	56(1)	77(1)	71(1)	-14(1)	-13(1)	-27(1)
C(11)	61(3)	60(3)	65(3)	-6(2)	-1(2)	-24(2)
C(21)	71(3)	65(3)	56(3)	-7(2)	-3(2)	-25(3)
C(31)	67(3)	77(3)	75(4)	-12(3)	-16(3)	-20(3)
C(41)	58(3)	74(3)	88(4)	-11(3)	-8(3)	-17(3)
C(51)	62(3)	71(3)	72(3)	-17(3)	5(3)	-24(3)
C(61)	57(3)	61(3)	61(3)	-12(2)	4(2)	-24(2)
F(71)	83(2)	99(2)	96(2)	-21(2)	-28(2)	-20(2)
C(81)	56(3)	66(3)	69(3)	-21(3)	12(2)	-22(2)
C(91)	67(3)	74(3)	66(3)	-21(3)	6(3)	-28(3)
C(101)	83(4)	90(4)	66(3)	-10(3)	-6(3)	-45(3)
C(111)	81(4)	96(4)	69(4)	-17(3)	-3(3)	-39(3)
C(121)	73(4)	80(4)	97(4)	-28(3)	2(3)	-36(3)
C(131)	67(3)	66(3)	80(4)	-18(3)	6(3)	-23(3)
C(141)	84(4)	88(4)	65(3)	-9(3)	-4(3)	-51(3)
C(151)	78(4)	111(5)	88(4)	-6(4)	-3(3)	-47(4)
C(161)	91(4)	82(4)	104(5)	-9(3)	-8(4)	-42(3)
C(171)	126(6)	147(7)	91(5)	-27(5)	-8(4)	-88(6)
C(181)	144(8)	166(9)	144(8)	-14(7)	-77(6)	-43(7)
C(191)	207(12)	283(15)	140(9)	-121(10)	-21(8)	-76(11)
C(201)	84(4)	78(4)	94(4)	-4(3)	-7(3)	-39(3)
C(211)	132(7)	83(5)	180(9)	0(5)	-2(6)	-32(5)
C(221)	101(5)	122(6)	113(5)	5(4)	5(4)	-55(4)
C(12)	46(2)	75(3)	53(3)	-19(2)	-1(2)	-24(2)
C(22)	50(3)	70(3)	56(3)	-15(2)	-5(2)	-13(2)

C(32)	51(3)	82(4)	67(3)	-18(3)	-17(2)	-14(2)
C(42)	61(3)	91(4)	84(4)	-33(3)	-8(3)	-28(3)
C(52)	62(3)	75(3)	74(3)	-23(3)	3(3)	-26(3)
C(62)	53(3)	69(3)	62(3)	-12(2)	-7(2)	-21(2)
F(72)	67(2)	103(2)	96(2)	-21(2)	-36(2)	-18(2)
C(82)	57(3)	69(3)	67(3)	-11(3)	-5(2)	-22(2)
C(92)	68(3)	76(3)	70(3)	-6(3)	-7(3)	-22(3)
C(102)	79(4)	82(4)	65(3)	-4(3)	-9(3)	-22(3)
C(112)	78(4)	81(4)	78(4)	-3(3)	-18(3)	-29(3)
C(122)	59(3)	78(4)	92(4)	-12(3)	-12(3)	-11(3)
C(132)	58(3)	70(3)	73(3)	-8(3)	-4(3)	-15(3)
C(142)	70(3)	96(4)	62(3)	-9(3)	4(3)	-15(3)
C(152)	101(5)	93(4)	96(5)	-26(4)	18(4)	-28(4)
C(162)	82(4)	128(5)	91(4)	-27(4)	7(3)	-41(4)
C(172)	91(5)	88(4)	92(4)	6(4)	-34(4)	-12(3)
C(182)	142(9)	202(11)	243(13)	86(10)	-113(9)	-88(8)
C(192)	215(11)	95(6)	203(11)	29(6)	-123(9)	-16(6)
C(202)	59(3)	84(4)	75(4)	-12(3)	-5(3)	-7(3)
C(212)	77(4)	108(5)	104(5)	-19(4)	11(3)	-34(4)
C(222)	81(4)	124(5)	88(4)	-35(4)	-2(3)	-28(4)
C(13)	58(3)	80(3)	47(3)	-8(2)	-11(2)	-23(2)
C(23)	62(3)	73(3)	57(3)	-12(3)	-7(2)	-13(2)
C(33)	84(4)	92(4)	58(3)	-19(3)	-7(3)	-12(3)
C(43)	113(5)	82(4)	60(3)	-2(3)	-22(3)	-20(4)
C(53)	106(5)	73(4)	74(4)	-5(3)	-24(3)	-17(3)
C(63)	76(3)	66(3)	60(3)	-5(3)	-10(3)	-20(3)
K(1)	54(1)	89(1)	101(1)	-26(1)	0(1)	-27(1)
O(10)	105(4)	99(3)	111(4)	-19(3)	-8(3)	-30(3)
C(20)	94(5)	104(5)	163(8)	-38(5)	-8(5)	-10(5)
C(30)	131(7)	99(5)	134(7)	-13(5)	4(5)	-24(5)
O(40)	87(3)	118(4)	124(4)	-34(3)	6(3)	-26(3)
C(50)	63(4)	112(5)	115(5)	-1(4)	13(3)	-36(4)
C(60)	83(5)	168(8)	112(6)	-23(6)	4(4)	-42(5)
O(70)	89(3)	139(4)	134(4)	-17(4)	-9(3)	-45(3)
C(80)	138(7)	131(7)	128(6)	-42(5)	3(5)	-83(6)
C(90)	126(7)	143(7)	165(9)	-46(7)	-4(7)	-58(7)
O(100)	114(4)	109(4)	138(4)	-12(3)	-1(3)	-55(3)
C(110)	90(6)	121(6)	217(11)	-59(7)	-1(6)	-25(5)
C(120)	124(7)	120(7)	169(9)	-43(6)	33(6)	-35(6)
O(130)	86(3)	106(4)	155(5)	-41(3)	20(3)	-23(3)
C(140)	62(4)	129(6)	101(5)	-14(4)	3(3)	-29(4)
C(150)	76(4)	136(6)	108(5)	-15(5)	-29(4)	-34(4)
O(160)	86(3)	118(3)	102(3)	-16(3)	-17(2)	-46(3)
C(170)	101(5)	117(5)	107(5)	-24(4)	-22(4)	-54(4)
C(180)	119(6)	115(6)	123(6)	-17(5)	-37(5)	-43(5)
O(190)	304(12)	204(8)	127(6)	-10(5)	-83(6)	-81(8)
C(200)	346(13)	240(14)	179(9)	-78(9)	-100(9)	-75(9)
C(210)	378(17)	230(14)	178(9)	-22(10)	-107(10)	-82(13)
C(220)	394(18)	350(20)	157(9)	47(11)	-89(10)	-92(15)
C(230)	340(14)	166(10)	127(8)	-39(7)	-69(8)	-77(9)
O(240)	163(6)	300(9)	104(4)	-49(5)	-21(4)	-93(6)
C(250)	166(8)	335(13)	115(7)	-70(8)	-4(6)	-82(8)
C(260)	180(9)	264(12)	130(8)	-28(8)	-10(7)	-99(8)
C(270)	162(8)	258(12)	105(7)	-6(7)	-5(6)	-88(7)
C(280)	216(10)	252(10)	98(7)	-12(6)	-23(6)	-87(7)
K(2)	83(1)	75(1)	78(1)	-3(1)	-5(1)	-25(1)

O(290)	108(4)	121(4)	162(5)	-45(4)	17(4)	-41(3)
C(300)	113(7)	130(7)	167(9)	9(7)	-42(7)	-31(6)
C(310)	121(7)	125(7)	185(10)	-42(7)	-47(7)	-12(6)
O(320)	156(5)	97(4)	142(5)	-12(4)	-49(4)	-30(4)
C(330)	208(11)	90(5)	111(6)	19(5)	-24(6)	-75(7)
C(340)	209(11)	108(6)	99(6)	12(5)	-21(7)	-77(7)
O(350)	199(7)	112(4)	96(4)	-4(3)	5(4)	-73(4)
C(360)	126(8)	158(9)	169(10)	-53(8)	54(7)	-48(7)
C(370)	153(9)	141(8)	204(12)	-39(8)	75(9)	-73(7)
C(390)	206(9)	125(7)	152(7)	-20(6)	-38(6)	-57(6)
C(400)	264(12)	138(9)	165(8)	-25(6)	-14(7)	-62(8)
C(410)	204(9)	138(8)	224(9)	-26(7)	-20(7)	-75(7)
C(420)	272(11)	106(6)	181(8)	-5(6)	-92(7)	-53(6)
O(380)	260(8)	107(4)	133(5)	-15(4)	-38(5)	-52(4)
K(3)	55(1)	106(1)	73(1)	-32(1)	3(1)	-37(1)
O(430)	53(2)	116(3)	71(2)	-30(2)	-2(2)	-35(2)
C(440)	70(4)	124(5)	76(4)	-35(3)	1(3)	-43(3)
C(450)	58(3)	115(4)	73(3)	-36(3)	4(3)	-31(3)
C(470)	55(3)	92(4)	80(4)	-24(3)	4(3)	-25(3)
C(480)	51(3)	93(4)	78(4)	-14(3)	2(2)	-31(3)
O(490)	54(2)	104(3)	70(2)	-23(2)	-1(2)	-36(2)
C(500)	55(3)	123(5)	90(4)	-39(4)	2(3)	-44(3)
C(510)	58(3)	138(5)	80(4)	-37(4)	0(3)	-40(3)
O(520)	137(5)	115(4)	171(6)	-28(4)	-3(4)	-31(4)
C(530)	164(8)	146(8)	244(13)	-35(8)	-36(8)	-56(6)
C(540)	209(10)	184(9)	243(14)	-82(10)	-11(10)	-58(8)
C(550)	199(10)	228(12)	540(30)	-162(18)	-118(13)	3(10)
C(560)	180(8)	147(8)	256(14)	-11(8)	-69(8)	-61(6)
O(460)	48(2)	102(3)	72(2)	-34(2)	3(2)	-26(2)

Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for [$LFeN_2$][K(18-crown-6)$(THF)_2$]$_2$ (3).

	x	y	z	U(eq)
H(41)	1922	8908	7559	90
H(51)	3046	8857	8263	81
H(101)	5638	7223	9802	92
H(121)	6437	8844	8906	95
H(141)	4140	7102	8725	89
H(15A)	3666	7291	9851	136
H(15B)	3060	6955	9522	136
H(15C)	3000	7746	9300	136
H(16A)	5637	6211	9078	136
H(16B)	4635	6030	9368	136
H(16C)	5323	6297	9711	136
H(171)	7200	8319	9795	132
H(18A)	6984	7021	10337	228
H(18B)	7776	7348	10530	228

H(18C)	7920	7140	9929	228
H(19A)	5544	8797	10196	294
H(19B)	6405	8394	10675	294
H(19C)	5586	8043	10551	294
H(201)	5066	8995	7641	101
H(21A)	4175	9851	8153	205
H(21B)	4840	10158	7650	205
H(21C)	5253	9936	8287	205
H(22A)	6933	9153	7968	169
H(22B)	6490	9387	7336	169
H(22C)	6895	8586	7638	169
H(42)	4328	4148	6695	90
H(52)	5639	3447	7349	82
H(102)	7289	3106	9226	93
H(122)	9373	2752	7990	95
H(142)	5287	4339	8310	96
H(15D)	6183	4112	9397	146
H(15E)	5061	4640	9211	146
H(15F)	6073	4776	8893	146
H(16D)	4983	3288	8591	147
H(16E)	4391	3770	9011	147
H(16F)	5447	3167	9206	147
H(172)	8876	2348	9480	116
H(18D)	10371	2623	8754	307
H(18E)	10667	2040	9325	307
H(18F)	10017	2813	9354	307
H(19D)	8703	1494	9164	274
H(19E)	9895	1280	9336	274
H(19F)	9565	1544	8683	274
H(202)	7800	3979	6872	93
H(21D)	9456	3931	7195	144
H(21E)	9500	3767	6581	144
H(21F)	9896	3152	7124	144
H(22D)	8715	2529	7001	145
H(22E)	8365	3069	6411	145
H(22F)	7513	2931	6875	145
H(13)	4680	6370	7431	74
H(33)	5235	6121	5798	97
H(43)	4478	7274	5469	106
H(53)	3869	8019	6106	105
H(20A)	12229	3828	7944	148
H(20B)	12275	3960	8566	148
H(30A)	13464	4368	7931	152
H(30B)	12521	4880	7539	152
H(50A)	13192	5762	7600	120
H(50B)	14056	5266	8056	120
H(60A)	13158	5889	8738	146
H(60B)	13624	6347	8226	146
H(80A)	12391	7386	8258	145
H(80B)	11874	7031	8812	145
H(90A)	10712	8050	8279	167
H(90B)	10816	7665	7771	167
H(11A)	9025	7714	7860	169
H(11B)	8894	8127	8352	169
H(12A)	8486	7226	8995	166
H(12B)	7676	7554	8483	166

H(14A)	7231	6590	8714	120
H(14B)	8148	6110	9146	120
H(15G)	7564	5493	8610	128
H(15H)	7979	5910	8051	128
H(17A)	9120	4867	7869	123
H(17B)	8785	4412	8437	123
H(18G)	10474	4107	8791	140
H(18H)	10456	3836	8230	140
H(20C)	9047	6646	6846	297
H(20D)	9090	7305	7062	297
H(21G)	9579	7038	6025	316
H(21H)	9515	7726	6222	316
H(22G)	11112	7480	6162	381
H(22H)	11180	6775	5987	381
H(23A)	11847	6230	6810	248
H(23B)	11602	6936	7016	248
H(25A)	10173	5748	10110	241
H(25B)	10289	6385	9617	241
H(26A)	11870	6263	9910	223
H(26B)	11585	5803	10491	223
H(27A)	13002	5362	9710	210
H(27B)	12750	4908	10304	210
H(28A)	12335	4756	9340	226
H(28B)	11731	4539	9913	226
H(30C)	7804	9486	5474	172
H(30D)	8427	8828	5225	172
H(31A)	7102	8337	5545	175
H(31B)	7648	8456	6056	175
H(33A)	6176	8464	6635	163
H(33B)	5635	8321	6132	163
H(34A)	4354	8908	6741	164
H(34B)	4810	9545	6578	164
H(36A)	3162	10217	6272	180
H(36B)	2764	9555	6399	180
H(37A)	8249	9648	4333	196
H(37B)	7504	10259	4600	196
H(39A)	3401	9100	3980	191
H(39B)	3800	9757	3778	191
H(40A)	4949	9245	3301	228
H(40B)	4468	8615	3454	228
H(41A)	6099	8762	3909	222
H(41B)	5834	8073	3902	222
H(42A)	4875	8113	4713	225
H(42B)	5719	8456	4838	225
H(44A)	10455	5339	6717	102
H(44B)	10469	4649	6536	102
H(45A)	8755	5358	6702	94
H(45B)	8909	5935	6168	94
H(47A)	7465	5786	5695	89
H(47B)	7379	5232	6264	89
H(48A)	7830	4369	5730	88
H(48B)	6754	4952	5529	88
H(50C)	6970	4708	4613	100
H(50D)	8058	4125	4793	100
H(51A)	7960	4626	3789	105
H(51B)	7889	5348	3930	105

H(53A)	10160	6993	4390	219
H(53B)	10092	6636	5050	219
H(54A)	8622	7389	5155	247
H(54B)	8861	7839	4556	247
H(55A)	7417	7285	4777	381
H(55B)	7754	7645	4165	381
H(56A)	7927	6382	4551	233
H(56B)	8331	6735	3958	233

Torsion angles [°] for $[LFeN_2][K(18\text{-crown-}6)(THF)_2]_2$ (3).

Fe(1)-S(11)-C(11)-C(61)	172.6(3)
Fe(1)-S(11)-C(11)-C(21)	-10.5(5)
C(61)-C(11)-C(21)-C(31)	1.5(7)
S(11)-C(11)-C(21)-C(31)	-175.3(4)
C(61)-C(11)-C(21)-C(63)	-178.2(4)
S(11)-C(11)-C(21)-C(63)	4.9(7)
C(11)-C(21)-C(31)-F(71)	-178.7(5)
C(63)-C(21)-C(31)-F(71)	1.0(8)
C(11)-C(21)-C(31)-C(41)	0.0(8)
C(63)-C(21)-C(31)-C(41)	179.7(5)
C(21)-C(31)-C(41)-C(51)	-0.6(9)
F(71)-C(31)-C(41)-C(51)	178.2(5)
C(31)-C(41)-C(51)-C(61)	-0.4(8)
C(41)-C(51)-C(61)-C(11)	1.8(7)
C(41)-C(51)-C(61)-C(81)	-177.9(5)
C(21)-C(11)-C(61)-C(51)	-2.4(7)
S(11)-C(11)-C(61)-C(51)	174.6(4)
C(21)-C(11)-C(61)-C(81)	177.3(4)
S(11)-C(11)-C(61)-C(81)	-5.7(6)
C(51)-C(61)-C(81)-C(131)	-81.6(6)
C(11)-C(61)-C(81)-C(131)	98.7(6)
C(51)-C(61)-C(81)-C(91)	94.8(6)
C(11)-C(61)-C(81)-C(91)	-84.9(6)
C(131)-C(81)-C(91)-C(101)	-1.2(8)
C(61)-C(81)-C(91)-C(101)	-177.6(5)
C(131)-C(81)-C(91)-C(141)	176.8(5)
C(61)-C(81)-C(91)-C(141)	0.4(7)
C(81)-C(91)-C(101)-C(111)	2.2(9)
C(141)-C(91)-C(101)-C(111)	-175.8(5)
C(91)-C(101)-C(111)-C(121)	-2.7(9)
C(91)-C(101)-C(111)-C(171)	178.8(6)
C(101)-C(111)-C(121)-C(131)	2.3(9)
C(171)-C(111)-C(121)-C(131)	-179.3(6)
C(91)-C(81)-C(131)-C(121)	0.8(7)
C(61)-C(81)-C(131)-C(121)	177.2(5)
C(91)-C(81)-C(131)-C(201)	178.6(5)
C(61)-C(81)-C(131)-C(201)	-5.0(7)
C(111)-C(121)-C(131)-C(81)	-1.4(8)
C(111)-C(121)-C(131)-C(201)	-179.3(5)
C(101)-C(91)-C(141)-C(161)	-50.8(7)

C(81)-C(91)-C(141)-C(161)	131.2(5)
C(101)-C(91)-C(141)-C(151)	74.5(7)
C(81)-C(91)-C(141)-C(151)	-103.5(6)
C(121)-C(111)-C(171)-C(181)	-133.4(8)
C(101)-C(111)-C(171)-C(181)	45.0(10)
C(121)-C(111)-C(171)-C(191)	103.3(9)
C(101)-C(111)-C(171)-C(191)	-78.3(10)
C(81)-C(131)-C(201)-C(221)	-122.7(6)
C(121)-C(131)-C(201)-C(221)	55.2(8)
C(81)-C(131)-C(201)-C(211)	113.8(6)
C(121)-C(131)-C(201)-C(211)	-68.3(7)
Fe(1)-S(21)-C(12)-C(62)	-176.8(4)
Fe(1)-S(21)-C(12)-C(22)	3.7(4)
C(62)-C(12)-C(22)-C(32)	-2.3(7)
S(21)-C(12)-C(22)-C(32)	177.1(4)
C(62)-C(12)-C(22)-C(23)	178.0(4)
S(21)-C(12)-C(22)-C(23)	-2.6(6)
C(12)-C(22)-C(32)-C(42)	2.4(8)
C(23)-C(22)-C(32)-C(42)	-177.9(5)
C(12)-C(22)-C(32)-F(72)	178.6(4)
C(23)-C(22)-C(32)-F(72)	-1.7(7)
F(72)-C(32)-C(42)-C(52)	-178.0(4)
C(22)-C(32)-C(42)-C(52)	-1.7(9)
C(32)-C(42)-C(52)-C(62)	1.0(8)
C(42)-C(52)-C(62)-C(12)	-1.1(8)
C(42)-C(52)-C(62)-C(82)	178.7(5)
C(22)-C(12)-C(62)-C(52)	1.8(7)
S(21)-C(12)-C(62)-C(52)	-177.6(4)
C(22)-C(12)-C(62)-C(82)	-178.0(4)
S(21)-C(12)-C(62)-C(82)	2.6(6)
C(52)-C(62)-C(82)-C(92)	-87.0(6)
C(12)-C(62)-C(82)-C(92)	92.8(6)
C(52)-C(62)-C(82)-C(132)	90.0(6)
C(12)-C(62)-C(82)-C(132)	-90.2(6)
C(132)-C(82)-C(92)-C(102)	-1.4(8)
C(62)-C(82)-C(92)-C(102)	175.7(5)
C(132)-C(82)-C(92)-C(142)	179.3(5)
C(62)-C(82)-C(92)-C(142)	-3.6(8)
C(82)-C(92)-C(102)-C(112)	-0.2(9)
C(142)-C(92)-C(102)-C(112)	179.1(5)
C(92)-C(102)-C(112)-C(122)	2.8(9)
C(92)-C(102)-C(112)-C(172)	-178.1(6)
C(102)-C(112)-C(122)-C(132)	-4.0(9)
C(172)-C(112)-C(122)-C(132)	176.9(5)
C(112)-C(122)-C(132)-C(82)	2.5(9)
C(112)-C(122)-C(132)-C(202)	-178.5(5)
C(92)-C(82)-C(132)-C(122)	0.3(8)
C(62)-C(82)-C(132)-C(122)	-176.7(5)
C(92)-C(82)-C(132)-C(202)	-178.7(5)
C(62)-C(82)-C(132)-C(202)	4.3(8)
C(102)-C(92)-C(142)-C(162)	-66.9(7)
C(82)-C(92)-C(142)-C(162)	112.4(6)
C(102)-C(92)-C(142)-C(152)	58.3(7)
C(82)-C(92)-C(142)-C(152)	-122.5(6)
C(102)-C(112)-C(172)-C(182)	-119.6(10)
C(122)-C(112)-C(172)-C(182)	59.4(11)

