Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

Direct Monitoring of Spin Transition at a High $T_{1/2}$ Value in a Dinuclear Triple-Stranded Helicate Iron(II) Complex Through X-ray Photoelectron Spectroscopy

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Cotents

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Materials

All chemicals and solvents used were of commercial grade and used without further purification.

Experimental Section

L 4, 4'-Oxydianiline (210 mg, 1.05 mmol) in 10 mL of ethanol was added to the solution of thiazole-4-carboxaldehyde (250 mg, 2.21 mmol)) in 10 mL of ethanol leading to a clear yellow solution. The mixture was heated to reflux with overnight stirring and then the yellow precipate was collected by filtration and washed with cold ethanol (3 × 5 mL) to give a yellow powder in 84.5% yield. ^{1}H NMR ($CDCl_3$, 300 MHz) δ (ppm) 8.92 (s, 2H), 8.71 (s, 2H), 8.05 (s, 2H), 7.31 (d, 4H), 7.08 (d, 4H); ^{13}C NMR (DMSO, 75.5 MHz) δ (ppm) 156.19, 154.93, 153.67, 152.54, 146.70, 122.73, 119.63; UV/Vis (solid state in nujol): λ_{max} 271, 325(sh) nm; FT-IR (ATR ν_{max} /cm^{-1}): 3039, 1621, 1498, 1425, 1244, 1200, 940, 850, 537; ESI-HRMS (positive-ion detection, CH_3OH): *m/z* = 804.1400 [Na+2**L**]$^{+}$, 413.0550 [Na+**L**]$^{+}$ and 319.0853 [H+**L**]$^{+}$.

1 $[Fe_2\mathbf{L}_3](BF_4)_4 \cdot 2(CH_3CN)\ 0.3(H_2O)$ Iron(II) tetrafluoroborate hexahydrate (14 mg, 0.04 mmol) in 5 mL of acetonitrile was slowly added to the suspension of **L** (25 mg, 0.06 mmol) in 10 mL of acetonitrile, there was an immediate colour changed from yellow to red. The reaction mixture was heated at 50 °C with stirring for 4 h, then cooled to room temperature and filtered. Slow diffusion of diethyl ether into the filtrate of the product resulted in the formation of dark red needle crystals and air dry in 65% yield. Elemental analysis (%) (calcd., found for $C_{60}H_{42}B_4F_{16}Fe_2N_{12}O_3S_6 \cdot 2(CH_3CN)\ 0.3(H_2O)$: C (44.75, 44.59), H (2.85, 2.87), N(11.42, 11.57), S(11.20, 10.78); UV/Vis (solid state in nujol): λmax 264, 330, 499 nm; FT-IR (ATR νmax /cm^{-1}): 3113, 1594, 1488, 1235, 1203, 1030, 834, 521; ESI-HRMS (positive-ion detection, CH_3CN): *m/z* = 320.4999 $[Fe_2\mathbf{L}_3]^{4+}$. Single crystals were taken from the same sample and used directly for the X-ray study.

General physical measurements

^{1}H NMR and ^{13}C NMR spectra were recorded on a Bruker 300 MHz spectrometer. High resolution ESI-MS data were acquired using a Waters Xevo QToF mass spectrometer, operating in positive ion mode. FT-IR measurements were undertaken on a Bruker Vertex 70 with a diamond ATR stage. The solid state UV-vis spectra were measured in nujol at ambient temperature using a Agilent Cary 100 UV-Vis with WinUV software. Spectra were determined from 800-250 nm with a scan rate of 600nm per minute.

Magnetic measurements

Susceptibility data were collected using a Quantum Design SQUID magnetometer calibrated against a standard palladium sample. The data were collected between 5 and 400 K and the scan rate of the temperature was fixed at 2.0 K min^{-1}.

Mössbauer Studies

Mössbauer experiments were carried out using a Wissel MVT-1000 Mössbauer spectrometer with a ^{57}Co/Rh source in a constant-acceleration transmission spectrometer (Topologic Systems) equipped with a closed-cycle helium refrigerator cryostat (Iwatani Co., Ltd.). All isomer shifts are given relative to α-Fe at room temperature. Measurements at low temperature were performed.

Single crystal X-ray diffraction measurements

1 at 100(2) K and 298(2) K were with collected at beamline MX1 of the Australian Synchrotron with Silicon Double Crystal monochromated radiation.[1,2] Data integration and reduction were undertaken

with XDS.[3] An empirical absorption correction was then applied using SADABS at the Australian Synchrotron.[4] The structures were solved by direct methods and the full-matrix least-squares refinements were carried out using a suite of SHELX programs[5,6] via the Olex2 interface.[7] Non-hydrogen atoms were refined anisotropically. Carbon-bound hydrogen atoms were included in idealised positions and refined using a riding model. The crystallographic data in CIF format has been deposited at the Cambridge Crystallographic Data Centre with CCDC 1540558-1540559. It is available free of charge from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1 EZ, UK; fax: (+44) 1223-336-033; or e-mail: deposit@ccdc.cam.ac.uk. Specific refinement details and crystallographic data for each structure are present above and in the supporting information.

XPS Experimental

X-ray photoelectron spectroscopy (XPS) was performed on an ESCALAB250Xi (Thermo Scientific, UK) using a monochromated Al K alpha line (energy 1486.68 eV) at 150W (13 kV x 12 mA) with a spot size of 500 micrometre on the sample. Electron optics are arranged at 90 degrees with respect to the surface plane. Survey scans were performed with a pass energy of 100 eV with high-resolution scans performed at 20 eV. The complex was measured at room temperature, then 170K, then allowed to warm to room temperature and remeasured to ensure the sample had not undergone X-ray damage. Data was processed using the Avantage software package (Thermo Scientific, UK). Peaks were calibrated using the C 1s peak at 284.8 eV and background corrected using the Shirley method.[8]

Regular solution model

Cooperativity was estimated from the measured $\chi_m T$ *versus* T curves (χ_m; molar magnetic susceptibility, T; temperature) by applying the regular solution model (eq 1),[9] where ΔH, ΔS and Γ are the enthalpy and the entropy variations and the parameter accounting for cooperativity based on SCO, respectively. The HS molar fraction, γ_{HS}, is shown as a function of the magnetic susceptibility through (eq 2), where $(\chi_m T)_m$ is the $\chi_m T$ value at any temperature, $(\chi_m T)_{HS}$ and $(\chi_m T)_{LS}$ are the pure LS and HS states, respectively. R is the gas constant unit, 8.314 J K^{-1} mol^{-1}. The cooperativity value, C, is given by eq 3.

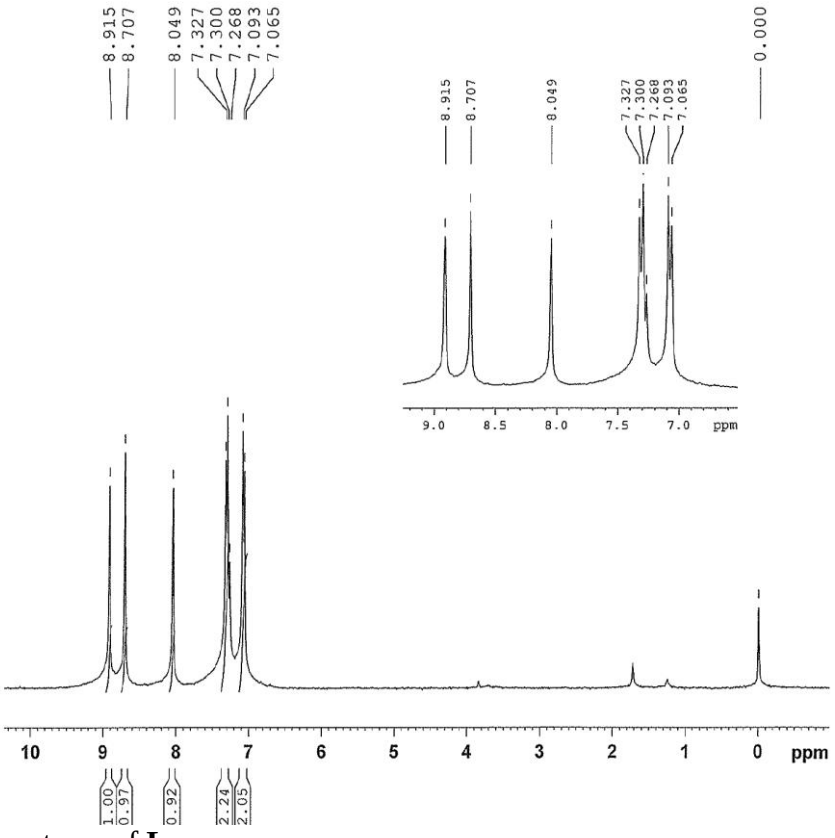
$$\ln[(1-\gamma_{HS})/(\gamma_{HS})] = [\{\Delta H+\Gamma(1-2\gamma_{HS})\}/RT]-\Delta S/R \quad \text{(eq 1)}$$

$$\gamma_{HS} = [(\chi_m T)_m-(\chi_m T)_{LS}]/[(\chi_m T)_{HS}-(\chi_m T)_{LS}] \quad \text{(eq 2)}$$

$$C = \Gamma/(2RT_{1/2}),\ T_{1/2} = \Delta H/\Delta S \quad \text{(eq 3)}$$

Table S1. Crystallographic data and refinement details for the complex **1** at 100 and 298 K.

	100K	**298 K**
Empirical formula	$[C_{60}H_{42}N_{12}O_3S_6Fe_2]4(BF_4).4(CH_3CN).0.5(H_2O)$	$[C_{60}H_{42}N_{12}O_3S_6Fe_2]4(BF_4).2(CH_3CN).0.3(H_2O)$
Formula weight	1803.58	1717.07
Temperature/K	100(2)	298
Crystal system	triclinic	triclinic
Space group	$P\bar{1}$	$P\bar{1}$
a/Å	11.724(2)	11.806(2)
b/Å	15.555(3)	15.605(3)
c/Å	21.641(4)	22.029(4)
α/°	89.79(3)	89.52(3)
β/°	85.72(3)	85.48(3)
γ/°	73.09(3)	73.49(3)
Volume/Å3	3764.8(14)	3878.6(15)
Z	2	2
ρcalcg/cm3	1.591	1.470
μ/mm 1	0.652	0.627
F(000)	1830.0	1737.0
Radiation	0.03 × 0.02 × 0.01	0.03 × 0.02 × 0.01
2Θ range for data collection/°	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
Index ranges	2.736 to 52.998	2.722 to 49.996
Reflections collected	$-14 \le h \le 14, -19 \le k \le 19, -27 \le l \le 27$	$-14 \le h \le 14, -18 \le k \le 18, -26 \le l \le 26$
Independent reflections	54362	47455
Data/restraints/parameters	14128 [Rint = 0.0247, Rsigma = 0.0194]	12382 [Rint = 0.0341, Rsigma = 0.0286]
Goodness-of-fit on F2	14128/0/1115	12382/399/1153
Final R indexes [I>=2σ (I)]	1.048	1.045
Final R indexes [all data]	R1 = 0.0369, wR2 = 0.0944	R1 = 0.0695, wR2 = 0.2157
Largest diff. peak/hole / e Å-3	R1 = 0.0424, wR2 = 0.0981	R1 = 0.0804, wR2 = 0.2289
Flack parameter		



FigureS1 ^{1}H-NMR spectrum of **L**.

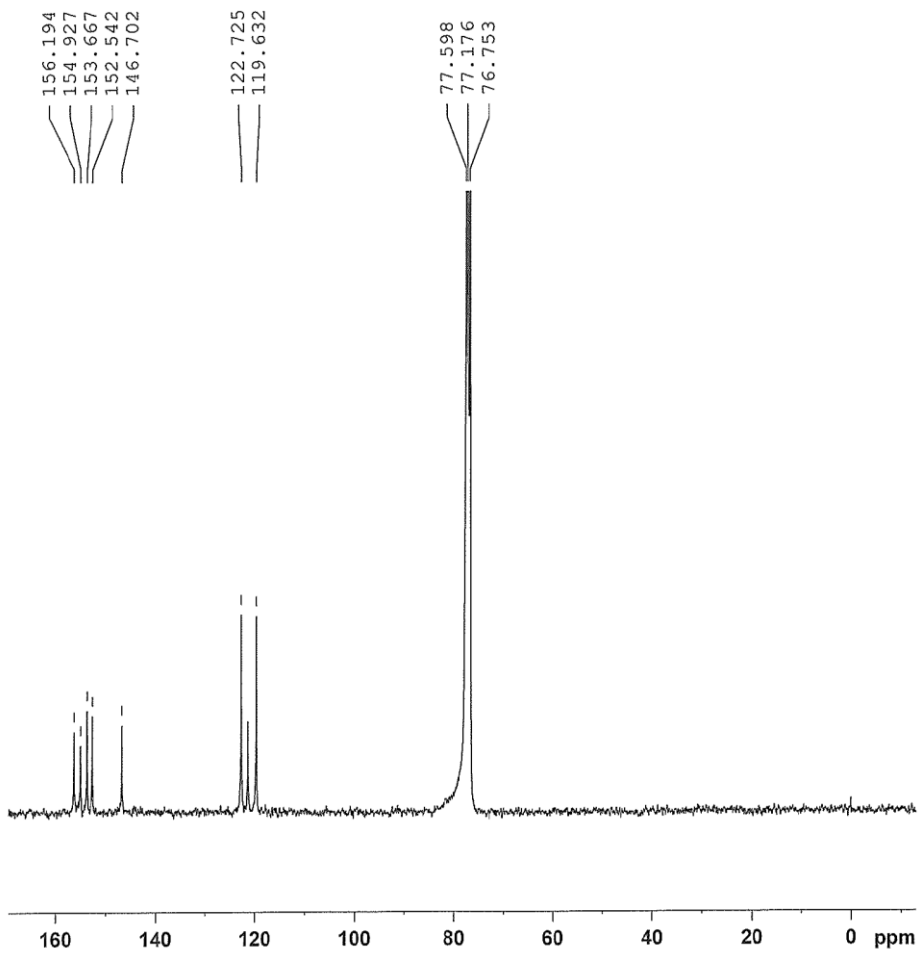


Figure S2 ^{13}C-NMR spectrum of **L**.