C(102)-C(112)-C(172)-C(192)	106.7(9)
C(122)-C(112)-C(172)-C(192)	-74.2(10)
C(122)-C(132)-C(202)-C(222)	82.2(7)
C(82)-C(132)-C(202)-C(222)	-98.8(6)
C(122)-C(132)-C(202)-C(212)	-41.2(8)
C(82)-C(132)-C(202)-C(212)	137.8(5)
C(63)-C(13)-C(23)-C(33)	-4.8(7)
Fe(1)-C(13)-C(23)-C(33)	-102.3(5)
C(63)-C(13)-C(23)-C(22)	-163.4(5)
Fe(1)-C(13)-C(23)-C(22)	99.0(4)
C(63)-C(13)-C(23)-Fe(1)	97.5(5)
C(32)-C(22)-C(23)-C(13)	109.9(6)
C(12)-C(22)-C(23)-C(13)	-70.4(6)
C(32)-C(22)-C(23)-C(33)	-48.0(7)
C(12)-C(22)-C(23)-C(33)	131.8(5)
C(32)-C(22)-C(23)-Fe(1)	-180.0(4)
C(12)-C(22)-C(23)-Fe(1)	-0.3(6)
C(13)-C(23)-C(33)-C(43)	2.2(8)
C(22)-C(23)-C(33)-C(43)	161.1(6)
Fe(1)-C(23)-C(33)-C(43)	-67.2(7)
C(23)-C(33)-C(43)-C(53)	0.6(10)
C(33)-C(43)-C(53)-C(63)	-0.9(10)
C(43)-C(53)-C(63)-C(13)	-1.7(9)
C(43)-C(53)-C(63)-C(21)	176.1(6)
C(23)-C(13)-C(63)-C(53)	4.7(8)
Fe(1)-C(13)-C(63)-C(53)	88.4(5)
C(23)-C(13)-C(63)-C(21)	-173.2(5)
Fe(1)-C(13)-C(63)-C(21)	-89.6(5)
C(31)-C(21)-C(63)-C(53)	55.2(8)
C(11)-C(21)-C(63)-C(53)	-125.0(6)
C(31)-C(21)-C(63)-C(13)	-126.9(5)
C(11)-C(21)-C(63)-C(13)	52.8(7)
C(180)-O(10)-C(20)-C(30)	-172.4(7)
K(1)-O(10)-C(20)-C(30)	-36.3(9)
C(180)-O(10)-C(20)-K(1)	-136.2(7)
O(10)-C(20)-C(30)-O(40)	63.4(10)
K(1)-C(20)-C(30)-O(40)	38.5(6)
O(10)-C(20)-C(30)-K(1)	25.0(6)
C(20)-C(30)-O(40)-C(50)	176.6(7)
K(1)-C(30)-O(40)-C(50)	-129.9(7)
C(20)-C(30)-O(40)-K(1)	-53.6(9)
C(30)-O(40)-C(50)-C(60)	175.7(7)
K(1)-O(40)-C(50)-C(60)	48.1(7)
C(30)-O(40)-C(50)-K(1)	127.6(7)
O(40)-C(50)-C(60)-O(70)	-67.5(8)
K(1)-C(50)-C(60)-O(70)	-34.4(5)
O(40)-C(50)-C(60)-K(1)	-33.1(5)
C(50)-C(60)-O(70)-C(80)	-170.2(6)
K(1)-C(60)-O(70)-C(80)	138.5(8)
C(50)-C(60)-O(70)-K(1)	51.3(7)
C(60)-O(70)-C(80)-C(90)	175.7(7)
K(1)-O(70)-C(80)-C(90)	-46.9(9)
C(60)-O(70)-C(80)-K(1)	-137.4(8)
O(70)-C(80)-C(90)-O(100)	68.0(10)
K(1)-C(80)-C(90)-O(100)	37.2(6)
O(70)-C(80)-C(90)-K(1)	30.8(6)

C(80)-C(90)-O(100)-C(110)	-178.0(7)
K(1)-C(90)-O(100)-C(110)	-125.7(8)
C(80)-C(90)-O(100)-K(1)	-52.3(8)
C(90)-O(100)-C(110)-C(120)	-179.5(8)
K(1)-O(100)-C(110)-C(120)	54.0(9)
C(90)-O(100)-C(110)-K(1)	126.5(8)
O(100)-C(110)-C(120)-O(130)	-62.6(11)
K(1)-C(110)-C(120)-O(130)	-23.6(7)
O(100)-C(110)-C(120)-K(1)	-39.0(6)
C(110)-C(120)-O(130)-C(140)	-178.6(8)
K(1)-C(120)-O(130)-C(140)	143.9(9)
C(110)-C(120)-O(130)-K(1)	37.5(11)
C(120)-O(130)-C(140)-C(150)	165.3(7)
K(1)-O(130)-C(140)-C(150)	-48.4(7)
C(120)-O(130)-C(140)-K(1)	-146.2(9)
O(130)-C(140)-C(150)-O(160)	67.6(8)
K(1)-C(140)-C(150)-O(160)	35.7(5)
O(130)-C(140)-C(150)-K(1)	32.0(4)
C(140)-C(150)-O(160)-C(170)	-178.4(6)
K(1)-C(150)-O(160)-C(170)	-127.6(6)
C(140)-C(150)-O(160)-K(1)	-50.8(7)
C(150)-O(160)-C(170)-C(180)	175.6(6)
K(1)-O(160)-C(170)-C(180)	49.2(7)
C(150)-O(160)-C(170)-K(1)	126.4(6)
C(20)-O(10)-C(180)-C(170)	-175.6(7)
K(1)-O(10)-C(180)-C(170)	46.6(7)
C(20)-O(10)-C(180)-K(1)	137.8(7)
O(160)-C(170)-C(180)-O(10)	-65.6(8)
K(1)-C(170)-C(180)-O(10)	-31.8(5)
O(160)-C(170)-C(180)-K(1)	-33.7(5)
C(230)-O(190)-C(200)-C(210)	10.4(15)
K(1)-O(190)-C(200)-C(210)	172.2(9)
C(230)-O(190)-C(200)-K(1)	-161.8(14)
O(190)-C(200)-C(210)-C(220)	-5(2)
K(1)-C(200)-C(210)-C(220)	2(3)
C(200)-C(210)-C(220)-C(230)	-2(3)
C(200)-O(190)-C(230)-C(220)	-12.1(17)
K(1)-O(190)-C(230)-C(220)	-174.0(12)
C(200)-O(190)-C(230)-K(1)	161.9(14)
C(210)-C(220)-C(230)-O(190)	9(2)
C(210)-C(220)-C(230)-K(1)	2(3)
C(280)-O(240)-C(250)-C(260)	29.4(13)
K(1)-O(240)-C(250)-C(260)	-120.9(9)
C(280)-O(240)-C(250)-K(1)	150.3(12)
O(240)-C(250)-C(260)-C(270)	-16.4(14)
K(1)-C(250)-C(260)-C(270)	-53.7(13)
C(250)-C(260)-C(270)-C(280)	-2.3(14)
C(250)-O(240)-C(280)-C(270)	-32.3(13)
K(1)-O(240)-C(280)-C(270)	118.3(8)
C(250)-O(240)-C(280)-K(1)	-150.7(12)
C(260)-C(270)-C(280)-O(240)	20.3(13)
C(260)-C(270)-C(280)-K(1)	60.1(12)
C(370)-O(290)-C(300)-C(310)	172.9(8)
K(2)-O(290)-C(300)-C(310)	46.0(10)
C(370)-O(290)-C(300)-K(2)	127.0(8)
O(290)-C(300)-C(310)-O(320)	-64.1(11)

K(2)-C(300)-C(310)-O(320)	-31.8(6)
O(290)-C(300)-C(310)-K(2)	-32.2(7)
C(300)-C(310)-O(320)-C(330)	-178.7(8)
K(2)-C(310)-O(320)-C(330)	133.8(8)
C(300)-C(310)-O(320)-K(2)	47.5(9)
C(310)-O(320)-C(330)-C(340)	-179.4(8)
K(2)-O(320)-C(330)-C(340)	-45.3(8)
C(310)-O(320)-C(330)-K(2)	-134.1(8)
O(320)-C(330)-C(340)-O(350)	63.7(9)
K(2)-C(330)-C(340)-O(350)	32.8(5)
O(320)-C(330)-C(340)-K(2)	30.9(6)
C(330)-C(340)-O(350)-C(360)	176.1(7)
K(2)-C(340)-O(350)-C(360)	-133.5(8)
C(330)-C(340)-O(350)-K(2)	-50.3(8)
C(340)-O(350)-C(360)-C(370)#1	179.0(8)
K(2)-O(350)-C(360)-C(370)#1	44.4(10)
C(340)-O(350)-C(360)-K(2)	134.5(8)
C(300)-O(290)-C(370)-C(360)#1	178.5(8)
K(2)-O(290)-C(370)-C(360)#1	-53.6(10)
C(300)-O(290)-C(370)-K(2)	-128.0(8)
O(380)-C(390)-C(400)-C(410)	5.6(15)
K(2)-C(390)-C(400)-C(410)	41.7(13)
C(390)-C(400)-C(410)-C(420)	17.3(15)
C(390)-C(400)-C(410)-K(2)	-32.2(10)
C(400)-C(410)-C(420)-O(380)	-32.3(13)
K(2)-C(410)-C(420)-O(380)	47.9(5)
C(400)-C(410)-C(420)-K(2)	-80.2(11)
C(400)-C(390)-O(380)-C(420)	-26.8(14)
K(2)-C(390)-O(380)-C(420)	-131.3(13)
C(400)-C(390)-O(380)-K(2)	104.5(11)
C(410)-C(420)-O(380)-C(390)	33.1(11)
K(2)-C(420)-O(380)-C(390)	143.1(9)
C(410)-C(420)-O(380)-K(2)	-110.0(7)
C(510)#2-O(430)-C(440)-C(450)	176.9(5)
K(3)-O(430)-C(440)-C(450)	-53.1(5)
C(510)#2-O(430)-C(440)-K(3)	-130.0(5)
O(430)-C(440)-C(450)-O(460)	68.1(6)
K(3)-C(440)-C(450)-O(460)	31.4(4)
O(430)-C(440)-C(450)-K(3)	36.7(4)
O(460)-C(470)-C(480)-O(490)	-65.9(6)
K(3)-C(470)-C(480)-O(490)	-33.9(3)
O(460)-C(470)-C(480)-K(3)	-32.0(3)
C(470)-C(480)-O(490)-C(500)	-178.7(5)
K(3)-C(480)-O(490)-C(500)	131.9(5)
C(470)-C(480)-O(490)-K(3)	49.3(5)
C(480)-O(490)-C(500)-C(510)	178.1(5)
K(3)-O(490)-C(500)-C(510)	-51.0(5)
C(480)-O(490)-C(500)-K(3)	-130.9(5)
O(490)-C(500)-C(510)-O(430)#2	67.0(6)
K(3)-C(500)-C(510)-O(430)#2	33.1(4)
O(490)-C(500)-C(510)-K(3)	33.9(4)
C(560)-O(520)-C(530)-C(540)	16.6(15)
K(3)-O(520)-C(530)-C(540)	-135.1(9)
C(560)-O(520)-C(530)-K(3)	151.7(12)
O(520)-C(530)-C(540)-C(550)	-14(2)
K(3)-C(530)-C(540)-C(550)	-47(2)

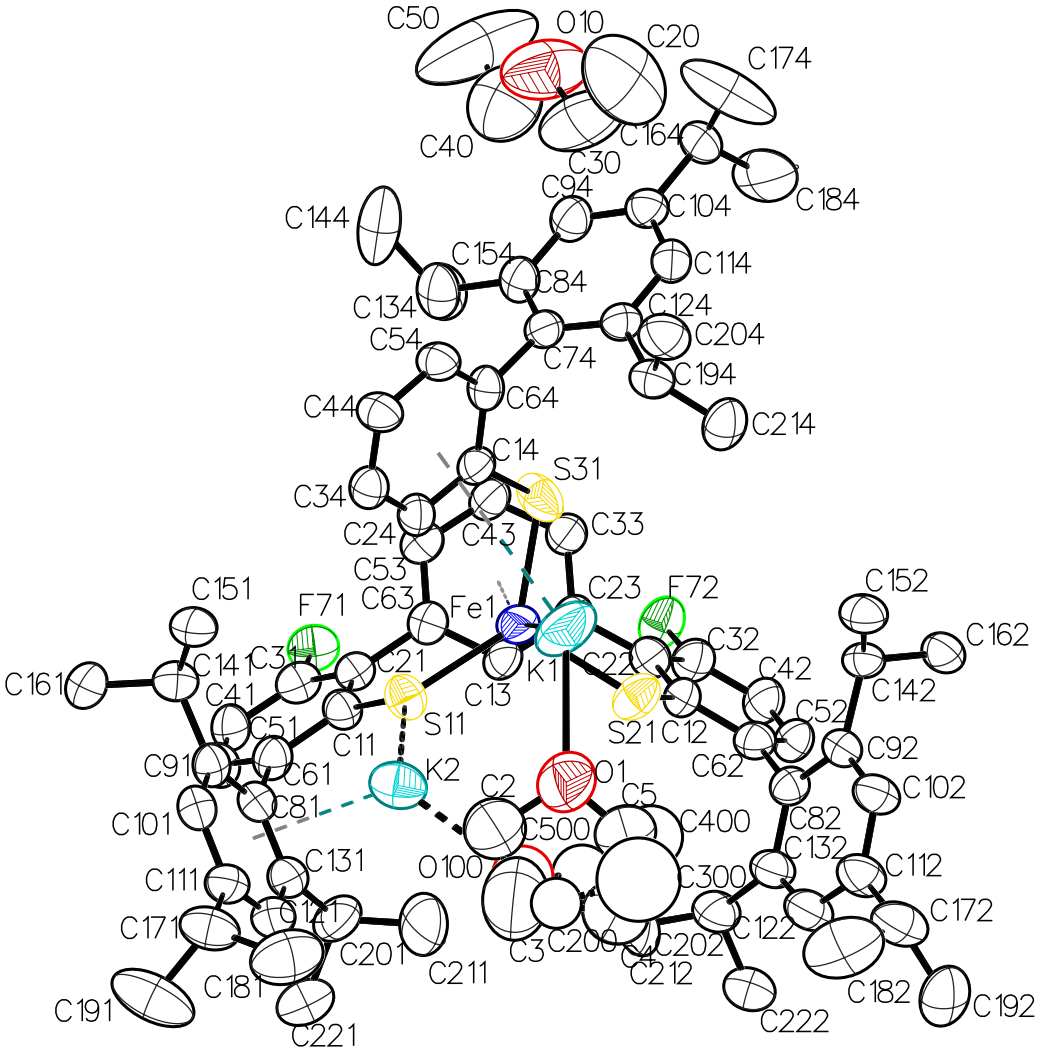
C(530)-C(540)-C(550)-C(560)	7(3)
C(530)-O(520)-C(560)-C(550)	-13(2)
K(3)-O(520)-C(560)-C(550)	139.2(15)
C(530)-O(520)-C(560)-K(3)	-152.4(12)
C(540)-C(550)-C(560)-O(520)	4(3)
C(540)-C(550)-C(560)-K(3)	41(3)
C(440)-C(450)-O(460)-C(470)	176.0(5)
K(3)-C(450)-O(460)-C(470)	-136.2(5)
C(440)-C(450)-O(460)-K(3)	-47.8(6)
C(480)-C(470)-O(460)-C(450)	-174.4(5)
K(3)-C(470)-O(460)-C(450)	136.1(5)
C(480)-C(470)-O(460)-K(3)	49.5(5)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+2,-z+1 #2 -x+2,-y+1,-z+1

Experimental and Refinement Details for [LFeSC$_6$H$_4$Ar]K (5)

Single crystals for X-ray analysis were obtained by slow evaporation of a solution of [LFeSC$_6$H$_4$Ar]K (**5**) (30 mg, crude product after concentration of the reaction mixture) in Et_2O (0.2 mL) at room temperature. Low-temperature diffraction data (ω-scans) were collected on a Rigaku MicroMax-007HF diffractometer coupled to a Saturn994+ CCD detector with Cu Kα (λ = 1.54178 Å). All structures were solved by direct methods and were refined against F^2 on all data by full-matrix least squares[50]. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included in the model at geometrically calculated positions and refined using a riding model. The isotropic displacement parameters of all hydrogen atoms were fixed to 1.2 times the U value of the atoms to which they are linked (1.5 times for methyl groups).

The diffraction of the crystal was weak. Long exposure times were used to compensate for this fact. However, numerous OMIT statements were needed to exclude overexposed reflections that were improperly recorded by the CCD detector. There are a number of elongated thermal ellipsoids in the terminal isopropyl groups. Numerous attempts to model these groups as disordered resulted in unstable refinements. This difficulty required the incorporation of some rigid bond restraints to aid in the refinement of the groups {C184, C164, C174, C104}, {C191, C171, C181, C111}, and {C212, C202, C222, C132}. The THF-potassium moiety is disordered over two positions. The site occupancy factors of the two positions were freely refined and converged at the values of 0.65(7) and 0.35(7). The major position involves atoms {K1, O1, C2, C3, C4, C5}; the minor component contains {K2, O100, C200, C300, C400, C500}. Free refinement of the THF-potassium moiety was not possible due to the close proximity of the atoms in the disordered model. Rigid bond restraints were used to aid the refinement of the major site, while the geometries of the minor site were constrained to be the same as the major site. The minor site was also left isotropic due to the small amount of electron density modeled and to aid in convergence.



The full numbering scheme of [LFeSC$_6$H$_4$Ar]K (**5**). All atoms shown are depicted with 50% thermal contours. The hydrogen atoms have been removed for clarity.

Crystal data and structure refinement for [$LFeSC_6H_4Ar$]K (5).

Identification code	007-14192	
Empirical formula	$C_{77}H_{99}F_2FeKO_2S_3$	
Formula weight	1285.69	
Temperature	93(2) K	
Wavelength	1.54187 Å	
Crystal system	Monoclinic	
Space group	$P2_1$	
Unit cell dimensions	a = 9.1551(2) Å	a = 90°
	b = 22.2274(4) Å	b = 91.735(7)°
	c = 17.4467(12) Å	g = 90°
Volume	3548.7(3) $Å^3$	
Z	2	
Density (calculated)	1.203 g/cm^3	
Absorption coefficient	3.432 mm^{-1}	
F(000)	1376	
Crystal size	0.150 x 0.150 x 0.080 mm^3	
Crystal color and habit	Orange block	
Θ range for data collection	2.534 to 65.087°.	
Index ranges	$-10 \le h \le 10$, $-26 \le k \le 26$, $-20 \le l \le 20$	
Reflections collected	124330	
Independent reflections	11975 [R(int) = 0.2102]	
Completeness to θ = 65.087°	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.771 and 0.655	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	11975 / 95 / 825	
Goodness-of-fit on F^2	0.973	
Final R indices [I>2σ(I)]	R1 = 0.0706, wR2 = 0.1620	
R indices (all data)	R1 = 0.1132, wR2 = 0.1894	
Absolute structure parameter	0.095(5)	
Largest diff. peak and hole	1.161 and -0.533 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for [$LFeSC_6H_4Ar$]K (5). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Fe(1)	5148(2)	5033(1)	4400(1)	70(1)
S(11)	5427(3)	4186(1)	3673(1)	54(1)
S(21)	5388(3)	5933(1)	3742(2)	61(1)
S(31)	5956(3)	5129(1)	5636(1)	76(1)
F(72)	18(6)	6351(2)	4362(3)	64(2)
F(71)	-15(6)	3726(2)	4020(3)	62(1)
C(24)	7713(9)	4120(3)	5458(5)	47(2)
C(61)	3867(10)	3266(4)	3025(5)	50(2)
C(81)	5218(10)	3098(4)	2625(5)	49(2)
C(53)	1923(10)	4436(4)	5093(5)	51(2)
C(194)	9246(10)	5798(4)	6859(5)	50(2)
C(34)	8750(9)	3707(4)	5724(5)	48(2)
C(41)	1318(11)	3059(4)	3259(5)	58(2)
C(22)	2482(10)	6160(4)	4073(5)	47(2)
C(32)	1294(10)	6543(4)	4037(5)	53(2)
C(142)	6005(10)	7613(4)	4171(4)	45(2)
C(91)	6203(9)	2698(4)	2981(5)	46(2)
C(141)	5934(10)	2422(4)	3767(5)	52(2)
C(111)	7777(11)	2773(4)	1878(5)	55(2)
C(84)	6085(9)	4918(3)	7711(5)	51(2)
C(92)	6149(9)	7467(3)	3328(5)	43(2)
C(51)	2602(10)	2921(4)	2917(5)	53(2)
C(74)	7279(8)	5062(4)	7265(4)	45(2)
C(42)	1258(11)	7085(4)	3670(5)	56(2)
C(43)	1765(9)	4942(4)	5527(5)	52(2)
C(124)	8019(10)	5608(4)	7372(5)	47(2)
C(104)	6476(10)	5847(4)	8439(5)	51(2)
C(101)	7439(10)	2543(4)	2589(5)	51(2)
C(214)	8913(13)	6375(4)	6441(6)	71(3)
C(114)	7598(10)	5992(4)	7960(5)	53(2)
C(94)	5715(10)	5310(4)	8300(5)	56(2)
C(52)	2514(10)	7267(4)	3323(5)	47(2)
C(63)	2322(9)	4478(4)	4336(5)	46(2)
C(64)	7815(9)	4609(3)	6696(5)	44(2)
C(31)	1270(10)	3563(4)	3708(5)	51(2)
C(132)	5210(10)	7012(4)	2135(5)	53(2)
C(14)	7211(9)	4584(3)	5940(5)	44(2)
C(12)	3785(10)	6352(4)	3722(5)	47(2)
C(171)	9150(12)	2591(5)	1470(6)	76(3)
C(164)	6011(11)	6261(4)	9078(5)	56(2)
C(121)	6775(11)	3177(4)	1549(5)	60(3)
C(44)	9346(10)	3745(4)	6458(5)	53(2)
C(152)	7439(11)	7537(4)	4640(5)	57(2)
C(13)	2516(8)	5046(4)	4010(4)	47(2)
C(23)	2327(11)	5572(4)	4448(5)	51(2)
C(62)	3736(10)	6913(4)	3334(5)	47(2)
C(54)	8828(10)	4199(4)	6950(5)	50(2)
C(102)	7301(10)	7685(4)	2919(5)	55(2)

C(222)	3567(11)	6942(4)	951(5)	65(3)
C(82)	5075(9)	7128(4)	2930(5)	44(2)
C(21)	2482(10)	3934(4)	3852(5)	47(2)
C(161)	5484(12)	1769(4)	3689(6)	65(3)
C(162)	5388(11)	8242(4)	4259(5)	56(2)
C(11)	3805(10)	3787(4)	3505(5)	47(2)
C(122)	6407(12)	7239(4)	1773(5)	64(3)
C(112)	7473(11)	7581(5)	2139(6)	63(3)
C(202)	4071(12)	6648(5)	1691(5)	71(3)
C(201)	4432(13)	3768(4)	1516(6)	74(3)
C(204)	10676(12)	5817(5)	7292(6)	71(3)
C(134)	5216(11)	4346(4)	7565(7)	69(3)
C(33)	1987(10)	5521(4)	5219(5)	51(2)
C(131)	5497(11)	3336(4)	1913(5)	54(2)
C(154)	3600(12)	4451(5)	7529(7)	80(3)
C(151)	7260(12)	2484(4)	4313(5)	64(3)
C(192)	8245(14)	8205(5)	1024(8)	92(4)
C(172)	8749(13)	7823(6)	1711(6)	80(4)
C(221)	4003(13)	3566(5)	700(6)	79(3)
C(144)	5593(15)	3866(5)	8177(10)	110(5)
C(182)	9799(15)	7357(8)	1487(9)	124(6)
C(191)	8759(17)	2196(8)	783(8)	131(5)
C(181)	10043(16)	3140(7)	1233(8)	113(4)
C(212)	4606(19)	6028(5)	1543(8)	120(5)
C(211)	5020(20)	4396(5)	1500(9)	132(6)
C(174)	7260(20)	6399(11)	9594(10)	173(8)
O(10)	9946(15)	4882(7)	9797(6)	159(5)
C(30)	10930(20)	5131(11)	9336(10)	156(7)
C(20)	12130(20)	5383(11)	9764(15)	198(11)
C(40)	8840(20)	4639(10)	9443(13)	153(7)
C(50)	7640(30)	4471(16)	9950(14)	280(20)
K(1)	8778(5)	5228(2)	4433(3)	108(2)
K(2)	8199(7)	4024(3)	2876(4)	72(3)
C(184)	5210(20)	6789(7)	8768(8)	163(8)
O(1)	9139(16)	5250(6)	2973(8)	108(4)
C(2)	9280(30)	4715(11)	2512(15)	134(9)
C(3)	10170(70)	4848(15)	1860(30)	260(20)
C(4)	9610(90)	5635(15)	1750(20)	280(30)
C(5)	9180(50)	5710(13)	2508(15)	146(13)
O(100)	9040(30)	4946(12)	2060(18)	108(9)
C(200)	10450(30)	5143(15)	1840(20)	74(9)
C(300)	10710(60)	5750(30)	2090(50)	200(30)
C(400)	8890(50)	5920(20)	2470(30)	115(19)
C(500)	8220(40)	5436(16)	2070(30)	105(12)

Bond lengths [Å] and angles [°] for [LFeSC$_6$H$_4$Ar]K (5).

Fe(1)-S(31)	2.269(3)
Fe(1)-S(11)	2.288(3)
Fe(1)-S(21)	2.319(3)
Fe(1)-C(13)	2.484(8)

Fe(1)-K(1)	3.350(5)
S(11)-C(11)	1.747(10)
S(11)-K(2)	2.953(7)
S(21)-C(12)	1.737(9)
S(21)-K(1)	3.649(6)
S(31)-C(14)	1.741(8)
S(31)-K(1)	3.384(5)
F(72)-C(32)	1.381(10)
F(72)-K(1)#1	2.747(7)
F(71)-C(31)	1.359(10)
F(71)-K(2)#1	2.628(8)
C(24)-C(34)	1.390(11)
C(24)-C(14)	1.416(11)
C(24)-K(1)	3.212(9)
C(24)-H(24)	0.9500
C(61)-C(51)	1.396(12)
C(61)-C(11)	1.431(12)
C(61)-C(81)	1.486(13)
C(81)-C(131)	1.382(12)
C(81)-C(91)	1.399(12)
C(81)-K(2)	3.436(11)
C(53)-C(43)	1.367(12)
C(53)-C(63)	1.384(12)
C(53)-K(1)#1	3.538(10)
C(53)-H(53)	0.9500
C(194)-C(204)	1.492(14)
C(194)-C(214)	1.503(13)
C(194)-C(124)	1.518(12)
C(194)-H(194)	1.0000
C(34)-C(44)	1.381(12)
C(34)-H(34)	0.9500
C(41)-C(51)	1.369(13)
C(41)-C(31)	1.370(13)
C(41)-H(41)	0.9500
C(22)-C(32)	1.382(12)
C(22)-C(12)	1.424(12)
C(22)-C(23)	1.469(12)
C(32)-C(42)	1.364(12)
C(142)-C(92)	1.515(11)
C(142)-C(162)	1.518(11)
C(142)-C(152)	1.535(12)
C(142)-H(142)	1.0000
C(91)-C(101)	1.382(12)
C(91)-C(141)	1.529(12)
C(91)-K(2)	3.476(11)
C(141)-C(161)	1.513(12)
C(141)-C(151)	1.527(13)
C(141)-H(141)	1.0000
C(111)-C(101)	1.385(12)
C(111)-C(121)	1.394(13)
C(111)-C(171)	1.518(14)
C(111)-K(2)	3.298(11)
C(84)-C(94)	1.397(11)
C(84)-C(74)	1.398(11)
C(84)-C(134)	1.517(13)
C(92)-C(102)	1.379(12)

C(92)-C(82)	1.405(11)
C(51)-H(51)	0.9500
C(74)-C(124)	1.399(12)
C(74)-C(64)	1.506(11)
C(42)-C(52)	1.376(12)
C(42)-H(42)	0.9500
C(43)-C(33)	1.412(12)
C(43)-K(1)#1	3.349(10)
C(43)-H(43)	0.9500
C(124)-C(114)	1.398(11)
C(104)-C(114)	1.382(12)
C(104)-C(94)	1.398(12)
C(104)-C(164)	1.518(12)
C(101)-K(2)	3.398(11)
C(101)-H(101)	0.9500
C(214)-H(21A)	0.9800
C(214)-H(21B)	0.9800
C(214)-H(21C)	0.9800
C(114)-H(114)	0.9500
C(94)-H(94)	0.9500
C(52)-C(62)	1.367(12)
C(52)-H(52)	0.9500
C(63)-C(13)	1.399(12)
C(63)-C(21)	1.484(12)
C(64)-C(54)	1.366(11)
C(64)-C(14)	1.416(11)
C(31)-C(21)	1.399(12)
C(31)-K(2)#1	3.288(11)
C(132)-C(122)	1.377(13)
C(132)-C(82)	1.421(11)
C(132)-C(202)	1.514(13)
C(14)-K(1)	3.353(9)
C(12)-C(62)	1.418(11)
C(171)-C(191)	1.521(17)
C(171)-C(181)	1.532(17)
C(171)-H(171)	1.0000
C(164)-C(174)	1.466(18)
C(164)-C(184)	1.477(16)
C(164)-H(164)	1.0000
C(121)-C(131)	1.394(13)
C(121)-K(2)	3.228(11)
C(121)-H(121)	0.9500
C(44)-C(54)	1.415(12)
C(44)-H(44)	0.9500
C(152)-H(15A)	0.9800
C(152)-H(15B)	0.9800
C(152)-H(15C)	0.9800
C(13)-C(23)	1.410(12)
C(13)-H(13)	0.9500
C(23)-C(33)	1.394(12)
C(23)-K(1)#1	3.337(11)
C(62)-C(82)	1.510(12)
C(54)-H(54)	0.9500
C(102)-C(112)	1.393(12)
C(102)-H(102)	0.9500
C(222)-C(202)	1.506(13)

C(222)-H(22A)	0.9800
C(222)-H(22B)	0.9800
C(222)-H(22C)	0.9800
C(21)-C(11)	1.408(12)
C(161)-H(16A)	0.9800
C(161)-H(16B)	0.9800
C(161)-H(16C)	0.9800
C(162)-H(16D)	0.9800
C(162)-H(16E)	0.9800
C(162)-H(16F)	0.9800
C(122)-C(112)	1.378(13)
C(122)-H(122)	0.9500
C(112)-C(172)	1.504(14)
C(202)-C(212)	1.489(16)
C(202)-H(202)	1.0000
C(201)-C(211)	1.497(17)
C(201)-C(131)	1.519(13)
C(201)-C(221)	1.533(15)
C(201)-H(201)	1.0000
C(204)-H(20A)	0.9800
C(204)-H(20B)	0.9800
C(204)-H(20C)	0.9800
C(134)-C(154)	1.497(14)
C(134)-C(144)	1.542(17)
C(134)-H(134)	1.0000
C(33)-K(1)#1	3.270(11)
C(33)-H(33)	0.9500
C(131)-K(2)	3.320(12)
C(154)-H(15D)	0.9800
C(154)-H(15E)	0.9800
C(154)-H(15F)	0.9800
C(151)-H(15G)	0.9800
C(151)-H(15H)	0.9800
C(151)-H(15I)	0.9800
C(192)-C(172)	1.528(17)
C(192)-H(19A)	0.9800
C(192)-H(19B)	0.9800
C(192)-H(19C)	0.9800
C(172)-C(182)	1.473(17)
C(172)-H(172)	1.0000
C(221)-H(22D)	0.9800
C(221)-H(22E)	0.9800
C(221)-H(22F)	0.9800
C(144)-H(14A)	0.9800
C(144)-H(14B)	0.9800
C(144)-H(14C)	0.9800
C(182)-H(18A)	0.9800
C(182)-H(18B)	0.9800
C(182)-H(18C)	0.9800
C(191)-H(19D)	0.9800
C(191)-H(19E)	0.9800
C(191)-H(19F)	0.9800
C(181)-H(18D)	0.9800
C(181)-H(18E)	0.9800
C(181)-H(18F)	0.9800
C(212)-H(21D)	0.9800

C(212)-H(21E)	0.9800
C(212)-H(21F)	0.9800
C(211)-H(21G)	0.9800
C(211)-H(21H)	0.9800
C(211)-H(21I)	0.9800
C(174)-H(17A)	0.9800
C(174)-H(17B)	0.9800
C(174)-H(17C)	0.9800
O(10)-C(40)	1.29(2)
O(10)-C(30)	1.347(19)
C(30)-C(20)	1.42(3)
C(30)-H(30C)	0.9900
C(30)-H(30D)	0.9900
C(20)-H(20F)	0.9800
C(20)-H(20G)	0.9800
C(20)-H(20H)	0.9800
C(40)-C(50)	1.48(3)
C(40)-H(40C)	0.9900
C(40)-H(40D)	0.9900
C(50)-H(50C)	0.9800
C(50)-H(50D)	0.9800
C(50)-H(50E)	0.9800
K(1)-O(1)	2.579(15)
K(1)-F(72)#2	2.747(7)
K(1)-C(33)#2	3.270(11)
K(1)-C(23)#2	3.337(11)
K(1)-C(43)#2	3.349(10)
K(1)-C(53)#2	3.538(10)
K(2)-O(100)	2.62(3)
K(2)-F(71)#2	2.628(8)
K(2)-C(31)#2	3.288(11)
K(2)-C(500)	3.44(4)
C(184)-H(18G)	0.9800
C(184)-H(18H)	0.9800
C(184)-H(18I)	0.9800
O(1)-C(5)	1.31(3)
O(1)-C(2)	1.45(2)
C(2)-C(3)	1.45(4)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-C(4)	1.83(5)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-C(5)	1.40(4)
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(5)-H(5A)	0.9900
C(5)-H(5B)	0.9900
O(100)-C(500)	1.32(3)
O(100)-C(200)	1.42(3)
C(200)-C(300)	1.44(4)
C(200)-H(20D)	0.9900
C(200)-H(20E)	0.9900
C(300)-C(400)	1.85(6)
C(300)-H(30A)	0.9900
C(300)-H(30B)	0.9900

C(400)-C(500)	1.41(4)
C(400)-H(40A)	0.9900
C(400)-H(40B)	0.9900
C(500)-H(50A)	0.9900
C(500)-H(50B)	0.9900

S(31)-Fe(1)-S(11)	124.40(10)
S(31)-Fe(1)-S(21)	110.87(12)
S(11)-Fe(1)-S(21)	114.97(10)
S(31)-Fe(1)-C(13)	123.0(2)
S(11)-Fe(1)-C(13)	89.0(2)
S(21)-Fe(1)-C(13)	87.7(2)
S(31)-Fe(1)-K(1)	71.13(12)
S(11)-Fe(1)-K(1)	89.36(11)
S(21)-Fe(1)-K(1)	77.80(11)
C(13)-Fe(1)-K(1)	163.1(2)
C(11)-S(11)-Fe(1)	113.7(3)
C(11)-S(11)-K(2)	126.7(3)
Fe(1)-S(11)-K(2)	118.24(17)
C(12)-S(21)-Fe(1)	112.4(3)
C(12)-S(21)-K(1)	161.2(3)
Fe(1)-S(21)-K(1)	63.81(9)
C(14)-S(31)-Fe(1)	114.7(3)
C(14)-S(31)-K(1)	74.0(3)
Fe(1)-S(31)-K(1)	69.50(12)
C(32)-F(72)-K(1)#1	130.9(5)
C(31)-F(71)-K(2)#1	106.8(5)
C(34)-C(24)-C(14)	120.9(8)
C(34)-C(24)-K(1)	118.4(5)
C(14)-C(24)-K(1)	83.2(4)
C(34)-C(24)-H(24)	119.5
C(14)-C(24)-H(24)	119.5
K(1)-C(24)-H(24)	68.8
C(51)-C(61)-C(11)	118.4(8)
C(51)-C(61)-C(81)	119.8(8)
C(11)-C(61)-C(81)	121.8(8)
C(131)-C(81)-C(91)	120.5(8)
C(131)-C(81)-C(61)	120.3(8)
C(91)-C(81)-C(61)	119.1(8)
C(131)-C(81)-K(2)	73.5(6)
C(91)-C(81)-K(2)	79.9(5)
C(61)-C(81)-K(2)	117.3(5)
C(43)-C(53)-C(63)	120.6(8)
C(43)-C(53)-K(1)#1	70.9(5)
C(63)-C(53)-K(1)#1	83.8(5)
C(43)-C(53)-H(53)	119.7
C(63)-C(53)-H(53)	119.7
K(1)#1-C(53)-H(53)	116.1
C(204)-C(194)-C(214)	112.5(9)
C(204)-C(194)-C(124)	111.3(7)
C(214)-C(194)-C(124)	112.4(7)
C(204)-C(194)-H(194)	106.7
C(214)-C(194)-H(194)	106.7
C(124)-C(194)-H(194)	106.7
C(44)-C(34)-C(24)	121.1(8)
C(44)-C(34)-H(34)	119.5

C(24)-C(34)-H(34)	119.5
C(51)-C(41)-C(31)	118.4(9)
C(51)-C(41)-H(41)	120.8
C(31)-C(41)-H(41)	120.8
C(32)-C(22)-C(12)	117.7(8)
C(32)-C(22)-C(23)	118.8(8)
C(12)-C(22)-C(23)	123.5(8)
C(42)-C(32)-F(72)	117.2(8)
C(42)-C(32)-C(22)	125.0(9)
F(72)-C(32)-C(22)	117.8(7)
C(92)-C(142)-C(162)	109.8(7)
C(92)-C(142)-C(152)	113.3(7)
C(162)-C(142)-C(152)	111.2(7)
C(92)-C(142)-H(142)	107.4
C(162)-C(142)-H(142)	107.4
C(152)-C(142)-H(142)	107.4
C(101)-C(91)-C(81)	117.7(8)
C(101)-C(91)-C(141)	120.0(8)
C(81)-C(91)-C(141)	122.2(8)
C(101)-C(91)-K(2)	75.2(5)
C(81)-C(91)-K(2)	76.7(5)
C(141)-C(91)-K(2)	119.1(5)
C(161)-C(141)-C(151)	110.6(8)
C(161)-C(141)-C(91)	110.8(7)
C(151)-C(141)-C(91)	112.1(8)
C(161)-C(141)-H(141)	107.7
C(151)-C(141)-H(141)	107.7
C(91)-C(141)-H(141)	107.7
C(101)-C(111)-C(121)	116.3(9)
C(101)-C(111)-C(171)	122.1(9)
C(121)-C(111)-C(171)	121.5(9)
C(101)-C(111)-K(2)	82.2(5)
C(121)-C(111)-K(2)	74.9(5)
C(171)-C(111)-K(2)	112.7(6)
C(94)-C(84)-C(74)	118.5(8)
C(94)-C(84)-C(134)	120.6(8)
C(74)-C(84)-C(134)	120.8(8)
C(102)-C(92)-C(82)	117.8(7)
C(102)-C(92)-C(142)	121.2(8)
C(82)-C(92)-C(142)	120.9(7)
C(41)-C(51)-C(61)	122.6(8)
C(41)-C(51)-H(51)	118.7
C(61)-C(51)-H(51)	118.7
C(84)-C(74)-C(124)	120.5(7)
C(84)-C(74)-C(64)	119.3(8)
C(124)-C(74)-C(64)	120.1(7)
C(32)-C(42)-C(52)	117.2(8)
C(32)-C(42)-H(42)	121.4
C(52)-C(42)-H(42)	121.4
C(53)-C(43)-C(33)	121.3(8)
C(53)-C(43)-K(1)#1	86.5(6)
C(33)-C(43)-K(1)#1	74.6(5)
C(53)-C(43)-H(43)	119.3
C(33)-C(43)-H(43)	119.3
K(1)#1-C(43)-H(43)	109.5
C(114)-C(124)-C(74)	119.0(7)

C(114)-C(124)-C(194)	119.2(8)
C(74)-C(124)-C(194)	121.8(7)
C(114)-C(104)-C(94)	118.1(8)
C(114)-C(104)-C(164)	122.2(8)
C(94)-C(104)-C(164)	119.7(8)
C(91)-C(101)-C(111)	124.0(9)
C(91)-C(101)-K(2)	81.6(5)
C(111)-C(101)-K(2)	74.0(5)
C(91)-C(101)-H(101)	118.0
C(111)-C(101)-H(101)	118.0
K(2)-C(101)-H(101)	116.7
C(194)-C(214)-H(21A)	109.5
C(194)-C(214)-H(21B)	109.5
H(21A)-C(214)-H(21B)	109.5
C(194)-C(214)-H(21C)	109.5
H(21A)-C(214)-H(21C)	109.5
H(21B)-C(214)-H(21C)	109.5
C(104)-C(114)-C(124)	121.8(8)
C(104)-C(114)-H(114)	119.1
C(124)-C(114)-H(114)	119.1
C(84)-C(94)-C(104)	121.9(8)
C(84)-C(94)-H(94)	119.0
C(104)-C(94)-H(94)	119.0
C(62)-C(52)-C(42)	121.3(8)
C(62)-C(52)-H(52)	119.4
C(42)-C(52)-H(52)	119.4
C(53)-C(63)-C(13)	119.3(8)
C(53)-C(63)-C(21)	121.4(7)
C(13)-C(63)-C(21)	119.3(7)
C(54)-C(64)-C(14)	121.3(7)
C(54)-C(64)-C(74)	117.6(7)
C(14)-C(64)-C(74)	120.9(7)
F(71)-C(31)-C(41)	119.3(8)
F(71)-C(31)-C(21)	117.6(8)
C(41)-C(31)-C(21)	123.1(9)
F(71)-C(31)-K(2)#1	49.9(4)
C(41)-C(31)-K(2)#1	92.5(6)
C(21)-C(31)-K(2)#1	124.0(6)
C(122)-C(132)-C(82)	118.4(8)
C(122)-C(132)-C(202)	120.5(8)
C(82)-C(132)-C(202)	121.1(8)
C(24)-C(14)-C(64)	117.2(7)
C(24)-C(14)-S(31)	123.3(6)
C(64)-C(14)-S(31)	119.5(6)
C(24)-C(14)-K(1)	72.0(4)
C(64)-C(14)-K(1)	123.3(5)
S(31)-C(14)-K(1)	76.0(3)
C(62)-C(12)-C(22)	117.0(8)
C(62)-C(12)-S(21)	119.8(7)
C(22)-C(12)-S(21)	123.2(6)
C(111)-C(171)-C(191)	110.2(10)
C(111)-C(171)-C(181)	111.8(10)
C(191)-C(171)-C(181)	111.2(11)
C(111)-C(171)-H(171)	107.9
C(191)-C(171)-H(171)	107.9
C(181)-C(171)-H(171)	107.9