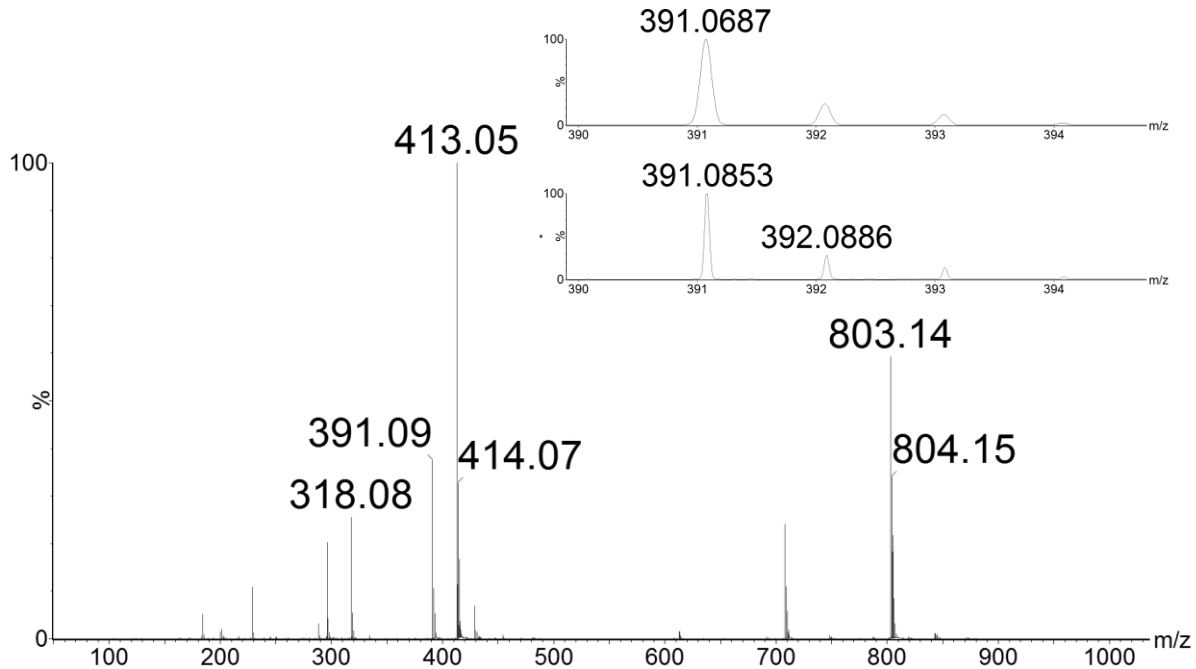


Figure S3 ESI-HRMS spectrum of **L**. The inset shows the isotope pattern for {[Na+**L**]$^+$. The inset shows the isotope pattern (bottom) with the simulated distribution (top)

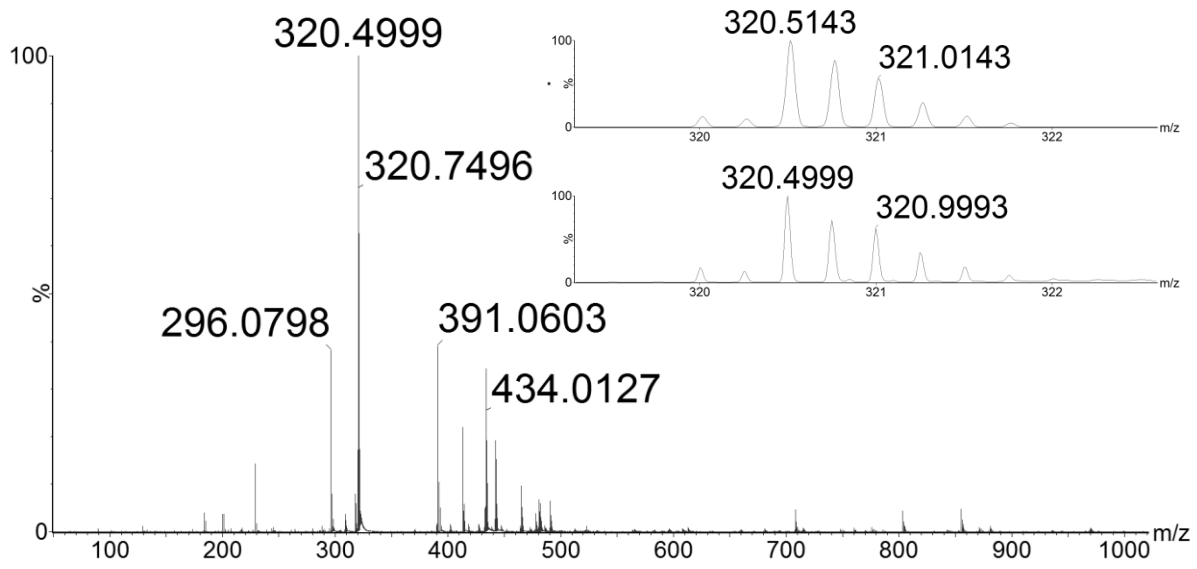


Figure S4 ESI-HRMS spectrum of **1**. The inset shows the isotope pattern for $\{[Fe_2\mathbf{L}_3]^{4+}$. The inset shows the isotope pattern (bottom) with the simulated distribution (top)

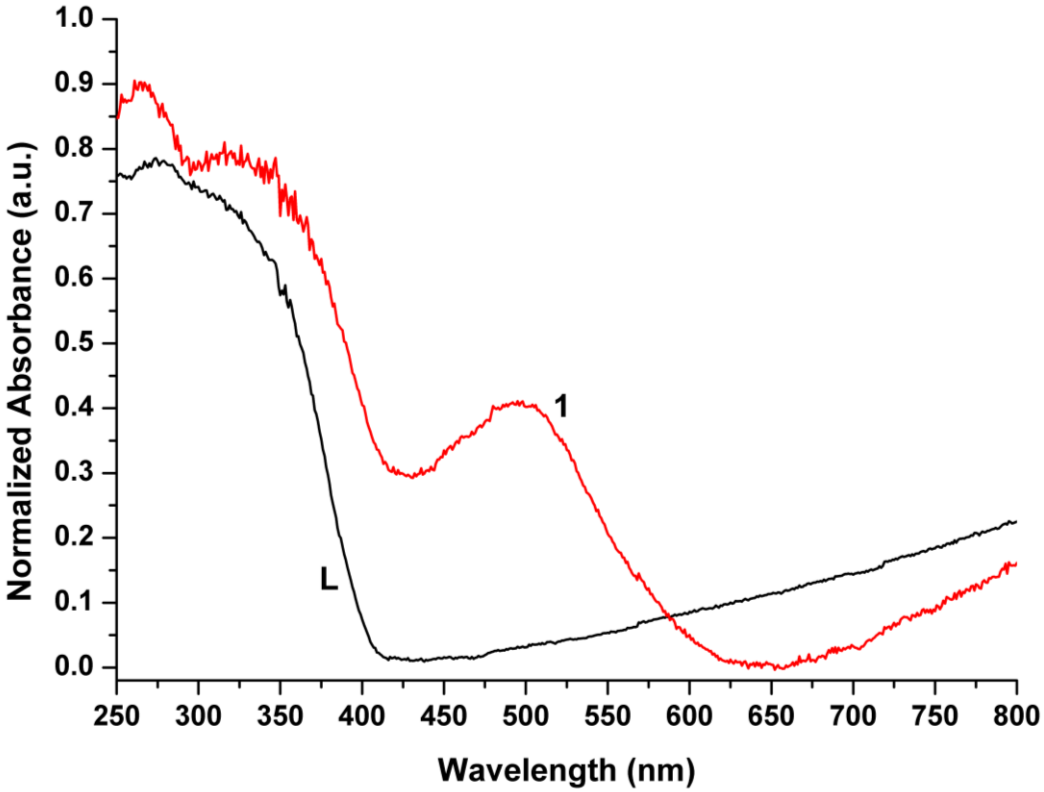


Figure S5. Solid state UV-vis absorption spectra of **L**(black) and **1** (Black) in nujol.

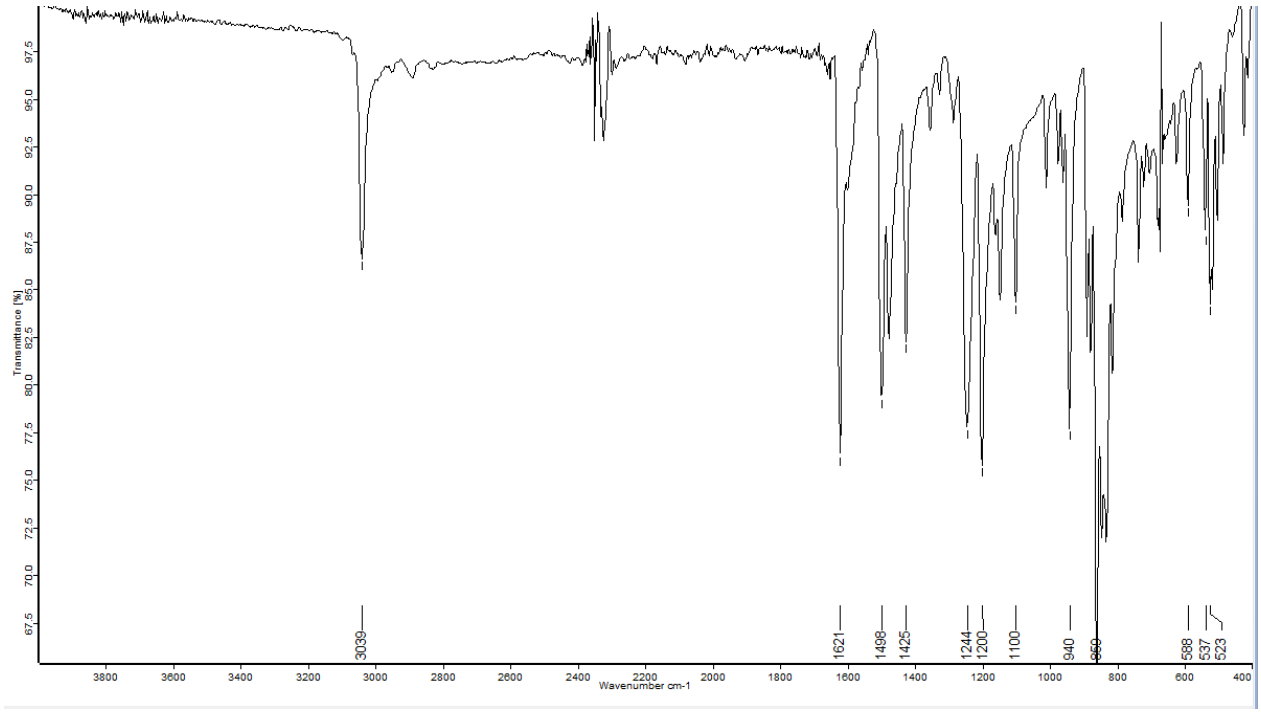


Figure S6: FT-IR spectra of **L**.

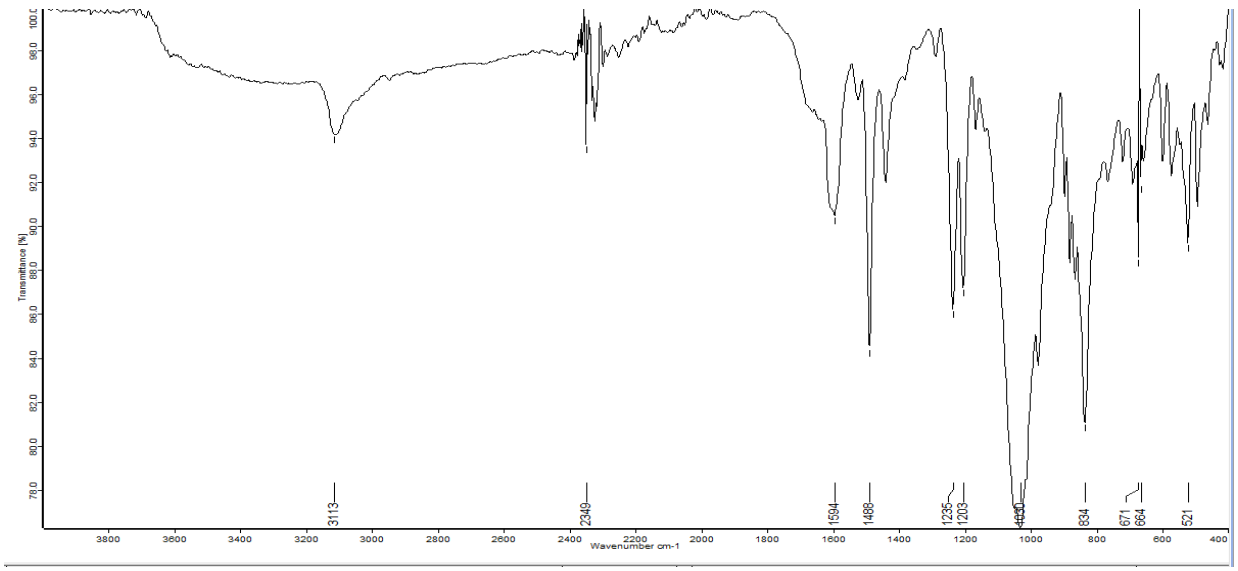


Figure S7: FT-IR spectra of **1**.

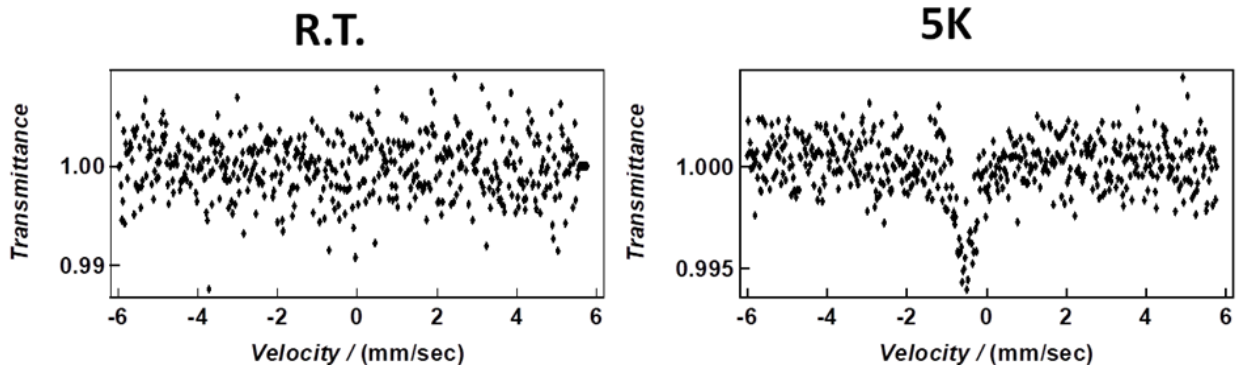


Figure S8 Mössbauer spectrum of **1** at RT and 5 K.

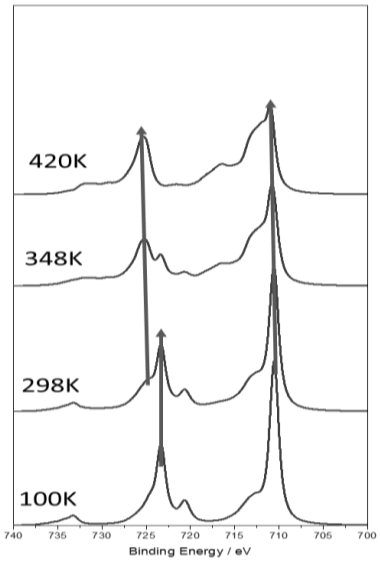


Figure S9. The simulation of VT-XPS of the Fe 2p region.