C(174)-C(164)-C(184)	115.3(14)
C(174)-C(164)-C(104)	110.3(9)
C(184)-C(164)-C(104)	111.1(8)
C(174)-C(164)-H(164)	106.5
C(184)-C(164)-H(164)	106.5
C(104)-C(164)-H(164)	106.5
C(131)-C(121)-C(111)	121.8(9)
C(131)-C(121)-K(2)	81.5(5)
C(111)-C(121)-K(2)	80.5(5)
C(131)-C(121)-H(121)	119.1
C(111)-C(121)-H(121)	119.1
K(2)-C(121)-H(121)	108.8
C(34)-C(44)-C(54)	118.5(8)
C(34)-C(44)-H(44)	120.8
C(54)-C(44)-H(44)	120.8
C(142)-C(152)-H(15A)	109.5
C(142)-C(152)-H(15B)	109.5
H(15A)-C(152)-H(15B)	109.5
C(142)-C(152)-H(15C)	109.5
H(15A)-C(152)-H(15C)	109.5
H(15B)-C(152)-H(15C)	109.5
C(63)-C(13)-C(23)	120.7(7)
C(63)-C(13)-Fe(1)	90.7(5)
C(23)-C(13)-Fe(1)	89.8(6)
C(63)-C(13)-H(13)	119.7
C(23)-C(13)-H(13)	119.7
Fe(1)-C(13)-H(13)	89.5
C(33)-C(23)-C(13)	119.3(7)
C(33)-C(23)-C(22)	122.0(8)
C(13)-C(23)-C(22)	118.7(7)
C(33)-C(23)-K(1)#1	75.1(6)
C(13)-C(23)-K(1)#1	86.6(5)
C(22)-C(23)-K(1)#1	107.9(6)
C(52)-C(62)-C(12)	121.8(8)
C(52)-C(62)-C(82)	119.1(7)
C(12)-C(62)-C(82)	119.1(8)
C(64)-C(54)-C(44)	121.0(8)
C(64)-C(54)-H(54)	119.5
C(44)-C(54)-H(54)	119.5
C(92)-C(102)-C(112)	124.0(9)
C(92)-C(102)-H(102)	118.0
C(112)-C(102)-H(102)	118.0
C(202)-C(222)-H(22A)	109.5
C(202)-C(222)-H(22B)	109.5
H(22A)-C(222)-H(22B)	109.5
C(202)-C(222)-H(22C)	109.5
H(22A)-C(222)-H(22C)	109.5
H(22B)-C(222)-H(22C)	109.5
C(92)-C(82)-C(132)	119.9(8)
C(92)-C(82)-C(62)	120.3(7)
C(132)-C(82)-C(62)	119.7(8)
C(31)-C(21)-C(11)	118.3(8)
C(31)-C(21)-C(63)	119.4(8)
C(11)-C(21)-C(63)	122.3(8)
C(141)-C(161)-H(16A)	109.5
C(141)-C(161)-H(16B)	109.5

H(16A)-C(161)-H(16B)	109.5
C(141)-C(161)-H(16C)	109.5
H(16A)-C(161)-H(16C)	109.5
H(16B)-C(161)-H(16C)	109.5
C(142)-C(162)-H(16D)	109.5
C(142)-C(162)-H(16E)	109.5
H(16D)-C(162)-H(16E)	109.5
C(142)-C(162)-H(16F)	109.5
H(16D)-C(162)-H(16F)	109.5
H(16E)-C(162)-H(16F)	109.5
C(21)-C(11)-C(61)	119.3(8)
C(21)-C(11)-S(11)	123.2(6)
C(61)-C(11)-S(11)	117.4(7)
C(132)-C(122)-C(112)	123.5(9)
C(132)-C(122)-H(122)	118.2
C(112)-C(122)-H(122)	118.2
C(122)-C(112)-C(102)	116.4(9)
C(122)-C(112)-C(172)	121.1(9)
C(102)-C(112)-C(172)	122.5(9)
C(212)-C(202)-C(222)	110.3(9)
C(212)-C(202)-C(132)	111.0(10)
C(222)-C(202)-C(132)	113.3(8)
C(212)-C(202)-H(202)	107.4
C(222)-C(202)-H(202)	107.4
C(132)-C(202)-H(202)	107.4
C(211)-C(201)-C(131)	111.8(10)
C(211)-C(201)-C(221)	109.7(9)
C(131)-C(201)-C(221)	112.5(8)
C(211)-C(201)-H(201)	107.5
C(131)-C(201)-H(201)	107.5
C(221)-C(201)-H(201)	107.5
C(194)-C(204)-H(20A)	109.5
C(194)-C(204)-H(20B)	109.5
H(20A)-C(204)-H(20B)	109.5
C(194)-C(204)-H(20C)	109.5
H(20A)-C(204)-H(20C)	109.5
H(20B)-C(204)-H(20C)	109.5
C(154)-C(134)-C(84)	112.9(8)
C(154)-C(134)-C(144)	109.7(9)
C(84)-C(134)-C(144)	111.0(10)
C(154)-C(134)-H(134)	107.7
C(84)-C(134)-H(134)	107.7
C(144)-C(134)-H(134)	107.7
C(23)-C(33)-C(43)	118.8(8)
C(23)-C(33)-K(1)#1	80.6(6)
C(43)-C(33)-K(1)#1	80.8(6)
C(23)-C(33)-H(33)	120.6
C(43)-C(33)-H(33)	120.6
K(1)#1-C(33)-H(33)	108.5
C(81)-C(131)-C(121)	119.5(9)
C(81)-C(131)-C(201)	121.2(9)
C(121)-C(131)-C(201)	119.3(8)
C(81)-C(131)-K(2)	82.9(6)
C(121)-C(131)-K(2)	74.0(6)
C(201)-C(131)-K(2)	113.4(6)
C(134)-C(154)-H(15D)	109.5

C(134)-C(154)-H(15E)	109.5
H(15D)-C(154)-H(15E)	109.5
C(134)-C(154)-H(15F)	109.5
H(15D)-C(154)-H(15F)	109.5
H(15E)-C(154)-H(15F)	109.5
C(141)-C(151)-H(15G)	109.5
C(141)-C(151)-H(15H)	109.5
H(15G)-C(151)-H(15H)	109.5
C(141)-C(151)-H(15I)	109.5
H(15G)-C(151)-H(15I)	109.5
H(15H)-C(151)-H(15I)	109.5
C(172)-C(192)-H(19A)	109.5
C(172)-C(192)-H(19B)	109.5
H(19A)-C(192)-H(19B)	109.5
C(172)-C(192)-H(19C)	109.5
H(19A)-C(192)-H(19C)	109.5
H(19B)-C(192)-H(19C)	109.5
C(182)-C(172)-C(112)	113.8(10)
C(182)-C(172)-C(192)	111.5(10)
C(112)-C(172)-C(192)	111.5(10)
C(182)-C(172)-H(172)	106.5
C(112)-C(172)-H(172)	106.5
C(192)-C(172)-H(172)	106.5
C(201)-C(221)-H(22D)	109.5
C(201)-C(221)-H(22E)	109.5
H(22D)-C(221)-H(22E)	109.5
C(201)-C(221)-H(22F)	109.5
H(22D)-C(221)-H(22F)	109.5
H(22E)-C(221)-H(22F)	109.5
C(134)-C(144)-H(14A)	109.5
C(134)-C(144)-H(14B)	109.5
H(14A)-C(144)-H(14B)	109.5
C(134)-C(144)-H(14C)	109.5
H(14A)-C(144)-H(14C)	109.5
H(14B)-C(144)-H(14C)	109.5
C(172)-C(182)-H(18A)	109.5
C(172)-C(182)-H(18B)	109.5
H(18A)-C(182)-H(18B)	109.5
C(172)-C(182)-H(18C)	109.5
H(18A)-C(182)-H(18C)	109.5
H(18B)-C(182)-H(18C)	109.5
C(171)-C(191)-H(19D)	109.5
C(171)-C(191)-H(19E)	109.5
H(19D)-C(191)-H(19E)	109.5
C(171)-C(191)-H(19F)	109.5
H(19D)-C(191)-H(19F)	109.5
H(19E)-C(191)-H(19F)	109.5
C(171)-C(181)-H(18D)	109.5
C(171)-C(181)-H(18E)	109.5
H(18D)-C(181)-H(18E)	109.5
C(171)-C(181)-H(18F)	109.5
H(18D)-C(181)-H(18F)	109.5
H(18E)-C(181)-H(18F)	109.5
C(202)-C(212)-H(21D)	109.5
C(202)-C(212)-H(21E)	109.5
H(21D)-C(212)-H(21E)	109.5

C(202)-C(212)-H(21F)	109.5
H(21D)-C(212)-H(21F)	109.5
H(21E)-C(212)-H(21F)	109.5
C(201)-C(211)-H(21G)	109.5
C(201)-C(211)-H(21H)	109.5
H(21G)-C(211)-H(21H)	109.5
C(201)-C(211)-H(21I)	109.5
H(21G)-C(211)-H(21I)	109.5
H(21H)-C(211)-H(21I)	109.5
C(164)-C(174)-H(17A)	109.5
C(164)-C(174)-H(17B)	109.5
H(17A)-C(174)-H(17B)	109.5
C(164)-C(174)-H(17C)	109.5
H(17A)-C(174)-H(17C)	109.5
H(17B)-C(174)-H(17C)	109.5
C(40)-O(10)-C(30)	114.6(17)
O(10)-C(30)-C(20)	111.6(17)
O(10)-C(30)-H(30C)	109.3
C(20)-C(30)-H(30C)	109.3
O(10)-C(30)-H(30D)	109.3
C(20)-C(30)-H(30D)	109.3
H(30C)-C(30)-H(30D)	108.0
C(30)-C(20)-H(20F)	109.5
C(30)-C(20)-H(20G)	109.5
H(20F)-C(20)-H(20G)	109.5
C(30)-C(20)-H(20H)	109.5
H(20F)-C(20)-H(20H)	109.5
H(20G)-C(20)-H(20H)	109.5
O(10)-C(40)-C(50)	114(2)
O(10)-C(40)-H(40C)	108.8
C(50)-C(40)-H(40C)	108.8
O(10)-C(40)-H(40D)	108.8
C(50)-C(40)-H(40D)	108.8
H(40C)-C(40)-H(40D)	107.7
C(40)-C(50)-H(50C)	109.5
C(40)-C(50)-H(50D)	109.5
H(50C)-C(50)-H(50D)	109.5
C(40)-C(50)-H(50E)	109.5
H(50C)-C(50)-H(50E)	109.5
H(50D)-C(50)-H(50E)	109.5
O(1)-K(1)-F(72)#2	82.7(3)
O(1)-K(1)-C(24)	127.9(4)
F(72)#2-K(1)-C(24)	148.7(3)
O(1)-K(1)-C(33)#2	105.6(4)
F(72)#2-K(1)-C(33)#2	58.0(2)
C(24)-K(1)-C(33)#2	101.7(3)
O(1)-K(1)-C(23)#2	81.3(4)
F(72)#2-K(1)-C(23)#2	52.3(2)
C(24)-K(1)-C(23)#2	118.9(3)
C(33)#2-K(1)-C(23)#2	24.3(2)
O(1)-K(1)-C(43)#2	116.1(4)
F(72)#2-K(1)-C(43)#2	82.3(2)
C(24)-K(1)-C(43)#2	78.1(2)
C(33)#2-K(1)-C(43)#2	24.6(2)
C(23)#2-K(1)-C(43)#2	42.3(2)
O(1)-K(1)-Fe(1)	98.2(4)

F(72)#2-K(1)-Fe(1)	121.87(19)
C(24)-K(1)-Fe(1)	65.98(17)
C(33)#2-K(1)-Fe(1)	155.7(2)
C(23)#2-K(1)-Fe(1)	174.2(2)
C(43)#2-K(1)-Fe(1)	141.09(19)
O(1)-K(1)-C(14)	148.6(4)
F(72)#2-K(1)-C(14)	127.6(2)
C(24)-K(1)-C(14)	24.78(19)
C(33)#2-K(1)-C(14)	99.0(2)
C(23)#2-K(1)-C(14)	122.1(3)
C(43)#2-K(1)-C(14)	80.4(2)
Fe(1)-K(1)-C(14)	60.72(16)
O(1)-K(1)-S(31)	137.5(4)
F(72)#2-K(1)-S(31)	114.30(18)
C(24)-K(1)-S(31)	49.81(15)
C(33)#2-K(1)-S(31)	116.5(2)
C(23)#2-K(1)-S(31)	140.5(2)
C(43)#2-K(1)-S(31)	105.07(19)
Fe(1)-K(1)-S(31)	39.37(7)
C(14)-K(1)-S(31)	29.95(15)
O(1)-K(1)-C(53)#2	101.7(4)
F(72)#2-K(1)-C(53)#2	97.7(2)
C(24)-K(1)-C(53)#2	72.2(2)
C(33)#2-K(1)-C(53)#2	41.4(2)
C(23)#2-K(1)-C(53)#2	47.9(2)
C(43)#2-K(1)-C(53)#2	22.7(2)
Fe(1)-K(1)-C(53)#2	137.60(19)
C(14)-K(1)-C(53)#2	84.0(2)
S(31)-K(1)-C(53)#2	113.26(19)
O(1)-K(1)-S(21)	78.4(3)
F(72)#2-K(1)-S(21)	86.77(17)
C(24)-K(1)-S(21)	104.1(2)
C(33)#2-K(1)-S(21)	142.9(2)
C(23)#2-K(1)-S(21)	136.25(19)
C(43)#2-K(1)-S(21)	160.4(2)
Fe(1)-K(1)-S(21)	38.40(7)
C(14)-K(1)-S(21)	93.58(18)
S(31)-K(1)-S(21)	64.85(10)
C(53)#2-K(1)-S(21)	175.5(2)
O(100)-K(2)-F(71)#2	115.0(7)
O(100)-K(2)-S(11)	115.6(7)
F(71)#2-K(2)-S(11)	101.3(2)
O(100)-K(2)-C(121)	100.7(7)
F(71)#2-K(2)-C(121)	128.8(3)
S(11)-K(2)-C(121)	94.3(3)
O(100)-K(2)-C(31)#2	102.8(7)
F(71)#2-K(2)-C(31)#2	23.31(19)
S(11)-K(2)-C(31)#2	124.4(3)
C(121)-K(2)-C(31)#2	117.1(3)
O(100)-K(2)-C(111)	113.8(7)
F(71)#2-K(2)-C(111)	104.4(3)
S(11)-K(2)-C(111)	105.2(3)
C(121)-K(2)-C(111)	24.6(2)
C(31)#2-K(2)-C(111)	93.2(3)
O(100)-K(2)-C(131)	108.2(7)
F(71)#2-K(2)-C(131)	134.8(3)

S(11)-K(2)-C(131)	69.9(2)
C(121)-K(2)-C(131)	24.5(2)
C(31)#2-K(2)-C(131)	133.9(3)
C(111)-K(2)-C(131)	43.2(2)
O(100)-K(2)-C(101)	137.6(7)
F(71)#2-K(2)-C(101)	89.3(3)
S(11)-K(2)-C(101)	90.7(2)
C(121)-K(2)-C(101)	41.7(2)
C(31)#2-K(2)-C(101)	86.1(3)
C(111)-K(2)-C(101)	23.8(2)
C(131)-K(2)-C(101)	48.2(2)
O(100)-K(2)-C(500)	20.1(8)
F(71)#2-K(2)-C(500)	121.9(7)
S(11)-K(2)-C(500)	95.5(7)
C(121)-K(2)-C(500)	104.4(7)
C(31)#2-K(2)-C(500)	116.7(6)
C(111)-K(2)-C(500)	123.9(7)
C(131)-K(2)-C(500)	103.2(7)
C(101)-K(2)-C(500)	145.9(7)
O(100)-K(2)-C(81)	130.1(7)
F(71)#2-K(2)-C(81)	114.8(3)
S(11)-K(2)-C(81)	56.10(19)
C(121)-K(2)-C(81)	42.0(2)
C(31)#2-K(2)-C(81)	122.3(3)
C(111)-K(2)-C(81)	49.3(2)
C(131)-K(2)-C(81)	23.5(2)
C(101)-K(2)-C(81)	40.8(2)
C(500)-K(2)-C(81)	120.7(6)
O(100)-K(2)-C(91)	148.7(7)
F(71)#2-K(2)-C(91)	93.5(3)
S(11)-K(2)-C(91)	67.5(2)
C(121)-K(2)-C(91)	48.8(2)
C(31)#2-K(2)-C(91)	99.0(3)
C(111)-K(2)-C(91)	42.2(2)
C(131)-K(2)-C(91)	41.5(2)
C(101)-K(2)-C(91)	23.2(2)
C(500)-K(2)-C(91)	143.7(7)
C(81)-K(2)-C(91)	23.3(2)
C(164)-C(184)-H(18G)	109.5
C(164)-C(184)-H(18H)	109.5
H(18G)-C(184)-H(18H)	109.5
C(164)-C(184)-H(18I)	109.5
H(18G)-C(184)-H(18I)	109.5
H(18H)-C(184)-H(18I)	109.5
C(5)-O(1)-C(2)	107.0(18)
C(5)-O(1)-K(1)	129.5(14)
C(2)-O(1)-K(1)	123.5(13)
O(1)-C(2)-C(3)	109(2)
O(1)-C(2)-H(2A)	109.8
C(3)-C(2)-H(2A)	109.8
O(1)-C(2)-H(2B)	109.8
C(3)-C(2)-H(2B)	109.8
H(2A)-C(2)-H(2B)	108.2
C(2)-C(3)-C(4)	96(3)
C(2)-C(3)-H(3A)	112.5
C(4)-C(3)-H(3A)	112.5

C(2)-C(3)-H(3B)	112.5
C(4)-C(3)-H(3B)	112.5
H(3A)-C(3)-H(3B)	110.0
C(5)-C(4)-C(3)	96(3)
C(5)-C(4)-H(4A)	112.6
C(3)-C(4)-H(4A)	112.6
C(5)-C(4)-H(4B)	112.6
C(3)-C(4)-H(4B)	112.6
H(4A)-C(4)-H(4B)	110.1
O(1)-C(5)-C(4)	121(3)
O(1)-C(5)-H(5A)	107.2
C(4)-C(5)-H(5A)	107.2
O(1)-C(5)-H(5B)	107.2
C(4)-C(5)-H(5B)	107.2
H(5A)-C(5)-H(5B)	106.8
C(500)-O(100)-C(200)	106(2)
C(500)-O(100)-K(2)	117(2)
C(200)-O(100)-K(2)	132(2)
O(100)-C(200)-C(300)	110(3)
O(100)-C(200)-H(20D)	109.6
C(300)-C(200)-H(20D)	109.6
O(100)-C(200)-H(20E)	109.6
C(300)-C(200)-H(20E)	109.6
H(20D)-C(200)-H(20E)	108.1
C(200)-C(300)-C(400)	99(3)
C(200)-C(300)-H(30A)	111.9
C(400)-C(300)-H(30A)	111.9
C(200)-C(300)-H(30B)	111.9
C(400)-C(300)-H(30B)	111.9
H(30A)-C(300)-H(30B)	109.6
C(500)-C(400)-C(300)	93(3)
C(500)-C(400)-H(40A)	113.1
C(300)-C(400)-H(40A)	113.1
C(500)-C(400)-H(40B)	113.1
C(300)-C(400)-H(40B)	113.1
H(40A)-C(400)-H(40B)	110.5
O(100)-C(500)-C(400)	113(3)
O(100)-C(500)-K(2)	42.8(18)
C(400)-C(500)-K(2)	120(3)
O(100)-C(500)-H(50A)	108.9
C(400)-C(500)-H(50A)	108.9
K(2)-C(500)-H(50A)	66.8
O(100)-C(500)-H(50B)	108.9
C(400)-C(500)-H(50B)	108.9
K(2)-C(500)-H(50B)	129.7
H(50A)-C(500)-H(50B)	107.7

Symmetry transformations used to generate equivalent atoms:
#1 x-1,y,z #2 x+1,y,z

Anisotropic displacement parameters ($Å^2 x\ 10^3$) for [$LFeSC_6H_4Ar$]K (5). The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Fe(1)	118(1)	50(1)	43(1)	4(1)	4(1)	26(1)
S(11)	48(2)	52(1)	61(1)	-9(1)	5(1)	2(1)
S(21)	55(2)	63(2)	66(2)	19(1)	10(1)	13(1)
S(31)	97(2)	61(2)	67(2)	-20(1)	-29(1)	34(2)
F(72)	52(3)	58(3)	85(4)	13(3)	27(3)	6(2)
F(71)	47(3)	77(3)	62(3)	2(3)	10(3)	-1(3)
C(24)	51(5)	38(4)	51(5)	0(4)	3(4)	1(4)
C(61)	48(6)	46(5)	56(6)	2(4)	7(5)	-4(4)
C(81)	59(6)	43(5)	46(5)	-6(4)	3(4)	-2(4)
C(53)	49(6)	53(5)	50(5)	7(4)	5(4)	0(4)
C(194)	51(6)	57(5)	42(5)	-4(4)	2(4)	5(4)
C(34)	47(5)	43(5)	53(5)	1(4)	4(4)	3(4)
C(41)	67(7)	46(5)	61(6)	0(5)	-2(5)	-13(5)
C(22)	43(6)	48(5)	49(5)	-3(4)	4(4)	3(4)
C(32)	51(6)	52(5)	56(5)	4(4)	16(5)	2(4)
C(142)	47(5)	52(5)	36(4)	0(4)	5(4)	7(4)
C(91)	41(5)	42(5)	55(5)	-3(4)	8(4)	-4(4)
C(141)	49(6)	60(6)	46(5)	0(4)	3(4)	0(4)
C(111)	65(6)	56(5)	44(5)	-2(4)	6(4)	4(5)
C(84)	47(5)	44(5)	61(5)	1(4)	11(4)	6(4)
C(92)	45(5)	45(5)	40(5)	-4(4)	0(4)	2(4)
C(51)	52(6)	50(5)	57(6)	-5(4)	2(5)	-1(5)
C(74)	50(5)	43(4)	41(4)	3(4)	7(4)	7(5)
C(42)	60(6)	46(5)	62(6)	6(4)	10(5)	14(4)
C(43)	57(5)	46(5)	53(5)	9(4)	14(4)	7(4)
C(124)	52(6)	49(5)	41(5)	2(4)	9(4)	0(4)
C(104)	57(6)	52(5)	44(5)	1(4)	7(4)	8(4)
C(101)	54(6)	44(5)	56(6)	-5(4)	0(5)	0(4)
C(214)	76(8)	56(6)	84(7)	8(5)	36(6)	-1(5)
C(114)	60(6)	45(5)	54(5)	0(4)	7(5)	-1(4)
C(94)	59(6)	49(5)	62(6)	3(4)	14(5)	4(4)
C(52)	44(5)	45(5)	53(5)	7(4)	5(4)	7(4)
C(63)	40(5)	46(5)	52(5)	2(4)	1(4)	3(4)
C(64)	39(5)	36(4)	58(5)	0(4)	5(4)	7(4)
C(31)	46(6)	58(5)	49(5)	6(4)	1(4)	-1(5)
C(132)	59(6)	60(5)	40(5)	-6(4)	-1(4)	-5(4)
C(14)	49(5)	41(4)	42(5)	6(4)	-5(4)	-2(4)
C(12)	58(6)	38(4)	44(5)	3(4)	-2(4)	3(4)
C(171)	68(7)	103(7)	56(6)	-13(5)	14(5)	10(5)
C(164)	66(6)	50(5)	52(5)	-10(4)	13(4)	6(4)
C(121)	73(7)	58(5)	49(5)	-1(4)	13(5)	-8(5)
C(44)	54(6)	60(5)	44(5)	-4(4)	-6(4)	14(4)
C(152)	62(6)	66(6)	44(5)	-2(4)	-6(5)	11(5)
C(13)	53(5)	41(4)	48(4)	8(4)	8(4)	11(5)
C(23)	59(6)	43(5)	51(5)	7(4)	15(4)	4(4)
C(62)	48(6)	51(5)	40(5)	1(4)	-4(4)	1(4)
C(54)	55(6)	54(5)	41(5)	-1(4)	0(4)	13(5)
C(102)	52(6)	68(6)	46(5)	-11(4)	7(5)	-11(5)
C(222)	62(6)	78(6)	54(5)	-8(4)	4(4)	4(5)
C(82)	43(5)	46(5)	43(5)	3(4)	2(4)	-2(4)

C(21)	56(6)	44(5)	41(5)	3(4)	-1(4)	2(4)
C(161)	80(7)	54(6)	62(6)	8(5)	6(5)	-13(5)
C(162)	68(7)	54(5)	47(5)	-7(4)	3(5)	11(5)
C(11)	51(6)	43(5)	45(5)	-3(4)	0(4)	4(4)
C(122)	69(7)	75(6)	48(5)	-15(5)	8(5)	-19(5)
C(112)	61(7)	74(6)	55(6)	-15(5)	20(5)	-11(5)
C(202)	89(7)	75(6)	48(5)	-3(4)	-9(5)	-27(5)
C(201)	96(9)	62(6)	63(7)	19(5)	14(6)	24(6)
C(204)	71(7)	81(7)	62(6)	-8(5)	17(6)	-10(6)
C(134)	64(7)	52(6)	93(8)	-7(5)	29(6)	5(5)
C(33)	59(6)	46(5)	50(5)	2(4)	15(4)	8(4)
C(131)	69(7)	46(5)	48(5)	-3(4)	6(5)	11(4)
C(154)	71(8)	76(7)	92(8)	-11(6)	15(6)	-18(6)
C(151)	80(8)	66(6)	44(5)	0(4)	-6(5)	-8(5)
C(192)	88(9)	74(7)	116(10)	7(7)	51(8)	-8(6)
C(172)	72(8)	109(9)	60(7)	-22(6)	20(6)	-39(7)
C(221)	79(8)	94(8)	65(7)	21(6)	1(6)	3(6)
C(144)	98(10)	53(6)	182(15)	13(8)	27(10)	-3(6)
C(182)	73(9)	182(15)	118(11)	27(11)	46(8)	23(10)
C(191)	100(10)	198(13)	94(9)	-66(9)	8(7)	31(9)
C(181)	90(9)	159(11)	91(9)	22(8)	13(7)	-12(8)
C(212)	180(13)	61(6)	114(10)	-12(6)	-87(9)	-11(7)
C(211)	214(18)	63(8)	116(11)	2(7)	-53(11)	35(9)
C(174)	139(12)	270(20)	113(11)	-114(13)	-1(8)	7(11)
O(10)	126(9)	247(16)	104(8)	26(9)	-16(7)	-65(10)
C(30)	143(15)	207(18)	119(13)	50(15)	58(13)	18(17)
C(20)	131(15)	230(30)	230(30)	-63(19)	5(17)	-68(16)
C(40)	129(16)	159(15)	169(19)	21(14)	-20(16)	13(14)
C(50)	190(20)	480(50)	170(20)	180(30)	-44(18)	-140(30)
K(1)	127(4)	105(4)	95(3)	35(2)	45(3)	-1(3)
K(2)	59(4)	94(5)	64(4)	-8(3)	9(3)	14(3)
C(184)	286(19)	121(10)	83(9)	2(7)	43(10)	120(13)
O(1)	122(10)	97(9)	105(10)	14(6)	-22(8)	7(7)
C(2)	180(30)	108(12)	107(15)	3(10)	-25(14)	16(12)
C(3)	440(50)	132(19)	220(30)	-12(15)	140(30)	-30(20)
C(4)	590(80)	127(18)	124(15)	-11(13)	80(30)	-10(30)
C(5)	240(40)	108(13)	90(13)	10(10)	-29(14)	-2(13)

Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for [$LFeSC_6H_4Ar$]K (5).

	x	y	z	U(eq)
H(24)	7335	4091	4947	56
H(53)	1757	4052	5313	61
H(194)	9331	5478	6460	60
H(34)	9053	3394	5394	57
H(41)	481	2810	3187	70
H(142)	5280	7325	4383	54
H(141)	5105	2645	3996	62

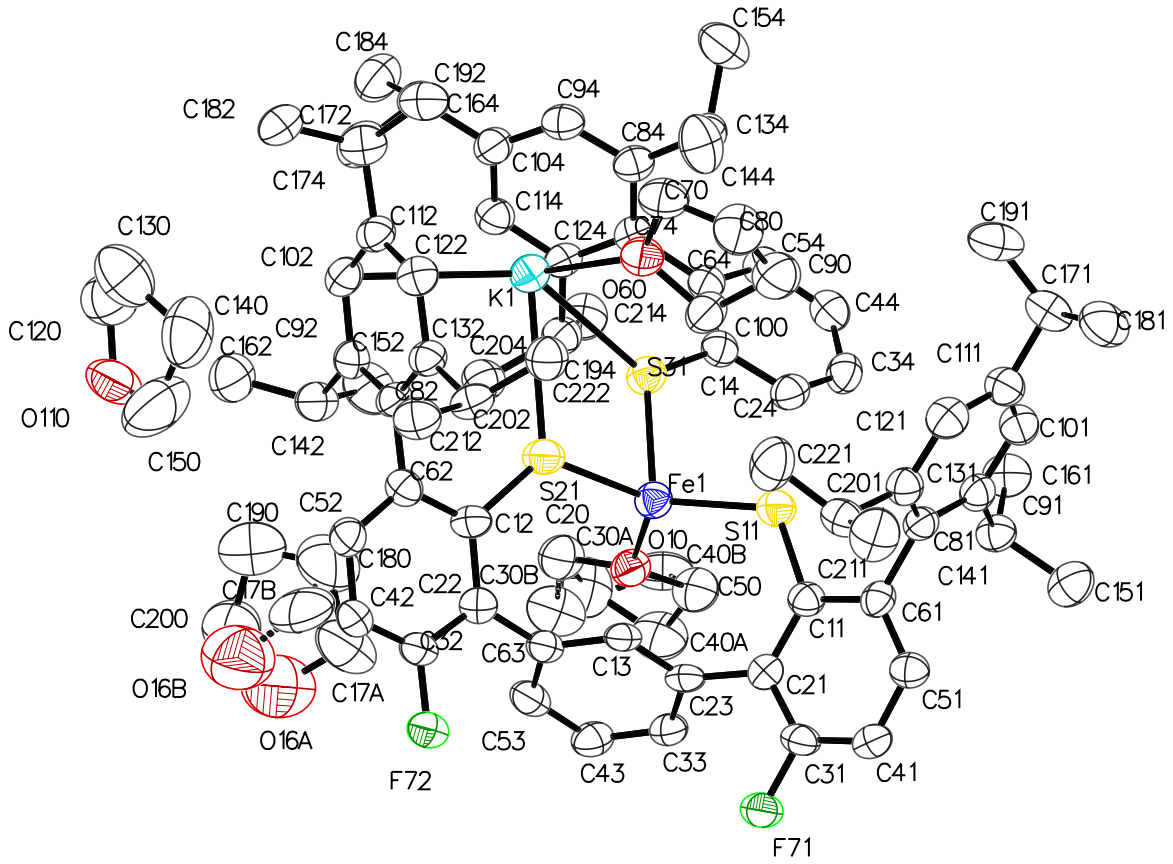
H(51)	2634	2578	2594	64
H(42)	403	7327	3655	67
H(43)	1501	4904	6047	62
H(101)	8096	2262	2822	61
H(21A)	8006	6329	6133	107
H(21B)	9717	6471	6103	107
H(21C)	8799	6701	6813	107
H(114)	8098	6363	8033	63
H(94)	4922	5210	8615	68
H(52)	2532	7645	3071	57
H(171)	9769	2348	1837	91
H(164)	5301	6029	9387	67
H(121)	6970	3348	1064	71
H(44)	10088	3474	6630	63
H(15A)	7811	7127	4573	86
H(15B)	7262	7609	5183	86
H(15C)	8161	7827	4462	86
H(13)	2778	5078	3489	57
H(54)	9190	4218	7466	60
H(102)	8020	7920	3184	66
H(22A)	3253	7355	1054	97
H(22B)	2747	6713	724	97
H(22C)	4374	6948	595	97
H(16A)	4660	1736	3320	98
H(16B)	5191	1617	4189	98
H(16C)	6309	1532	3510	98
H(16D)	6008	8531	3995	84
H(16E)	5364	8345	4805	84
H(16F)	4395	8257	4034	84
H(122)	6503	7157	1243	77
H(202)	3200	6612	2020	85
H(201)	3523	3774	1820	88
H(20A)	10663	6143	7670	107
H(20B)	11463	5888	6934	107
H(20C)	10841	5432	7555	107
H(134)	5502	4183	7057	83
H(33)	1906	5869	5531	62
H(15D)	3278	4583	8033	119
H(15E)	3099	4076	7385	119
H(15F)	3366	4761	7147	119
H(15G)	8057	2232	4132	95
H(15H)	6997	2354	4828	95
H(15I)	7575	2905	4330	95
H(19A)	7833	7943	621	137
H(19B)	9080	8426	827	137
H(19C)	7498	8490	1185	137
H(172)	9290	8099	2072	96
H(22D)	4847	3605	371	118
H(22E)	3204	3820	498	118
H(22F)	3683	3146	708	118
H(14A)	6623	3752	8144	165
H(14B)	4976	3511	8089	165
H(14C)	5420	4030	8688	165
H(18A)	10173	7146	1945	185
H(18B)	10613	7547	1226	185
H(18C)	9310	7069	1140	185

H(19D)	8146	1861	946	196
H(19E)	9656	2038	565	196
H(19F)	8224	2435	395	196
H(18D)	9455	3389	877	170
H(18E)	10927	3005	981	170
H(18F)	10316	3376	1689	170
H(21D)	5426	6045	1195	180
H(21E)	3814	5788	1308	180
H(21F)	4932	5842	2028	180
H(21G)	5086	4556	2023	198
H(21H)	4362	4650	1185	198
H(21I)	5992	4394	1281	198
H(17A)	7552	6819	9523	260
H(17B)	8078	6134	9477	260
H(17C)	6983	6337	10126	260
H(30C)	10451	5449	9022	187
H(30D)	11298	4820	8983	187
H(20F)	12851	5538	9411	296
H(20G)	12580	5072	10091	296
H(20H)	11778	5712	10083	296
H(40C)	9177	4274	9175	184
H(40D)	8459	4923	9049	184
H(50C)	6743	4678	9780	422
H(50D)	7897	4588	10478	422
H(50E)	7487	4035	9926	422
H(18G)	5688	7158	8954	244
H(18H)	4201	6779	8937	244
H(18I)	5216	6780	8206	244
H(2A)	8307	4575	2331	161
H(2B)	9746	4391	2823	161
H(3A)	9901	4601	1406	313
H(3B)	11231	4807	1983	313
H(4A)	10424	5903	1619	333
H(4B)	8784	5685	1375	333
H(5A)	9838	6013	2749	176
H(5B)	8187	5889	2488	176
H(20D)	10500	5126	1270	88
H(20E)	11206	4873	2058	88
H(30A)	10960	6019	1666	246
H(30B)	11489	5767	2499	246
H(40A)	8858	5879	3035	138
H(40B)	8512	6317	2304	138
H(50A)	7290	5338	2320	126
H(50B)	7986	5562	1541	126

Experimental and Refinement Details for [LFeSC$_6$H$_4$Ar(THF)]K (5·THF)

Single crystals of [LFeSC$_6$H$_4$Ar(THF)]K (**5**·THF) for X-ray analysis were obtained at -40 °C from a concentrated solution of [LFeSC$_6$H$_4$Ar]K (**5**) in THF. Crystals were taken into cold Fomblin Y oil in the cold well (-70 °C) and transported cold (-78 °C) in a closed jar. Suitable crystal was selected under microscope while keeping the sample under cold nitrogen stream (< -80 °C). The pin with the crystal was immediately placed in the cold (liquid N_2) cryo-tongs, transported on dry ice, and the crystal was placed on the goniometer under a cold nitrogen stream. Low-temperature diffraction data (ω-scans) were collected on a Rigaku MicroMax-007HF diffractometer coupled to a Saturn994+ CCD detector with Cu Kα (λ = 1.54178 Å). All structures were solved by direct methods and were refined against F^2 on all data by full-matrix least squares[50]. All non-hydrogen atoms were refined anisotropically. Unless stated otherwise, hydrogen atoms were included in the model at geometrically calculated positions and refined using a riding model. The isotropic displacement parameters of all hydrogen atoms were fixed to 1.2 times the U value of the atoms to which they are linked (1.5 times for methyl groups).

Two of the four THF solvents were disordered. Atoms {C30, C40} were modeled with a major and minor component delineated with the suffixes "a" and "b", respectively. The site occupancies were freely refined to convergence at values of 0.77(8) and 0.23(1). The RIGU command was used to aid in the convergence of C30 and C40. This rigid bond restraint was needed due to the near superposition of the carbon atoms positions as a result of disorder. Atoms {O16 C17} were modeled with major and minor components delineated with the suffixes "a" and "b", respectively. The site occupancies were refined, and converged at values of 0.67(1) and 0.33(1). The rigid bond restraint was used in this model for similar reasons as mentioned previously with atoms C30 and C40. However, the bond distances were chemically unreasonable and therefore required additional similarity restraints. A SIMU command with a standard deviation of 0.002 was used to establish the {C200-C190, C190-C180, C180-C17B, C180-C17A} bonds as similar.



The full numbering scheme of [LFeSC$_6$H$_4$Ar(THF)]K (**5**·THF). All atoms shown are depicted with 50% thermal contours. The hydrogen atoms have been removed for clarity.

Crystal data and structure refinement for [$LFeSC_6H_4Ar(THF)$]K (5·THF).

Identification code	007-15021	
Empirical formula	C85 H113 F2 Fe K O4 S3	
Formula weight	1427.88	
Temperature	93(2) K	
Wavelength	1.54187 Å	
Crystal system	Monoclinic	
Space group	P 2_1/c	
Unit cell dimensions	a = 17.371(5) Å	α = 90°.
	b = 16.4629(3) Å	β = 107.059(10)°.
	c = 28.368(2) Å	γ = 90°.
Volume	7756(2) $Å^3$	
Z	4	
Density (calculated)	1.223 g/cm^3	
Absorption coefficient	3.210 mm^{-1}	
F(000)	3064	
Crystal size	0.190 x 0.180 x 0.020 mm^3	
Crystal color and habit	Yellow plate	
Diffractometer	Rigaku Saturn 944+ CCD	
Θ range for data collection	2.661 to 66.603°.	
Index ranges	$-20 \le h \le 20$, $-19 \le k \le 19$, $-32 \le l \le 31$	
Reflections collected	172297	
Independent reflections	13584 [R(int) = 0.2073]	
Observed reflections (I > 2σ(I))	6660	
Completeness to θ = 66.603°	99.1 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.939 and 0.572	
Solution method	SHELXS-2013 (Sheldrick, 2013)	
Refinement method	SHELXL-2014/7 (Sheldrick, 2014)	
Data / restraints / parameters	13584 / 87 / 921	
Goodness-of-fit on F^2	0.906	
Final R indices [I>2σ(I)]	R1 = 0.0663, wR2 = 0.1469	
R indices (all data)	R1 = 0.1314, wR2 = 0.1720	
Largest diff. peak and hole	0.880 and -0.492 e.$Å^{-3}$	

Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for [$LFeSC_6H_4Ar(THF)$]K (5·THF). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Fe(1)	7030(1)	3166(1)	6990(1)	41(1)
S(11)	5753(1)	3337(1)	7060(1)	45(1)
S(21)	7385(1)	2030(1)	6618(1)	54(1)
S(31)	7068(1)	3846(1)	6262(1)	45(1)
C(11)	5553(2)	3022(2)	7606(2)	38(1)
C(21)	6150(2)	2774(2)	8041(2)	37(1)
C(31)	5915(3)	2622(2)	8456(2)	41(1)
C(41)	5135(3)	2687(2)	8476(2)	43(1)
C(51)	4554(3)	2893(2)	8046(2)	42(1)
C(61)	4742(2)	3046(2)	7612(2)	39(1)
F(71)	6481(1)	2378(1)	8878(1)	49(1)
C(81)	4058(2)	3218(3)	7151(2)	38(1)
C(91)	3809(3)	4018(2)	7026(2)	41(1)
C(101)	3148(3)	4150(3)	6611(2)	48(1)
C(111)	2749(3)	3526(3)	6318(2)	48(1)
C(121)	3017(3)	2733(3)	6448(2)	49(1)
C(131)	3670(3)	2562(3)	6864(2)	44(1)
C(141)	4219(3)	4725(2)	7341(2)	44(1)
C(151)	3720(3)	4973(3)	7684(2)	60(1)
C(161)	4347(3)	5453(3)	7038(2)	59(1)
C(171)	2050(3)	3693(3)	5858(2)	58(1)
C(181)	1257(3)	3378(3)	5918(2)	72(2)
C(191)	2192(3)	3394(3)	5395(2)	69(2)
C(201)	3942(3)	1697(3)	6984(2)	50(1)
C(211)	3271(3)	1140(3)	7045(2)	76(2)
C(221)	4311(3)	1337(3)	6614(2)	75(2)
C(12)	7951(3)	1229(2)	6958(2)	42(1)
C(22)	8162(2)	1177(2)	7478(2)	41(1)
C(32)	8565(3)	480(3)	7694(2)	44(1)
C(42)	8773(3)	-151(3)	7446(2)	46(1)
C(52)	8578(2)	-79(3)	6939(2)	46(1)
C(62)	8173(2)	592(2)	6687(2)	40(1)
F(72)	8734(1)	408(1)	8196(1)	57(1)
C(82)	7962(3)	624(2)	6135(2)	41(1)
C(92)	8506(3)	945(2)	5908(2)	43(1)
C(102)	8283(3)	964(2)	5389(2)	45(1)
C(112)	7551(3)	673(2)	5098(2)	43(1)
C(122)	7027(3)	356(2)	5337(2)	45(1)
C(132)	7212(3)	330(2)	5852(2)	42(1)
C(142)	9314(3)	1300(3)	6201(2)	51(1)
C(152)	9268(3)	2237(3)	6198(2)	75(2)
C(162)	10017(3)	1027(3)	6025(2)	72(2)
C(172)	7359(3)	691(3)	4538(2)	53(1)
C(182)	7799(3)	26(3)	4354(2)	74(2)
C(192)	6461(3)	663(3)	4264(2)	62(1)
C(202)	6626(3)	-42(2)	6094(2)	47(1)
C(212)	6720(3)	-968(3)	6122(2)	57(1)
C(222)	5750(3)	201(3)	5847(2)	56(1)

C(13)	7186(2)	2041(2)	7756(1)	35(1)
C(23)	7006(3)	2621(2)	8065(1)	38(1)
C(33)	7645(3)	2991(3)	8418(2)	43(1)
C(43)	8431(3)	2790(3)	8458(2)	46(1)
C(53)	8603(3)	2198(3)	8151(2)	47(1)
C(63)	7978(3)	1817(2)	7794(2)	40(1)
C(14)	6794(2)	4877(2)	6182(2)	40(1)
C(24)	6410(2)	5274(3)	6490(2)	43(1)
C(34)	6250(2)	6093(3)	6444(2)	45(1)
C(44)	6467(2)	6543(3)	6087(2)	47(1)
C(54)	6818(2)	6161(2)	5771(2)	43(1)
C(64)	6987(2)	5330(2)	5807(2)	38(1)
C(74)	7375(3)	4927(2)	5464(2)	39(1)
C(84)	6911(3)	4656(2)	4996(2)	44(1)
C(94)	7307(3)	4262(2)	4699(2)	46(1)
C(104)	8118(3)	4121(3)	4837(2)	45(1)
C(114)	8566(3)	4410(3)	5301(2)	46(1)
C(124)	8212(3)	4808(2)	5615(2)	40(1)
C(134)	6009(3)	4766(3)	4816(2)	48(1)
C(144)	5599(3)	3961(3)	4818(2)	71(2)
C(154)	5712(3)	5118(3)	4298(2)	74(2)
C(164)	8512(3)	3677(3)	4504(2)	49(1)
C(174)	8798(3)	2844(3)	4714(2)	78(2)
C(184)	9198(3)	4139(3)	4405(2)	70(2)
C(194)	8731(3)	5118(3)	6115(2)	48(1)
C(204)	9466(3)	4597(3)	6347(2)	55(1)
C(214)	8980(3)	5998(3)	6070(2)	62(1)
K(1)	7130(1)	2505(1)	5504(1)	52(1)
O(10)	7970(2)	3787(2)	7467(1)	45(1)
C(20)	8767(3)	3839(3)	7401(2)	63(1)
C(30A)	9117(5)	4638(7)	7660(4)	83(3)
C(40A)	8608(4)	4853(5)	7985(4)	77(3)
C(30B)	9303(19)	4236(19)	7774(12)	75(7)
C(40B)	8503(15)	5138(15)	7600(11)	72(7)
C(50)	7813(3)	4556(3)	7671(2)	58(1)
O(60)	5559(2)	2193(2)	5376(1)	53(1)
C(70)	4891(3)	1906(3)	4987(2)	61(1)
C(80)	4172(3)	1941(3)	5189(2)	72(2)
C(90)	4373(3)	2640(3)	5539(2)	72(2)
C(100)	5271(3)	2547(3)	5761(2)	57(1)
O(110)	9960(3)	-1160(2)	5864(2)	95(1)
C(120)	9756(4)	-1060(4)	5353(2)	92(2)
C(130)	9105(4)	-1638(4)	5158(3)	102(2)
C(140)	8621(4)	-1606(5)	5519(3)	116(2)
C(150)	9323(5)	-1537(6)	5989(3)	140(3)
O(16A)	11613(5)	2412(8)	8084(3)	148(4)
C(17A)	10800(6)	2600(7)	7854(3)	99(4)
O(16B)	11561(12)	1796(15)	7849(8)	152(7)
C(17B)	10722(14)	1930(7)	7565(8)	121(6)
C(180)	10754(4)	2716(6)	7339(2)	141(3)
C(190)	11522(4)	2637(6)	7236(2)	153(3)
C(200)	12086(4)	2661(4)	7730(2)	106(2)

Bond lengths [Å] and angles [°] for [LFeSC$_6$H$_4$Ar(THF)]K (5·THF).