Crystallographic details:

1 at 298 K:

Empirical formula	$C_{64}H_{48.6}B_4F_{16}Fe_2N_{14}O_{3.3}S_6$
Formula weight	1717.07
Temperature/K	298
Crystal system	triclinic
Space group	$P\bar{1}$
a/Å	11.806(2)
b/Å	15.605(3)
c/Å	22.029(4)
α/°	89.52(3)
β/°	85.48(3)
γ/°	73.49(3)
Volume/Å^3	3878.6(15)
Z	2
ρ_{calc}g/cm^3	1.470
μ/mm^{-1}	0.627
F(000)	1737.0
Crystal size/mm^3	0.03 × 0.02 × 0.01
Radiation	Synchrotron (λ = 0.7108)
2Θ range for data collection/°	2.722 to 49.996
Index ranges	$-14 \le h \le 14$, $-18 \le k \le 18$, $-26 \le l \le 26$
Reflections collected	47455
Independent reflections	12382 [R_{int} = 0.0341, R_{sigma} = 0.0286]
Data/restraints/parameters	12382/399/1153
Goodness-of-fit on F^2	1.045
Final R indexes [I>=2σ (I)]	R_1 = 0.0695, wR_2 = 0.2157
Final R indexes [all data]	R_1 = 0.0804, wR_2 = 0.2289
Largest diff. peak/hole / e Å^{-3}	0.93/-0.55

Table S2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **1** at 298 K U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Fe01	5025.6(5)	2411.3(4)	8596.3(3)	37.87(19)
Fe02	10081.1(6)	6992.0(4)	6406.6(3)	39.36(19)
S1A	4523.3(15)	-18.1(9)	7685.9(7)	64.5(4)
S2A	11351.1(14)	8840.0(11)	7604.7(7)	67.4(4)
S1B	1298.8(12)	3049.0(11)	9455.7(8)	66.6(4)

S2B	13609(2)	6179.1(18)	5269.2(8)	100.3(7)
S1C	6341.7(14)	620.2(10)	10156.2(6)	63.5(4)
S2C	9012.3(17)	9292.4(10)	5088.9(9)	76.7(5)
O1A	4272(3)	6531(2)	7164.9(18)	53.7(9)
O1B	9018(3)	4825(2)	9114.0(14)	49.2(8)
O1C	8643(4)	2951(2)	6038.2(16)	69.2(12)
N1A	4755(3)	1402(2)	8153.0(17)	43.9(9)
N2A	4383(3)	3050(2)	7844.3(17)	41.6(8)
N3A	8518(3)	7478(2)	6947.6(17)	40.8(8)
N4A	10557(3)	7832(3)	6962.7(17)	44.1(9)
N1B	3413(3)	2752(3)	9012.4(17)	42.8(9)
N2B	5095(3)	3496(3)	9063.2(17)	41.7(8)
N3B	10868(4)	5886(3)	6910.4(16)	45.0(9)
N4B	11682(5)	6571(3)	5939.4(18)	58.2(11)
N1C	5708(3)	1626(3)	9260.2(17)	42.7(8)
N2C	6721(3)	2032(2)	8266.3(17)	41.9(8)
N3C	9258(3)	6359(2)	5814.8(16)	41.7(8)
N4C	9540(4)	7975(3)	5799(2)	51.5(10)
C1A	4933(5)	541(3)	8251(2)	54.9(12)
C2A	4090(5)	939(4)	7291(3)	57.6(13)
C3A	4269(4)	1628(3)	7606(2)	46.7(11)
C4A	4081(4)	2561(3)	7455(2)	48.3(11)
C5A	4313(4)	3952(3)	7666(2)	42.6(10)
C6A	3540(4)	4682(3)	7982(2)	44.5(10)
C7A	3535(4)	5548(3)	7814(2)	46.3(11)
C8A	4296(4)	5664(3)	7333(2)	45.9(11)
C9A	5033(4)	4946(3)	7014(2)	50.6(11)
C10A	5046(4)	4084(3)	7177(2)	48.0(11)
C11A	5366(4)	6714(3)	7085(2)	46.9(11)
C12A	5481(5)	7348(3)	6674(3)	60.2(14)
C13A	6526(5)	7600(4)	6622(3)	62.1(15)
C14A	7435(4)	7206(3)	6968(2)	40.8(10)
C15A	7325(5)	6542(4)	7354(3)	69.1(17)
C16A	6289(5)	6290(4)	7410(3)	71.7(18)
C17A	8500(4)	8118(3)	7307(2)	46(1)
C18A	9614(4)	8339(3)	7342(2)	45(1)
C19A	9884(5)	8914(4)	7718(2)	57.5(13)
C20A	11515(5)	8038(4)	7058(2)	54.9(12)
C1B	2500(4)	2437(3)	9014(2)	51.6(12)
C2B	2052(5)	3765(4)	9659(3)	64.7(15)
C3B	3178(4)	3506(3)	9378(2)	48.3(11)
C4B	4161(4)	3879(3)	9397(2)	49.1(11)

C5B	7076(5)	3382(4)	9359(3)	59.0(14)
C6B	8051(5)	3712(4)	9362(3)	59.2(14)
C7B	8038(4)	4504(3)	9088.3(19)	42.8(10)
C8B	7040(5)	4997(4)	8833(3)	67.0(16)
C9B	6062(5)	4665(4)	8830(3)	67.7(17)
C10B	9475(4)	5076(3)	8555.1(19)	43.5(10)
C11B	9805(6)	4480(4)	8071(2)	60.9(14)
C12B	10289(6)	4738(4)	7523(2)	61.1(14)
C13B	10408(4)	5599(3)	7474(2)	44(1)
C14B	10119(4)	6169(3)	7972(2)	47.1(11)
C15B	9658(5)	5908(3)	8517(2)	47.5(11)
C16B	11890(5)	5420(4)	6682(2)	50.5(12)
C17B	12381(5)	5758(4)	6136(2)	53.5(12)
C18B	13423(6)	5436(5)	5821(3)	75.0(18)
C19B	12241(7)	6861(5)	5482(3)	80.2(19)
C1C	5299(5)	1373(3)	9774(2)	52.3(12)
C2C	7401(5)	653(4)	9606(2)	59.5(13)
C3C	6909(4)	1218(3)	9152(2)	48.8(11)
C4C	7436(4)	1469(3)	8590(2)	49.6(11)
C5C	7200(5)	1813(3)	7166(2)	54.1(12)
C6C	7663(6)	2055(4)	6614(2)	59.6(14)
C7C	8155(5)	2762(3)	6598(2)	50.7(12)
C8C	8182(5)	3224(3)	7125(2)	53.2(12)
C9C	7710(5)	2975(3)	7674(2)	53.0(12)
C10C	8801(6)	3802(3)	5975(2)	54.7(13)
C11C	7806(6)	4533(4)	5946(3)	60.8(14)
C12C	7968(5)	5375(4)	5889(3)	58.1(13)
C13C	9097(5)	5487(3)	5858.6(19)	44.7(10)
C14C	10063(5)	4745(3)	5865(2)	46.7(11)
C15C	9920(5)	3896(3)	5933(2)	52.3(12)
C16C	8709(4)	6881(3)	5410(2)	45.8(11)
C17C	8866(5)	7769(3)	5366(2)	49.3(11)
C18C	8499(5)	8408(4)	4947(3)	60.3(14)
C19C	9678(6)	8755(4)	5700(3)	69.9(17)
C00T	7210(4)	2280(3)	7694(2)	42.5(10)
C00X	6092(4)	3855(3)	9082(2)	43.5(10)
C2	9710(20)	1605(15)	10511(10)	41(5)
N5AA	8247(17)	3254(13)	10937(9)	56(4)
N3	8376(17)	2857(14)	11104(8)	59(5)
C1AA	8968(14)	2297(12)	10845(6)	22(3)
N02V	4719(11)	6802(7)	9324(5)	77(3)
C033	4078(10)	7881(7)	8485(4)	53(2)

C02W	4425(9)	7258(7)	8959(5)	50(2)
N0AA	11354(15)	2571(11)	7120(8)	47(4)
C1	11058(15)	1966(11)	7132(9)	32(4)
C4AA	10690(20)	1190(18)	7116(14)	53(7)
F6AA	3712(14)	8857(9)	5728(5)	162(5)
F7AA	2899(12)	8620(7)	5840(6)	129(4)
F8AA	3216(18)	9211(14)	6669(6)	83(4)
F9AA	3009(12)	10060(9)	5696(6)	114(4)
F0BA	1739(11)	9366(12)	6063(7)	124(5)
F02K	2929(13)	10296(7)	6011(6)	109(4)
F00M	3220(20)	9438(14)	6660(6)	94(5)
F01Q	1512(8)	9729(9)	6209(7)	91(3)
N1	7121(9)	-184(5)	6531(4)	53(2)
C2AA	6526(9)	7(6)	6180(5)	44(2)
C3AA	5728(11)	170(13)	5691(7)	94(5)
F00N	10184(4)	298(3)	8602(2)	109.8(16)
F00W	10277(5)	1609(3)	8938(3)	122.7(18)
B3	7094(6)	8463(5)	8924(3)	83.0(19)
F1	6083(10)	9068(9)	9168(6)	116(4)
F2	8003(13)	8725(14)	8683(7)	162(7)
F3	7483(14)	7963(11)	9421(6)	162(6)
F4	6701(14)	8111(14)	8431(6)	168(5)
F0AA	5904(8)	8814(7)	8921(6)	90(3)
F5	7548(10)	9121(7)	8632(6)	94(3)
F7	7407(14)	7659(7)	8657(7)	147(5)
F8	7266(11)	8500(9)	9552(4)	109(3)
F5BA	11905(5)	624(5)	8577(4)	157(3)
F9BA	11052(7)	402(5)	9450(3)	171(3)
B02P	10865(6)	720(4)	8888(3)	67.3(18)
B02Z	2803(7)	9447(5)	6101(3)	82.0(18)
O1	6851(16)	1879(11)	5283(7)	67(4)
C1AB	8731(18)	2607(15)	10795(8)	37(5)
C0AA	9410(30)	1807(18)	10580(14)	68(9)
N0AB	11409(15)	2640(11)	7435(9)	50(4)
C5AA	11158(15)	2100(11)	7319(9)	28(4)
C4AB	10740(20)	1271(18)	7275(13)	52(7)
B0AA	3758(8)	2973(7)	5706(4)	123(2)
F2AA	4821(11)	2761(10)	5927(8)	141(4)
F1AA	3042(11)	3552(8)	6169(5)	130(3)
F4AA	3649(13)	3473(10)	5195(5)	144(3)
F3AA	3350(14)	2274(9)	5655(8)	164(4)
F2BA	2691(10)	3550(9)	5814(7)	148(4)

F5AA	3897(11)	2706(11)	5107(5)	147(4)
F1BA	4683(11)	3200(8)	5893(8)	125(4)
F3AB	3736(15)	2162(8)	5985(6)	159(4)

Table S3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **1** at 298 K. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
Fe01	31.8(4)	46.1(4)	39.0(3)	7.2(2)	-5.2(3)	-15.8(3)
Fe02	43.0(4)	43.8(3)	35.1(3)	6.3(2)	-6.2(3)	-17.8(3)
S1A	76.8(10)	49.6(7)	72.4(9)	-0.2(6)	-5.3(8)	-26.6(6)
S2A	62.9(9)	93.1(11)	63.9(8)	3.5(7)	-14.0(7)	-48.2(8)
S1B	35.0(7)	85.3(10)	83.7(10)	-5.0(8)	5.1(7)	-26.5(7)
S2B	102.2(16)	161(2)	53.6(9)	3.3(10)	18.6(9)	-69.6(15)
S1C	71.1(10)	69.7(8)	48.9(7)	21.6(6)	-9.0(6)	-18.3(7)
S2C	85.1(12)	61.3(9)	93.7(11)	34.8(8)	-27.5(9)	-32.4(8)
O1A	28.6(18)	48.5(18)	88(2)	17.0(17)	-15.3(17)	-15.6(13)
O1B	48(2)	77(2)	36.7(15)	12.3(14)	-9.0(14)	-38.8(17)
O1C	116(4)	54(2)	45.7(19)	-8.3(15)	25(2)	-45(2)
N1A	41(2)	45(2)	48(2)	8.0(16)	-3.8(17)	-15.8(16)
N2A	38(2)	46(2)	44.6(19)	6.0(16)	-7.6(16)	-16.7(16)
N3A	37(2)	45(2)	45.4(19)	4.3(16)	-5.9(16)	-19.2(15)
N4A	37(2)	53(2)	44(2)	11.1(16)	-3.3(17)	-16.4(17)
N1B	32(2)	54(2)	47(2)	8.4(16)	-7.5(16)	-18.6(16)
N2B	33(2)	57(2)	41.0(19)	7.0(16)	-6.1(16)	-21.8(17)
N3B	50(2)	61(2)	32.9(17)	3.8(16)	-3.3(17)	-29.3(19)
N4B	78(3)	69(3)	36.6(19)	6.9(18)	-2.1(19)	-37(2)
N1C	39(2)	52(2)	40.9(19)	8.1(16)	-3.6(16)	-18.2(16)
N2C	38(2)	49(2)	41.5(19)	5.7(16)	-2.3(16)	-17.4(16)
N3C	44(2)	43.8(19)	38.5(18)	4.4(15)	-3.2(16)	-15.2(16)
N4C	53(3)	47(2)	60(2)	10.1(18)	-17(2)	-19.3(18)
C1A	54(3)	54(3)	59(3)	11(2)	-3(2)	-19(2)
C2A	62(3)	58(3)	57(3)	0(2)	-10(3)	-23(2)
C3A	43(3)	53(3)	49(2)	4(2)	-7(2)	-21(2)
C4A	47(3)	53(3)	50(3)	10(2)	-14(2)	-21(2)
C5A	41(3)	47(2)	44(2)	8.7(18)	-15(2)	-17.5(19)
C6A	34(2)	56(3)	47(2)	10(2)	-9(2)	-18(2)
C7A	33(2)	50(3)	57(3)	1(2)	-12(2)	-11.9(19)
C8A	33(3)	48(2)	62(3)	13(2)	-16(2)	-16.6(19)
C9A	39(3)	56(3)	59(3)	14(2)	-3(2)	-18(2)
C10A	45(3)	50(3)	49(3)	8(2)	-5(2)	-13(2)
C11A	35(3)	47(2)	63(3)	9(2)	-13(2)	-16.6(19)

C12A	43(3)	55(3)	87(4)	26(3)	-25(3)	-17(2)
C13A	50(3)	63(3)	82(4)	34(3)	-19(3)	-27(2)
C14A	34(2)	46(2)	46(2)	2.5(18)	-4.8(19)	-15.8(18)
C15A	47(3)	85(4)	89(4)	43(3)	-32(3)	-36(3)
C16A	59(4)	87(4)	86(4)	51(3)	-35(3)	-43(3)
C17A	38(3)	54(3)	49(2)	1(2)	2(2)	-20(2)
C18A	45(3)	50(3)	44(2)	2.7(19)	-3(2)	-21(2)
C19A	58(3)	71(3)	54(3)	-4(2)	-1(3)	-36(3)
C20A	42(3)	72(3)	54(3)	14(2)	-7(2)	-23(2)
C1B	41(3)	59(3)	59(3)	6(2)	-9(2)	-20(2)
C2B	44(3)	80(4)	73(4)	-14(3)	7(3)	-23(3)
C3B	37(3)	64(3)	47(2)	-1(2)	-2(2)	-20(2)
C4B	40(3)	61(3)	50(3)	-4(2)	-3(2)	-21(2)
C5B	46(3)	68(3)	73(3)	31(3)	-19(3)	-30(2)
C6B	40(3)	76(3)	70(3)	28(3)	-19(3)	-27(2)
C7B	38(3)	64(3)	35(2)	2.7(19)	-4.3(19)	-27(2)
C8B	65(4)	69(3)	84(4)	34(3)	-36(3)	-39(3)
C9B	54(3)	71(3)	93(4)	31(3)	-42(3)	-33(3)
C10B	40(3)	65(3)	34(2)	11.2(19)	-8.9(19)	-29(2)
C11B	89(4)	58(3)	47(3)	7(2)	-6(3)	-40(3)
C12B	88(4)	65(3)	39(2)	0(2)	2(3)	-37(3)
C13B	46(3)	56(3)	37(2)	6.3(19)	-7(2)	-24(2)
C14B	50(3)	57(3)	43(2)	7(2)	-6(2)	-29(2)
C15B	50(3)	59(3)	38(2)	1.1(19)	-3(2)	-24(2)
C16B	52(3)	68(3)	37(2)	8(2)	-10(2)	-25(2)
C17B	51(3)	79(3)	37(2)	2(2)	-3(2)	-30(3)
C18B	62(4)	122(5)	47(3)	2(3)	3(3)	-36(4)
C19B	105(6)	100(5)	48(3)	9(3)	8(3)	-53(4)
C1C	53(3)	61(3)	46(3)	15(2)	-5(2)	-21(2)
C2C	55(3)	64(3)	57(3)	16(2)	-12(3)	-12(2)
C3C	43(3)	53(3)	48(2)	12(2)	-6(2)	-10(2)
C4C	38(3)	59(3)	48(3)	9(2)	-1(2)	-10(2)
C5C	63(3)	55(3)	50(3)	1(2)	3(2)	-29(2)
C6C	83(4)	59(3)	45(3)	-8(2)	11(3)	-36(3)
C7C	61(3)	50(3)	43(2)	-2.7(19)	14(2)	-22(2)
C8C	68(4)	56(3)	45(3)	-2(2)	2(2)	-34(2)
C9C	64(3)	61(3)	41(2)	-5(2)	1(2)	-31(2)
C10C	82(4)	53(3)	34(2)	-5.5(19)	12(2)	-30(3)
C11C	64(4)	65(3)	62(3)	-6(2)	12(3)	-35(3)
C12C	61(4)	53(3)	62(3)	-5(2)	-1(3)	-22(2)
C13C	53(3)	50(2)	35(2)	1.8(18)	-1(2)	-21(2)
C14C	56(3)	50(3)	36(2)	3.0(18)	0(2)	-19(2)

C15C	72(4)	50(3)	36(2)	1.8(19)	2(2)	-20(2)
C16C	49(3)	53(3)	40(2)	6.3(19)	-9(2)	-22(2)
C17C	52(3)	50(3)	48(3)	9(2)	-13(2)	-16(2)
C18C	66(4)	63(3)	58(3)	21(2)	-19(3)	-25(3)
C19C	75(4)	55(3)	91(4)	22(3)	-32(3)	-31(3)
C00T	38(3)	49(2)	39(2)	7.3(18)	1.4(19)	-13.4(19)
C00X	39(3)	57(3)	40(2)	4.4(19)	-6.7(19)	-22(2)
N02V	79(8)	64(6)	79(7)	5(5)	-2(6)	-8(5)
C033	52(6)	71(6)	43(5)	-1(4)	-13(4)	-25(5)
C02W	39(5)	61(6)	52(5)	-19(5)	3(4)	-16(4)
F6AA	188(10)	161(8)	105(7)	4(6)	19(7)	-4(7)
F7AA	123(9)	109(6)	161(9)	-26(6)	14(7)	-50(6)
F8AA	68(7)	86(8)	95(5)	28(4)	-14(5)	-22(5)
F9AA	98(7)	154(8)	114(8)	75(7)	-44(7)	-68(6)
F0BA	134(7)	172(15)	103(10)	32(9)	-36(6)	-94(8)
F02K	134(9)	102(6)	111(8)	60(6)	-53(7)	-56(6)
F00M	108(10)	103(11)	86(5)	14(5)	-33(5)	-50(8)
F01Q	78(5)	105(7)	95(7)	-13(5)	-18(4)	-30(4)
N1	67(6)	36(4)	60(5)	-2(4)	2(5)	-21(4)
C2AA	36(5)	38(5)	56(6)	-6(4)	18(5)	-15(4)
C3AA	34(7)	160(15)	79(8)	10(9)	5(6)	-17(8)
F00N	85(3)	111(3)	145(4)	-33(3)	-37(3)	-39(2)
F00W	135(4)	80(3)	157(5)	-7(3)	-40(4)	-30(3)
B3	67(4)	99(4)	77(4)	-2(3)	3(3)	-16(3)
F1	111(7)	116(8)	105(9)	19(6)	32(6)	-19(6)
F2	124(9)	307(19)	88(7)	-19(10)	21(7)	-124(11)
F3	140(10)	174(12)	134(8)	42(8)	-14(7)	17(9)
F4	148(11)	279(15)	115(7)	-31(8)	8(7)	-126(11)
F0AA	80(5)	89(6)	102(8)	29(5)	-21(4)	-21(4)
F5	83(6)	101(6)	95(6)	-14(4)	20(5)	-30(5)
F7	169(11)	87(5)	152(10)	-27(5)	-7(8)	15(5)
F8	105(8)	142(9)	77(4)	-8(5)	-7(4)	-31(7)
F5BA	84(4)	180(6)	217(7)	-50(5)	34(4)	-64(4)
F9BA	222(8)	171(6)	110(4)	29(4)	-83(5)	-25(5)
B02P	55(4)	81(5)	73(4)	-2(3)	-15(3)	-29(3)
B02Z	98(5)	78(4)	74(4)	22(3)	-13(3)	-30(3)
O1	87(12)	87(11)	46(7)	18(7)	-17(8)	-53(9)
B0AA	113(4)	142(5)	112(4)	1(4)	-52(3)	-21(3)
F2AA	123(5)	163(10)	132(7)	-13(7)	-60(5)	-21(5)
F1AA	139(6)	131(6)	112(5)	17(4)	-42(4)	-19(5)
F4AA	147(8)	169(7)	120(5)	14(5)	-59(5)	-41(6)
F3AA	165(9)	162(6)	177(10)	1(6)	-68(7)	-53(6)

F2BA	116(5)	155(7)	166(9)	-11(6)	-48(5)	-18(4)
F5AA	130(7)	186(9)	120(5)	-9(5)	-50(4)	-27(7)
F1BA	115(5)	129(8)	127(7)	7(6)	-60(5)	-12(5)
F3AB	195(10)	149(6)	129(7)	-2(5)	-37(6)	-38(5)

Table S4 Bond Lengths for **1** at 298 K.

Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**
Fe01	N1A	1.974(4)	C3B	C4B	1.442(7)
Fe01	N2A	2.013(4)	C5B	C6B	1.389(7)
Fe01	N1B	1.977(4)	C5B	C00X	1.372(7)
Fe01	N2B	2.013(4)	C6B	C7B	1.367(7)
Fe01	N1C	1.971(4)	C7B	C8B	1.371(7)
Fe01	N2C	1.998(4)	C8B	C9B	1.395(7)
Fe02	N3A	2.067(4)	C9B	C00X	1.369(7)
Fe02	N4A	2.022(4)	C10B	C11B	1.377(7)
Fe02	N3B	2.072(4)	C10B	C15B	1.375(7)
Fe02	N4B	2.016(5)	C11B	C12B	1.401(7)
Fe02	N3C	2.095(4)	C12B	C13B	1.392(7)
Fe02	N4C	2.023(4)	C13B	C14B	1.377(7)
S1A	C1A	1.703(6)	C14B	C15B	1.386(7)
S1A	C2A	1.692(6)	C16B	C17B	1.454(7)
S2A	C19A	1.702(6)	C17B	C18B	1.328(8)
S2A	C20A	1.703(6)	C2C	C3C	1.379(7)
S1B	C1B	1.702(6)	C3C	C4C	1.444(7)
S1B	C2B	1.696(6)	C5C	C6C	1.388(7)
S2B	C18B	1.718(7)	C5C	C00T	1.379(7)
S2B	C19B	1.694(8)	C6C	C7C	1.383(7)
S1C	C1C	1.712(5)	C7C	C8C	1.378(7)
S1C	C2C	1.683(6)	C8C	C9C	1.391(7)
S2C	C18C	1.698(6)	C9C	C00T	1.373(7)
S2C	C19C	1.705(6)	C10C	C11C	1.391(8)
O1A	C8A	1.394(6)	C10C	C15C	1.365(8)
O1A	C11A	1.397(6)	C11C	C12C	1.383(7)
O1B	C7B	1.389(5)	C12C	C13C	1.390(8)
O1B	C10B	1.403(5)	C13C	C14C	1.375(7)
O1C	C7C	1.385(6)	C14C	C15C	1.388(7)
O1C	C10C	1.398(6)	C16C	C17C	1.451(7)
N1A	C1A	1.319(6)	C17C	C18C	1.355(7)
N1A	C3A	1.376(6)	C2	C1AA	1.36(2)
N2A	C4A	1.287(6)	N5AA	C1AB	1.04(2)
N2A	C5A	1.440(6)	N3	C1AA	1.08(2)

N3A	C14A	1.454(6)	N02V	C02W	1.081(14)
N3A	C17A	1.275(6)	C033	C02W	1.423(16)
N4A	C18A	1.388(6)	N0AA	C1	1.09(3)
N4A	C20A	1.294(6)	C1	C4AA	1.40(3)
N1B	C1B	1.305(6)	F6AA	B02Z	1.411(10)
N1B	C3B	1.380(6)	F7AA	B02Z	1.389(10)
N2B	C4B	1.272(6)	F8AA	B02Z	1.388(11)
N2B	C00X	1.444(6)	F9AA	B02Z	1.362(10)
N3B	C13B	1.435(6)	F0BA	B02Z	1.307(11)
N3B	C16B	1.284(7)	F02K	B02Z	1.386(10)
N4B	C17B	1.389(7)	F00M	B02Z	1.359(11)
N4B	C19B	1.309(7)	F01Q	B02Z	1.461(10)
N1C	C1C	1.299(6)	N1	C2AA	1.069(13)
N1C	C3C	1.381(6)	C2AA	C3AA	1.460(17)
N2C	C4C	1.286(6)	F00N	B02P	1.367(7)
N2C	C00T	1.441(6)	F00W	B02P	1.364(7)
N3C	C13C	1.427(6)	B3	F1	1.368(10)
N3C	C16C	1.287(6)	B3	F2	1.325(11)
N4C	C17C	1.385(6)	B3	F3	1.369(11)
N4C	C19C	1.288(7)	B3	F4	1.390(10)
C2A	C3A	1.359(7)	B3	F0AA	1.356(10)
C3A	C4A	1.449(7)	B3	F5	1.414(10)
C5A	C6A	1.392(7)	B3	F7	1.331(10)
C5A	C10A	1.379(7)	B3	F8	1.416(10)
C6A	C7A	1.398(7)	F5BA	B02P	1.328(8)
C7A	C8A	1.378(7)	F9BA	B02P	1.341(8)
C8A	C9A	1.367(7)	C1AB	C0AA	1.34(3)
C9A	C10A	1.386(7)	N0AB	C5AA	1.01(2)
C11A	C12A	1.363(7)	C5AA	C4AB	1.52(3)
C11A	C16A	1.359(7)	B0AA	F2AA	1.335(11)
C12A	C13A	1.394(8)	B0AA	F1AA	1.420(11)
C13A	C14A	1.363(7)	B0AA	F4AA	1.357(11)
C14A	C15A	1.364(7)	B0AA	F3AA	1.321(11)
C15A	C16A	1.383(8)	B0AA	F2BA	1.329(11)
C17A	C18A	1.458(7)	B0AA	F5AA	1.370(11)
C18A	C19A	1.346(7)	B0AA	F1BA	1.334(11)
C2B	C3B	1.372(8)	B0AA	F3AB	1.409(11)

Table S5 Bond Angles for **1** at 298 K.

Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
N1A	Fe01	N2A	80.55(15)	C2B	C3B	N1B	114.2(5)

N1A	Fe01	N1B	93.14(16)	C2B	C3B	C4B	131.5(5)
N1A	Fe01	N2B	173.33(16)	N2B	C4B	C3B	116.5(4)
N1A	Fe01	N2C	89.42(16)	C00X	C5B	C6B	119.8(5)
N1B	Fe01	N2A	90.05(16)	C7B	C6B	C5B	120.4(5)
N1B	Fe01	N2B	80.55(16)	C6B	C7B	O1B	118.7(4)
N1B	Fe01	N2C	173.67(15)	C6B	C7B	C8B	120.0(5)
N2B	Fe01	N2A	97.19(15)	C8B	C7B	O1B	121.1(4)
N1C	Fe01	N1A	91.65(15)	C7B	C8B	C9B	119.5(5)
N1C	Fe01	N2A	171.67(16)	C00X	C9B	C8B	120.4(5)
N1C	Fe01	N1B	93.30(16)	C11B	C10B	O1B	120.5(4)
N1C	Fe01	N2B	90.88(15)	C15B	C10B	O1B	118.2(4)
N1C	Fe01	N2C	80.82(16)	C15B	C10B	C11B	121.1(4)
N2C	Fe01	N2A	96.08(16)	C10B	C11B	C12B	119.5(5)
N2C	Fe01	N2B	97.08(16)	C13B	C12B	C11B	119.3(5)
N3A	Fe02	N3B	99.12(16)	C12B	C13B	N3B	120.2(4)
N3A	Fe02	N3C	91.58(15)	C14B	C13B	N3B	119.7(4)
N4A	Fe02	N3A	79.74(15)	C14B	C13B	C12B	120.1(4)
N4A	Fe02	N3B	92.40(15)	C13B	C14B	C15B	120.5(4)
N4A	Fe02	N3C	167.45(15)	C10B	C15B	C14B	119.3(4)
N4A	Fe02	N4C	91.41(16)	N3B	C16B	C17B	117.1(5)
N3B	Fe02	N3C	97.95(14)	N4B	C17B	C16B	114.6(5)
N4B	Fe02	N3A	174.38(16)	C18B	C17B	N4B	115.5(5)
N4B	Fe02	N4A	94.78(17)	C18B	C17B	C16B	129.8(6)
N4B	Fe02	N3B	79.71(17)	C17B	C18B	S2B	109.8(5)
N4B	Fe02	N3C	94.03(17)	N4B	C19B	S2B	114.4(6)
N4B	Fe02	N4C	90.67(18)	N1C	C1C	S1C	114.1(4)
N4C	Fe02	N3A	90.74(17)	C3C	C2C	S1C	109.7(4)
N4C	Fe02	N3B	169.92(17)	N1C	C3C	C4C	114.5(4)
N4C	Fe02	N3C	79.57(15)	C2C	C3C	N1C	114.3(4)
C2A	S1A	C1A	90.5(3)	C2C	C3C	C4C	131.1(5)
C19A	S2A	C20A	89.9(3)	N2C	C4C	C3C	115.5(4)
C2B	S1B	C1B	91.2(3)	C00T	C5C	C6C	120.5(5)
C19B	S2B	C18B	90.0(3)	C7C	C6C	C5C	119.4(5)
C2C	S1C	C1C	90.8(3)	C6C	C7C	O1C	116.8(4)
C18C	S2C	C19C	90.0(3)	C8C	C7C	O1C	122.8(4)
C8A	O1A	C11A	116.5(3)	C8C	C7C	C6C	120.3(4)
C7B	O1B	C10B	115.6(3)	C7C	C8C	C9C	119.5(5)
C7C	O1C	C10C	116.6(4)	C00T	C9C	C8C	120.5(4)
C1A	N1A	Fe01	135.4(3)	C11C	C10C	O1C	118.6(6)
C1A	N1A	C3A	110.3(4)	C15C	C10C	O1C	119.7(5)
C3A	N1A	Fe01	114.3(3)	C15C	C10C	C11C	121.7(5)
C4A	N2A	Fe01	115.0(3)	C12C	C11C	C10C	118.4(6)

C4A	N2A	C5A	116.4(4)	C11C	C12C	C13C	120.8(5)
C5A	N2A	Fe01	128.4(3)	C12C	C13C	N3C	120.6(4)
C14A	N3A	Fe02	129.4(3)	C14C	C13C	N3C	120.3(5)
C17A	N3A	Fe02	114.9(3)	C14C	C13C	C12C	119.1(5)
C17A	N3A	C14A	115.7(4)	C13C	C14C	C15C	120.9(5)
C18A	N4A	Fe02	112.9(3)	C10C	C15C	C14C	118.9(5)
C20A	N4A	Fe02	137.0(4)	N3C	C16C	C17C	117.6(4)
C20A	N4A	C18A	110.1(4)	N4C	C17C	C16C	115.0(4)
C1B	N1B	Fe01	134.7(4)	C18C	C17C	N4C	115.4(5)
C1B	N1B	C3B	111.9(4)	C18C	C17C	C16C	129.5(5)
C3B	N1B	Fe01	113.4(3)	C17C	C18C	S2C	109.4(4)
C4B	N2B	Fe01	115.3(3)	N4C	C19C	S2C	115.2(4)
C4B	N2B	C00X	117.2(4)	C5C	C00T	N2C	120.5(4)
C00X	N2B	Fe01	127.4(3)	C9C	C00T	N2C	119.9(4)
C13B	N3B	Fe02	127.7(3)	C9C	C00T	C5C	119.7(4)
C16B	N3B	Fe02	114.5(3)	C5B	C00X	N2B	119.7(4)
C16B	N3B	C13B	117.9(4)	C9B	C00X	N2B	120.6(4)
C17B	N4B	Fe02	113.5(3)	C9B	C00X	C5B	119.7(5)
C19B	N4B	Fe02	136.2(5)	N3	C1AA	C2	179(2)
C19B	N4B	C17B	110.2(6)	N02V	C02W	C033	177.2(12)
C1C	N1C	Fe01	135.6(4)	N0AA	C1	C4AA	177(3)
C1C	N1C	C3C	111.1(4)	N1	C2AA	C3AA	174.1(12)
C3C	N1C	Fe01	113.3(3)	F1	B3	F3	102.0(9)
C4C	N2C	Fe01	115.7(3)	F1	B3	F4	102.6(10)
C4C	N2C	C00T	117.1(4)	F2	B3	F1	121.2(13)
C00T	N2C	Fe01	127.1(3)	F2	B3	F3	106.4(11)
C13C	N3C	Fe02	128.4(3)	F2	B3	F4	103.8(10)
C16C	N3C	Fe02	113.6(3)	F3	B3	F4	122.4(14)
C16C	N3C	C13C	117.4(4)	F0AA	B3	F5	103.4(8)
C17C	N4C	Fe02	113.7(3)	F0AA	B3	F8	102.1(8)
C19C	N4C	Fe02	136.3(4)	F5	B3	F8	107.2(9)
C19C	N4C	C17C	110.0(4)	F7	B3	F0AA	108.8(9)
N1A	C1A	S1A	114.1(4)	F7	B3	F5	116.4(10)
C3A	C2A	S1A	110.0(4)	F7	B3	F8	117.2(10)
N1A	C3A	C4A	113.7(4)	F00W	B02P	F00N	108.5(5)
C2A	C3A	N1A	115.1(4)	F5BA	B02P	F00N	111.5(6)
C2A	C3A	C4A	131.2(4)	F5BA	B02P	F00W	108.7(6)
N2A	C4A	C3A	116.4(4)	F5BA	B02P	F9BA	108.9(7)
C6A	C5A	N2A	121.3(4)	F9BA	B02P	F00N	110.9(6)
C10A	C5A	N2A	118.5(4)	F9BA	B02P	F00W	108.2(6)
C10A	C5A	C6A	120.1(4)	F7AA	B02Z	F01Q	96.7(8)
C5A	C6A	C7A	119.7(5)	F8AA	B02Z	F7AA	102.0(10)

C8A	C7A	C6A	119.1(5)	F8AA	B02Z	F01Q	105.0(11)
C7A	C8A	O1A	118.6(4)	F9AA	B02Z	F6AA	82.4(9)
C9A	C8A	O1A	120.4(5)	F0BA	B02Z	F6AA	115.6(11)
C9A	C8A	C7A	121.0(4)	F0BA	B02Z	F9AA	110.2(10)
C8A	C9A	C10A	120.4(5)	F0BA	B02Z	F00M	118.8(13)
C5A	C10A	C9A	119.6(5)	F02K	B02Z	F7AA	146.4(10)
C12A	C11A	O1A	118.0(4)	F02K	B02Z	F8AA	104.4(11)
C16A	C11A	O1A	121.7(5)	F02K	B02Z	F01Q	96.2(9)
C16A	C11A	C12A	120.3(5)	F00M	B02Z	F6AA	106.4(12)
C11A	C12A	C13A	119.3(5)	F00M	B02Z	F9AA	117.8(12)
C14A	C13A	C12A	120.6(5)	N5AA	C1AB	C0AA	175(3)
C13A	C14A	N3A	122.3(4)	N0AB	C5AA	C4AB	169(2)
C13A	C14A	C15A	119.1(5)	F2AA	B0AA	F1AA	102.0(10)
C15A	C14A	N3A	118.5(4)	F2AA	B0AA	F4AA	115.8(12)
C14A	C15A	C16A	120.6(5)	F4AA	B0AA	F1AA	104.8(10)
C11A	C16A	C15A	119.9(5)	F3AA	B0AA	F2AA	112.5(11)
N3A	C17A	C18A	116.6(4)	F3AA	B0AA	F1AA	108.5(11)
N4A	C18A	C17A	115.2(4)	F3AA	B0AA	F4AA	112.2(10)
C19A	C18A	N4A	115.2(5)	F2BA	B0AA	F5AA	108.6(9)
C19A	C18A	C17A	129.5(5)	F2BA	B0AA	F1BA	117.7(11)
C18A	C19A	S2A	109.8(4)	F2BA	B0AA	F3AB	107.8(11)
N4A	C20A	S2A	115.0(4)	F5AA	B0AA	F3AB	99.6(10)
N1B	C1B	S1B	113.4(4)	F1BA	B0AA	F5AA	113.8(12)
C3B	C2B	S1B	109.3(4)	F1BA	B0AA	F3AB	107.6(10)
N1B	C3B	C4B	114.3(4)				

Table S6 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **1** at 298 K.

Atom	***x***	***y***	***z***	**U(eq)**
H1A	5255	263	8599	66
H2A	3775	986	6914	69
H4A	3759	2795	7097	58
H6A	3028	4593	8304	53
H7A	3026	6041	8024	56
H9A	5529	5037	6686	61
H10A	5547	3597	6959	58
H12A	4868	7610	6431	72
H13A	6604	8041	6349	75
H15A	7951	6256	7582	83
H16A	6225	5831	7671	86
H17A	7812	8430	7536	55

H19A	9348	9294	7999	69
H20A	12240	7769	6845	66
H1B	2506	1928	8796	62
H2B	1749	4256	9920	78
H4B	4115	4374	9641	59
H5B	7090	2841	9543	71
H6B	8716	3393	9552	71
H8B	7015	5550	8664	80
H9B	5385	4995	8654	81
H11B	9707	3911	8109	73
H12B	10528	4339	7195	73
H14B	10234	6734	7942	57
H15B	9473	6291	8855	57
H16B	12297	4890	6858	61
H18B	13969	4891	5890	90
H19B	11915	7398	5289	96
H1C	4508	1583	9922	63
H2C	8199	338	9609	71
H4C	8238	1240	8470	59
H5C	6879	1333	7181	65
H6C	7644	1745	6258	71
H8C	8514	3698	7113	64
H9C	7732	3282	8031	64
H11C	7051	4458	5964	73
H12C	7312	5872	5872	70
H14C	10822	4814	5823	56
H15C	10576	3399	5949	63
H16C	8229	6695	5156	55
H18C	8037	8368	4631	72
H19C	10111	9007	5944	84
H2D	9583	1699	10088	61
H2E	9543	1058	10636	61
H2F	10512	1570	10575	61
H03A	3399	8356	8633	79
H03B	3880	7584	8146	79
H03C	4719	8123	8358	79
H4AA	10381	1142	6731	79
H4AB	10077	1219	7437	79
H4AC	11346	676	7171	79
H3AA	6161	-86	5317	140
H3AB	5398	802	5645	140
H3AC	5101	-99	5790	140

H0AA	9228	1343	10825	102
H0AB	10229	1776	10597	102
H0AC	9251	1731	10166	102
H4AD	10803	1086	6856	78
H4AE	9930	1402	7438	78
H4AF	11225	800	7504	78

Table S7 Atomic Occupancy for **1** at 298 K.

Atom	***Occupancy***	**Atom**	***Occupancy***	**Atom**	***Occupancy***
C2	0.25	H2D	0.25	H2E	0.25
H2F	0.25	N5AA	0.25	N3	0.25
C1AA	0.25	N02V	0.5	C033	0.5
H03A	0.5	H03B	0.5	H03C	0.5
C02W	0.5	N0AA	0.25	C1	0.25
C4AA	0.25	H4AA	0.25	H4AB	0.25
H4AC	0.25	F6AA	0.5	F7AA	0.5
F8AA	0.5	F9AA	0.5	F0BA	0.5
F02K	0.5	F00M	0.5	F01Q	0.5
N1	0.5	C2AA	0.5	C3AA	0.5
H3AA	0.5	H3AB	0.5	H3AC	0.5
F1	0.5	F2	0.5	F3	0.5
F4	0.5	F0AA	0.5	F5	0.5
F7	0.5	F8	0.5	O1	0.25
C1AB	0.25	C0AA	0.25	H0AA	0.25
H0AB	0.25	H0AC	0.25	N0AB	0.25
C5AA	0.25	C4AB	0.25	H4AD	0.25
H4AE	0.25	H4AF	0.25	F2AA	0.5
F1AA	0.5	F4AA	0.5	F3AA	0.5
F2BA	0.5	F5AA	0.5	F1BA	0.5
F3AB	0.5				

Crystal structure determination of **1** at 298 K

Crystal Data for $C_{64}H_{48.6}B_4F_{16}Fe_2N_{14}O_{3.3}S_6$ (*M* =1717.07 g/mol): triclinic, space group P-1 (no. 2), a = 11.806(2) Å, b = 15.605(3) Å, c = 22.029(4) Å, α = 89.52(3)°, β = 85.48(3)°, γ = 73.49(3)°, V = 3878.6(15) Å^3, Z = 2, T = ? K, μ(MoKα) = 0.627 mm^{-1}, *Dcalc* = 1.470 g/cm^3, 47455 reflections measured (2.722° ≤ 2Θ ≤ 49.996°), 12382 unique (R_{int} = 0.0341, R_{sigma} = 0.0286) which were used in all calculations. The final R_1 was 0.0695 (I > 2σ(I)) and wR_2 was 0.2289 (all data).

Refinement model description

Number of restraints - 399, number of constraints - unknown.

Details:

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1. Fixed Uiso
 At 1.2 times of:
  All C(H) groups
 At 1.5 times of:
  All C(H,H,H) groups
2. Restrained distances
 F7AA-F8AA ≈ F7AA-F01Q ≈ F8AA-F02K ≈ F8AA-F01Q ≈ F02K-F01Q
 with sigma of 0.04
 F1-F3 ≈ F1-F4 ≈ F2-F3 ≈ F2-F4
 with sigma of 0.04
 B3-F1 ≈ B3-F2 ≈ B3-F3 ≈ B3-F4
 with sigma of 0.02
 F6AA-F9AA ≈ F6AA-F0BA ≈ F6AA-F00M ≈ F9AA-F0BA ≈ F0BA-F00M
 with sigma of 0.04
 B02Z-F6AA ≈ B02Z-F9AA ≈ B02Z-F0BA ≈ B02Z-F00M
 with sigma of 0.02
 F00N-F00W ≈ F00N-F5BA ≈ F00N-F9BA ≈ F00W-F5BA ≈ F00W-F9BA
≈ F5BA-F9BA
 with sigma of 0.04
 B02P-F00N ≈ B02P-F00W ≈ B02P-F5BA ≈ B02P-F9BA
 with sigma of 0.02
 F0AA-F5 ≈ F0AA-F7 ≈ F0AA-F8
 with sigma of 0.04
 F6AA-F9AA ≈ F6AA-F0BA ≈ F6AA-F00M ≈ F7AA-F8AA ≈ F7AA-F01Q
≈ F8AA-F02K ≈ F9AA-
 F0BA ≈ F0BA-F00M ≈ F02K-F01Q
 with sigma of 0.04
 B02Z-F6AA ≈ B02Z-F7AA ≈ B02Z-F8AA ≈ B02Z-F9AA ≈ B02Z-F0BA
≈ B02Z-F02K ≈ B02Z-
 F00M ≈ B02Z-F01Q
 with sigma of 0.02
 F1-F3 ≈ F1-F4 ≈ F2-F3 ≈ F2-F4 ≈ F0AA-F5 ≈ F0AA-F7 ≈
F0AA-F8 ≈ F5-F8
 with sigma of 0.04
 B3-F1 ≈ B3-F2 ≈ B3-F3 ≈ B3-F4 ≈ B3-F0AA ≈ B3-F5 ≈
B3-F7 ≈ B3-F8
 with sigma of 0.02
 C1AB-C0AA ≈ C2-C1AA
 with sigma of 0.02
 N5AA-C1AB ≈ N3-C1AA
 with sigma of 0.02
 F2AA-F1AA ≈ F2AA-F4AA ≈ F2AA-F3AA ≈ F1AA-F3AA ≈ F4AA-F3AA
≈ F2BA-F5AA ≈ F2BA-
 F3AB ≈ F5AA-F3AB ≈ F1BA-F3AB
 with sigma of 0.04
 B0AA-F2AA ≈ B0AA-F1AA ≈ B0AA-F4AA ≈ B0AA-F3AA ≈ B0AA-F2BA
≈ B0AA-F5AA ≈ B0AA-
 F1BA ≈ B0AA-F3AB
 with sigma of 0.02
3. Rigid bond restraints
 F4AA, F5AA, F2BA, F1AA, F3AA, F3AB, F2AA, F1BA
 with sigma for 1-2 distances of 0.01 and sigma for 1-3 distances of 0.01
4. Rigid body (RIGU) restrains
 F00M, F01Q, F7AA, F9AA
 with sigma for 1-2 distances of 0.004 and sigma for 1-3 distances of 0.004
 F02K, F6AA, F8AA, F0BA
 with sigma for 1-2 distances of 0.004 and sigma for 1-3 distances of 0.004
 C1AA
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 with sigma for 1-2 distances of 0.004 and sigma for 1-3 distances of 0.004
 C1AA, N3, N5AA
 with sigma for 1-2 distances of 0.004 and sigma for 1-3 distances of 0.004
 F6AA, F7AA, F8AA, F9AA, F0BA, F02K, F00M, F01Q, B02Z
 with sigma for 1-2 distances of 0.004 and sigma for 1-3 distances of 0.004
 B3, F1, F2, F3, F4, F0AA, F5, F7, F8
 with sigma for 1-2 distances of 0.004 and sigma for 1-3 distances of 0.004
 C2, N5AA, N3, C1AA, C1AB, C0AA
 with sigma for 1-2 distances of 0.004 and sigma for 1-3 distances of 0.004
 B0AA, F2AA, F1AA, F4AA, F3AA, F2BA, F5AA, F1BA, F3AB
 with sigma for 1-2 distances of 0.002 and sigma for 1-3 distances of 0.002
 Fe02, N4B
 with sigma for 1-2 distances of 0.002 and sigma for 1-3 distances of 0.002
5. Others
 Fixed Sof: C2(0.25) H2D(0.25) H2E(0.25) H2F(0.25) N5AA(0.25) N3(0.25)
 C1AA(0.25) N02V(0.5) C033(0.5) H03A(0.5) H03B(0.5) H03C(0.5) C02W(0.5)
 N0AA(0.25) C1(0.25) C4AA(0.25) H4AA(0.25) H4AB(0.25) H4AC(0.25) F6AA(0.5)
 F7AA(0.5) F8AA(0.5) F9AA(0.5) F0BA(0.5) F02K(0.5) F00M(0.5) F01Q(0.5) N1(0.5)
 C2AA(0.5) C3AA(0.5) H3AA(0.5) H3AB(0.5) H3AC(0.5) F1(0.5) F2(0.5) F3(0.5)
 F4(0.5) F0AA(0.5) F5(0.5) F7(0.5) F8(0.5) O1(0.25) C1AB(0.25) C0AA(0.25)
 H0AA(0.25) H0AB(0.25) H0AC(0.25) N0AB(0.25) C5AA(0.25) C4AB(0.25) H4AD(0.25)
 H4AE(0.25) H4AF(0.25) F2AA(0.5) F1AA(0.5) F4AA(0.5) F3AA(0.5) F2BA(0.5)
 F5AA(0.5) F1BA(0.5) F3AB(0.5)
6.a Aromatic/amide H refined with riding coordinates:
 C1A(H1A), C2A(H2A), C4A(H4A), C6A(H6A), C7A(H7A), C9A(H9A), C10A(H10A),
 C12A(H12A), C13A(H13A), C15A(H15A), C16A(H16A), C17A(H17A), C19A(H19A),
 C20A(H20A), C1B(H1B), C2B(H2B), C4B(H4B), C5B(H5B), C6B(H6B), C8B(H8B),
 C9B(H9B), C11B(H11B), C12B(H12B), C14B(H14B), C15B(H15B), C16B(H16B),
 C18B(H18B), C19B(H19B), C1C(H1C), C2C(H2C), C4C(H4C), C5C(H5C), C6C(H6C),
 C8C(H8C), C9C(H9C), C11C(H11C), C12C(H12C), C14C(H14C), C15C(H15C), C16C(H16C),
  C18C(H18C), C19C(H19C)
6.b Idealised Me refined as rotating group:
 C2(H2D,H2E,H2F), C033(H03A,H03B,H03C), C4AA(H4AA,H4AB,H4AC), C3AA(H3AA,H3AB,
 H3AC), C0AA(H0AA,H0AB,H0AC), C4AB(H4AD,H4AE,H4AF
```

1 at 100 K:

Empirical formula	$C_{68}H_{55}B_4F_{16}Fe_2N_{16}O_{3.5}S_6$
Formula weight	1803.58
Temperature/K	100(2)
Crystal system	triclinic
Space group	P-1
a/Å	11.724(2)
b/Å	15.555(3)
c/Å	21.641(4)
α/°	89.79(3)
β/°	85.72(3)
γ/°	73.09(3)
Volume/Å^3	3764.8(14)
Z	2

ρ_{calc}g/cm^3	1.591
μ/mm^{-1}	0.652
F(000)	1830.0
Crystal size/mm^3	0.03 × 0.02 × 0.01
Radiation	Synchrotron (λ = 0.7108)
2Θ range for data collection/°	2.736 to 52.998
Index ranges	$-14 \leq h \leq 14$, $-19 \leq k \leq 19$, $-27 \leq l \leq 27$
Reflections collected	54362
Independent reflections	14128 [R_{int} = 0.0247, R_{sigma} = 0.0194]
Data/restraints/parameters	14128/0/1115
Goodness-of-fit on F^2	1.035
Final R indexes [I>=2σ (I)]	R_1 = 0.0369, wR_2 = 0.0944
Final R indexes [all data]	R_1 = 0.0424, wR_2 = 0.0982
Largest diff. peak/hole / e Å^{-3}	0.63/-0.67

Table S8 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **1** at 100 K. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
Fe01	4937.8(3)	2984.4(2)	8588.3(2)	11.95(7)
Fe02	9958.2(3)	7587.9(2)	6410.6(2)	12.19(7)
S1A	8670.3(5)	9402.2(4)	4823.3(2)	21.11(12)
S2A	6027.5(6)	680.1(4)	9894.1(3)	22.26(12)
S1B	10418.4(5)	10050.9(3)	7322.4(3)	20.98(12)
S2B	3636.9(5)	1151.3(4)	7394.3(2)	18.30(11)
S1C	13758.2(5)	6935.1(4)	5602.7(3)	20.01(12)
S2C	1438.4(6)	3750.1(4)	9757.5(3)	25.87(13)
O1A	6198.5(17)	7091(1)	8970.4(7)	24.2(4)
O1B	10743.3(13)	3471.8(10)	7883.7(7)	17.8(3)
O1C	5979.9(13)	5156.3(10)	5848.9(6)	15.5(3)
N1A	9287.7(16)	8369.9(11)	5731.6(8)	14.5(4)
N2A	8252.6(16)	7957.1(11)	6727.5(8)	14.7(4)
N3A	5716.3(16)	3620.4(11)	9165.5(8)	13.2(3)
N4A	5505.3(16)	2010.7(12)	9173.6(8)	14.9(4)
N1B	10200.0(16)	8609.5(12)	6859.5(8)	15.5(4)
N2B	10592.6(16)	6965.5(11)	7178.9(8)	13.6(3)
N3B	6472.4(16)	2527.6(11)	8057.7(8)	13.4(3)
N4B	4453.4(16)	2171.5(11)	8039.7(8)	13.7(3)
N1C	11591.3(16)	7248.6(12)	6010.2(8)	15.1(4)
N2C	9920.1(16)	6493.9(12)	5933.1(8)	14.1(3)

N3C	4165.1(16)	4053.8(11)	8086.7(8)	13.4(3)
N4C	3374.5(17)	3380.0(12)	9063.0(8)	16.6(4)
C1A	9718(2)	8637.7(14)	5215.2(10)	18.2(4)
C2A	7583(2)	9363.9(15)	5381.6(10)	21.3(5)
C3A	8062(2)	8782.8(14)	5830(1)	17.5(4)
C4A	7529(2)	8528.9(14)	6396(1)	17.8(4)
C5A	7738.7(19)	7713.4(14)	7304.1(9)	15.0(4)
C6A	7724(2)	8202.4(15)	7842.1(10)	19.3(4)
C7A	7221(2)	7974.2(15)	8397.6(10)	20.7(5)
C8A	6738(2)	7256.9(14)	8406.9(10)	18.2(4)
C9A	6749(2)	6769.8(14)	7870.6(10)	18.1(4)
C10A	7254(2)	7000.6(14)	7315.6(10)	17.9(4)
C11A	6073(2)	6225.4(14)	9032.3(9)	18.6(5)
C12A	4946(2)	6119.1(14)	9078.2(9)	18.2(4)
C13A	4828(2)	5254.3(14)	9138.5(9)	15.9(4)
C14A	5845(2)	4513.9(13)	9128.7(9)	15.0(4)
C15A	6975(2)	4636.6(14)	9092.9(9)	17.8(4)
C16A	7090(2)	5498.2(15)	9050.5(10)	20.5(5)
C17A	6310.5(19)	3110.4(14)	9577.4(9)	15.3(4)
C18A	6186.4(19)	2215.1(14)	9618.4(9)	15.2(4)
C19A	6556(2)	1565.8(15)	10042.9(10)	19.5(4)
C20A	5355(2)	1216.5(15)	9266.1(10)	19.6(4)
C1B	10001(2)	9473.6(14)	6754.2(10)	18.3(4)
C2B	10886(2)	9087.8(14)	7733.2(10)	19.0(4)
C3B	10702.7(19)	8388.7(14)	7421.2(9)	15.9(4)
C4B	10898.6(19)	7455.3(14)	7578.3(10)	16.3(4)
C5B	10671.6(19)	6058.6(13)	7357.2(9)	14.2(4)
C6B	11459.3(19)	5322.6(14)	7036.9(9)	14.7(4)
C7B	11472.7(19)	4449.6(14)	7209.1(10)	15.4(4)
C8B	10713.9(19)	4338.4(13)	7700.7(10)	15.2(4)
C9B	9945.5(19)	5072.7(14)	8031.3(10)	16.2(4)
C10B	9929.7(19)	5934.8(14)	7859.6(10)	16.1(4)
C11B	9641.2(19)	3292.5(13)	7953.7(10)	15.3(4)
C12B	9531(2)	2627.6(14)	8363.1(11)	19.7(5)
C13B	8484(2)	2378.8(14)	8403.6(11)	20.0(5)
C14B	7550.0(19)	2803.2(13)	8049.6(9)	13.6(4)
C15B	7658(2)	3483.3(15)	7657.8(11)	20.7(5)
C16B	8701(2)	3730.8(15)	7607.6(11)	21.2(5)
C17B	6512.1(19)	1875.0(14)	7687.2(9)	15.5(4)
C18B	5407.5(19)	1652.6(14)	7650.5(9)	15.2(4)
C19B	5117(2)	1073.0(15)	7268(1)	18.0(4)
C20B	3473.0(19)	1967.5(14)	7948.8(9)	16.1(4)

C1C	12512.6(19)	7558.6(14)	6029.6(10)	16.3(4)
C2C	13009(2)	6216.4(15)	5375.9(10)	19.8(4)
C3C	11861.9(19)	6482.8(14)	5635.6(9)	16.0(4)
C4C	10884.6(19)	6101.6(14)	5596.3(10)	16.5(4)
C5C	8927.9(19)	6132.5(14)	5901.7(9)	15.2(4)
C6C	7942(2)	6597.1(15)	5592.5(10)	20.0(4)
C7C	6965(2)	6269.0(15)	5580.2(10)	19.7(4)
C8C	6970.9(19)	5477.7(14)	5878.9(9)	14.6(4)
C9C	7970(2)	4989.6(15)	6163.7(11)	20.5(5)
C10C	8947(2)	5318.8(15)	6175.7(11)	21.1(5)
C11C	5531.6(19)	4893.9(14)	6414.6(9)	14.7(4)
C12C	5374.8(19)	4045.7(14)	6445.4(9)	15.7(4)
C13C	4915.8(19)	3773.2(14)	6998.5(9)	15.0(4)
C14C	4614.6(18)	4352.4(14)	7512.3(9)	13.4(4)
C15C	4739(2)	5214.6(14)	7468.5(9)	17.9(4)
C16C	5198(2)	5487.9(14)	6915.4(10)	19.2(4)
C17C	3130.1(19)	4538.9(14)	8319.6(9)	16.2(4)
C18C	2652(2)	4201.1(14)	8871.8(9)	16.7(4)
C19C	1584(2)	4511.5(16)	9208.7(10)	21.8(5)
C20C	2836(2)	3073.7(16)	9530.1(10)	21.5(5)
N025	2110(2)	-183.9(15)	11542.2(11)	35.6(5)
C1	704(3)	334(5)	10672.6(19)	117(3)
C030	1497(3)	53(2)	11160.9(13)	34.5(6)
F2	-2261(9)	3569(8)	10842(7)	57(3)
F3	-1400(12)	2132(7)	10878(6)	73(3)
F15	-80(20)	2780(20)	10880(11)	54(7)
F2AA	-1112(9)	2790(12)	10044(4)	72(4)
F02H	-1587(4)	2343(3)	10611(2)	60.8(11)
F00K	-150(9)	2991(8)	10877(3)	39.8(17)
F01T	-1342(2)	3557(2)	10146.6(11)	57.9(7)
F00X	-2014(2)	3636.0(17)	11156.7(12)	42.4(6)
B037	-1247(3)	3064(2)	10690.8(14)	33.7(7)
F1	1927(5)	-113(3)	9213(2)	46.2(12)
F011	3500(4)	329(3)	8821(2)	37.1(10)
F034	1900(4)	1359(2)	9244.2(18)	49.8(10)
F035	1159(4)	1053(2)	9267.3(14)	46.4(10)
F01A	2107(4)	-386(3)	8953.0(19)	32.1(10)
F0AA	3097(6)	666(4)	8950(3)	35.6(14)
F00B	1753.1(13)	710.5(10)	8290.2(7)	29.8(3)
B036	2157(3)	539(2)	8875.2(14)	35.6(8)
N031	13578(3)	7336.1(18)	7697(2)	66.1(10)
C032	14224(3)	8770.4(18)	7828.6(14)	36.9(6)

C02Z	13865(2)	7963.2(18)	7755.3(15)	35.6(6)
N02T	6763(3)	-2911(2)	3860.8(14)	53.4(8)
C02S	6133(2)	-2334.2(19)	4146.6(11)	29.5(6)
C02X	5328(3)	-1597.7(18)	4508.5(13)	34.5(6)
N02O	9818(2)	6816.8(17)	4358.0(11)	41.9(6)
C02U	9531(2)	7276.6(17)	3952.2(12)	30.4(6)
C02Y	9174(3)	7862.1(18)	3431.8(12)	32.6(6)
F00G	10884.6(14)	8890.4(11)	3994.0(8)	41.3(4)
F00H	12726.0(17)	8982.3(13)	3671.1(7)	44.9(4)
F00T	12442.6(17)	8171.5(18)	4519.7(9)	65.7(7)
F00Y	12239(2)	7688.2(13)	3556.9(10)	66.5(6)
B033	12095(3)	8426.0(19)	3936.1(12)	23.9(6)
F009	4717.4(14)	-1652.9(9)	6098.7(7)	29.4(3)
F1AA	4775.6(13)	-290.4(10)	6435.4(7)	30.8(3)
F00E	3015.2(15)	-635.1(12)	6507.0(8)	42.3(4)
F00F	3858.6(17)	-397.9(11)	5571.7(7)	43.9(4)
B02V	4084(2)	-745.2(17)	6152.9(12)	19.4(5)
O1	1901(4)	1797(3)	10282.7(19)	38.8(9)

Table S9 Anisotropic Displacement Parameters ($Å^2×10^3$) for **1** at 100 K. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
Fe01	11.34(15)	15.13(14)	10.85(13)	1.73(10)	-1.57(11)	-6.04(11)
Fe02	9.22(15)	15.52(14)	12.94(14)	2.7(1)	-1.41(11)	-5.26(11)
S1A	22.2(3)	22.9(3)	17.0(2)	7.5(2)	-1.6(2)	-4.6(2)
S2A	25.5(3)	19.9(3)	24.2(3)	9.5(2)	-5.3(2)	-10.3(2)
S1B	23.0(3)	15.7(2)	25.7(3)	0.3(2)	0.2(2)	-8.3(2)
S2B	17.4(3)	24.3(3)	17.8(2)	-0.53(19)	-3.5(2)	-12.8(2)
S1C	10.5(3)	24.8(3)	26.2(3)	-1.6(2)	1.3(2)	-8.1(2)
S2C	19.1(3)	40.6(3)	17.2(3)	2.6(2)	5.0(2)	-9.2(3)
O1A	39.6(11)	17.7(8)	17.7(7)	-3.9(6)	12.6(7)	-15.7(7)
O1B	9.5(8)	15.6(7)	31.0(8)	6.1(6)	-5.9(6)	-7.1(6)
O1C	13.6(8)	25.7(8)	11.3(6)	2.4(5)	-1.7(6)	-12.1(6)
N1A	12.4(9)	16.8(8)	15.8(8)	2.6(6)	-1.8(7)	-6.2(7)
N2A	13.9(9)	17.6(8)	14.5(8)	1.6(6)	-1.1(7)	-7.5(7)
N3A	12.5(9)	16.0(8)	12.2(8)	0.6(6)	0.7(6)	-6.4(7)
N4A	12.0(9)	19.3(8)	15.2(8)	2.3(7)	-0.4(7)	-7.5(7)
N1B	11.8(9)	17.8(8)	17.2(8)	4.0(7)	-0.7(7)	-4.6(7)
N2B	11.3(9)	14.1(8)	16.1(8)	3.1(6)	-0.9(7)	-5.1(7)
N3B	12.5(9)	16.3(8)	14.3(8)	1.9(6)	-2.5(7)	-8.0(7)
N4B	12.8(9)	17.1(8)	13.3(8)	4.6(6)	-1.7(7)	-7.7(7)

N1C	13.9(9)	18.6(8)	14.2(8)	3.1(7)	-2.4(7)	-6.7(7)
N2C	10.0(9)	19.8(8)	14.9(8)	2.9(6)	-1.8(7)	-8.1(7)
N3C	11.5(9)	19.7(8)	11.0(8)	1.4(6)	-1.9(6)	-7.3(7)
N4C	16.2(9)	23.0(9)	12.4(8)	1.3(7)	-2.6(7)	-8.1(7)
C1A	17.5(11)	19.6(10)	17.7(10)	4.1(8)	-1.5(8)	-5.9(8)
C2A	17.5(12)	24.8(11)	19.1(10)	4.2(8)	-0.9(9)	-2.5(9)
C3A	13.0(11)	21.3(10)	18(1)	3.3(8)	-0.8(8)	-4.7(8)
C4A	11.9(11)	22.2(10)	18.1(10)	2.6(8)	0.3(8)	-3.4(8)
C5A	10.5(10)	19.1(10)	15.2(9)	2.4(8)	0.7(8)	-4.4(8)
C6A	20.3(12)	19.8(10)	20.2(10)	0.0(8)	1.9(9)	-10.5(9)
C7A	28.4(13)	19.7(10)	16.5(10)	-2.9(8)	2.4(9)	-11.7(9)
C8A	20.6(12)	17.5(10)	15.9(10)	1.8(8)	4.9(8)	-6.0(9)
C9A	20.6(12)	18(1)	17.9(10)	-0.4(8)	2.0(8)	-9.9(9)
C10A	17.8(11)	20.6(10)	16.4(10)	-0.7(8)	1.1(8)	-7.8(9)
C11A	30.8(13)	16(1)	11.3(9)	-1.7(7)	5.1(9)	-12.0(9)
C12A	25.4(12)	17.8(10)	10.5(9)	0.2(7)	1.3(8)	-5.6(9)
C13A	18.9(11)	18.8(10)	11.3(9)	1.0(7)	-0.7(8)	-7.5(8)
C14A	21.9(12)	15.6(9)	9.8(9)	-0.1(7)	-1.2(8)	-9.0(8)
C15A	18.2(11)	20.3(10)	16.2(10)	-1.0(8)	1.4(8)	-8.0(9)
C16A	22.8(12)	23.0(11)	19.4(10)	-3.5(8)	4.6(9)	-14.1(9)
C17A	15.2(11)	18.2(10)	14.3(9)	1.1(7)	-1.1(8)	-8.0(8)
C18A	12.7(10)	18.9(10)	15.3(9)	2.1(8)	-2.2(8)	-6.5(8)
C19A	18.3(12)	22.0(11)	19.3(10)	4.4(8)	-3.1(9)	-7.3(9)
C20A	20.4(12)	20.7(10)	20.9(10)	5.3(8)	-4.1(9)	-10.6(9)
C1B	18.2(11)	17.1(10)	20.4(10)	2.9(8)	0.7(8)	-6.9(8)
C2B	17.7(11)	20.1(10)	21.2(10)	0.6(8)	-1.7(9)	-8.5(9)
C3B	14.3(11)	18.9(10)	15.7(9)	2.0(8)	-1.4(8)	-6.8(8)
C4B	13.9(11)	18.8(10)	18.3(10)	3.2(8)	-2.5(8)	-7.4(8)
C5B	13.6(10)	15.4(9)	15.9(9)	3.2(7)	-7.2(8)	-6.6(8)
C6B	10.5(10)	20.5(10)	15.3(9)	2.4(8)	-3.8(8)	-7.1(8)
C7B	10.4(10)	16.8(10)	19.4(10)	0.2(8)	-4.9(8)	-3.8(8)
C8B	12.6(11)	16.1(9)	20.3(10)	4.0(8)	-7.5(8)	-8.0(8)
C9B	12.0(11)	18.5(10)	19.2(10)	3.7(8)	-1.2(8)	-6.0(8)
C10B	12.6(11)	18.1(10)	17.6(10)	1.9(8)	-1.9(8)	-4.4(8)
C11B	11(1)	16.6(9)	21.1(10)	0.1(8)	-2.3(8)	-8.1(8)
C12B	13.2(11)	19.3(10)	28.6(11)	6.8(9)	-8.0(9)	-6.5(8)
C13B	17.6(12)	18.6(10)	25.9(11)	7.7(8)	-5.3(9)	-7.7(9)
C14B	10.5(10)	16.6(9)	15.4(9)	-1.6(7)	0.4(8)	-7.0(8)
C15B	16.0(12)	24.1(11)	25.9(11)	8.3(9)	-9.2(9)	-9.9(9)
C16B	18.9(12)	23.7(11)	26.1(11)	11.7(9)	-8.2(9)	-12.7(9)
C17B	14.2(11)	17.6(10)	16.0(9)	0.2(8)	-1.0(8)	-6.8(8)
C18B	15.0(11)	18.8(10)	13.9(9)	1.0(7)	-0.1(8)	-8.6(8)

C19B	17.2(11)	22.7(10)	17.5(10)	-0.8(8)	-0.1(8)	-11.5(9)
C20B	13.1(11)	20.6(10)	16.6(9)	3.1(8)	-2.1(8)	-8.0(8)
C1C	11.7(11)	18.5(10)	21(1)	1.7(8)	-1.9(8)	-7.7(8)
C2C	14.8(11)	23.8(11)	21.5(10)	-3.7(8)	1.2(9)	-7.3(9)
C3C	14.5(11)	19.2(10)	15.2(9)	-0.8(8)	-1.8(8)	-6.3(8)
C4C	13.6(11)	21(1)	16.6(10)	0.0(8)	-1.5(8)	-7.7(8)
C5C	13.8(11)	19.8(10)	14.0(9)	-0.2(7)	-1.4(8)	-7.9(8)
C6C	14.4(11)	24.2(11)	24.2(11)	8.6(9)	-3.6(9)	-9.6(9)
C7C	13.6(11)	25.4(11)	22(1)	8.4(9)	-5.4(9)	-7.6(9)
C8C	12.4(10)	22.5(10)	11.9(9)	-1.1(7)	-0.3(8)	-9.6(8)
C9C	20.4(12)	19.6(10)	25.3(11)	6.9(8)	-9.3(9)	-9.9(9)
C10C	17.2(12)	21.8(11)	28.0(11)	6.7(9)	-11.2(9)	-9.3(9)
C11C	10.4(10)	24.2(10)	12.2(9)	4.6(8)	-1.9(8)	-9.1(8)
C12C	14.3(11)	21.2(10)	13.5(9)	-1.6(8)	-1.7(8)	-7.9(8)
C13C	13.7(11)	19.1(10)	15.0(9)	1.4(8)	-3.0(8)	-8.7(8)
C14C	10(1)	19.3(10)	11.0(9)	3.1(7)	-2.2(7)	-4.3(8)
C15C	22.8(12)	19.8(10)	12.3(9)	-0.6(8)	1.1(8)	-8.6(9)
C16C	24.9(12)	18.9(10)	16.3(10)	2.1(8)	-3.0(9)	-9.9(9)
C17C	13.3(11)	21.9(10)	14.1(9)	1.5(8)	-2.9(8)	-5.8(8)
C18C	14.3(11)	23.9(10)	12.8(9)	0.3(8)	-2.7(8)	-6.5(8)
C19C	16.5(12)	31.3(12)	16.7(10)	0.7(9)	-0.3(8)	-5.8(9)
C20C	21.2(12)	29.7(12)	15(1)	3.1(8)	2.1(8)	-10.5(10)
N025	41.4(15)	30.3(12)	34.7(12)	-0.6(9)	1.7(11)	-11(1)
C1	26.9(19)	260(8)	40(2)	9(3)	-3.4(16)	-5(3)
C030	24.9(14)	45.8(16)	32.9(14)	-5.3(12)	7.3(12)	-12.5(12)
F2	24(5)	49(6)	94(10)	-30(7)	-6(6)	-2(4)
F3	98(8)	30(4)	95(9)	6(5)	-29(6)	-19(4)
F15	25(5)	60(12)	70(8)	-11(6)	-28(5)	7(6)
F2AA	31(5)	166(14)	26(5)	-7(7)	-10(4)	-37(7)
F02H	65(2)	42(2)	88(3)	-3.4(19)	-29(2)	-29.2(19)
F00K	32(4)	66(5)	27(2)	0(2)	-7.7(18)	-21(3)
F01T	55.7(17)	89(2)	31.0(12)	13.9(13)	-15.7(11)	-21.5(15)
F00X	41.9(16)	34.6(12)	41.2(14)	1.1(11)	3.9(11)	1.9(10)
B037	22.8(16)	47.8(18)	30.9(15)	3.3(13)	-7.0(12)	-9.7(14)
F1	36(3)	47(3)	59(3)	37(2)	-5(3)	-18(2)
F011	31(2)	54(3)	34(2)	6.3(17)	-11.6(17)	-21.7(18)
F034	60(3)	36.7(19)	48(2)	-16.5(16)	-7.6(19)	-5.4(18)
F035	62(3)	44(2)	19.7(15)	-2.8(14)	2.8(16)	4.0(19)
F01A	34(2)	30(2)	34(2)	15.3(16)	-7.2(19)	-10.6(17)
F0AA	34(4)	54(4)	31(3)	12(3)	-14(3)	-30(3)
F00B	26.6(8)	34.3(8)	30.1(7)	4.2(6)	-3.4(6)	-11.1(6)
B036	49(2)	24.8(14)	23.3(14)	8.3(11)	8.4(13)	1.3(13)

N031	25.3(15)	30.3(14)	138(3)	6.3(16)	2.1(17)	-3.4(11)
C032	32.4(16)	30.6(13)	46.0(16)	4.6(12)	-4.2(12)	-5.9(11)
C02Z	20.0(14)	26.7(13)	54.7(17)	7.7(12)	2.6(12)	0.1(11)
N02T	37.0(15)	66.1(19)	56.8(17)	-30.2(15)	5.5(13)	-16.2(14)
C02S	26.5(14)	42.9(15)	24.0(12)	-2.2(11)	-0.6(10)	-18.0(12)
C02X	35.0(16)	31.9(13)	37.0(14)	-0.8(11)	1.1(12)	-11.6(12)
N02O	47.7(16)	41.1(13)	33.8(13)	3.3(11)	-4.4(11)	-7.9(12)
C02U	31.1(15)	31.1(13)	28.9(13)	-3.1(11)	-3.5(11)	-8.8(11)
C02Y	36.8(16)	34.9(14)	28.6(13)	0.6(10)	-7.6(11)	-13.0(12)
F00G	25.3(9)	44.5(9)	47.6(10)	26.8(8)	5.3(7)	-2.3(7)
F00H	46.2(11)	69.9(12)	31.0(8)	-6.9(8)	11.3(7)	-39.7(9)
F00T	35.3(11)	123.4(19)	39.8(10)	37.1(11)	-15.0(8)	-23.0(12)
F00Y	91.9(18)	43.7(11)	60.9(13)	-18.8(9)	32.2(12)	-24.0(11)
B033	19.2(14)	30.6(14)	20.5(12)	2.4(10)	1.4(10)	-5.5(11)
F009	31.3(8)	20.7(7)	37.4(8)	-0.3(6)	-7.3(6)	-8.3(6)
F1AA	20.6(7)	31.6(8)	43.2(8)	-14.0(6)	-5.4(6)	-11.3(6)
F00E	24.0(9)	51.3(10)	54.6(10)	-15.6(8)	11.6(7)	-19.0(8)
F00F	53.8(11)	42.8(9)	28.3(8)	7.3(7)	-15.8(7)	-0.3(8)
B02V	18.3(13)	21.2(12)	20.1(11)	-2.5(9)	-3.8(10)	-7.3(10)
O1	43(3)	45(2)	34(2)	4.4(17)	-2.3(18)	-23(2)

Table S10 Bond Lengths for **1** at 100 K.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Fe01	N3A	2.0190(18)	C15A	C16A	1.387(3)
Fe01	N4A	1.9664(19)	C17A	C18A	1.443(3)
Fe01	N3B	2.004(2)	C18A	C19A	1.360(3)
Fe01	N4B	1.9648(18)	C2B	C3B	1.359(3)
Fe01	N3C	2.0058(18)	C3B	C4B	1.446(3)
Fe01	N4C	1.965(2)	C5B	C6B	1.393(3)
Fe02	N1A	1.9646(18)	C5B	C10B	1.389(3)
Fe02	N2A	1.982(2)	C6B	C7B	1.403(3)
Fe02	N1B	1.9656(19)	C7B	C8B	1.378(3)
Fe02	N2B	2.0023(18)	C8B	C9B	1.393(3)
Fe02	N1C	1.965(2)	C9B	C10B	1.385(3)
Fe02	N2C	2.0074(18)	C11B	C12B	1.387(3)
S1A	C1A	1.715(2)	C11B	C16B	1.387(3)
S1A	C2A	1.703(2)	C12B	C13B	1.388(3)
S2A	C19A	1.707(2)	C13B	C14B	1.386(3)
S2A	C20A	1.713(2)	C14B	C15B	1.382(3)
S1B	C1B	1.706(2)	C15B	C16B	1.381(3)
S1B	C2B	1.709(2)	C17B	C18B	1.442(3)

S2B	C19B	1.705(2)	C18B	C19B	1.357(3)
S2B	C20B	1.710(2)	C2C	C3C	1.364(3)
S1C	C1C	1.705(2)	C3C	C4C	1.443(3)
S1C	C2C	1.703(2)	C5C	C6C	1.390(3)
S2C	C19C	1.709(2)	C5C	C10C	1.391(3)
S2C	C20C	1.708(3)	C6C	C7C	1.386(3)
O1A	C8A	1.390(3)	C7C	C8C	1.386(3)
O1A	C11A	1.401(3)	C8C	C9C	1.384(3)
O1B	C8B	1.395(2)	C9C	C10C	1.386(3)
O1B	C11B	1.397(3)	C11C	C12C	1.385(3)
O1C	C8C	1.398(3)	C11C	C16C	1.384(3)
O1C	C11C	1.402(2)	C12C	C13C	1.391(3)
N1A	C1A	1.308(3)	C13C	C14C	1.391(3)
N1A	C3A	1.394(3)	C14C	C15C	1.393(3)
N2A	C4A	1.293(3)	C15C	C16C	1.391(3)
N2A	C5A	1.443(3)	C17C	C18C	1.444(3)
N3A	C14A	1.442(3)	C18C	C19C	1.359(3)
N3A	C17A	1.294(3)	N025	C030	1.125(4)
N4A	C18A	1.389(3)	C1	C030	1.442(5)
N4A	C20A	1.310(3)	F2	B037	1.241(11)
N1B	C1B	1.318(3)	F3	B037	1.560(11)
N1B	C3B	1.389(3)	F15	B037	1.41(3)
N2B	C4B	1.291(3)	F2AA	B037	1.449(10)
N2B	C5B	1.440(3)	F02H	B037	1.310(5)
N3B	C14B	1.446(3)	F00K	B037	1.349(12)
N3B	C17B	1.284(3)	F01T	B037	1.397(4)
N4B	C18B	1.397(3)	F00X	B037	1.423(4)
N4B	C20B	1.306(3)	F1	B036	1.326(6)
N1C	C1C	1.308(3)	F011	B036	1.507(6)
N1C	C3C	1.388(3)	F034	B036	1.450(5)
N2C	C4C	1.289(3)	F035	B036	1.429(5)
N2C	C5C	1.438(3)	F01A	B036	1.466(6)
N3C	C14C	1.442(3)	F0AA	B036	1.196(8)
N3C	C17C	1.294(3)	F00B	B036	1.383(3)
N4C	C18C	1.392(3)	N031	C02Z	1.130(4)
N4C	C20C	1.313(3)	C032	C02Z	1.449(4)
C2A	C3A	1.361(3)	N02T	C02S	1.132(4)
C3A	C4A	1.439(3)	C02S	C02X	1.444(4)
C5A	C6A	1.389(3)	N02O	C02U	1.138(4)
C5A	C10A	1.384(3)	C02U	C02Y	1.454(4)
C6A	C7A	1.390(3)	F00G	B033	1.389(3)
C7A	C8A	1.390(3)	F00H	B033	1.389(3)

C8A	C9A	1.386(3)	F00T	B033	1.377(3)		
C9A	C10A	1.392(3)	F00Y	B033	1.376(3)		
C11A	C12A	1.375(3)	F009	B02V	1.392(3)		
C11A	C16A	1.387(3)	F1AA	B02V	1.394(3)		
C12A	C13A	1.397(3)	F00E	B02V	1.385(3)		
C13A	C14A	1.395(3)	F00F	B02V	1.380(3)		
C14A	C15A	1.389(3)					

Table S11 Bond Angles for FL199_a.

Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
N4A	Fe01	N3A	80.92(7)	N4A	C20A	S2A	113.94(17)
N4A	Fe01	N3B	89.93(8)	N1B	C1B	S1B	114.12(16)
N4A	Fe01	N3C	171.62(7)	C3B	C2B	S1B	109.86(16)
N3B	Fe01	N3A	91.19(7)	N1B	C3B	C4B	113.61(18)
N3B	Fe01	N3C	98.30(8)	C2B	C3B	N1B	114.81(19)
N4B	Fe01	N3A	169.09(7)	C2B	C3B	C4B	131.54(19)
N4B	Fe01	N4A	91.08(7)	N2B	C4B	C3B	115.73(18)
N4B	Fe01	N3B	81.33(8)	C6B	C5B	N2B	121.5(2)
N4B	Fe01	N3C	91.71(7)	C10B	C5B	N2B	117.99(19)
N4B	Fe01	N4C	94.05(8)	C10B	C5B	C6B	120.53(19)
N3C	Fe01	N3A	97.25(7)	C5B	C6B	C7B	119.7(2)
N4C	Fe01	N3A	93.46(8)	C8B	C7B	C6B	119.0(2)
N4C	Fe01	N4A	90.73(8)	C7B	C8B	O1B	119.33(19)
N4C	Fe01	N3B	175.35(7)	C7B	C8B	C9B	121.39(19)
N4C	Fe01	N3C	81.20(8)	C9B	C8B	O1B	119.3(2)
N1A	Fe02	N2A	81.09(8)	C10B	C9B	C8B	119.5(2)
N1A	Fe02	N1B	91.08(7)	C9B	C10B	C5B	119.8(2)
N1A	Fe02	N2B	171.21(7)	C12B	C11B	O1B	117.66(18)
N1A	Fe02	N1C	93.51(8)	C16B	C11B	O1B	121.61(19)
N1A	Fe02	N2C	91.07(7)	C16B	C11B	C12B	120.7(2)
N2A	Fe02	N2B	96.14(8)	C11B	C12B	C13B	119.1(2)
N2A	Fe02	N2C	96.77(8)	C14B	C13B	C12B	120.4(2)
N1B	Fe02	N2A	89.84(8)	C13B	C14B	N3B	121.66(19)
N1B	Fe02	N2B	80.54(7)	C15B	C14B	N3B	118.43(18)
N1B	Fe02	N2C	173.29(7)	C15B	C14B	C13B	119.9(2)
N2B	Fe02	N2C	97.56(7)	C16B	C15B	C14B	120.4(2)
N1C	Fe02	N2A	174.08(7)	C15B	C16B	C11B	119.6(2)
N1C	Fe02	N1B	92.72(8)	N3B	C17B	C18B	115.97(19)
N1C	Fe02	N2B	89.55(8)	N4B	C18B	C17B	114.49(18)
N1C	Fe02	N2C	80.81(8)	C19B	C18B	N4B	114.6(2)
C2A	S1A	C1A	90.52(11)	C19B	C18B	C17B	130.7(2)

C19A	S2A	C20A	90.58(11)	C18B	C19B	S2B	110.16(17)
C1B	S1B	C2B	90.50(11)	N4B	C20B	S2B	114.52(16)
C19B	S2B	C20B	90.22(11)	N1C	C1C	S1C	113.78(16)
C2C	S1C	C1C	90.79(11)	C3C	C2C	S1C	109.69(16)
C20C	S2C	C19C	90.37(12)	N1C	C3C	C4C	114.29(19)
C8A	O1A	C11A	115.45(16)	C2C	C3C	N1C	114.36(19)
C8B	O1B	C11B	116.07(16)	C2C	C3C	C4C	131.3(2)
C8C	O1C	C11C	115.50(15)	N2C	C4C	C3C	115.70(19)
C1A	N1A	Fe02	135.65(16)	C6C	C5C	N2C	119.80(19)
C1A	N1A	C3A	110.89(18)	C6C	C5C	C10C	119.6(2)
C3A	N1A	Fe02	113.36(14)	C10C	C5C	N2C	120.58(19)
C4A	N2A	Fe02	115.90(15)	C7C	C6C	C5C	120.1(2)
C4A	N2A	C5A	116.27(18)	C6C	C7C	C8C	119.8(2)
C5A	N2A	Fe02	127.67(13)	C7C	C8C	O1C	118.43(19)
C14A	N3A	Fe01	129.19(13)	C9C	C8C	O1C	120.94(19)
C17A	N3A	Fe01	114.40(14)	C9C	C8C	C7C	120.5(2)
C17A	N3A	C14A	115.75(18)	C8C	C9C	C10C	119.6(2)
C18A	N4A	Fe01	113.71(14)	C9C	C10C	C5C	120.3(2)
C20A	N4A	Fe01	135.34(15)	C12C	C11C	O1C	118.10(18)
C20A	N4A	C18A	110.87(18)	C16C	C11C	O1C	120.48(19)
C1B	N1B	Fe02	135.06(15)	C16C	C11C	C12C	121.3(2)
C1B	N1B	C3B	110.70(18)	C11C	C12C	C13C	119.27(19)
C3B	N1B	Fe02	114.24(14)	C12C	C13C	C14C	119.99(19)
C4B	N2B	Fe02	115.78(14)	C13C	C14C	N3C	119.40(18)
C4B	N2B	C5B	116.24(17)	C13C	C14C	C15C	120.09(19)
C5B	N2B	Fe02	127.83(13)	C15C	C14C	N3C	120.51(18)
C14B	N3B	Fe01	129.40(13)	C16C	C15C	C14C	119.94(19)
C17B	N3B	Fe01	114.82(15)	C11C	C16C	C15C	119.3(2)
C17B	N3B	C14B	115.73(18)	N3C	C17C	C18C	116.08(19)
C18B	N4B	Fe01	112.52(14)	N4C	C18C	C17C	114.11(19)
C20B	N4B	Fe01	136.93(15)	C19C	C18C	N4C	114.6(2)
C20B	N4B	C18B	110.53(18)	C19C	C18C	C17C	131.1(2)
C1C	N1C	Fe02	134.89(15)	C18C	C19C	S2C	109.99(17)
C1C	N1C	C3C	111.37(18)	N4C	C20C	S2C	114.24(17)
C3C	N1C	Fe02	113.68(15)	N025	C030	C1	178.5(4)
C4C	N2C	Fe02	115.45(15)	F2	B037	F3	101.1(9)
C4C	N2C	C5C	117.03(18)	F2	B037	F15	142.4(13)
C5C	N2C	Fe02	127.44(14)	F2	B037	F2AA	112.0(8)
C14C	N3C	Fe01	128.72(13)	F15	B037	F3	88.9(13)
C17C	N3C	Fe01	114.73(14)	F15	B037	F2AA	104.0(11)
C17C	N3C	C14C	116.55(17)	F2AA	B037	F3	89.8(8)
C18C	N4C	Fe01	113.17(15)	F02H	B037	F00K	120.3(6)

C20C	N4C	Fe01	136.03(16)	F02H	B037	F01T	109.9(3)
C20C	N4C	C18C	110.78(19)	F02H	B037	F00X	110.3(4)
N1A	C1A	S1A	114.01(17)	F00K	B037	F01T	106.3(5)
C3A	C2A	S1A	109.93(17)	F00K	B037	F00X	102.5(5)
N1A	C3A	C4A	113.93(18)	F01T	B037	F00X	106.5(3)
C2A	C3A	N1A	114.7(2)	F1	B036	F011	105.3(4)
C2A	C3A	C4A	131.4(2)	F1	B036	F034	110.5(4)
N2A	C4A	C3A	115.6(2)	F1	B036	F00B	121.0(4)
C6A	C5A	N2A	119.63(19)	F034	B036	F011	97.3(4)
C10A	C5A	N2A	119.76(18)	F035	B036	F01A	103.4(3)
C10A	C5A	C6A	120.6(2)	F0AA	B036	F035	116.0(5)
C5A	C6A	C7A	119.8(2)	F0AA	B036	F01A	116.2(4)
C8A	C7A	C6A	119.4(2)	F0AA	B036	F00B	116.0(4)
O1A	C8A	C7A	116.47(19)	F00B	B036	F011	108.5(3)
C9A	C8A	O1A	122.5(2)	F00B	B036	F034	111.4(3)
C9A	C8A	C7A	120.9(2)	F00B	B036	F035	102.6(3)
C8A	C9A	C10A	119.5(2)	F00B	B036	F01A	100.5(3)
C5A	C10A	C9A	119.81(19)	N031	C02Z	C032	179.6(4)
C12A	C11A	O1A	119.2(2)	N02T	C02S	C02X	179.7(4)
C12A	C11A	C16A	121.7(2)	N02O	C02U	C02Y	179.5(3)
C16A	C11A	O1A	119.1(2)	F00G	B033	F00H	109.1(2)
C11A	C12A	C13A	118.9(2)	F00T	B033	F00G	107.8(2)
C14A	C13A	C12A	119.9(2)	F00T	B033	F00H	111.2(2)
C13A	C14A	N3A	119.6(2)	F00Y	B033	F00G	107.6(2)
C15A	C14A	N3A	120.15(19)	F00Y	B033	F00H	110.0(2)
C15A	C14A	C13A	120.2(2)	F00Y	B033	F00T	111.1(2)
C16A	C15A	C14A	119.7(2)	F009	B02V	F1AA	108.80(19)
C11A	C16A	C15A	119.4(2)	F00E	B02V	F009	110.1(2)
N3A	C17A	C18A	116.17(19)	F00E	B02V	F1AA	109.74(19)
N4A	C18A	C17A	114.15(18)	F00F	B02V	F009	109.69(19)
C19A	C18A	N4A	114.98(19)	F00F	B02V	F1AA	108.7(2)
C19A	C18A	C17A	130.7(2)	F00F	B02V	F00E	109.8(2)
C18A	C19A	S2A	109.63(17)				

Table S12 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **1** at 100 K.

Atom	***x***	***y***	***z***	**U(eq)**
H1A	10521	8432	5073	22
H2A	6781	9691	5380	26
H4A	6719	8761	6516	21
H6A	8050	8681	7831	23

H7A	7208	8299	8760	25
H9A	6420	6292	7881	22
H10A	7266	6677	6954	22
H12A	4273	6615	9069	22
H13A	4072	5172	9185	19
H15A	7651	4144	9097	21
H16A	7842	5587	9034	25
H17A	6790	3309	9832	18
H19A	7024	1599	10365	23
H20A	4922	967	9014	23
H1B	9663	9745	6401	22
H2B	11218	9048	8113	23
H4B	11224	7223	7944	20
H6B	11974	5410	6710	18
H7B	11986	3953	6995	18
H9B	9446	4985	8365	19
H10B	9424	6429	8080	19
H12B	10151	2352	8607	24
H13B	8407	1925	8670	24
H15B	7026	3776	7427	25
H16B	8772	4188	7343	25
H17B	7211	1564	7456	19
H19B	5648	689	6979	22
H20B	2745	2244	8168	19
H1C	12490	8072	6255	20
H2C	13333	5718	5115	24
H4C	10947	5605	5344	20
H6C	7939	7129	5394	24
H7C	6306	6579	5372	24
H9C	7985	4444	6346	25
H10C	9619	4994	6368	25
H12C	5574	3662	6100	19
H13C	4810	3204	7025	18
H15C	4516	5607	7809	21
H16C	5280	6064	6883	23
H17C	2718	5074	8142	19
H19C	1016	5058	9149	26
H20C	3186	2534	9721	26
H1D	69	859	10808	175
H1E	374	-140	10574	175
H1F	1141	472	10312	175
H03A	14959	8714	7582	55

H03B	14339	8853	8257	55
H03C	13614	9279	7696	55
H02A	5478	-1045	4385	52
H02B	5452	-1691	4940	52
H02C	4517	-1568	4441	52
H02D	8766	7590	3158	49
H02E	9871	7952	3212	49
H02F	8650	8431	3582	49
H1G	1267	2128	10475	58
H1H	2426	2077	10251	58

Table S13 Atomic Occupancy for **1** at 100 K.

Atom	***Occupancy***	**Atom**	***Occupancy***	**Atom**	***Occupancy***
F2	0.2	F3	0.3	F15	0.3
F2AA	0.2	F02H	0.7	F00K	0.7
F01T	0.8	F00X	0.8	F1	0.5
F011	0.6	F034	0.5	F035	0.5
F01A	0.5	F0AA	0.4	O1	0.5
H1G	0.5	H1H	0.5		

Crystal structure determination of **1** at 100 K

Crystal Data for (M =1803.58 g/mol): triclinic, space group P-1 (no. 2), a = 11.724(2) Å, b = 15.555(3) Å, c = 21.641(4) Å, α = 89.79(3)°, β = 85.72(3)°, γ = 73.09(3)°, V = 3764.8(14) Å^3, Z = 2, T = 293(2) K, μ(MoKα) = 0.652 mm^{-1}, *Dcalc* = 1.591 g/cm^3, 54362 reflections measured (2.736° ≤ 2Θ ≤ 52.998°), 14128 unique (R_{int} = 0.0247, R_{sigma} = 0.0194) which were used in all calculations. The final R_1 was 0.0369 (I > 2σ(I)) and wR_2 was 0.0982 (all data).

Refinement model description

Number of restraints - 0, number of constraints - unknown.

Details:

```
1. Fixed Uiso
 At 1.2 times of:
  All C(H) groups
 At 1.5 times of:
  All C(H,H,H) groups, All O(H,H) groups
2. Others
 Fixed Sof: F2(0.2) F3(0.3) F15(0.3) F2AA(0.2) F02H(0.7) F00K(0.7) F01T(0.8)
 F00X(0.8) F1(0.5) F011(0.6) F034(0.5) F035(0.5) F01A(0.5) F0AA(0.4) O1(0.5)
 H1G(0.5) H1H(0.5)
3.a Free rotating group:
 O1(H1G,H1H)
3.b Aromatic/amide H refined with riding coordinates:
 C1A(H1A), C2A(H2A), C4A(H4A), C6A(H6A), C7A(H7A), C9A(H9A), C10A(H10A),
 C12A(H12A), C13A(H13A), C15A(H15A), C16A(H16A), C17A(H17A), C19A(H19A),
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 C20A(H20A), C1B(H1B), C2B(H2B), C4B(H4B), C6B(H6B), C7B(H7B), C9B(H9B),
 C10B(H10B), C12B(H12B), C13B(H13B), C15B(H15B), C16B(H16B), C17B(H17B),
 C19B(H19B), C20B(H20B), C1C(H1C), C2C(H2C), C4C(H4C), C6C(H6C), C7C(H7C),
 C9C(H9C), C10C(H10C), C12C(H12C), C13C(H13C), C15C(H15C), C16C(H16C),
 C17C(H17C), C19C(H19C), C20C(H20C)
3.c Idealised Me refined as rotating group:
 C1(H1D,H1E,H1F), C032(H03A,H03B,H03C), C02X(H02A,H02B,H02C), C02Y(H02D,H02E,
 H02F)
```

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