Fe(1)-O(10)	2.061(3)
Fe(1)-S(11)	2.3029(14)
Fe(1)-S(21)	2.3174(12)
Fe(1)-S(31)	2.3671(12)
S(11)-C(11)	1.762(4)
S(21)-C(12)	1.754(4)
S(21)-K(1)	3.1611(15)
S(31)-C(14)	1.759(4)
S(31)-K(1)	3.1063(14)
C(11)-C(61)	1.413(5)
C(11)-C(21)	1.419(5)
C(21)-C(31)	1.379(5)
C(21)-C(23)	1.490(5)
C(31)-F(71)	1.368(4)
C(31)-C(41)	1.376(6)
C(41)-C(51)	1.377(5)
C(41)-H(41)	0.9500
C(51)-C(61)	1.388(5)
C(51)-H(51)	0.9500
C(61)-C(81)	1.513(6)
C(81)-C(91)	1.398(5)
C(81)-C(131)	1.402(5)
C(91)-C(101)	1.399(6)
C(91)-C(141)	1.512(5)
C(101)-C(111)	1.375(6)
C(101)-H(101)	0.9500
C(111)-C(121)	1.399(6)
C(111)-C(171)	1.523(6)
C(121)-C(131)	1.404(6)
C(121)-H(121)	0.9500
C(131)-C(201)	1.508(6)
C(141)-C(161)	1.528(6)
C(141)-C(151)	1.538(6)
C(141)-H(141)	1.0000
C(151)-H(15A)	0.9800
C(151)-H(15B)	0.9800
C(151)-H(15C)	0.9800
C(161)-H(16A)	0.9800
C(161)-H(16B)	0.9800
C(161)-H(16C)	0.9800
C(171)-C(191)	1.489(6)
C(171)-C(181)	1.526(6)
C(171)-H(171)	1.0000
C(181)-H(18A)	0.9800
C(181)-H(18B)	0.9800
C(181)-H(18C)	0.9800
C(191)-H(19A)	0.9800
C(191)-H(19B)	0.9800
C(191)-H(19C)	0.9800
C(201)-C(221)	1.503(6)
C(201)-C(211)	1.531(6)
C(201)-H(201)	1.0000
C(211)-H(21A)	0.9800
C(211)-H(21B)	0.9800

C(211)-H(21C)	0.9800
C(221)-H(22A)	0.9800
C(221)-H(22B)	0.9800
C(221)-H(22C)	0.9800
C(12)-C(22)	1.416(5)
C(12)-C(62)	1.418(5)
C(22)-C(32)	1.388(5)
C(22)-C(63)	1.477(6)
C(32)-C(42)	1.361(6)
C(32)-F(72)	1.374(5)
C(42)-C(52)	1.383(5)
C(42)-H(42)	0.9500
C(52)-C(62)	1.389(5)
C(52)-H(52)	0.9500
C(62)-C(82)	1.503(6)
C(82)-C(92)	1.395(6)
C(82)-C(132)	1.401(6)
C(92)-C(102)	1.408(6)
C(92)-C(142)	1.522(6)
C(92)-K(1)	3.467(4)
C(102)-C(112)	1.383(6)
C(102)-K(1)	3.307(4)
C(102)-H(102)	0.9500
C(112)-C(122)	1.387(6)
C(112)-C(172)	1.523(6)
C(112)-K(1)	3.384(4)
C(122)-C(132)	1.402(5)
C(122)-H(122)	0.9500
C(132)-C(202)	1.514(6)
C(142)-C(162)	1.516(6)
C(142)-C(152)	1.544(6)
C(142)-H(142)	1.0000
C(152)-H(15D)	0.9800
C(152)-H(15E)	0.9800
C(152)-H(15F)	0.9800
C(162)-H(16D)	0.9800
C(162)-H(16E)	0.9800
C(162)-H(16F)	0.9800
C(172)-C(182)	1.511(6)
C(172)-C(192)	1.526(6)
C(172)-H(172)	1.0000
C(182)-H(18D)	0.9800
C(182)-H(18E)	0.9800
C(182)-H(18F)	0.9800
C(192)-H(19D)	0.9800
C(192)-H(19E)	0.9800
C(192)-H(19F)	0.9800
C(202)-C(222)	1.530(6)
C(202)-C(212)	1.533(6)
C(202)-H(202)	1.0000
C(212)-H(21D)	0.9800
C(212)-H(21E)	0.9800
C(212)-H(21F)	0.9800
C(222)-H(22D)	0.9800
C(222)-H(22E)	0.9800
C(222)-H(22F)	0.9800

C(13)-C(23)	1.392(5)
C(13)-C(63)	1.398(5)
C(13)-H(13)	0.9500
C(23)-C(33)	1.397(5)
C(33)-C(43)	1.377(5)
C(33)-H(33)	0.9500
C(43)-C(53)	1.397(6)
C(43)-H(43)	0.9500
C(53)-C(63)	1.398(5)
C(53)-H(53)	0.9500
C(14)-C(24)	1.408(5)
C(14)-C(64)	1.418(5)
C(24)-C(34)	1.375(5)
C(24)-H(24)	0.9500
C(34)-C(44)	1.393(6)
C(34)-H(34)	0.9500
C(44)-C(54)	1.375(5)
C(44)-H(44)	0.9500
C(54)-C(64)	1.396(5)
C(54)-H(54)	0.9500
C(64)-C(74)	1.491(5)
C(74)-C(124)	1.404(6)
C(74)-C(84)	1.410(5)
C(84)-C(94)	1.393(6)
C(84)-C(134)	1.510(6)
C(94)-C(104)	1.366(6)
C(94)-H(94)	0.9500
C(104)-C(114)	1.402(6)
C(104)-C(164)	1.508(6)
C(114)-C(124)	1.387(5)
C(114)-H(114)	0.9500
C(124)-C(194)	1.528(6)
C(134)-C(144)	1.505(6)
C(134)-C(154)	1.523(6)
C(134)-H(134)	1.0000
C(144)-H(14A)	0.9800
C(144)-H(14B)	0.9800
C(144)-H(14C)	0.9800
C(154)-H(15G)	0.9800
C(154)-H(15H)	0.9800
C(154)-H(15I)	0.9800
C(164)-C(184)	1.507(6)
C(164)-C(174)	1.520(6)
C(164)-H(164)	1.0000
C(174)-H(17A)	0.9800
C(174)-H(17B)	0.9800
C(174)-H(17C)	0.9800
C(184)-H(18G)	0.9800
C(184)-H(18H)	0.9800
C(184)-H(18I)	0.9800
C(194)-C(204)	1.519(6)
C(194)-C(214)	1.529(6)
C(194)-H(194)	1.0000
C(204)-H(20A)	0.9800
C(204)-H(20B)	0.9800
C(204)-H(20C)	0.9800

C(214)-H(21G)	0.9800
C(214)-H(21H)	0.9800
C(214)-H(21I)	0.9800
K(1)-O(60)	2.696(3)
O(10)-C(50)	1.451(5)
O(10)-C(20)	1.452(5)
C(20)-C(30B)	1.36(3)
C(20)-C(30A)	1.542(10)
C(20)-H(20D)	0.9900
C(20)-H(20E)	0.9900
C(20)-H(20F)	0.9900
C(20)-H(20G)	0.9900
C(30A)-C(40A)	1.496(12)
C(30A)-H(30A)	0.9900
C(30A)-H(30B)	0.9900
C(40A)-C(50)	1.489(8)
C(40A)-H(40A)	0.9900
C(40A)-H(40B)	0.9900
C(30B)-C(40B)	1.99(4)
C(30B)-H(30C)	0.9900
C(30B)-H(30D)	0.9900
C(40B)-C(50)	1.59(2)
C(40B)-H(40C)	0.9900
C(40B)-H(40D)	0.9900
C(50)-H(50A)	0.9900
C(50)-H(50B)	0.9900
C(50)-H(50C)	0.9900
C(50)-H(50D)	0.9900
O(60)-C(70)	1.425(5)
O(60)-C(100)	1.449(5)
C(70)-C(80)	1.521(6)
C(70)-H(70A)	0.9900
C(70)-H(70B)	0.9900
C(80)-C(90)	1.492(6)
C(80)-H(80A)	0.9900
C(80)-H(80B)	0.9900
C(90)-C(100)	1.508(6)
C(90)-H(90A)	0.9900
C(90)-H(90B)	0.9900
C(100)-H(10A)	0.9900
C(100)-H(10B)	0.9900
O(110)-C(120)	1.396(6)
O(110)-C(150)	1.401(8)
C(120)-C(130)	1.456(8)
C(120)-H(12A)	0.9900
C(120)-H(12B)	0.9900
C(130)-C(140)	1.504(8)
C(130)-H(13A)	0.9900
C(130)-H(13B)	0.9900
C(140)-C(150)	1.524(9)
C(140)-H(14D)	0.9900
C(140)-H(14E)	0.9900
C(150)-H(15J)	0.9900
C(150)-H(15K)	0.9900
O(16A)-C(17A)	1.405(11)
O(16A)-C(200)	1.530(10)

C(17A)-C(180)	1.454(5)
C(17A)-H(17D)	0.9900
C(17A)-H(17E)	0.9900
O(16B)-C(17B)	1.46(3)
O(16B)-C(200)	1.78(2)
C(17B)-C(180)	1.452(5)
C(17B)-H(17F)	0.9900
C(17B)-H(17G)	0.9900
C(180)-C(190)	1.452(5)
C(180)-H(18L)	0.9900
C(180)-H(18M)	0.9900
C(180)-H(18J)	0.9900
C(180)-H(18K)	0.9900
C(190)-C(200)	1.454(5)
C(190)-H(19G)	0.9900
C(190)-H(19H)	0.9900
C(200)-H(20J)	0.9900
C(200)-H(20K)	0.9900
C(200)-H(20H)	0.9900
C(200)-H(20I)	0.9900

O(10)-Fe(1)-S(11)	118.70(9)
O(10)-Fe(1)-S(21)	115.73(9)
S(11)-Fe(1)-S(21)	121.96(5)
O(10)-Fe(1)-S(31)	96.83(8)
S(11)-Fe(1)-S(31)	106.99(5)
S(21)-Fe(1)-S(31)	84.63(4)
C(11)-S(11)-Fe(1)	118.95(14)
C(12)-S(21)-Fe(1)	122.58(15)
C(12)-S(21)-K(1)	128.80(15)
Fe(1)-S(21)-K(1)	106.07(4)
C(14)-S(31)-Fe(1)	119.55(15)
C(14)-S(31)-K(1)	131.25(15)
Fe(1)-S(31)-K(1)	106.46(4)
C(61)-C(11)-C(21)	118.5(4)
C(61)-C(11)-S(11)	117.1(3)
C(21)-C(11)-S(11)	124.5(3)
C(31)-C(21)-C(11)	118.0(4)
C(31)-C(21)-C(23)	118.2(4)
C(11)-C(21)-C(23)	123.7(4)
F(71)-C(31)-C(41)	116.9(4)
F(71)-C(31)-C(21)	118.9(4)
C(41)-C(31)-C(21)	124.2(4)
C(31)-C(41)-C(51)	117.3(4)
C(31)-C(41)-H(41)	121.4
C(51)-C(41)-H(41)	121.4
C(41)-C(51)-C(61)	121.9(4)
C(41)-C(51)-H(51)	119.1
C(61)-C(51)-H(51)	119.1
C(51)-C(61)-C(11)	119.9(4)
C(51)-C(61)-C(81)	118.1(4)
C(11)-C(61)-C(81)	121.9(4)
C(91)-C(81)-C(131)	121.2(4)
C(91)-C(81)-C(61)	120.1(4)
C(131)-C(81)-C(61)	118.7(4)
C(81)-C(91)-C(101)	118.4(4)

C(81)-C(91)-C(141)	121.1(4)
C(101)-C(91)-C(141)	120.4(4)
C(111)-C(101)-C(91)	122.5(4)
C(111)-C(101)-H(101)	118.8
C(91)-C(101)-H(101)	118.8
C(101)-C(111)-C(121)	117.9(4)
C(101)-C(111)-C(171)	121.1(4)
C(121)-C(111)-C(171)	121.0(4)
C(111)-C(121)-C(131)	122.2(4)
C(111)-C(121)-H(121)	118.9
C(131)-C(121)-H(121)	118.9
C(81)-C(131)-C(121)	117.8(4)
C(81)-C(131)-C(201)	122.1(4)
C(121)-C(131)-C(201)	120.1(4)
C(91)-C(141)-C(161)	113.1(3)
C(91)-C(141)-C(151)	108.9(3)
C(161)-C(141)-C(151)	110.4(3)
C(91)-C(141)-H(141)	108.1
C(161)-C(141)-H(141)	108.1
C(151)-C(141)-H(141)	108.1
C(141)-C(151)-H(15A)	109.5
C(141)-C(151)-H(15B)	109.5
H(15A)-C(151)-H(15B)	109.5
C(141)-C(151)-H(15C)	109.5
H(15A)-C(151)-H(15C)	109.5
H(15B)-C(151)-H(15C)	109.5
C(141)-C(161)-H(16A)	109.5
C(141)-C(161)-H(16B)	109.5
H(16A)-C(161)-H(16B)	109.5
C(141)-C(161)-H(16C)	109.5
H(16A)-C(161)-H(16C)	109.5
H(16B)-C(161)-H(16C)	109.5
C(191)-C(171)-C(111)	113.5(4)
C(191)-C(171)-C(181)	111.9(4)
C(111)-C(171)-C(181)	111.2(4)
C(191)-C(171)-H(171)	106.6
C(111)-C(171)-H(171)	106.6
C(181)-C(171)-H(171)	106.6
C(171)-C(181)-H(18A)	109.5
C(171)-C(181)-H(18B)	109.5
H(18A)-C(181)-H(18B)	109.5
C(171)-C(181)-H(18C)	109.5
H(18A)-C(181)-H(18C)	109.5
H(18B)-C(181)-H(18C)	109.5
C(171)-C(191)-H(19A)	109.5
C(171)-C(191)-H(19B)	109.5
H(19A)-C(191)-H(19B)	109.5
C(171)-C(191)-H(19C)	109.5
H(19A)-C(191)-H(19C)	109.5
H(19B)-C(191)-H(19C)	109.5
C(221)-C(201)-C(131)	112.6(4)
C(221)-C(201)-C(211)	109.7(4)
C(131)-C(201)-C(211)	113.1(4)
C(221)-C(201)-H(201)	107.0
C(131)-C(201)-H(201)	107.0
C(211)-C(201)-H(201)	107.0

C(201)-C(211)-H(21A)	109.5
C(201)-C(211)-H(21B)	109.5
H(21A)-C(211)-H(21B)	109.5
C(201)-C(211)-H(21C)	109.5
H(21A)-C(211)-H(21C)	109.5
H(21B)-C(211)-H(21C)	109.5
C(201)-C(221)-H(22A)	109.5
C(201)-C(221)-H(22B)	109.5
H(22A)-C(221)-H(22B)	109.5
C(201)-C(221)-H(22C)	109.5
H(22A)-C(221)-H(22C)	109.5
H(22B)-C(221)-H(22C)	109.5
C(22)-C(12)-C(62)	119.4(4)
C(22)-C(12)-S(21)	123.3(3)
C(62)-C(12)-S(21)	117.2(3)
C(32)-C(22)-C(12)	116.8(4)
C(32)-C(22)-C(63)	119.6(4)
C(12)-C(22)-C(63)	123.6(4)
C(42)-C(32)-F(72)	117.4(4)
C(42)-C(32)-C(22)	125.5(4)
F(72)-C(32)-C(22)	117.0(4)
C(32)-C(42)-C(52)	116.8(4)
C(32)-C(42)-H(42)	121.6
C(52)-C(42)-H(42)	121.6
C(42)-C(52)-C(62)	122.3(4)
C(42)-C(52)-H(52)	118.8
C(62)-C(52)-H(52)	118.8
C(52)-C(62)-C(12)	119.2(4)
C(52)-C(62)-C(82)	119.7(4)
C(12)-C(62)-C(82)	121.1(4)
C(92)-C(82)-C(132)	120.6(4)
C(92)-C(82)-C(62)	120.3(4)
C(132)-C(82)-C(62)	119.1(4)
C(82)-C(92)-C(102)	118.3(4)
C(82)-C(92)-C(142)	122.3(4)
C(102)-C(92)-C(142)	119.4(4)
C(82)-C(92)-K(1)	86.5(2)
C(102)-C(92)-K(1)	71.7(2)
C(142)-C(92)-K(1)	109.4(2)
C(112)-C(102)-C(92)	122.8(4)
C(112)-C(102)-K(1)	81.2(2)
C(92)-C(102)-K(1)	84.4(2)
C(112)-C(102)-H(102)	118.6
C(92)-C(102)-H(102)	118.6
K(1)-C(102)-H(102)	105.1
C(102)-C(112)-C(122)	117.3(4)
C(102)-C(112)-C(172)	119.9(4)
C(122)-C(112)-C(172)	122.9(4)
C(102)-C(112)-K(1)	75.0(2)
C(122)-C(112)-K(1)	86.0(2)
C(172)-C(112)-K(1)	109.6(3)
C(112)-C(122)-C(132)	122.6(4)
C(112)-C(122)-H(122)	118.7
C(132)-C(122)-H(122)	118.7
C(82)-C(132)-C(122)	118.5(4)
C(82)-C(132)-C(202)	121.1(4)

C(122)-C(132)-C(202)	120.4(4)
C(162)-C(142)-C(92)	114.1(4)
C(162)-C(142)-C(152)	109.8(4)
C(92)-C(142)-C(152)	110.0(4)
C(162)-C(142)-H(142)	107.6
C(92)-C(142)-H(142)	107.6
C(152)-C(142)-H(142)	107.6
C(142)-C(152)-H(15D)	109.5
C(142)-C(152)-H(15E)	109.5
H(15D)-C(152)-H(15E)	109.5
C(142)-C(152)-H(15F)	109.5
H(15D)-C(152)-H(15F)	109.5
H(15E)-C(152)-H(15F)	109.5
C(142)-C(162)-H(16D)	109.5
C(142)-C(162)-H(16E)	109.5
H(16D)-C(162)-H(16E)	109.5
C(142)-C(162)-H(16F)	109.5
H(16D)-C(162)-H(16F)	109.5
H(16E)-C(162)-H(16F)	109.5
C(182)-C(172)-C(112)	111.6(4)
C(182)-C(172)-C(192)	110.3(4)
C(112)-C(172)-C(192)	114.1(4)
C(182)-C(172)-H(172)	106.8
C(112)-C(172)-H(172)	106.8
C(192)-C(172)-H(172)	106.8
C(172)-C(182)-H(18D)	109.5
C(172)-C(182)-H(18E)	109.5
H(18D)-C(182)-H(18E)	109.5
C(172)-C(182)-H(18F)	109.5
H(18D)-C(182)-H(18F)	109.5
H(18E)-C(182)-H(18F)	109.5
C(172)-C(192)-H(19D)	109.5
C(172)-C(192)-H(19E)	109.5
H(19D)-C(192)-H(19E)	109.5
C(172)-C(192)-H(19F)	109.5
H(19D)-C(192)-H(19F)	109.5
H(19E)-C(192)-H(19F)	109.5
C(132)-C(202)-C(222)	113.4(4)
C(132)-C(202)-C(212)	110.5(4)
C(222)-C(202)-C(212)	111.1(4)
C(132)-C(202)-H(202)	107.2
C(222)-C(202)-H(202)	107.2
C(212)-C(202)-H(202)	107.2
C(202)-C(212)-H(21D)	109.5
C(202)-C(212)-H(21E)	109.5
H(21D)-C(212)-H(21E)	109.5
C(202)-C(212)-H(21F)	109.5
H(21D)-C(212)-H(21F)	109.5
H(21E)-C(212)-H(21F)	109.5
C(202)-C(222)-H(22D)	109.5
C(202)-C(222)-H(22E)	109.5
H(22D)-C(222)-H(22E)	109.5
C(202)-C(222)-H(22F)	109.5
H(22D)-C(222)-H(22F)	109.5
H(22E)-C(222)-H(22F)	109.5
C(23)-C(13)-C(63)	122.0(4)

C(23)-C(13)-H(13)	119.0
C(63)-C(13)-H(13)	119.0
C(13)-C(23)-C(33)	118.2(4)
C(13)-C(23)-C(21)	119.4(4)
C(33)-C(23)-C(21)	122.1(4)
C(43)-C(33)-C(23)	121.0(4)
C(43)-C(33)-H(33)	119.5
C(23)-C(33)-H(33)	119.5
C(33)-C(43)-C(53)	120.3(4)
C(33)-C(43)-H(43)	119.9
C(53)-C(43)-H(43)	119.9
C(43)-C(53)-C(63)	120.2(4)
C(43)-C(53)-H(53)	119.9
C(63)-C(53)-H(53)	119.9
C(53)-C(63)-C(13)	118.4(4)
C(53)-C(63)-C(22)	119.9(4)
C(13)-C(63)-C(22)	121.6(4)
C(24)-C(14)-C(64)	118.8(4)
C(24)-C(14)-S(31)	121.9(3)
C(64)-C(14)-S(31)	119.3(3)
C(34)-C(24)-C(14)	121.1(4)
C(34)-C(24)-H(24)	119.5
C(14)-C(24)-H(24)	119.5
C(24)-C(34)-C(44)	120.0(4)
C(24)-C(34)-H(34)	120.0
C(44)-C(34)-H(34)	120.0
C(54)-C(44)-C(34)	119.8(4)
C(54)-C(44)-H(44)	120.1
C(34)-C(44)-H(44)	120.1
C(44)-C(54)-C(64)	121.7(4)
C(44)-C(54)-H(54)	119.1
C(64)-C(54)-H(54)	119.1
C(54)-C(64)-C(14)	118.6(4)
C(54)-C(64)-C(74)	121.0(4)
C(14)-C(64)-C(74)	120.4(4)
C(124)-C(74)-C(84)	119.9(4)
C(124)-C(74)-C(64)	119.3(4)
C(84)-C(74)-C(64)	120.8(4)
C(94)-C(84)-C(74)	118.0(4)
C(94)-C(84)-C(134)	120.0(4)
C(74)-C(84)-C(134)	122.0(4)
C(104)-C(94)-C(84)	123.9(4)
C(104)-C(94)-H(94)	118.1
C(84)-C(94)-H(94)	118.1
C(94)-C(104)-C(114)	116.9(4)
C(94)-C(104)-C(164)	121.5(4)
C(114)-C(104)-C(164)	121.6(4)
C(124)-C(114)-C(104)	122.4(4)
C(124)-C(114)-H(114)	118.8
C(104)-C(114)-H(114)	118.8
C(114)-C(124)-C(74)	119.0(4)
C(114)-C(124)-C(194)	120.2(4)
C(74)-C(124)-C(194)	120.8(4)
C(144)-C(134)-C(84)	109.8(4)
C(144)-C(134)-C(154)	108.2(4)
C(84)-C(134)-C(154)	113.3(4)

C(144)-C(134)-H(134)	108.5
C(84)-C(134)-H(134)	108.5
C(154)-C(134)-H(134)	108.5
C(134)-C(144)-H(14A)	109.5
C(134)-C(144)-H(14B)	109.5
H(14A)-C(144)-H(14B)	109.5
C(134)-C(144)-H(14C)	109.5
H(14A)-C(144)-H(14C)	109.5
H(14B)-C(144)-H(14C)	109.5
C(134)-C(154)-H(15G)	109.5
C(134)-C(154)-H(15H)	109.5
H(15G)-C(154)-H(15H)	109.5
C(134)-C(154)-H(15I)	109.5
H(15G)-C(154)-H(15I)	109.5
H(15H)-C(154)-H(15I)	109.5
C(184)-C(164)-C(104)	113.6(4)
C(184)-C(164)-C(174)	110.1(4)
C(104)-C(164)-C(174)	110.3(4)
C(184)-C(164)-H(164)	107.5
C(104)-C(164)-H(164)	107.5
C(174)-C(164)-H(164)	107.5
C(164)-C(174)-H(17A)	109.5
C(164)-C(174)-H(17B)	109.5
H(17A)-C(174)-H(17B)	109.5
C(164)-C(174)-H(17C)	109.5
H(17A)-C(174)-H(17C)	109.5
H(17B)-C(174)-H(17C)	109.5
C(164)-C(184)-H(18G)	109.5
C(164)-C(184)-H(18H)	109.5
H(18G)-C(184)-H(18H)	109.5
C(164)-C(184)-H(18I)	109.5
H(18G)-C(184)-H(18I)	109.5
H(18H)-C(184)-H(18I)	109.5
C(204)-C(194)-C(124)	113.9(4)
C(204)-C(194)-C(214)	110.4(4)
C(124)-C(194)-C(214)	110.0(4)
C(204)-C(194)-H(194)	107.4
C(124)-C(194)-H(194)	107.4
C(214)-C(194)-H(194)	107.4
C(194)-C(204)-H(20A)	109.5
C(194)-C(204)-H(20B)	109.5
H(20A)-C(204)-H(20B)	109.5
C(194)-C(204)-H(20C)	109.5
H(20A)-C(204)-H(20C)	109.5
H(20B)-C(204)-H(20C)	109.5
C(194)-C(214)-H(21G)	109.5
C(194)-C(214)-H(21H)	109.5
H(21G)-C(214)-H(21H)	109.5
C(194)-C(214)-H(21I)	109.5
H(21G)-C(214)-H(21I)	109.5
H(21H)-C(214)-H(21I)	109.5
O(60)-K(1)-S(31)	89.38(7)
O(60)-K(1)-S(21)	85.77(7)
S(31)-K(1)-S(21)	60.42(3)
O(60)-K(1)-C(102)	117.32(10)
S(31)-K(1)-C(102)	139.32(9)

S(21)-K(1)-C(102)	89.83(8)
O(60)-K(1)-C(112)	95.48(10)
S(31)-K(1)-C(112)	157.51(8)
S(21)-K(1)-C(112)	97.98(8)
C(102)-K(1)-C(112)	23.82(10)
C(50)-O(10)-C(20)	107.4(3)
C(50)-O(10)-Fe(1)	119.3(2)
C(20)-O(10)-Fe(1)	123.1(2)
C(30B)-C(20)-O(10)	112.9(15)
O(10)-C(20)-C(30A)	104.3(5)
O(10)-C(20)-H(20D)	110.9
C(30A)-C(20)-H(20D)	110.9
O(10)-C(20)-H(20E)	110.9
C(30A)-C(20)-H(20E)	110.9
H(20D)-C(20)-H(20E)	108.9
C(30B)-C(20)-H(20F)	109.0
O(10)-C(20)-H(20F)	109.0
C(30B)-C(20)-H(20G)	109.0
O(10)-C(20)-H(20G)	109.0
H(20F)-C(20)-H(20G)	107.8
C(40A)-C(30A)-C(20)	105.9(7)
C(40A)-C(30A)-H(30A)	110.6
C(20)-C(30A)-H(30A)	110.6
C(40A)-C(30A)-H(30B)	110.6
C(20)-C(30A)-H(30B)	110.6
H(30A)-C(30A)-H(30B)	108.7
C(50)-C(40A)-C(30A)	99.6(6)
C(50)-C(40A)-H(40A)	111.9
C(30A)-C(40A)-H(40A)	111.9
C(50)-C(40A)-H(40B)	111.9
C(30A)-C(40A)-H(40B)	111.9
H(40A)-C(40A)-H(40B)	109.6
C(20)-C(30B)-C(40B)	84.1(18)
C(20)-C(30B)-H(30C)	114.6
C(40B)-C(30B)-H(30C)	114.6
C(20)-C(30B)-H(30D)	114.6
C(40B)-C(30B)-H(30D)	114.6
H(30C)-C(30B)-H(30D)	111.7
C(50)-C(40B)-C(30B)	90.9(16)
C(50)-C(40B)-H(40C)	113.5
C(30B)-C(40B)-H(40C)	113.5
C(50)-C(40B)-H(40D)	113.5
C(30B)-C(40B)-H(40D)	113.5
H(40C)-C(40B)-H(40D)	110.8
O(10)-C(50)-C(40A)	105.9(4)
O(10)-C(50)-C(40B)	103.7(10)
O(10)-C(50)-H(50A)	110.6
C(40A)-C(50)-H(50A)	110.6
O(10)-C(50)-H(50B)	110.6
C(40A)-C(50)-H(50B)	110.6
H(50A)-C(50)-H(50B)	108.7
O(10)-C(50)-H(50C)	111.0
C(40B)-C(50)-H(50C)	111.0
O(10)-C(50)-H(50D)	111.0
C(40B)-C(50)-H(50D)	111.0
H(50C)-C(50)-H(50D)	109.0

C(70)-O(60)-C(100)	109.5(3)
C(70)-O(60)-K(1)	136.8(3)
C(100)-O(60)-K(1)	112.4(2)
O(60)-C(70)-C(80)	105.6(4)
O(60)-C(70)-H(70A)	110.6
C(80)-C(70)-H(70A)	110.6
O(60)-C(70)-H(70B)	110.6
C(80)-C(70)-H(70B)	110.6
H(70A)-C(70)-H(70B)	108.8
C(90)-C(80)-C(70)	102.8(4)
C(90)-C(80)-H(80A)	111.2
C(70)-C(80)-H(80A)	111.2
C(90)-C(80)-H(80B)	111.2
C(70)-C(80)-H(80B)	111.2
H(80A)-C(80)-H(80B)	109.1
C(80)-C(90)-C(100)	102.2(4)
C(80)-C(90)-H(90A)	111.3
C(100)-C(90)-H(90A)	111.3
C(80)-C(90)-H(90B)	111.3
C(100)-C(90)-H(90B)	111.3
H(90A)-C(90)-H(90B)	109.2
O(60)-C(100)-C(90)	105.6(4)
O(60)-C(100)-K(1)	45.17(17)
C(90)-C(100)-K(1)	144.7(3)
O(60)-C(100)-H(10A)	110.6
C(90)-C(100)-H(10A)	110.6
K(1)-C(100)-H(10A)	73.5
O(60)-C(100)-H(10B)	110.6
C(90)-C(100)-H(10B)	110.6
K(1)-C(100)-H(10B)	100.2
H(10A)-C(100)-H(10B)	108.8
C(120)-O(110)-C(150)	109.6(5)
O(110)-C(120)-C(130)	104.5(5)
O(110)-C(120)-H(12A)	110.9
C(130)-C(120)-H(12A)	110.9
O(110)-C(120)-H(12B)	110.9
C(130)-C(120)-H(12B)	110.9
H(12A)-C(120)-H(12B)	108.9
C(120)-C(130)-C(140)	104.2(6)
C(120)-C(130)-H(13A)	110.9
C(140)-C(130)-H(13A)	110.9
C(120)-C(130)-H(13B)	110.9
C(140)-C(130)-H(13B)	110.9
H(13A)-C(130)-H(13B)	108.9
C(130)-C(140)-C(150)	97.7(5)
C(130)-C(140)-H(14D)	112.2
C(150)-C(140)-H(14D)	112.2
C(130)-C(140)-H(14E)	112.2
C(150)-C(140)-H(14E)	112.2
H(14D)-C(140)-H(14E)	109.8
O(110)-C(150)-C(140)	107.5(6)
O(110)-C(150)-H(15J)	110.2
C(140)-C(150)-H(15J)	110.2
O(110)-C(150)-H(15K)	110.2
C(140)-C(150)-H(15K)	110.2
H(15J)-C(150)-H(15K)	108.5

C(17A)-O(16A)-C(200)	107.2(7)
O(16A)-C(17A)-C(180)	104.4(7)
O(16A)-C(17A)-H(17D)	110.9
C(180)-C(17A)-H(17D)	110.9
O(16A)-C(17A)-H(17E)	110.9
C(180)-C(17A)-H(17E)	110.9
H(17D)-C(17A)-H(17E)	108.9
C(17B)-O(16B)-C(200)	105.0(13)
C(180)-C(17B)-O(16B)	102.6(15)
C(180)-C(17B)-H(17F)	111.3
O(16B)-C(17B)-H(17F)	111.3
C(180)-C(17B)-H(17G)	111.3
O(16B)-C(17B)-H(17G)	111.3
H(17F)-C(17B)-H(17G)	109.2
C(17B)-C(180)-C(190)	99.5(11)
C(190)-C(180)-C(17A)	114.0(6)
C(17B)-C(180)-H(18L)	111.9
C(190)-C(180)-H(18L)	111.9
C(17B)-C(180)-H(18M)	111.9
C(190)-C(180)-H(18M)	111.9
H(18L)-C(180)-H(18M)	109.6
C(190)-C(180)-H(18J)	108.8
C(17A)-C(180)-H(18J)	108.8
C(190)-C(180)-H(18K)	108.8
C(17A)-C(180)-H(18K)	108.8
H(18J)-C(180)-H(18K)	107.6
C(180)-C(190)-C(200)	101.8(6)
C(180)-C(190)-H(19G)	111.4
C(200)-C(190)-H(19G)	111.4
C(180)-C(190)-H(19H)	111.4
C(200)-C(190)-H(19H)	111.4
H(19G)-C(190)-H(19H)	109.3
C(190)-C(200)-O(16A)	106.6(6)
C(190)-C(200)-O(16B)	85.6(8)
C(190)-C(200)-H(20J)	114.4
O(16B)-C(200)-H(20J)	114.4
C(190)-C(200)-H(20K)	114.4
O(16B)-C(200)-H(20K)	114.4
H(20J)-C(200)-H(20K)	111.5
C(190)-C(200)-H(20H)	110.4
O(16A)-C(200)-H(20H)	110.4
C(190)-C(200)-H(20I)	110.4
O(16A)-C(200)-H(20I)	110.4
H(20H)-C(200)-H(20I)	108.6

Symmetry transformations used to generate equivalent atoms:

Anisotropic displacement parameters ($Å^2 x\ 10^3$) for [$LFeSC_6H_4Ar(THF)$]K (5·THF). The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Fe(1)	44(1)	39(1)	39(1)	-1(1)	13(1)	0(1)
S(11)	43(1)	53(1)	39(1)	5(1)	12(1)	2(1)
S(21)	79(1)	43(1)	36(1)	1(1)	13(1)	15(1)
S(31)	56(1)	40(1)	43(1)	0(1)	18(1)	2(1)
C(11)	38(3)	41(3)	34(3)	-3(2)	8(2)	-2(2)
C(21)	38(3)	37(2)	37(3)	-2(2)	13(2)	-2(2)
C(31)	46(3)	42(3)	29(3)	0(2)	1(2)	2(2)
C(41)	51(3)	45(3)	34(3)	-1(2)	16(2)	-2(2)
C(51)	45(3)	41(3)	37(3)	-2(2)	9(2)	-3(2)
C(61)	43(3)	37(2)	37(3)	-7(2)	13(2)	0(2)
F(71)	50(2)	58(2)	36(2)	5(1)	8(1)	1(1)
C(81)	36(2)	46(3)	33(3)	-1(2)	12(2)	-1(2)
C(91)	43(3)	42(3)	43(3)	4(2)	19(2)	2(2)
C(101)	47(3)	49(3)	49(3)	2(2)	14(3)	3(2)
C(111)	47(3)	51(3)	46(3)	4(2)	12(2)	2(2)
C(121)	47(3)	51(3)	49(3)	-9(2)	12(2)	-9(2)
C(131)	40(3)	49(3)	43(3)	-1(2)	13(2)	0(2)
C(141)	51(3)	39(3)	40(3)	-3(2)	12(2)	-2(2)
C(151)	82(4)	44(3)	61(3)	-4(2)	30(3)	-2(3)
C(161)	66(3)	54(3)	55(3)	-1(3)	15(3)	-8(3)
C(171)	54(3)	59(3)	52(4)	9(3)	1(3)	3(3)
C(181)	48(3)	95(4)	65(4)	12(3)	7(3)	-4(3)
C(191)	64(4)	87(4)	46(3)	10(3)	1(3)	-14(3)
C(201)	54(3)	44(3)	44(3)	0(2)	4(2)	-2(2)
C(211)	92(4)	56(3)	94(4)	14(3)	47(4)	-1(3)
C(221)	93(4)	56(3)	90(4)	5(3)	47(4)	12(3)
C(12)	51(3)	43(3)	32(3)	4(2)	12(2)	-2(2)
C(22)	42(3)	42(3)	39(3)	0(2)	11(2)	-1(2)
C(32)	49(3)	47(3)	34(3)	5(2)	8(2)	7(2)
C(42)	49(3)	46(3)	42(3)	5(2)	10(2)	12(2)
C(52)	45(3)	48(3)	44(3)	-7(2)	10(2)	5(2)
C(62)	41(3)	37(3)	42(3)	1(2)	9(2)	0(2)
F(72)	67(2)	63(2)	39(2)	6(1)	10(1)	18(1)
C(82)	51(3)	41(3)	34(3)	-2(2)	16(2)	6(2)
C(92)	44(3)	41(3)	44(3)	-1(2)	13(2)	4(2)
C(102)	51(3)	44(3)	46(3)	0(2)	23(3)	1(2)
C(112)	53(3)	39(3)	37(3)	-4(2)	15(2)	1(2)
C(122)	51(3)	39(3)	46(3)	-4(2)	14(2)	-5(2)
C(132)	48(3)	39(3)	37(3)	-4(2)	12(2)	1(2)
C(142)	51(3)	57(3)	45(3)	1(2)	13(2)	-3(2)
C(152)	60(3)	70(4)	83(4)	-8(3)	1(3)	-12(3)
C(162)	52(3)	92(4)	70(4)	-8(3)	17(3)	-3(3)
C(172)	61(3)	50(3)	47(3)	0(2)	15(3)	-10(2)
C(182)	90(4)	88(4)	47(3)	-9(3)	23(3)	23(3)
C(192)	74(4)	67(3)	44(3)	5(3)	14(3)	-1(3)
C(202)	60(3)	46(3)	37(3)	-5(2)	17(2)	-7(2)
C(212)	67(3)	52(3)	54(3)	5(2)	19(3)	-6(2)
C(222)	50(3)	61(3)	57(3)	0(2)	18(3)	-2(2)

C(13)	37(3)	43(3)	23(2)	2(2)	4(2)	-1(2)
C(23)	47(3)	42(3)	24(2)	7(2)	9(2)	0(2)
C(33)	42(3)	56(3)	30(3)	-4(2)	9(2)	2(2)
C(43)	48(3)	53(3)	35(3)	-7(2)	9(2)	-7(2)
C(53)	42(3)	53(3)	41(3)	11(2)	5(2)	4(2)
C(63)	43(3)	41(3)	32(3)	3(2)	7(2)	4(2)
C(14)	35(2)	42(3)	39(3)	-3(2)	7(2)	-2(2)
C(24)	44(3)	49(3)	37(3)	-4(2)	11(2)	-3(2)
C(34)	45(3)	45(3)	47(3)	-8(2)	14(2)	3(2)
C(44)	47(3)	38(3)	50(3)	-3(2)	6(2)	0(2)
C(54)	47(3)	40(3)	43(3)	-1(2)	14(2)	-2(2)
C(64)	36(2)	41(3)	37(3)	-4(2)	8(2)	-3(2)
C(74)	45(3)	35(2)	38(3)	-1(2)	14(2)	-3(2)
C(84)	46(3)	45(3)	38(3)	-3(2)	12(2)	-6(2)
C(94)	52(3)	45(3)	37(3)	-4(2)	9(2)	-4(2)
C(104)	46(3)	50(3)	41(3)	-3(2)	15(2)	0(2)
C(114)	40(3)	57(3)	40(3)	0(2)	9(2)	-1(2)
C(124)	43(3)	45(3)	34(3)	-3(2)	14(2)	-3(2)
C(134)	45(3)	55(3)	44(3)	-6(2)	11(2)	3(2)
C(144)	46(3)	60(3)	107(5)	5(3)	21(3)	-5(3)
C(154)	57(3)	87(4)	71(4)	25(3)	7(3)	5(3)
C(164)	50(3)	60(3)	38(3)	-4(2)	14(2)	-1(2)
C(174)	111(5)	66(4)	63(4)	-6(3)	37(3)	17(3)
C(184)	69(4)	83(4)	67(4)	-8(3)	32(3)	-1(3)
C(194)	40(3)	60(3)	42(3)	-5(2)	9(2)	-3(2)
C(204)	44(3)	70(3)	48(3)	1(3)	9(2)	-4(2)
C(214)	56(3)	63(3)	63(3)	-16(3)	9(3)	-10(3)
K(1)	56(1)	56(1)	42(1)	-5(1)	13(1)	7(1)
O(10)	46(2)	49(2)	40(2)	-3(1)	14(2)	-1(1)
C(20)	48(3)	84(4)	60(3)	6(3)	20(3)	-7(3)
C(30A)	55(5)	85(6)	104(7)	-24(6)	17(5)	-18(5)
C(40A)	80(5)	73(5)	68(6)	-14(4)	7(4)	-15(4)
C(30B)	62(9)	77(13)	79(11)	12(9)	11(7)	-29(8)
C(40B)	87(10)	76(9)	43(16)	-3(8)	4(9)	-24(7)
C(50)	72(3)	42(3)	56(3)	-10(2)	14(3)	-4(2)
O(60)	50(2)	61(2)	44(2)	-7(2)	7(2)	-1(2)
C(70)	66(4)	63(3)	48(3)	-6(3)	5(3)	-8(3)
C(80)	58(4)	76(4)	75(4)	-17(3)	10(3)	-12(3)
C(90)	67(4)	85(4)	66(4)	3(3)	22(3)	0(3)
C(100)	45(3)	80(4)	48(3)	-14(3)	15(3)	-3(3)
O(110)	108(4)	97(3)	63(3)	13(2)	-2(3)	31(3)
C(120)	110(5)	81(4)	83(5)	3(4)	27(4)	4(4)
C(130)	80(5)	91(5)	122(6)	15(4)	8(5)	-6(4)
C(140)	71(5)	136(6)	146(7)	-30(5)	42(5)	-7(4)
C(150)	133(7)	204(9)	103(7)	-20(6)	67(7)	-18(7)
O(16A)	111(5)	208(11)	121(6)	20(6)	30(5)	-26(6)
C(17A)	75(5)	114(9)	98(6)	43(6)	10(5)	-1(5)
O(16B)	137(10)	187(12)	123(12)	2(10)	24(8)	-4(8)
C(17B)	125(10)	178(12)	53(12)	-34(9)	16(8)	4(8)
C(180)	114(5)	179(7)	96(5)	-44(5)	-23(4)	30(5)
C(190)	158(6)	212(8)	83(5)	-1(5)	24(4)	43(6)
C(200)	95(4)	133(5)	83(4)	-14(4)	16(3)	3(4)

Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for [$LFeSC_6H_4Ar(THF)$]K (5·THF).

	x	y	z	U(eq)
H(41)	5002	2593	8773	51
H(51)	4009	2931	8047	50
H(101)	2968	4691	6529	58
H(121)	2748	2295	6249	59
H(141)	4758	4537	7550	53
H(15A)	3185	5153	7487	90
H(15B)	3992	5418	7899	90
H(15C)	3665	4507	7887	90
H(16A)	4706	5298	6844	88
H(16B)	4591	5899	7261	88
H(16C)	3828	5629	6817	88
H(171)	1997	4297	5827	70
H(18A)	1296	2790	5974	108
H(18B)	819	3494	5618	108
H(18C)	1149	3646	6200	108
H(19A)	2697	3621	5366	103
H(19B)	1745	3564	5112	103
H(19C)	2226	2800	5404	103
H(201)	4371	1707	7308	60
H(21A)	3026	1382	7282	115
H(21B)	3497	608	7165	115
H(21C)	2860	1075	6726	115
H(22A)	3919	1352	6286	113
H(22B)	4466	772	6704	113
H(22C)	4789	1650	6612	113
H(42)	9039	-618	7614	56
H(52)	8727	-504	6756	56
H(102)	8650	1185	5233	54
H(122)	6522	149	5144	54
H(142)	9423	1117	6551	61
H(15D)	9123	2433	5857	113
H(15E)	9793	2460	6383	113
H(15F)	8859	2411	6352	113
H(16D)	10035	432	6020	107
H(16E)	10520	1236	6249	107
H(16F)	9949	1237	5692	107
H(172)	7567	1219	4451	64
H(18D)	8381	97	4499	111
H(18E)	7664	56	3994	111
H(18F)	7637	-504	4451	111
H(19D)	6242	134	4317	93
H(19E)	6382	745	3911	93
H(19F)	6183	1093	4388	93
H(202)	6774	165	6440	56
H(21D)	6611	-1190	5788	86
H(21E)	6338	-1199	6280	86
H(21F)	7270	-1108	6315	86
H(22D)	5709	795	5827	84
H(22E)	5411	-5	6042	84

H(22F)	5570	-30	5514	84
H(13)	6757	1790	7512	42
H(33)	7536	3387	8634	51
H(43)	8859	3055	8696	55
H(53)	9146	2054	8185	56
H(24)	6258	4971	6734	52
H(34)	5992	6352	6657	54
H(44)	6372	7112	6062	56
H(54)	6948	6470	5523	52
H(94)	6996	4081	4383	55
H(114)	9133	4331	5404	55
H(134)	5846	5142	5047	58
H(14A)	5756	3584	4596	107
H(14B)	5013	4038	4707	107
H(14C)	5760	3738	5153	107
H(15G)	6043	5588	4271	111
H(15H)	5149	5289	4230	111
H(15I)	5751	4704	4058	111
H(164)	8093	3593	4180	59
H(17A)	9212	2906	5031	117
H(17B)	9023	2550	4484	117
H(17C)	8342	2538	4761	117
H(18G)	9008	4675	4270	105
H(18H)	9399	3838	4167	105
H(18I)	9633	4204	4713	105
H(194)	8389	5113	6344	58
H(20A)	9300	4030	6358	82
H(20B)	9731	4789	6682	82
H(20C)	9843	4636	6149	82
H(21G)	9273	6031	5823	93
H(21H)	9329	6185	6389	93
H(21I)	8499	6342	5968	93
H(20D)	8732	3856	7046	76
H(20E)	9102	3369	7555	76
H(20F)	8968	3283	7376	76
H(20G)	8726	4123	7087	76
H(30A)	9685	4563	7858	99
H(30B)	9092	5073	7414	99
H(40A)	8783	4564	8305	92
H(40B)	8603	5446	8043	92
H(30C)	9825	4356	7715	90
H(30D)	9376	3998	8105	90
H(40C)	8630	5596	7836	86
H(40D)	8402	5336	7257	86
H(50A)	7437	4480	7871	69
H(50B)	7573	4949	7404	69
H(50C)	7848	4500	8024	69
H(50D)	7272	4766	7490	69
H(70A)	4987	1342	4897	73
H(70B)	4801	2255	4692	73
H(80A)	3666	2042	4923	86
H(80B)	4118	1432	5362	86
H(90A)	4089	2599	5794	86
H(90B)	4237	3164	5363	86
H(10A)	5527	3081	5862	69
H(10B)	5393	2186	6052	69

H(12A)	10221	-1183	5231	110
H(12B)	9574	-498	5258	110
H(13A)	9320	-2191	5141	123
H(13B)	8773	-1475	4824	123
H(14D)	8303	-2108	5512	139
H(14E)	8262	-1126	5467	139
H(15J)	9164	-1210	6238	168
H(15K)	9488	-2083	6128	168
H(17D)	10642	3101	7995	119
H(17E)	10446	2150	7892	119
H(17F)	10530	1503	7312	145
H(17G)	10368	1946	7781	145
H(18L)	10757	3169	7569	169
H(18M)	10304	2789	7033	169
H(18J)	10374	2313	7138	169
H(18K)	10533	3263	7235	169
H(19G)	11614	3093	7032	184
H(19H)	11559	2117	7069	184
H(20J)	12038	3149	7923	127
H(20K)	12653	2555	7743	127
H(20H)	12308	3215	7808	127
H(20I)	12537	2280	7755	127

Torsion angles [°] for [LFeSC$_6$H$_4$Ar(THF)]K (5·THF).

Fe(1)-S(11)-C(11)-C(61)	-172.6(2)
Fe(1)-S(11)-C(11)-C(21)	9.6(4)
C(61)-C(11)-C(21)-C(31)	-4.2(5)
S(11)-C(11)-C(21)-C(31)	173.5(3)
C(61)-C(11)-C(21)-C(23)	171.9(4)
S(11)-C(11)-C(21)-C(23)	-10.3(6)
C(11)-C(21)-C(31)-F(71)	179.6(3)
C(23)-C(21)-C(31)-F(71)	3.2(5)
C(11)-C(21)-C(31)-C(41)	0.7(6)
C(23)-C(21)-C(31)-C(41)	-175.6(4)
F(71)-C(31)-C(41)-C(51)	-176.8(3)
C(21)-C(31)-C(41)-C(51)	2.1(6)
C(31)-C(41)-C(51)-C(61)	-1.3(6)
C(41)-C(51)-C(61)-C(11)	-2.3(6)
C(41)-C(51)-C(61)-C(81)	176.3(4)
C(21)-C(11)-C(61)-C(51)	5.0(5)
S(11)-C(11)-C(61)-C(51)	-172.9(3)
C(21)-C(11)-C(61)-C(81)	-173.5(4)
S(11)-C(11)-C(61)-C(81)	8.5(5)
C(51)-C(61)-C(81)-C(91)	91.9(5)
C(11)-C(61)-C(81)-C(91)	-89.5(5)
C(51)-C(61)-C(81)-C(131)	-86.4(5)
C(11)-C(61)-C(81)-C(131)	92.2(5)
C(131)-C(81)-C(91)-C(101)	1.5(6)
C(61)-C(81)-C(91)-C(101)	-176.8(4)
C(131)-C(81)-C(91)-C(141)	178.9(4)

C(61)-C(81)-C(91)-C(141)	0.7(6)
C(81)-C(91)-C(101)-C(111)	-1.6(6)
C(141)-C(91)-C(101)-C(111)	-179.0(4)
C(91)-C(101)-C(111)-C(121)	0.8(6)
C(91)-C(101)-C(111)-C(171)	-177.8(4)
C(101)-C(111)-C(121)-C(131)	0.1(6)
C(171)-C(111)-C(121)-C(131)	178.7(4)
C(91)-C(81)-C(131)-C(121)	-0.6(6)
C(61)-C(81)-C(131)-C(121)	177.6(4)
C(91)-C(81)-C(131)-C(201)	178.3(4)
C(61)-C(81)-C(131)-C(201)	-3.4(6)
C(111)-C(121)-C(131)-C(81)	-0.2(6)
C(111)-C(121)-C(131)-C(201)	-179.2(4)
C(81)-C(91)-C(141)-C(161)	138.9(4)
C(101)-C(91)-C(141)-C(161)	-43.7(5)
C(81)-C(91)-C(141)-C(151)	-97.9(5)
C(101)-C(91)-C(141)-C(151)	79.5(5)
C(101)-C(111)-C(171)-C(191)	119.8(5)
C(121)-C(111)-C(171)-C(191)	-58.7(6)
C(101)-C(111)-C(171)-C(181)	-112.9(5)
C(121)-C(111)-C(171)-C(181)	68.6(5)
C(81)-C(131)-C(201)-C(221)	-110.6(5)
C(121)-C(131)-C(201)-C(221)	68.3(5)
C(81)-C(131)-C(201)-C(211)	124.3(4)
C(121)-C(131)-C(201)-C(211)	-56.8(5)
Fe(1)-S(21)-C(12)-C(22)	6.6(4)
K(1)-S(21)-C(12)-C(22)	165.9(3)
Fe(1)-S(21)-C(12)-C(62)	-176.1(3)
K(1)-S(21)-C(12)-C(62)	-16.8(4)
C(62)-C(12)-C(22)-C(32)	-1.5(6)
S(21)-C(12)-C(22)-C(32)	175.7(3)
C(62)-C(12)-C(22)-C(63)	178.4(4)
S(21)-C(12)-C(22)-C(63)	-4.4(6)
C(12)-C(22)-C(32)-C(42)	0.1(7)
C(63)-C(22)-C(32)-C(42)	-179.8(4)
C(12)-C(22)-C(32)-F(72)	-176.7(4)
C(63)-C(22)-C(32)-F(72)	3.4(6)
F(72)-C(32)-C(42)-C(52)	178.2(4)
C(22)-C(32)-C(42)-C(52)	1.4(7)
C(32)-C(42)-C(52)-C(62)	-1.5(6)
C(42)-C(52)-C(62)-C(12)	0.2(6)
C(42)-C(52)-C(62)-C(82)	-178.6(4)
C(22)-C(12)-C(62)-C(52)	1.4(6)
S(21)-C(12)-C(62)-C(52)	-176.0(3)
C(22)-C(12)-C(62)-C(82)	-179.8(4)
S(21)-C(12)-C(62)-C(82)	2.7(5)
C(52)-C(62)-C(82)-C(92)	-88.4(5)
C(12)-C(62)-C(82)-C(92)	92.9(5)
C(52)-C(62)-C(82)-C(132)	91.8(5)
C(12)-C(62)-C(82)-C(132)	-86.9(5)
C(132)-C(82)-C(92)-C(102)	-0.2(6)
C(62)-C(82)-C(92)-C(102)	-180.0(4)
C(132)-C(82)-C(92)-C(142)	177.7(4)
C(62)-C(82)-C(92)-C(142)	-2.1(6)
C(132)-C(82)-C(92)-K(1)	66.9(4)
C(62)-C(82)-C(92)-K(1)	-112.9(3)

C(82)-C(92)-C(102)-C(112)	-0.3(6)
C(142)-C(92)-C(102)-C(112)	-178.3(4)
K(1)-C(92)-C(102)-C(112)	-75.8(4)
C(82)-C(92)-C(102)-K(1)	75.5(3)
C(142)-C(92)-C(102)-K(1)	-102.5(3)
C(92)-C(102)-C(112)-C(122)	0.2(6)
K(1)-C(102)-C(112)-C(122)	-77.4(3)
C(92)-C(102)-C(112)-C(172)	-178.3(4)
K(1)-C(102)-C(112)-C(172)	104.2(4)
C(92)-C(102)-C(112)-K(1)	77.5(4)
C(102)-C(112)-C(122)-C(132)	0.5(6)
C(172)-C(112)-C(122)-C(132)	178.9(4)
K(1)-C(112)-C(122)-C(132)	-70.3(4)
C(92)-C(82)-C(132)-C(122)	0.8(6)
C(62)-C(82)-C(132)-C(122)	-179.4(4)
C(92)-C(82)-C(132)-C(202)	178.3(4)
C(62)-C(82)-C(132)-C(202)	-1.9(6)
C(112)-C(122)-C(132)-C(82)	-1.0(6)
C(112)-C(122)-C(132)-C(202)	-178.5(4)
C(82)-C(92)-C(142)-C(162)	134.6(4)
C(102)-C(92)-C(142)-C(162)	-47.6(5)
K(1)-C(92)-C(142)-C(162)	-127.0(3)
C(82)-C(92)-C(142)-C(152)	-101.5(5)
C(102)-C(92)-C(142)-C(152)	76.4(5)
K(1)-C(92)-C(142)-C(152)	-3.1(4)
C(102)-C(112)-C(172)-C(182)	76.0(5)
C(122)-C(112)-C(172)-C(182)	-102.4(5)
K(1)-C(112)-C(172)-C(182)	159.5(3)
C(102)-C(112)-C(172)-C(192)	-158.2(4)
C(122)-C(112)-C(172)-C(192)	23.5(6)
K(1)-C(112)-C(172)-C(192)	-74.7(4)
C(82)-C(132)-C(202)-C(222)	139.7(4)
C(122)-C(132)-C(202)-C(222)	-42.9(5)
C(82)-C(132)-C(202)-C(212)	-94.8(5)
C(122)-C(132)-C(202)-C(212)	82.6(5)
C(63)-C(13)-C(23)-C(33)	0.8(6)
C(63)-C(13)-C(23)-C(21)	-173.9(4)
C(31)-C(21)-C(23)-C(13)	117.9(4)
C(11)-C(21)-C(23)-C(13)	-58.2(5)
C(31)-C(21)-C(23)-C(33)	-56.6(5)
C(11)-C(21)-C(23)-C(33)	127.3(4)
C(13)-C(23)-C(33)-C(43)	0.2(6)
C(21)-C(23)-C(33)-C(43)	174.8(4)
C(23)-C(33)-C(43)-C(53)	-1.2(6)
C(33)-C(43)-C(53)-C(63)	1.3(6)
C(43)-C(53)-C(63)-C(13)	-0.2(6)
C(43)-C(53)-C(63)-C(22)	-178.5(4)
C(23)-C(13)-C(63)-C(53)	-0.8(6)
C(23)-C(13)-C(63)-C(22)	177.4(4)
C(32)-C(22)-C(63)-C(53)	59.9(5)
C(12)-C(22)-C(63)-C(53)	-120.0(5)
C(32)-C(22)-C(63)-C(13)	-118.3(4)
C(12)-C(22)-C(63)-C(13)	61.8(6)
Fe(1)-S(31)-C(14)-C(24)	-12.1(4)
K(1)-S(31)-C(14)-C(24)	146.3(3)
Fe(1)-S(31)-C(14)-C(64)	165.8(3)

K(1)-S(31)-C(14)-C(64)	-35.7(4)
C(64)-C(14)-C(24)-C(34)	-2.6(6)
S(31)-C(14)-C(24)-C(34)	175.4(3)
C(14)-C(24)-C(34)-C(44)	0.3(6)
C(24)-C(34)-C(44)-C(54)	2.0(6)
C(34)-C(44)-C(54)-C(64)	-1.9(6)
C(44)-C(54)-C(64)-C(14)	-0.4(6)
C(44)-C(54)-C(64)-C(74)	-179.4(4)
C(24)-C(14)-C(64)-C(54)	2.6(6)
S(31)-C(14)-C(64)-C(54)	-175.4(3)
C(24)-C(14)-C(64)-C(74)	-178.4(4)
S(31)-C(14)-C(64)-C(74)	3.5(5)
C(54)-C(64)-C(74)-C(124)	96.5(5)
C(14)-C(64)-C(74)-C(124)	-82.4(5)
C(54)-C(64)-C(74)-C(84)	-84.4(5)
C(14)-C(64)-C(74)-C(84)	96.6(5)
C(124)-C(74)-C(84)-C(94)	1.0(6)
C(64)-C(74)-C(84)-C(94)	-178.1(4)
C(124)-C(74)-C(84)-C(134)	179.7(4)
C(64)-C(74)-C(84)-C(134)	0.7(6)
C(74)-C(84)-C(94)-C(104)	0.3(6)
C(134)-C(84)-C(94)-C(104)	-178.5(4)
C(84)-C(94)-C(104)-C(114)	-1.4(6)
C(84)-C(94)-C(104)-C(164)	178.9(4)
C(94)-C(104)-C(114)-C(124)	1.3(6)
C(164)-C(104)-C(114)-C(124)	-179.0(4)
C(104)-C(114)-C(124)-C(74)	-0.1(6)
C(104)-C(114)-C(124)-C(194)	-179.4(4)
C(84)-C(74)-C(124)-C(114)	-1.1(6)
C(64)-C(74)-C(124)-C(114)	178.0(4)
C(84)-C(74)-C(124)-C(194)	178.2(4)
C(64)-C(74)-C(124)-C(194)	-2.7(6)
C(94)-C(84)-C(134)-C(144)	71.5(5)
C(74)-C(84)-C(134)-C(144)	-107.2(5)
C(94)-C(84)-C(134)-C(154)	-49.6(6)
C(74)-C(84)-C(134)-C(154)	131.7(4)
C(94)-C(104)-C(164)-C(184)	125.7(5)
C(114)-C(104)-C(164)-C(184)	-54.0(6)
C(94)-C(104)-C(164)-C(174)	-110.1(5)
C(114)-C(104)-C(164)-C(174)	70.2(5)
C(114)-C(124)-C(194)-C(204)	-32.4(5)
C(74)-C(124)-C(194)-C(204)	148.3(4)
C(114)-C(124)-C(194)-C(214)	92.1(5)
C(74)-C(124)-C(194)-C(214)	-87.2(5)
C(50)-O(10)-C(20)-C(30B)	39.1(15)
Fe(1)-O(10)-C(20)-C(30B)	-176.3(15)
C(50)-O(10)-C(20)-C(30A)	9.0(6)
Fe(1)-O(10)-C(20)-C(30A)	153.6(5)
O(10)-C(20)-C(30A)-C(40A)	17.0(10)
C(20)-C(30A)-C(40A)-C(50)	-35.0(11)
O(10)-C(20)-C(30B)-C(40B)	-56.6(16)
C(20)-O(10)-C(50)-C(40A)	-32.3(6)
Fe(1)-O(10)-C(50)-C(40A)	-178.5(5)
C(20)-O(10)-C(50)-C(40B)	13.0(12)
Fe(1)-O(10)-C(50)-C(40B)	-133.2(12)
C(30A)-C(40A)-C(50)-O(10)	41.2(9)

C(30B)-C(40B)-C(50)-O(10)	-39.1(15)
C(100)-O(60)-C(70)-C(80)	-11.0(5)
K(1)-O(60)-C(70)-C(80)	-176.5(3)
O(60)-C(70)-C(80)-C(90)	30.7(5)
C(70)-C(80)-C(90)-C(100)	-37.4(5)
C(70)-O(60)-C(100)-C(90)	-12.9(5)
K(1)-O(60)-C(100)-C(90)	156.5(3)
C(70)-O(60)-C(100)-K(1)	-169.3(4)
C(80)-C(90)-C(100)-O(60)	31.6(5)
C(80)-C(90)-C(100)-K(1)	60.9(7)
C(150)-O(110)-C(120)-C(130)	-19.6(7)
O(110)-C(120)-C(130)-C(140)	37.8(6)
C(120)-C(130)-C(140)-C(150)	-38.9(7)
C(120)-O(110)-C(150)-C(140)	-6.0(8)
C(130)-C(140)-C(150)-O(110)	27.6(8)
C(200)-O(16A)-C(17A)-C(180)	16.3(11)
C(200)-O(16B)-C(17B)-C(180)	-1.1(18)
O(16B)-C(17B)-C(180)-C(190)	37.3(15)
O(16A)-C(17A)-C(180)-C(190)	-2.2(12)
C(17B)-C(180)-C(190)-C(200)	-69.9(11)
C(17A)-C(180)-C(190)-C(200)	-13.3(11)
C(180)-C(190)-C(200)-O(16A)	22.3(10)
C(180)-C(190)-C(200)-O(16B)	58.9(10)
C(17A)-O(16A)-C(200)-C(190)	-25.4(11)
C(17B)-O(16B)-C(200)-C(190)	-35.0(15)

Symmetry transformations used to generate equivalent atoms: