# Supplementary Materials : Investigation of the Spin Crossover Properties of Three Dinulear Fe(II) Triple Helicates by Variation of the Steric Nature of the Ligand Type
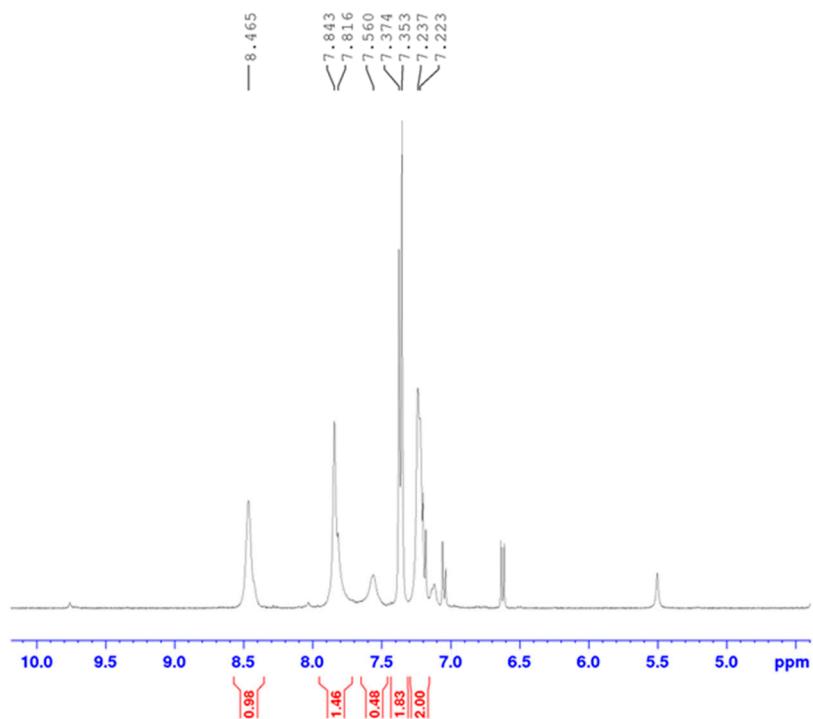
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¹H NMR:

Figure S1. ¹H-NMR spectrum of **L¹** (DMSO, 400 MHz).
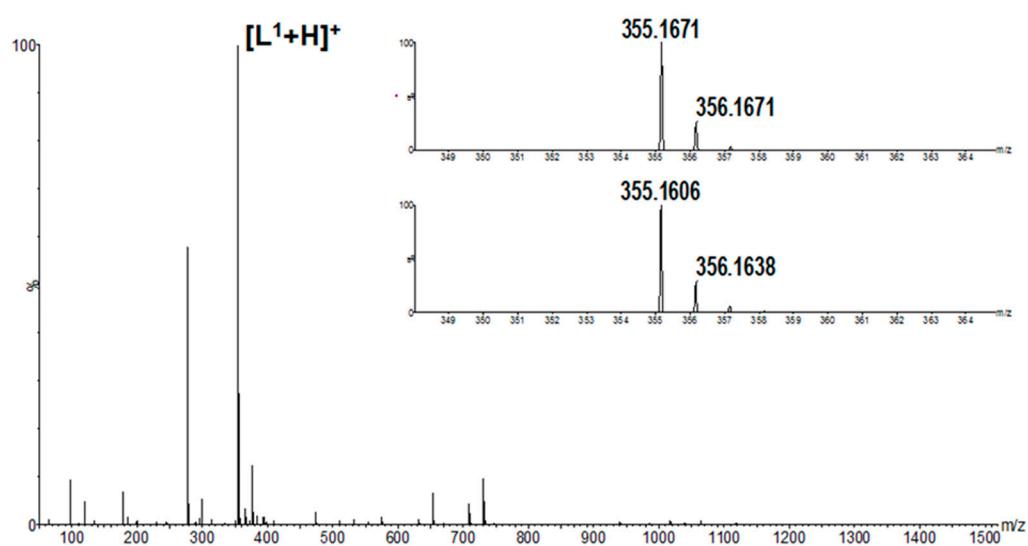
Figure S2. ¹H-NMR spectrum of **L²** (DMSO, 400 MHz).

2
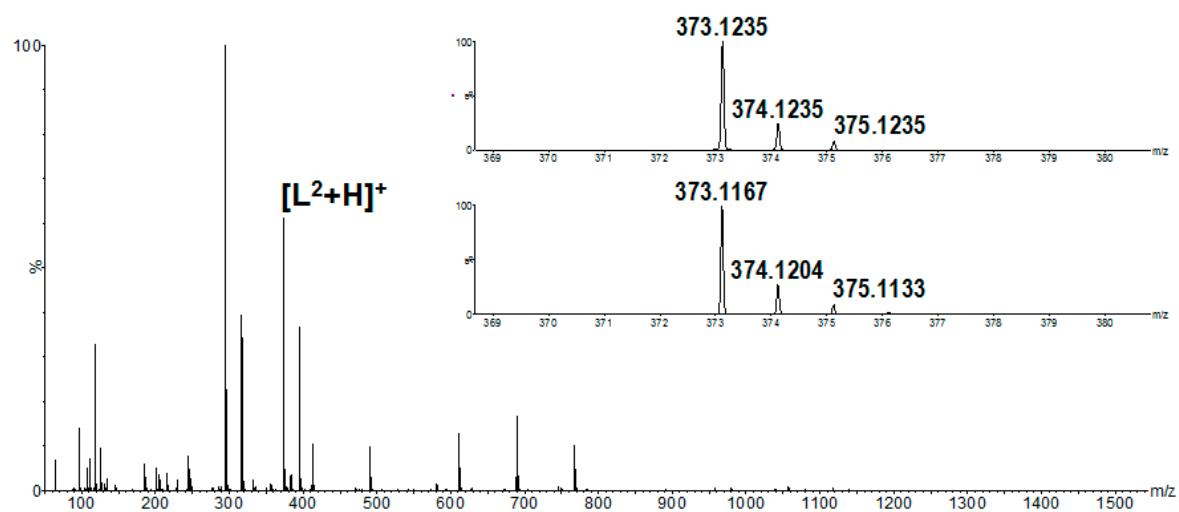
Figure S3. ¹H-NMR spectrum of **L³** (DMSO, 400 MHz).
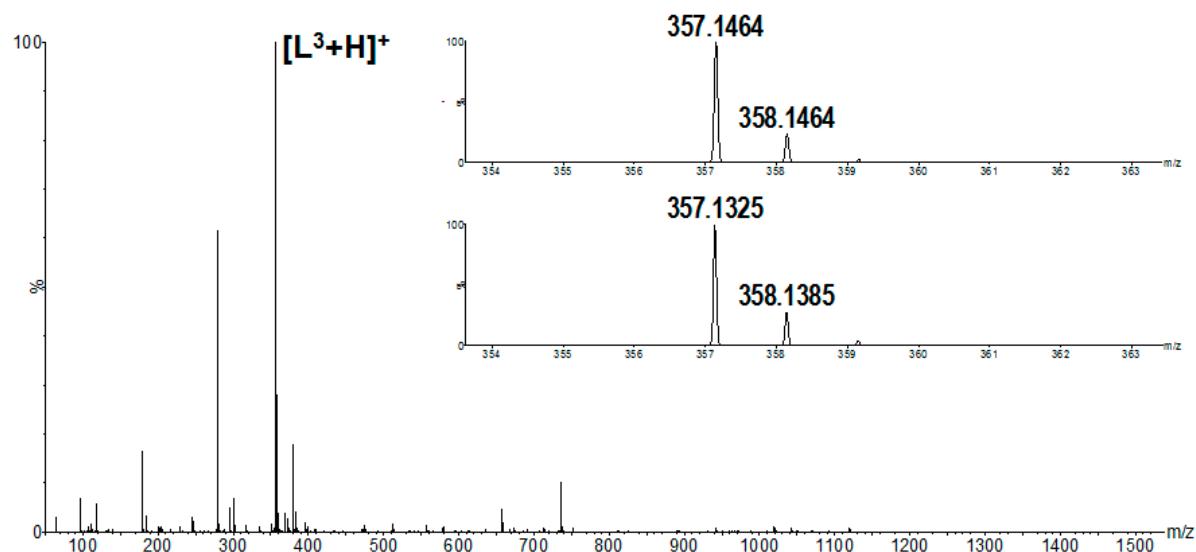
High resolution Electrospray Ionization Mass spectra:
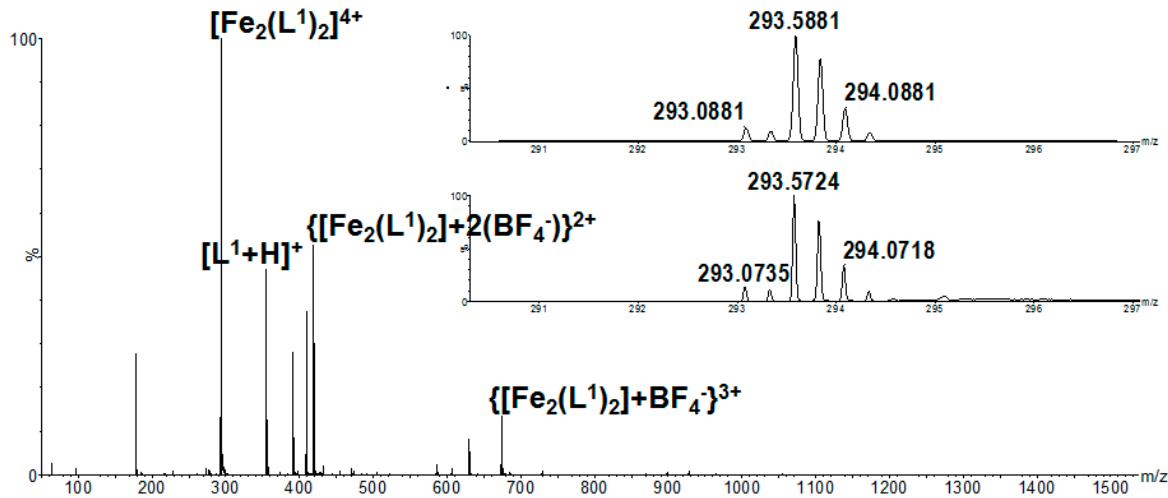
Figure S4. ESI-HRMS spectrum of **L¹**. The inset shows the isotope pattern for {[H+**L¹**]⁺ (bottom) with the simulated distribution (top).

3
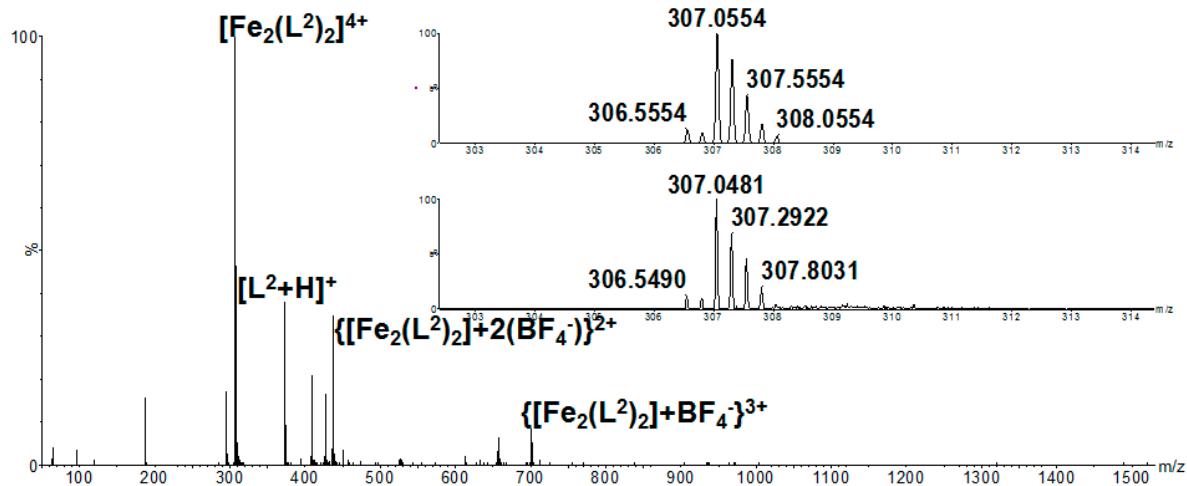
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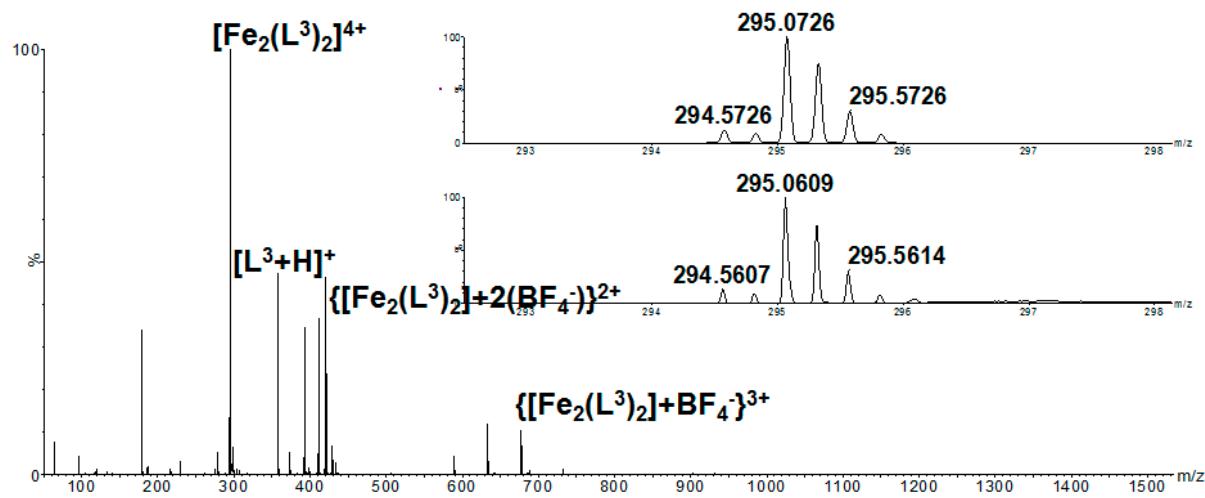
Figure S6. ESI-HRMS spectrum of L^3. The inset shows the isotope pattern for $\{[H+L^3]^+$ (bottom) with the simulated distribution (top).

Figure S7. ESI-HRMS spectrum of **1**. The inset shows the isotope pattern for $[Fe_2(\mathbf{L^1})_3]^{4+}$ (bottom) with the simulated distribution (top)
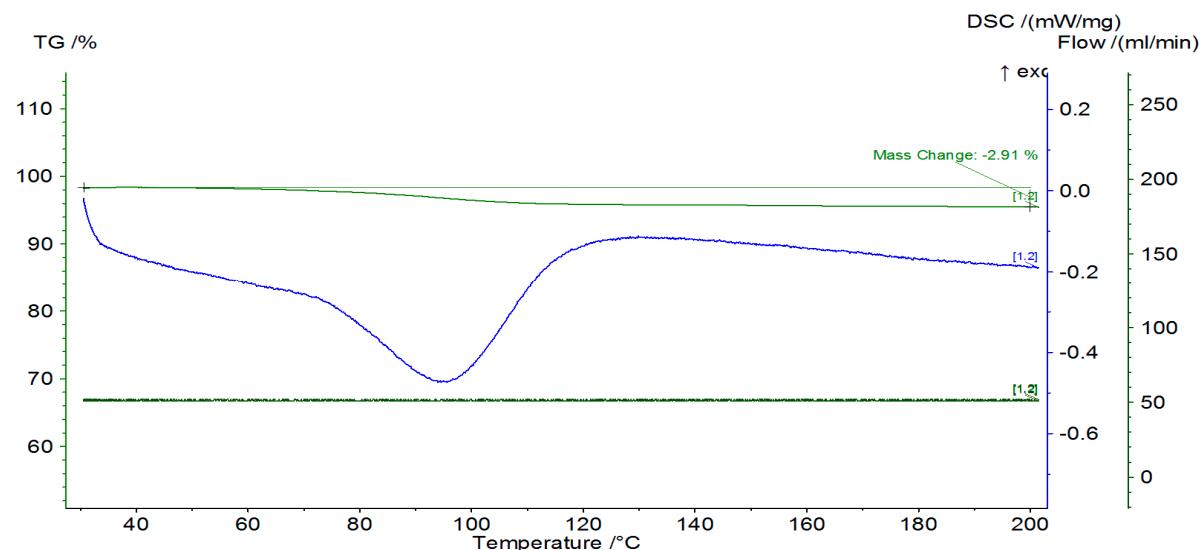
Figure S8. ESI-HRMS spectrum of **2**. The inset shows the isotope pattern for $[Fe_2(\mathbf{L^2})_3]^{4+}$ (bottom) with the simulated distribution (top)
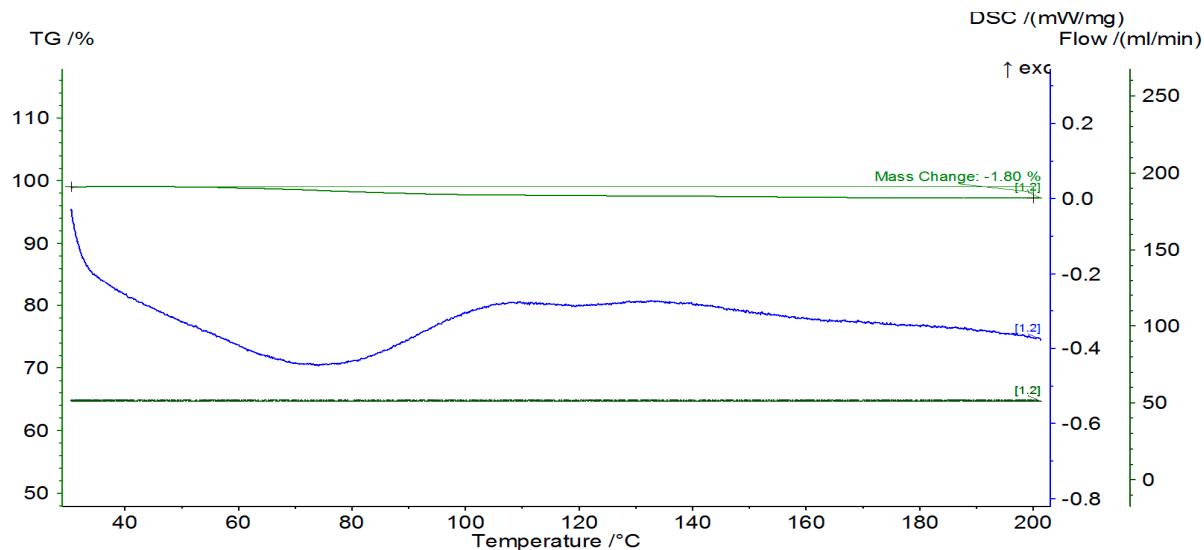
Figure 9. ESI-HRMS spectrum of **3**. The inset shows the isotope pattern for $[Fe_2(L^3)_3]^{4+}$ (bottom) with the simulated distribution (top)
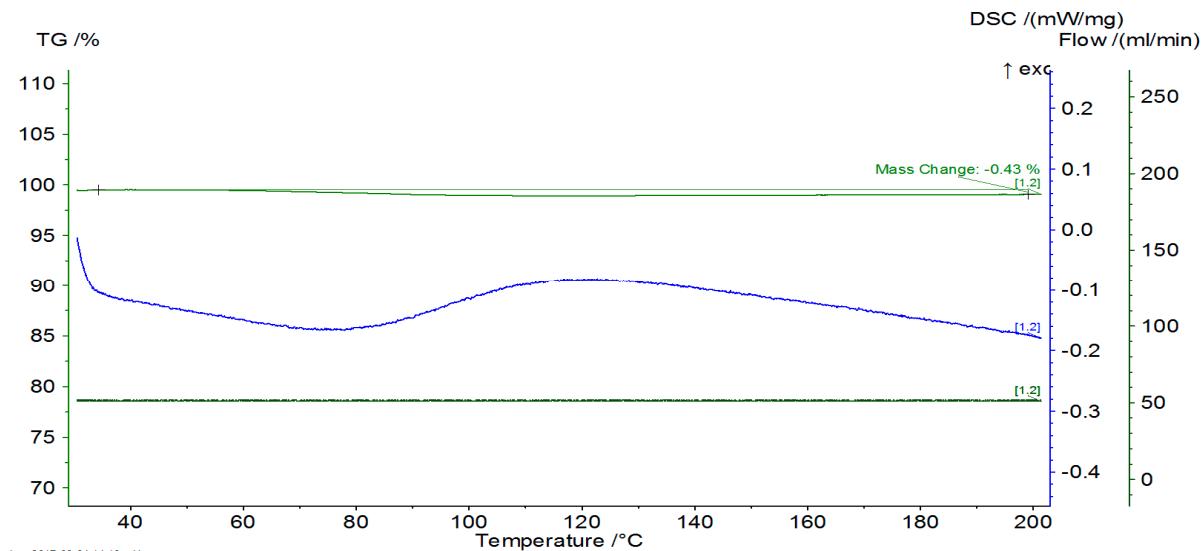
Simultaneous thermal analysis (STA) – DSC-TGA:

Figure S10. Thermogravimetric and differential thermal analysis results for **1**.
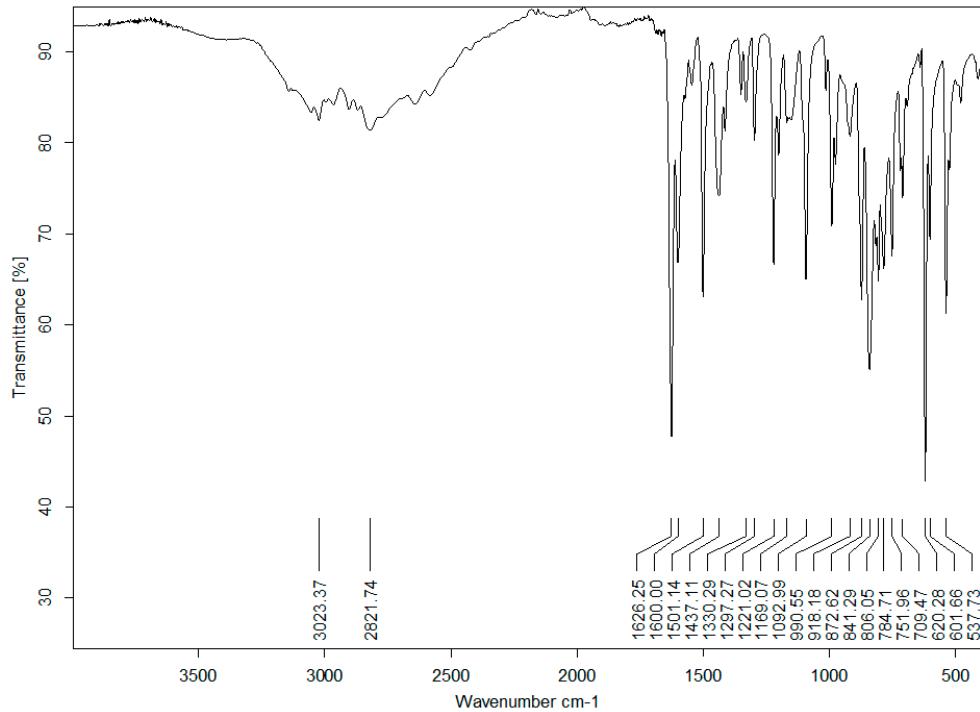
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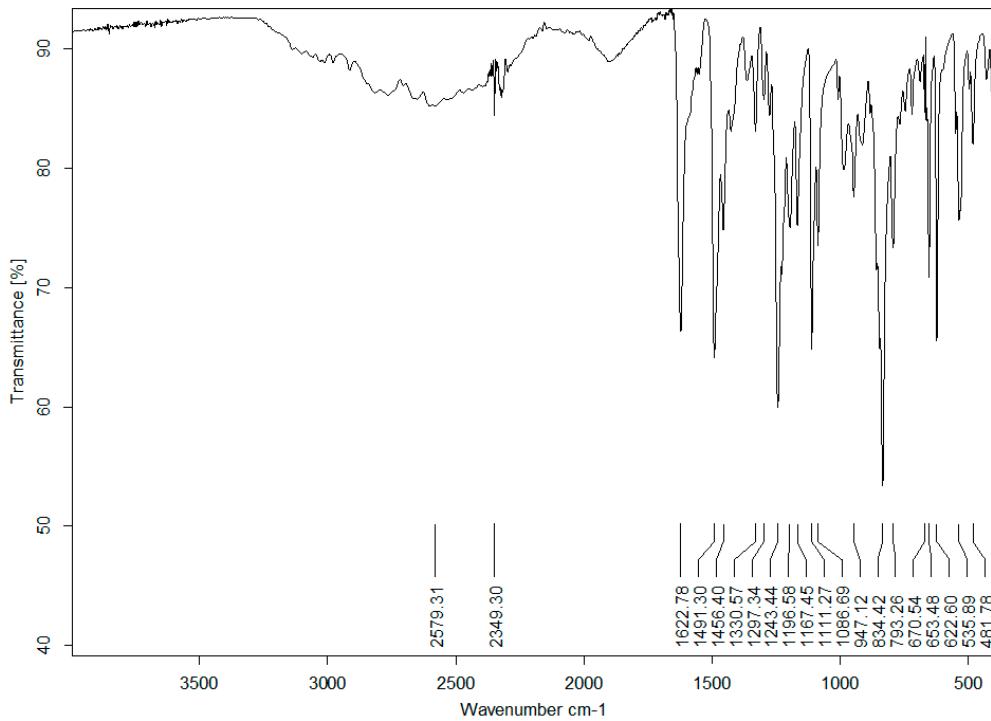
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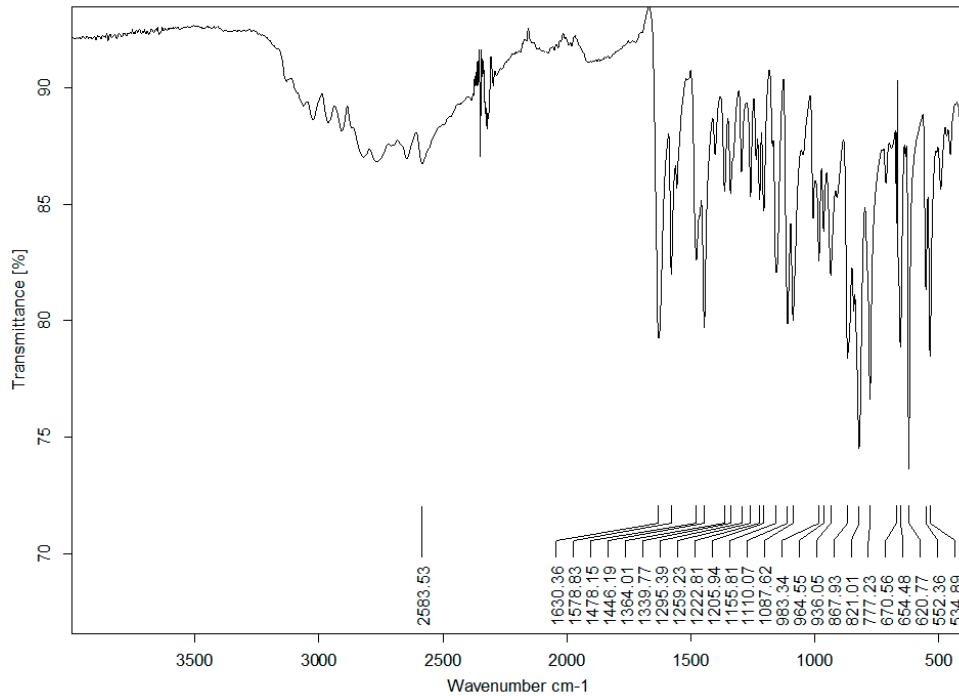
Note – acetonitrile solvent coming off between 50 and 100 degrees Celsius. Only a very small mass loss of 2.91, 1.80 and 0.43 % observed for **1**, **2** and **3** respectively.
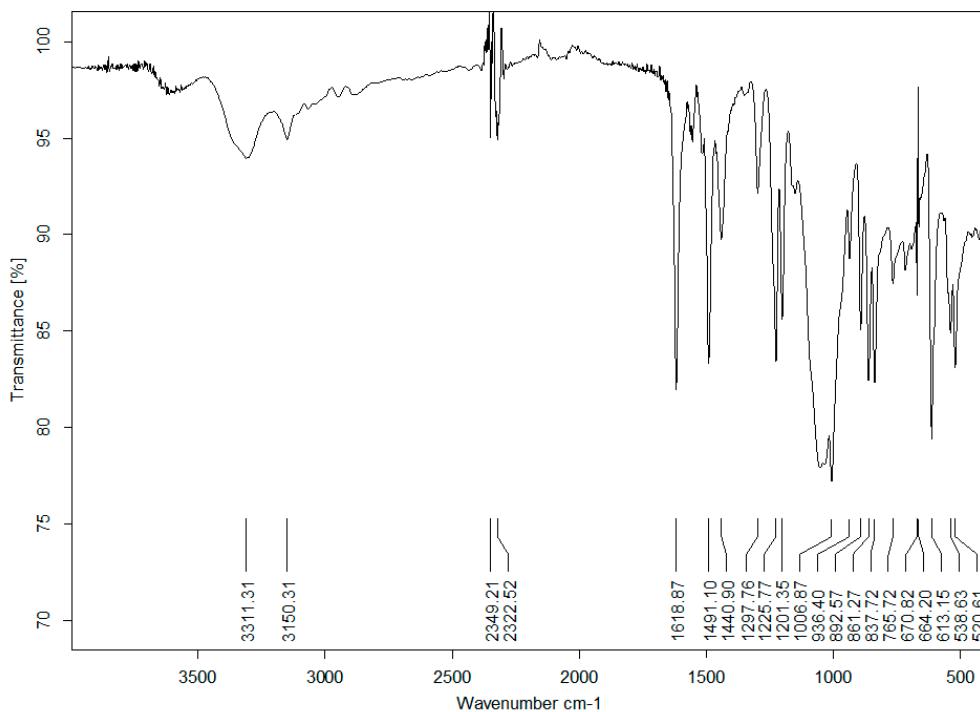
Figure S13. FT-IR spectrum of **L^1**.
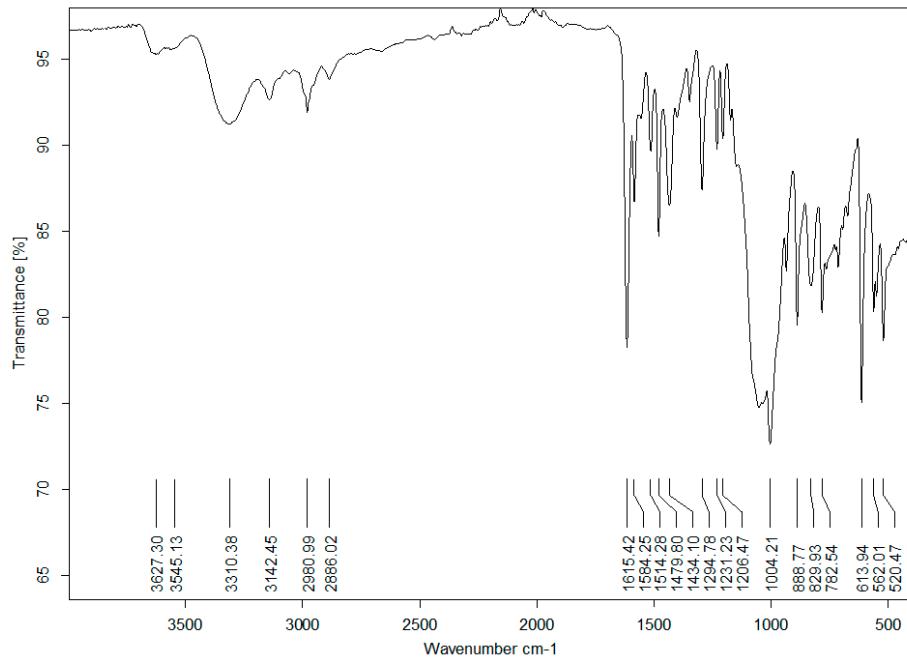
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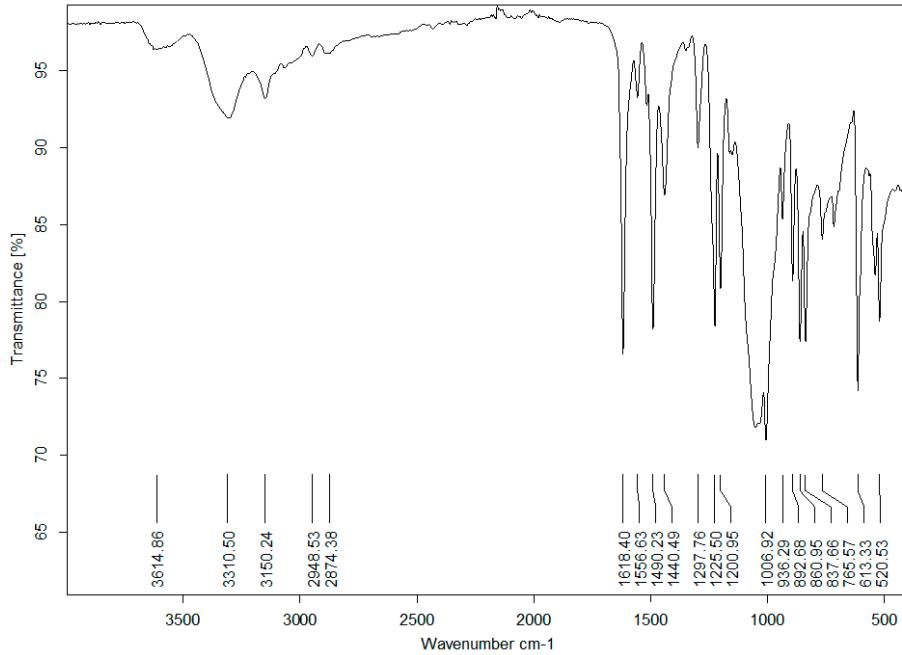
Figure S15. FT-IR spectrum of **L**^{3}.

Figure S16. FT-IR spectrum of **1**.

Figure S17. FT-IR spectrum of **2**.

Figure S18. FT-IR spectrum of **3**.

Crystallographic Details:

Crystal data and structure refinement for **1**.

Table 1 Crystal data and structure refinement for **1**.

Identification code	FL206_a
Empirical formula	$C_{65}H_{57}B_4F_{16}Fe_2N_{19.5}$
Formula weight	1570.24
Temperature/K	100
Crystal system	monoclinic
Space group	C2/c
a/Å	21.131(4)
b/Å	17.391(4)
c/Å	21.069(4)
α/°	90
β/°	107.00(3)
γ/°	90
Volume/Å^3	7404(3)
Z	4
ρ_{calc}g/cm^3	1.409
μ/mm^{-1}	0.486
F(000)	3198.0
Crystal size/mm^3	0.02 × 0.01 × 0.01
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.09 to 52.998
Index ranges	-26 ≤ h ≤ 26, -21 ≤ k ≤ 21, -26 ≤ l ≤ 26
Reflections collected	50460
Independent reflections	6995 [R_{int} = 0.0697, R_{sigma} = 0.0341]
Data/restraints/parameters	6995/218/630
Goodness-of-fit on F^2	1.096
Final R indexes [I>=2σ (I)]	R_1 = 0.1035, wR_2 = 0.2930
Final R indexes [all data]	R_1 = 0.1371, wR_2 = 0.3220
Largest diff. peak/hole / e Å^{-3}	1.37/-0.56

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

Atom	x	y	z	U(eq)
Fe$_{01}$	4398.4(5)	2776.3(6)	4604.0(5)	50.7(3)

N_{1A}	3882(4)	3668(4)	4013(3)	65.0(18)
N_{2A}	3417(4)	4647(6)	3368(4)	88(3)
N_{3A}	3649(3)	3069(4)	5090(3)	51.6(14)
N_{4A}	5214(3)	1771(4)	9804(3)	49.6(14)
N_{5A}	6784(4)	1039(6)	11601(4)	83(2)
N_{6A}	6155(3)	1892(4)	10965(3)	57.5(16)
N_{1B}	5256(11)	2769(13)	4175(11)	48(4)
N_{2B}	6108(10)	2669(11)	3780(11)	60(4)
N_{3B}	5135(3)	3527(4)	5208(3)	51.1(14)
$N_{1B'}$	5057(12)	2611(16)	4139(13)	67(6)
$N_{2B'}$	5802(11)	2410(11)	3593(8)	64(4)
C_1	3183(11)	1359(16)	7290(8)	76(7)
C_3	4705(7)	1811(10)	9185(4)	46(5)
C_5	4848(4)	1867(7)	8583(4)	48(3)
C_6	4337(5)	1867(8)	7991(4)	55(4)
C_{12A}	3684(4)	1812(8)	8001(5)	47(4)
C_7	3541(5)	1756(11)	8603(7)	48(5)
C_8	4052(8)	1756(12)	9195(5)	50(5)
C_{1A}	3848(6)	4061(7)	3468(4)	85(3)
C_{2A}	3144(5)	4628(6)	3883(5)	80(3)
C_{3A}	3427(4)	4021(5)	4271(4)	63(2)
C_{4A}	3314(4)	3674(5)	4850(4)	62(2)
C_{7A}	3339(9)	2925(8)	6713(8)	50(4)
C_{8A}	3240(10)	2137(8)	6735(7)	45(4)
C_{9A}	3288(12)	1672(10)	6215(9)	48(4)
C_9	3435(16)	1996(14)	5671(10)	50(6)
C_{5A}	3534(15)	2785(14)	5649(9)	47(5)
C_{6A}	3486(10)	3249(10)	6170(9)	47(4)
C_{11A}	3112(8)	1756(12)	7365(7)	52(5)
C_{15A}	4700(7)	1641(11)	9178(4)	45(5)
C_{16A}	4854(5)	1305(9)	8643(5)	69(5)
C_{17A}	4368(6)	1227(9)	8038(5)	73(4)
C_2	3729(5)	1485(9)	7967(5)	62(5)
C_{13A}	3575(6)	1821(11)	8502(7)	48(4)
C_{14A}	4060(8)	1899(12)	9108(6)	47(4)
C_{18A}	5456(4)	1135(5)	10076(3)	56.7(19)
C_{19A}	5976(4)	1179(5)	10699(3)	57.1(19)
C_{20A}	6377(5)	637(6)	11100(4)	79(3)
C_{21A}	6644(4)	1777(6)	11520(4)	70(2)
$C_{7A'}$	3437(11)	2607(9)	6793(8)	63(5)
$C_{8A'}$	3327(10)	1818(9)	6738(9)	54(5)

$C_{9A'}$	3314(12)	1440(11)	6153(11)	55(5)
C_{10A}	3411(17)	1850(16)	5623(10)	59(6)
$C_{5A'}$	3522(17)	2639(16)	5678(9)	55(6)
$C_{6A'}$	3535(13)	3017(10)	6263(10)	67(6)
C_{1B}	5476(13)	2467(13)	3712(11)	61(4)
C_{2B}	6314(11)	3109(11)	4312(11)	57(4)
C_{3B}	5793(11)	3182(13)	4578(11)	47(4)
C_{4B}	5680(20)	3630(20)	5132(18)	66(9)
C_{5B}	5108(3)	3948(4)	5789(4)	49.8(16)
C_{6B}	4680(4)	4571(4)	5716(4)	52.9(17)
C_{7B}	4646(4)	4971(4)	6279(4)	51.4(17)
C_{8B}	5027(4)	4764(4)	6908(4)	54.2(17)
C_{9B}	5440(5)	4148(5)	6959(4)	70(2)
C_{10B}	5487(4)	3742(5)	6412(4)	68(2)
C_{11B}	5000	5234(6)	7500	64(3)
$C_{1B'}$	5183(12)	2265(14)	3629(11)	69(5)
$C_{2B'}$	6089(12)	2893(14)	4051(11)	62(5)
$C_{3B'}$	5641(17)	3023(16)	4398(12)	60(6)
C_{4C}	5689(14)	3473(19)	5003(17)	43(5)
F_1	3220(50)	6120(20)	6700(40)	190(40)
F_3	2589(12)	5591(15)	6015(10)	77(7)
F_{10}	3280(20)	4653(15)	6580(20)	125(12)
F_{00X}	2514(12)	5252(14)	7000(12)	51(6)
B_{01B}	2995(5)	5359(6)	6637(5)	82(3)
F_{002}	7305(3)	3772(4)	7071(2)	83.7(16)
F_{003}	8042(3)	2906(3)	6903(3)	93.2(18)
F_{008}	7246(3)	3416(4)	6032(3)	104(2)
F_{00A}	8087(3)	4157(4)	6617(4)	108(2)
B_{01A}	7666(5)	3561(7)	6663(5)	69(3)
F_{009}	3272(4)	4763(4)	7040(3)	81.0(19)
F_{00H}	3414(7)	5982(7)	6871(5)	117(5)
F_{00T}	3011(5)	5125(6)	5993(3)	112(3)
F_{00Y}	2390(4)	5519(6)	6675(7)	138(5)
B_{01C}	2995(5)	5359(6)	6637(5)	82(3)
N_2	4363(9)	431(10)	10769(9)	88(5)
C_{1AA}	3917(11)	562(12)	10514(11)	29(4)
C_{2AA}	3289(12)	724(14)	10206(13)	40(5)
N_{01L}	5516(9)	−1381(10)	7422(10)	33(4)
C_4	5777(17)	31(17)	7357(17)	61(7)
C_{0AA}	5601(12)	−806(13)	7390(12)	35(5)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **1**. 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}
Fe_{01}	50.8(6)	72.7(7)	26.7(5)	0.8(4)	8.5(5)	0.8(5)
N_{1A}	63(4)	92(5)	34(3)	0(3)	6(4)	-13(4)
N_{2A}	79(6)	120(7)	46(4)	27(4)	-9(5)	-27(5)
N_{3A}	45(3)	78(4)	28(3)	1(3)	4(3)	-8(3)
N_{4A}	43(3)	77(4)	26(3)	1(3)	6(3)	5(3)
N_{5A}	74(5)	123(7)	43(4)	17(4)	4(4)	34(5)
N_{6A}	46(3)	86(4)	35(3)	0(3)	3(3)	-5(3)
N_{1B}	58(9)	59(8)	36(7)	13(6)	28(7)	12(6)
N_{2B}	67(8)	70(10)	56(9)	-1(7)	38(8)	9(6)
N_{3B}	41(3)	71(4)	46(4)	12(3)	20(3)	11(3)
$N_{1B'}$	73(10)	88(13)	43(8)	6(7)	21(8)	6(7)
$N_{2B'}$	74(10)	80(10)	43(7)	-4(7)	24(8)	2(7)
C_1	66(9)	130(20)	30(7)	-7(8)	11(6)	-29(10)
C_3	50(11)	62(11)	20(8)	-4(6)	0(8)	1(8)
C_5	38(6)	85(10)	19(5)	-3(6)	3(5)	-9(6)
C_6	42(5)	102(11)	16(5)	1(5)	2(4)	-11(5)
C_{12A}	39(5)	72(12)	28(6)	-1(5)	5(4)	-12(5)
C_7	50(8)	66(12)	29(6)	3(5)	10(5)	-10(7)
C_8	48(9)	69(12)	32(6)	1(6)	11(6)	-6(7)
C_{1A}	91(7)	117(8)	40(5)	9(5)	9(5)	-27(7)
C_{2A}	62(5)	90(6)	69(6)	13(5)	-12(5)	-10(5)
C_{3A}	55(5)	76(5)	48(5)	10(4)	-1(4)	-3(4)
C_{4A}	46(4)	82(5)	48(5)	-3(4)	-1(4)	2(4)
C_{7A}	46(8)	70(10)	35(7)	8(6)	15(7)	2(7)
C_{8A}	35(8)	71(10)	29(6)	8(6)	9(6)	3(7)
C_{9A}	43(10)	71(10)	30(7)	8(6)	10(6)	2(7)
C_9	48(15)	71(9)	32(8)	7(5)	14(9)	7(7)
C_{5A}	44(13)	70(9)	31(7)	9(5)	17(8)	4(7)
C_{6A}	41(9)	71(9)	33(7)	10(6)	14(6)	0(7)
C_{11A}	37(6)	101(16)	17(5)	-4(6)	5(5)	-21(7)
C_{15A}	42(8)	71(10)	21(7)	1(5)	5(6)	-6(6)
C_{16A}	47(7)	124(13)	36(6)	-21(7)	13(5)	-11(7)
C_{17A}	59(6)	127(13)	32(6)	-16(7)	10(5)	-20(7)
C_2	54(6)	96(13)	36(6)	-8(6)	11(5)	-29(6)
C_{13A}	46(7)	69(10)	23(6)	11(5)	1(5)	-16(6)
C_{14A}	44(8)	65(10)	28(6)	3(6)	6(5)	-8(6)

C_{18A}	66(5)	72(5)	26(3)	-4(3)	4(4)	-4(4)
C_{19A}	62(5)	75(5)	29(4)	3(3)	6(4)	9(4)
C_{20A}	85(7)	98(7)	37(4)	5(4)	-9(5)	25(5)
C_{21A}	57(5)	108(7)	41(5)	2(4)	5(5)	-7(5)
$C_{7A'}$	72(13)	83(12)	27(7)	5(7)	4(8)	-10(9)
$C_{8A'}$	35(9)	79(11)	38(7)	9(7)	-5(6)	-7(8)
$C_{9A'}$	36(10)	84(12)	38(7)	5(7)	1(7)	-8(8)
C_{10A}	43(14)	86(12)	43(8)	2(6)	5(8)	-14(9)
$C_{5A'}$	45(14)	86(12)	25(7)	4(6)	-4(8)	-14(9)
$C_{6A'}$	74(15)	86(12)	31(7)	5(7)	3(9)	-13(9)
C_{1B}	66(9)	79(10)	50(8)	1(7)	38(8)	5(7)
C_{2B}	61(8)	65(9)	57(9)	2(7)	37(7)	12(6)
C_{3B}	53(8)	55(9)	41(8)	11(6)	26(7)	15(6)
C_{4B}	100(20)	56(16)	56(14)	5(10)	41(13)	32(12)
C_{5B}	44(4)	56(4)	53(4)	5(3)	18(4)	-2(3)
C_{6B}	45(4)	65(4)	47(4)	8(3)	11(4)	5(3)
C_{7B}	45(4)	54(4)	52(4)	4(3)	10(4)	3(3)
C_{8B}	60(5)	55(4)	40(4)	1(3)	3(4)	-4(3)
C_{9B}	81(6)	68(5)	39(4)	-1(3)	-17(5)	13(4)
C_{10B}	65(5)	64(5)	63(5)	-2(4)	1(5)	19(4)
C_{11B}	86(9)	55(6)	43(6)	0	5(6)	0
$C_{1B'}$	73(10)	90(11)	45(7)	2(7)	21(7)	2(8)
$C_{2B'}$	68(9)	78(11)	42(10)	-3(8)	21(8)	7(7)
$C_{3B'}$	67(11)	78(12)	38(10)	6(8)	21(8)	15(8)
C_{4C}	36(9)	44(14)	65(14)	1(8)	38(10)	2(8)
B_{01B}	88(8)	88(8)	58(7)	6(5)	3(7)	-15(6)
F_{002}	64(3)	138(5)	48(3)	2(3)	14(3)	28(3)
F_{003}	101(4)	117(4)	72(4)	19(3)	41(3)	42(3)
F_{008}	117(5)	146(5)	41(3)	4(3)	12(3)	12(4)
F_{00A}	76(4)	124(5)	115(5)	37(4)	14(4)	4(4)
B_{01A}	59(6)	101(8)	46(5)	9(5)	16(5)	16(5)
F_{009}	96(5)	97(5)	50(4)	0(3)	21(4)	24(4)
F_{00H}	136(9)	138(8)	60(5)	8(5)	2(6)	-83(7)
F_{00T}	117(7)	155(7)	52(4)	3(4)	7(5)	27(6)
F_{00Y}	56(4)	110(7)	229(15)	-77(8)	10(7)	19(4)
B_{01C}	88(8)	88(8)	58(7)	6(5)	3(7)	-15(6)

Table 4 Bond Lengths for **1**.

Atom Atom Length/Å   Atom Atom Length/Å

15

Fe_{01}	N_{1A}	2.086(7)	C_{8A}	C_{9A}	1.3900
Fe_{01}	N_{3A}	2.183(6)	C_{8A}	C_{11A}	1.57(2)
Fe_{01}	N_{4A}^{1}	2.164(6)	C_{9A}	C_9	1.3900
Fe_{01}	N_{6A}^{1}	2.085(7)	C_9	C_{5A}	1.3900
Fe_{01}	N_{1B}	2.250(17)	C_{5A}	C_{6A}	1.3900
Fe_{01}	N_{3B}	2.142(7)	C_{15A}	C_{16A}	1.3900
Fe_{01}	$N_{1B'}$	1.94(2)	C_{15A}	C_{14A}	1.3900
N_{1A}	C_{1A}	1.320(11)	C_{16A}	C_{17A}	1.3900
N_{1A}	C_{3A}	1.381(11)	C_{17A}	C_2	1.3900
N_{2A}	C_{1A}	1.341(14)	C_2	C_{13A}	1.3900
N_{2A}	C_{2A}	1.371(13)	C_{13A}	C_{14A}	1.3900
N_{3A}	C_{4A}	1.286(10)	C_{18A}	C_{19A}	1.447(11)
N_{3A}	C_{5A}	1.363(14)	C_{19A}	C_{20A}	1.380(11)
N_{3A}	$C_{5A'}$	1.537(17)	$C_{7A'}$	$C_{8A'}$	1.3900
N_{4A}	Fe_{01}^{1}	2.164(6)	$C_{7A'}$	$C_{6A'}$	1.3900
N_{4A}	C_3	1.429(10)	$C_{8A'}$	$C_{9A'}$	1.3900
N_{4A}	C_{15A}	1.461(11)	$C_{9A'}$	C_{10A}	1.3900
N_{4A}	C_{18A}	1.282(10)	C_{10A}	$C_{5A'}$	1.3900
N_{5A}	C_{20A}	1.345(13)	$C_{5A'}$	$C_{6A'}$	1.3900
N_{5A}	C_{21A}	1.317(12)	C_{2B}	C_{3B}	1.38(2)
N_{6A}	Fe_{01}^{1}	2.085(7)	C_{3B}	C_{4B}	1.48(3)
N_{6A}	C_{19A}	1.367(10)	C_{5B}	C_{6B}	1.390(10)
N_{6A}	C_{21A}	1.330(11)	C_{5B}	C_{10B}	1.371(11)
N_{1B}	C_{1B}	1.31(2)	C_{6B}	C_{7B}	1.395(10)
N_{1B}	C_{3B}	1.40(3)	C_{7B}	C_{8B}	1.384(10)
N_{2B}	C_{1B}	1.35(3)	C_{8B}	C_{9B}	1.366(11)
N_{2B}	C_{2B}	1.32(3)	C_{8B}	C_{11B}	1.505(9)
N_{3B}	C_{4B}	1.22(4)	C_{9B}	C_{10B}	1.379(12)
N_{3B}	C_{5B}	1.442(9)	C_{11B}	C_{8B}^{1}	1.505(9)
N_{3B}	C_{4C}	1.36(2)	$C_{2B'}$	$C_{3B'}$	1.37(3)
$N_{1B'}$	$C_{1B'}$	1.33(3)	$C_{3B'}$	C_{4C}	1.47(3)
$N_{1B'}$	$C_{3B'}$	1.39(3)	F_1	B_{01B}	1.39(2)
$N_{2B'}$	$C_{1B'}$	1.36(3)	F_3	B_{01B}	1.400(17)
$N_{2B'}$	$C_{2B'}$	1.29(3)	F_{10}	B_{01B}	1.389(19)
C_1	C_2	1.567(16)	F_{00X}	B_{01B}	1.452(17)
C_1	$C_{8A'}$	1.51(3)	F_{002}	B_{01A}	1.356(10)
C_3	C_5	1.3900	F_{003}	B_{01A}	1.396(12)
C_3	C_8	1.3900	F_{008}	B_{01A}	1.389(12)
C_5	C_6	1.3900	F_{00A}	B_{01A}	1.389(13)
C_6	C_{12A}	1.3900	F_{009}	B_{01C}	1.359(11)
C_{12A}	C_7	1.3900	F_{00H}	B_{01C}	1.393(12)

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Atom	Atom		Atom	Atom	
C_{12A}	C_{11A}	1.523(15)	F_{00T}	B_{01C}	1.426(11)
C_7	C_8	1.3900	F_{00Y}	B_{01C}	1.333(12)
C_{2A}	C_{3A}	1.362(12)	N_2	C_{1AA}	0.97(2)
C_{3A}	C_{4A}	1.442(11)	C_{1AA}	C_{2AA}	1.32(3)
C_{7A}	C_{8A}	1.3900	N_{01L}	C_{0AA}	1.02(3)
C_{7A}	C_{6A}	1.3900	C_4	C_{0AA}	1.51(4)

[1] 1-X,+Y,3/2-Z

Table 5 Bond Angles for **1**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N_{1A}	Fe_{01}	N_{3A}	77.4(2)	N_{3A}	C_{5A}	C_9	117.0(15)
N_{1A}	Fe_{01}	N_{4A}[1]	171.2(2)	N_{3A}	C_{5A}	C_{6A}	122.9(15)
N_{1A}	Fe_{01}	N_{1B}	96.1(6)	C_{6A}	C_{5A}	C_9	120.0
N_{1A}	Fe_{01}	N_{3B}	93.7(3)	C_{5A}	C_{6A}	C_{7A}	120.0
N_{3A}	Fe_{01}	N_{1B}	166.0(6)	C_{12A}	C_{11A}	C_{8A}	115.3(14)
N_{4A}[1]	Fe_{01}	N_{3A}	97.0(2)	C_{16A}	C_{15A}	N_{4A}	120.6(9)
N_{4A}[1]	Fe_{01}	N_{1B}	90.8(6)	C_{16A}	C_{15A}	C_{14A}	120.0
N_{6A}[1]	Fe_{01}	N_{1A}	95.6(3)	C_{14A}	C_{15A}	N_{4A}	119.3(9)
N_{6A}[1]	Fe_{01}	N_{3A}	94.6(2)	C_{15A}	C_{16A}	C_{17A}	120.0
N_{6A}[1]	Fe_{01}	N_{4A}[1]	77.8(2)	C_2	C_{17A}	C_{16A}	120.0
N_{6A}[1]	Fe_{01}	N_{1B}	98.4(6)	C_{17A}	C_2	C_1	119.1(12)
N_{6A}[1]	Fe_{01}	N_{3B}	168.1(2)	C_{13A}	C_2	C_1	120.9(12)
N_{3B}	Fe_{01}	N_{3A}	94.6(2)	C_{13A}	C_2	C_{17A}	120.0
N_{3B}	Fe_{01}	N_{4A}[1]	93.6(2)	C_{14A}	C_{13A}	C_2	120.0
N_{3B}	Fe_{01}	N_{1B}	73.2(6)	C_{13A}	C_{14A}	C_{15A}	120.0
$N_{1B'}$	Fe_{01}	N_{1A}	97.8(9)	N_{4A}	C_{18A}	C_{19A}	117.2(7)
$N_{1B'}$	Fe_{01}	N_{3A}	174.7(9)	N_{6A}	C_{19A}	C_{18A}	117.8(7)
$N_{1B'}$	Fe_{01}	N_{4A}[1]	88.0(9)	N_{6A}	C_{19A}	C_{20A}	108.8(8)
$N_{1B'}$	Fe_{01}	N_{6A}[1]	88.0(7)	C_{20A}	C_{19A}	C_{18A}	133.4(8)
$N_{1B'}$	Fe_{01}	N_{3B}	83.5(7)	N_{5A}	C_{20A}	C_{19A}	105.3(9)
C_{1A}	N_{1A}	Fe_{01}	142.2(8)	N_{5A}	C_{21A}	N_{6A}	110.4(9)
C_{1A}	N_{1A}	C_{3A}	104.2(8)	$C_{8A'}$	$C_{7A'}$	$C_{6A'}$	120.0
C_{3A}	N_{1A}	Fe_{01}	113.5(5)	$C_{7A'}$	$C_{8A'}$	C_1	121.5(14)
C_{1A}	N_{2A}	C_{2A}	106.3(8)	$C_{7A'}$	$C_{8A'}$	$C_{9A'}$	120.0
C_{4A}	N_{3A}	Fe_{01}	113.5(5)	$C_{9A'}$	$C_{8A'}$	C_1	118.4(14)
C_{4A}	N_{3A}	C_{5A}	114.8(13)	C_{10A}	$C_{9A'}$	$C_{8A'}$	120.0
C_{4A}	N_{3A}	$C_{5A'}$	120.6(13)	$C_{9A'}$	C_{10A}	$C_{5A'}$	120.0
C_{5A}	N_{3A}	Fe_{01}	131.1(13)	C_{10A}	$C_{5A'}$	N_{3A}	118.5(15)
$C_{5A'}$	N_{3A}	Fe_{01}	125.9(13)	$C_{6A'}$	$C_{5A'}$	N_{3A}	121.4(15)

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C_3	N_{4A}	$Fe_{01}{}^1$	123.0(8)	$C_{6A'}$	$C_{5A'}$	C_{10A}	120.0
C_{15A}	N_{4A}	$Fe_{01}{}^1$	134.6(8)	$C_{5A'}$	$C_{6A'}$	$C_{7A'}$	120.0
C_{18A}	N_{4A}	$Fe_{01}{}^1$	113.9(5)	N_{1B}	C_{1B}	N_{2B}	112(2)
C_{18A}	N_{4A}	C_3	123.0(9)	N_{2B}	C_{2B}	C_{3B}	107.1(18)
C_{18A}	N_{4A}	C_{15A}	111.3(9)	N_{1B}	C_{3B}	C_{4B}	117(2)
C_{21A}	N_{5A}	C_{20A}	109.7(8)	C_{2B}	C_{3B}	N_{1B}	108.0(17)
C_{19A}	N_{6A}	$Fe_{01}{}^1$	113.1(5)	C_{2B}	C_{3B}	C_{4B}	135(3)
C_{21A}	N_{6A}	$Fe_{01}{}^1$	141.0(7)	N_{3B}	C_{4B}	C_{3B}	114(3)
C_{21A}	N_{6A}	C_{19A}	106.0(7)	C_{6B}	C_{5B}	N_{3B}	119.1(7)
C_{1B}	N_{1B}	Fe_{01}	143.8(19)	C_{10B}	C_{5B}	N_{3B}	121.6(7)
C_{1B}	N_{1B}	C_{3B}	104.8(18)	C_{10B}	C_{5B}	C_{6B}	119.3(7)
C_{3B}	N_{1B}	Fe_{01}	111.0(13)	C_{5B}	C_{6B}	C_{7B}	119.2(7)
C_{2B}	N_{2B}	C_{1B}	108.1(17)	C_{8B}	C_{7B}	C_{6B}	121.7(7)
C_{4B}	N_{3B}	Fe_{01}	124.2(15)	C_{7B}	C_{8B}	C_{11B}	120.0(7)
C_{4B}	N_{3B}	C_{5B}	108.0(15)	C_{9B}	C_{8B}	C_{7B}	117.3(7)
C_{5B}	N_{3B}	Fe_{01}	127.7(4)	C_{9B}	C_{8B}	C_{11B}	122.6(7)
C_{4C}	N_{3B}	Fe_{01}	108.2(12)	C_{8B}	C_{9B}	C_{10B}	122.4(8)
C_{4C}	N_{3B}	C_{5B}	123.6(13)	C_{5B}	C_{10B}	C_{9B}	120.1(7)
$C_{1B'}$	$N_{1B'}$	Fe_{01}	145.1(19)	$C_{8B}{}^1$	C_{11B}	C_{8B}	114.3(9)
$C_{1B'}$	$N_{1B'}$	$C_{3B'}$	100.7(19)	$N_{1B'}$	$C_{1B'}$	$N_{2B'}$	113(2)
$C_{3B'}$	$N_{1B'}$	Fe_{01}	114.2(17)	$N_{2B'}$	$C_{2B'}$	$C_{3B'}$	105(2)
$C_{2B'}$	$N_{2B'}$	$C_{1B'}$	109.2(19)	$N_{1B'}$	$C_{3B'}$	C_{4C}	116(2)
$C_{8A'}$	C_1	C_2	111.4(17)	$C_{2B'}$	$C_{3B'}$	$N_{1B'}$	112(2)
C_5	C_3	N_{4A}	122.0(9)	$C_{2B'}$	$C_{3B'}$	C_{4C}	132(3)
C_5	C_3	C_8	120.0	N_{3B}	C_{4C}	$C_{3B'}$	117(2)
C_8	C_3	N_{4A}	117.9(9)	F_1	B_{01B}	F_3	85(4)
C_6	C_5	C_3	120.0	F_1	B_{01B}	F_{00X}	110(4)
C_5	C_6	C_{12A}	120.0	F_3	B_{01B}	F_{00X}	101.5(16)
C_6	C_{12A}	C_{11A}	121.8(10)	F_{10}	B_{01B}	F_1	134(5)
C_7	C_{12A}	C_6	120.0	F_{10}	B_{01B}	F_3	110(2)
C_7	C_{12A}	C_{11A}	118.1(10)	F_{10}	B_{01B}	F_{00X}	109(2)
C_{12A}	C_7	C_8	120.0	F_{002}	B_{01A}	F_{003}	111.0(7)
C_7	C_8	C_3	120.0	F_{002}	B_{01A}	F_{008}	109.5(8)
N_{1A}	C_{1A}	N_{2A}	113.2(9)	F_{002}	B_{01A}	F_{00A}	109.5(9)
C_{3A}	C_{2A}	N_{2A}	106.4(9)	F_{008}	B_{01A}	F_{003}	109.7(9)
N_{1A}	C_{3A}	C_{4A}	117.0(7)	F_{00A}	B_{01A}	F_{003}	109.1(8)
C_{2A}	C_{3A}	N_{1A}	110.0(8)	F_{00A}	B_{01A}	F_{008}	108.1(8)
C_{2A}	C_{3A}	C_{4A}	132.9(9)	F_{009}	B_{01C}	F_{00H}	105.0(10)
N_{3A}	C_{4A}	C_{3A}	117.8(7)	F_{009}	B_{01C}	F_{00T}	104.5(8)
C_{8A}	C_{7A}	C_{6A}	120.0	F_{00H}	B_{01C}	F_{00T}	111.6(9)
C_{7A}	C_{8A}	C_{11A}	120.5(11)	F_{00Y}	B_{01C}	F_{009}	111.5(10)

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C$_{9A}$	C$_{8A}$	C$_{7A}$	120.0	F$_{00Y}$	B$_{01C}$	F$_{00H}$	109.7(11)
C$_{9A}$	C$_{8A}$	C$_{11A}$	119.4(11)	F$_{00Y}$	B$_{01C}$	F$_{00T}$	114.0(10)
C$_{8A}$	C$_{9A}$	C$_9$	120.0	N$_2$	C$_{1AA}$	C$_{2AA}$	175(3)
C$_{5A}$	C$_9$	C$_{9A}$	120.0	N$_{01L}$	C$_{0AA}$	C$_4$	176(3)

[1]1-X,+Y,3/2-Z

Table 6 Hydrogen Bonds for **1**.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
N$_{5A}$	H$_{5A}$	F$_{00X}$[1]	0.86	2.09	2.71(3)	128.8
N$_{2B}$	H$_{2B}$	F$_{003}$[2]	0.86	1.95	2.795(18)	167.7
C$_{2AA}$	H$_{2AB}$	F$_3$[3]	0.96	2.00	2.71(3)	128.4

[1]1/2+X,1/2-Y,1/2+Z; [2]3/2-X,1/2-Y,1-Z; [3]1/2-X,-1/2+Y,3/2-Z

Table 7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **1**.

Atom	x	y	z	U(eq)
H$_{2A}$	3330	4970	3044	105
H$_{5A}$	7090	843	11924	99
H$_{2B}$	6338	2535	3522	72
H$_{2B'}$	5975	2211	3309	77
H$_{1A}$	3159	817	7177	91
H$_{1B}$	2756	1512	7335	91
H$_5$	5285	1904	8576	58
H$_6$	4433	1905	7589	65
H$_7$	3104	1718	8610	58
H$_8$	3956	1718	9598	59
H$_{1AA}$	4097	3944	3183	102
H$_{2AA}$	2828	4964	3953	97
H$_{4A}$	3009	3881	5044	74
H$_{7A}$	3306	3236	7061	60
H$_{9A}$	3222	1144	6230	58
H$_9$	3468	1685	5323	60
H$_{6A}$	3551	3777	6154	57
H$_{11A}$	2727	1997	7441	63
H$_{11B}$	3008	1217	7270	63
H$_{16A}$	5282	1132	8690	83
H$_{17A}$	4471	1002	7680	88

H$_{13A}$	3147	1994	8455	58
H$_{14A}$	3957	2124	9466	56
H$_{18A}$	5304	664	9881	68
H$_{20A}$	6368	107	11038	95
H$_{21A}$	6856	2163	11809	84
H$_{7A'}$	3446	2860	7184	75
H$_{9A'}$	3240	912	6116	66
H$_{10A}$	3403	1597	5232	71
H$_{6A'}$	3608	3544	6300	80
H$_{1BA}$	5227	2151	3375	73
H$_{2BA}$	6731	3328	4477	68
H$_{4B}$	5991	3964	5396	79
H$_{6B}$	4419	4718	5296	63
H$_{7B}$	4360	5388	6229	62
H$_{9B}$	5698	3996	7378	84
H$_{10B}$	5777	3328	6467	81
H$_{11C}$	5387	5563	7630	77
H$_{11D}$	4613	5563	7370	77
H$_{1B'}$	4879	1957	3327	82
H$_{2BB}$	6508	3107	4129	74
H$_{4C}$	6083	3710	5237	52
H$_{2AB}$	3230	773	9738	60
H$_{2AC}$	3170	1198	10374	60
H$_{2AD}$	3013	317	10281	60
H$_{4D}$	5467	268	6981	92
H$_{4E}$	6215	72	7312	92
H$_{4F}$	5761	286	7756	92

Table 8 Atomic Occupancy for **1**.

Atom	*Occupancy*	Atom	*Occupancy*	Atom	*Occupancy*
N$_{1B}$	0.5	N$_{2B}$	0.5	H$_{2B}$	0.5
N$_{1B'}$	0.5	N$_{2B'}$	0.5	H$_{2B'}$	0.5
C$_1$	0.5	H$_{1A}$	0.5	H$_{1B}$	0.5
C$_3$	0.5	C$_5$	0.5	H$_5$	0.5
C$_6$	0.5	H$_6$	0.5	C$_{12A}$	0.5
C$_7$	0.5	H$_7$	0.5	C$_8$	0.5
H$_8$	0.5	C$_{7A}$	0.5	H$_{7A}$	0.5
C$_{8A}$	0.5	C$_{9A}$	0.5	H$_{9A}$	0.5
C$_9$	0.5	H$_9$	0.5	C$_{5A}$	0.5

C_{6A}	0.5	H_{6A}	0.5	C_{11A}	0.5
H_{11A}	0.5	H_{11B}	0.5	C_{15A}	0.5
C_{16A}	0.5	H_{16A}	0.5	C_{17A}	0.5
H_{17A}	0.5	C_2	0.5	C_{13A}	0.5
H_{13A}	0.5	C_{14A}	0.5	H_{14A}	0.5
$C_{7A'}$	0.5	$H_{7A'}$	0.5	$C_{8A'}$	0.5
$C_{9A'}$	0.5	$H_{9A'}$	0.5	C_{10A}	0.5
H_{10A}	0.5	$C_{5A'}$	0.5	$C_{6A'}$	0.5
$H_{6A'}$	0.5	C_{1B}	0.5	H_{1BA}	0.5
C_{2B}	0.5	H_{2BA}	0.5	C_{3B}	0.5
C_{4B}	0.5	H_{4B}	0.5	H_{11C}	0.5
H_{11D}	0.5	$C_{1B'}$	0.5	$H_{1B'}$	0.5
$C_{2B'}$	0.5	H_{2BB}	0.5	$C_{3B'}$	0.5
C_{4C}	0.5	H_{4C}	0.5	F_1	0.2
F_3	0.2	F_{10}	0.2	F_{00X}	0.2
B_{01B}	0.4	F_{009}	0.8	F_{00H}	0.8
F_{00T}	0.8	F_{00Y}	0.8	B_{01C}	0.6
N_2	0.5	C_{1AA}	0.25	C_{2AA}	0.25
H_{2AB}	0.25	H_{2AC}	0.25	H_{2AD}	0.25
N_{01L}	0.25	C_4	0.25	H_{4D}	0.25
H_{4E}	0.25	H_{4F}	0.25	C_{0AA}	0.25

Experimental

Single crystals of $C_{65}H_{57}B_4F_{16}Fe_2N_{19.5}$ **1** were crystallises using a diethyl ether vapour diffusion into acetonitrile. A suitable crystal was selected and [mounted in parafin oil] on a 'Bruker APEX-II CCD' diffractometer. The crystal was kept at 100 K during data collection. Using Olex2 [1], the structure was solved with the ShelXT [2] structure solution program using Intrinsic Phasing and refined with the ShelXL [3] refinement package using Least Squares minimisation.

1. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.
2. Sheldrick, G.M. (2015). Acta Cryst. A71, 3-8.
3. Sheldrick, G.M. (2015). Acta Cryst. C71, 3-8.

Crystal structure determination of **1**

Crystal Data for $C_{65}H_{57}B_4F_{16}Fe_2N_{19.5}$ (*M* = 1570.24 g/mol): monoclinic, space group C2/c (no. 15), *a* = 21.131(4) Å, *b* = 17.391(4) Å, *c* = 21.069(4) Å, β = 107.00(3)°, *V* = 7404(3) Å^3, *Z* = 4, *T* = 293(2) K, μ(MoKα) = 0.486 mm^{-1}, *Dcalc* = 1.409 g/cm^3, 50460 reflections measured (3.09° ≤ 2Θ ≤ 52.998°), 6995 unique (R_{int} = 0.0697, R_{sigma} = 0.0341) which were used in all calculations. The final R_1 was 0.1035 (I > 2σ(I)) and wR_2 was 0.3220 (all data).

Refinement model description

Number of restraints - 218, number of constraints - unknown.

Details:

```
1. Fixed Uiso
 At 1.2 times of:
  All C(H) groups, All C(H,H) groups, All N(H) groups
 At 1.5 times of:
  All C(H,H,H) groups
2. Shared sites
{B01C, B01B}
3. Restrained distances
 B01B-B01C
 1.42 with sigma of 0.02
 F00X-B01B = F00Y-B01C = F3-B01B = F009-B01C = F10-B01B = F00T-B01C = F00H-
 B01C = F1-B01B
 1.39 with sigma of 0.02
 C1-C2 ≈ C11A-C2
 with sigma of 0.02
4. Rigid bond restraints
 C3B', C4C
 with sigma for 1-2 distances of 0.01 and sigma for 1-3 distances of 0.01
5. Uiso/Uaniso restraints and constraints
Uanis(B01C) = Uanis(B01B)
6. Rigid body (RIGU) restrains
 N1B, N2B, N1B', N2B', C1B, C2B, C3B, C1B', C2B', C3B'
 with sigma for 1-2 distances of 0.004 and sigma for 1-3 distances of 0.004
 F009, F00H, F00T, F00Y
 with sigma for 1-2 distances of 0.004 and sigma for 1-3 distances of 0.004
 C1, C2, C5, C6, C7, C8, C11A, C12A, C13A, C14A, C15A, C16A, C17A
 with sigma for 1-2 distances of 0.004 and sigma for 1-3 distances of 0.004
 C3, C15A
 with sigma for 1-2 distances of 0.004 and sigma for 1-3 distances of 0.004
 C9, C5A, C6A, C7A, C8A, C9A, C10A, C5A', C6A', C7A', C8A', C9A'
 with sigma for 1-2 distances of 0.004 and sigma for 1-3 distances of 0.004
 C4B, C4C
 with sigma for 1-2 distances of 0.004 and sigma for 1-3 distances of 0.004
7. Others
 Fixed Sof: N1B(0.5) N2B(0.5) H2B(0.5) N1B'(0.5) N2B'(0.5) H2B'(0.5)
C1(0.5)
 H1A(0.5) H1B(0.5) C3(0.5) C5(0.5) H5(0.5) C6(0.5) H6(0.5) C12A(0.5)
C7(0.5)
 H7(0.5) C8(0.5) H8(0.5) C7A(0.5) H7A(0.5) C8A(0.5) C9A(0.5) H9A(0.5)
C9(0.5)
 H9(0.5) C5A(0.5) C6A(0.5) H6A(0.5) C11A(0.5) H11A(0.5) H11B(0.5) C15A(0.5)
 C16A(0.5) H16A(0.5) C17A(0.5) H17A(0.5) C2(0.5) C13A(0.5) H13A(0.5)
C14A(0.5)
 H14A(0.5) C7A'(0.5) H7A'(0.5) C8A'(0.5) C9A'(0.5) H9A'(0.5) C10A(0.5)
 H10A(0.5) C5A'(0.5) C6A'(0.5) H6A'(0.5) C1B(0.5) H1BA(0.5) C2B(0.5)
H2BA(0.5)
 C3B(0.5) C4B(0.5) H4B(0.5) H11C(0.5) H11D(0.5) C1B'(0.5) H1B'(0.5)
C2B'(0.5)
 H2BB(0.5) C3B'(0.5) C4C(0.5) H4C(0.5) F1(0.2) F3(0.2) F10(0.2) F00X(0.2)
 B01B(0.4) F009(0.8) F00H(0.8) F00T(0.8) F00Y(0.8) B01C(0.6) N2(0.5)
C1AA(0.25)
 C2AA(0.25) H2AB(0.25) H2AC(0.25) H2AD(0.25) N01L(0.25) C4(0.25) H4D(0.25)
 H4E(0.25) H4F(0.25) C0AA(0.25)
8.a Secondary CH2 refined with riding coordinates:
 C1(H1A,H1B), C11A(H11A,H11B), C11B(H11C,H11D)
8.b Aromatic/amide H refined with riding coordinates:
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 N2A(H2A), N5A(H5A), N2B(H2B), N2B'(H2B'), C5(H5), C6(H6), C7(H7), C8(H8),
 C1A(H1AA), C2A(H2AA), C4A(H4A), C7A(H7A), C9A(H9A), C9(H9), C6A(H6A),
 C16A(H16A), C17A(H17A), C13A(H13A), C14A(H14A), C18A(H18A), C20A(H20A),
 C21A(H21A), C7A'(H7A'), C9A'(H9A'), C10A(H10A), C6A'(H6A'), C1B(H1BA),
 C2B(H2BA), C4B(H4B), C6B(H6B), C7B(H7B), C9B(H9B), C10B(H10B), C1B'(H1B'),
 C2B'(H2BB), C4C(H4C)
8.c Fitted hexagon refined as free rotating group:
 C3(C5,C6,C12A,C7,C8), C7A(C8A,C9A,C9,C5A,C6A),
C15A(C16A,C17A,C2,C13A,C14A),
 C7A'(C8A',C9A',C10A,C5A',C6A')
8.d Idealised Me refined as rotating group:
 C2AA(H2AB,H2AC,H2AD), C4(H4D,H4E,H4F)
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Crystal data and structure refinement for **2**.

Table 9 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{Å}^2 \times 10^3$) for **2**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Fe01	7013.4(8)	7349.1(5)	7576.2(4)	44.7(3)
Fe02	3771.8(9)	7740.2(5)	2561.2(4)	46.3(3)
S1A	7790(2)	5268.3(10)	4688.2(10)	69.9(5)
S1B	8501.5(17)	9919.9(8)	5347.5(7)	50.0(4)
S1C	482.6(16)	7657.6(11)	5297.5(8)	55.0(4)
N1A	8789(6)	7773(3)	8094(3)	52.4(13)
N2A	10682(7)	8085(4)	8784(3)	74.2(19)
N3A	8434(5)	7024(3)	7057(3)	47.2(12)
N4A	3458(6)	6604(3)	2931(3)	53.4(13)
N5A	-142(8)	6688(4)	1429(4)	82(2)
N6A	1819(6)	7190(3)	2017(3)	55.4(13)
N1B	5891(5)	7715(3)	8160(2)	48.6(12)
N2B	4917(6)	8071(3)	8908(2)	56.3(13)
N3B	6518(5)	8437(3)	7315(2)	44.1(11)
N4B	5976(5)	8186(3)	3019(2)	46.0(11)
N5B	6013(7)	7396(4)	1139(3)	63.7(15)
N6B	5038(6)	7400(3)	1926(3)	54.3(13)
N1C	7223(5)	6298(3)	7906(2)	48.8(12)
N2C	7374(6)	5264(3)	8412(3)	55.8(14)
N3C	5263(5)	6717(3)	7082(2)	42.2(11)
N4C	2427(5)	8375(3)	3110(2)	43(1)
N5C	2462(6)	9640(3)	1521(2)	53.2(13)
N6C	3313(5)	8814(3)	2155(2)	47.6(11)
C1A	9230(7)	8109(4)	8621(3)	59.4(17)
C2A	11176(8)	7710(5)	8330(4)	69(2)
C3A	10014(7)	7502(4)	7899(3)	55.8(16)
C4A	9751(7)	7116(4)	7335(3)	55.7(16)
C5A	8178(6)	6609(3)	6489(3)	50.8(15)
C6A	8790(7)	5869(3)	6400(3)	58.0(18)
C7A	8603(8)	5483(4)	5850(4)	61.0(19)
C8A	7844(7)	5810(3)	5368(3)	53.6(16)
C9A	7246(7)	6538(3)	5474(3)	55.5(16)
C10A	7409(6)	6918(3)	6029(3)	49.2(15)
C11A	6471(7)	5697(3)	4205(3)	56.3(16)

C12A	5055(8)	5772(4)	4295(4)	64.9(19)
C13A	4050(7)	6079(3)	3882(3)	55.3(17)
C14A	4415(7)	6294(3)	3361(3)	57.0(17)
C15A	5835(7)	6207(3)	3278(3)	55.0(16)
C16A	6816(7)	5930(3)	3684(3)	57.9(17)
C17A	2204(8)	6225(4)	2717(4)	66(2)
C18A	1320(7)	6522(4)	2222(4)	60.9(17)
C19A	64(8)	6214(4)	1833(4)	72(2)
C20A	921(8)	7292(5)	1521(4)	67.0(18)
C1B	5575(7)	7496(4)	8658(3)	53.0(15)
C3B	4803(7)	8715(4)	8583(3)	53.8(15)
C4B	5425(6)	8487(4)	8115(3)	47.2(13)
C5B	5757(6)	8847(3)	7619(3)	45.6(13)
C6B	6939(6)	8782(3)	6830(3)	40.2(12)
C7B	5937(6)	9011(3)	6383(3)	47.9(14)
C8B	6387(6)	9344(3)	5915(3)	48.9(14)
C9B	7828(6)	9439(3)	5897(3)	43.9(13)
C10B	8840(6)	9214(3)	6347(3)	47.3(14)
C11B	8396(6)	8887(3)	6819(3)	42.7(12)
C12B	7616(6)	9395(3)	4690(3)	45.9(13)
C13B	7102(6)	8575(3)	4609(3)	46.5(13)
C14B	6541(6)	8194(3)	4075(3)	47.8(14)
C15B	6495(6)	8597(3)	3577(3)	44.6(13)
C16B	6968(6)	9416(3)	3644(3)	46.8(13)
C17B	7514(6)	9804(3)	4195(3)	47.4(14)
C18B	6819(6)	8203(3)	2637(3)	46.6(13)
C19B	6369(7)	7829(3)	2068(3)	47.0(13)
C20B	6972(7)	7824(4)	1576(3)	57.0(16)
C21B	4865(8)	7155(4)	1363(3)	63.3(18)
C1C	7988(7)	5995(4)	8337(3)	57.5(17)
C2C	6183(7)	5094(3)	7995(3)	51.8(15)
C3C	6065(6)	5735(3)	7673(3)	45.8(13)
C4C	5048(6)	5984(3)	7212(3)	45.3(13)
C5C	4177(5)	6966(3)	6637(3)	38.7(12)
C6C	3968(7)	6599(3)	6075(3)	44.9(13)
C7C	2873(7)	6808(3)	5648(3)	49.0(14)
C8C	1994(6)	7409(3)	5797(3)	43.0(12)
C9C	2230(6)	7781(3)	6367(3)	46.3(13)
C10C	3296(6)	7559(3)	6786(3)	44.6(13)
C11C	1177(6)	7785(3)	4657(3)	45.9(13)
C12C	2566(6)	8087(3)	4663(3)	48.3(13)

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C13C	2968(6)	8256(3)	4143(3)	44.9(13)
C14C	2001(6)	8154(3)	3632(3)	40.4(12)
C15C	612(7)	7845(4)	3625(3)	58.7(16)
C16C	223(7)	7649(4)	4145(3)	60.1(17)
C17C	1766(6)	8937(3)	2855(3)	43.9(12)
C18C	2191(6)	9173(3)	2337(3)	44.6(13)
C19C	1624(7)	9682(4)	1937(3)	51.5(14)
C20C	3468(7)	9117(4)	1668(3)	52.8(14)
F1	4241(17)	9051(12)	489(7)	94(4)
F2	2912(13)	8817(7)	-348(4)	76(3)
F4	2182(12)	8330(7)	463(6)	77(3)
F0AA	4362(19)	7951(11)	33(6)	136(5)
B9	3229(10)	8411(6)	155(4)	95(2)
F006	1142(4)	10367(2)	7510.1(19)	61.8(11)
F007	1551(5)	9524(2)	8204.0(19)	73.4(13)
F008	3417(4)	10153(2)	7910(2)	75.5(13)
F009	2086(5)	9167(3)	7329(2)	81.3(12)
B02Q	2067(8)	9802(4)	7745(3)	47.5(15)
F8	2568(14)	8021(8)	562(6)	97(4)
F10	2198(18)	8798(9)	-189(7)	144(6)
F11	4456(18)	8836(12)	445(9)	112(6)
F15	3448(13)	7702(6)	-174(6)	99(4)
B9A	3229(10)	8411(6)	155(4)	95(2)
F1AA	2700(20)	4855(12)	7852(13)	168(11)
F2AA	2638(8)	6268(4)	7782(4)	166(3)
F5AA	1920(15)	5540(10)	7136(7)	158(5)
F7AA	523(9)	5381(6)	7654(7)	121(5)
F1AB	2810(20)	4878(11)	7688(10)	106(5)
F0BA	1410(16)	5629(6)	8300(7)	143(6)
B2	1955(13)	5518(7)	7772(7)	153(8)
B2A	2003(16)	5468(10)	7735(10)	125(6)
F3AA	8189(9)	6220(4)	10292(4)	173(4)
F4AA	8542(11)	7487(5)	10456(4)	154(3)
F6AA	8383(9)	6993(7)	9540(3)	182(4)
F8AA	6488(9)	7057(7)	9958(3)	170(4)
B0AA	7933(13)	6919(9)	10026(5)	91(3)
N01B	1984(7)	5753(3)	665(3)	68.5(16)
C030	1397(17)	6093(11)	-413(6)	168(7)
C02V	1728(11)	5907(6)	194(4)	85(2)
N02E	11926(9)	10512(5)	10502(3)	88(2)
C02M	11870(10)	10571(5)	10031(4)	73(2)

| C02X | 11916(17) | 10643(6) | 9425(4) | 123(4) |

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

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe01	40.3(5)	47.2(4)	51.4(6)	14.0(4)	17.2(4)	2.2(3)
Fe02	40.9(5)	53.3(5)	48.3(5)	2.7(4)	19.2(4)	2.2(4)
S1A	77.6(13)	57.9(9)	77.4(14)	-3.4(9)	22.9(10)	21.8(8)
S1B	54.7(9)	49.5(7)	49.5(9)	9.6(6)	20.7(7)	-8.6(6)
S1C	36.5(8)	85(1)	50.4(10)	19.9(8)	19.5(7)	6.1(7)
N1A	54(3)	52(3)	52(3)	11(2)	12(3)	0(2)
N2A	71(4)	78(4)	66(4)	26(3)	-13(3)	-13(3)
N3A	36(3)	43(2)	66(4)	13(2)	17(2)	1.3(19)
N4A	48(3)	50(3)	65(4)	-3(2)	23(3)	0(2)
N5A	72(4)	80(4)	83(6)	-7(4)	-4(4)	4(3)
N6A	44(3)	63(3)	58(4)	-1(3)	10(2)	7(2)
N1B	45(3)	57(3)	47(3)	17(2)	13(2)	-3(2)
N2B	58(3)	75(3)	42(3)	16(3)	20(3)	6(3)
N3B	38(2)	52(2)	45(3)	12(2)	15(2)	-1(2)
N4B	45(3)	47(2)	50(3)	3(2)	21(2)	2(2)
N5B	69(4)	79(3)	47(3)	0(3)	25(3)	12(3)
N6B	53(3)	63(3)	51(3)	0(2)	24(3)	3(2)
N1C	44(3)	50(2)	55(3)	12(2)	11(2)	2(2)
N2C	61(3)	53(3)	58(4)	20(3)	14(3)	17(2)
N3C	36(2)	47(2)	50(3)	13(2)	19(2)	5.4(19)
N4C	35(2)	54(2)	43(3)	7(2)	13(2)	4.6(19)
N5C	56(3)	69(3)	39(3)	12(2)	17(2)	5(2)
N6C	41(3)	64(3)	41(3)	8(2)	13(2)	6(2)
C1A	58(4)	60(4)	61(5)	19(3)	10(3)	-2(3)
C2A	52(4)	80(4)	76(6)	22(4)	8(4)	2(3)
C3A	47(3)	57(3)	65(5)	18(3)	12(3)	-6(3)
C4A	56(4)	54(3)	65(5)	20(3)	25(3)	6(3)
C5A	47(3)	47(3)	67(4)	8(3)	32(3)	-2(2)
C6A	61(4)	48(3)	75(5)	18(3)	33(4)	9(3)
C7A	64(4)	47(3)	81(5)	5(3)	37(4)	9(3)
C8A	56(4)	44(3)	68(5)	10(3)	29(3)	5(3)
C9A	65(4)	41(3)	67(5)	7(3)	29(3)	2(3)
C10A	48(3)	41(3)	65(4)	9(3)	24(3)	4(2)
C11A	60(4)	40(3)	73(5)	-3(3)	26(3)	3(3)
C12A	79(5)	50(3)	73(5)	2(3)	37(4)	-5(3)

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C13A	46(3)	47(3)	80(5)	8(3)	29(3)	2(3)
C14A	58(4)	42(3)	75(5)	-2(3)	30(4)	-5(3)
C15A	48(4)	51(3)	67(5)	0(3)	22(3)	-7(3)
C16A	54(4)	46(3)	75(5)	-11(3)	25(3)	-5(3)
C17A	64(4)	44(3)	95(6)	-6(3)	37(4)	-8(3)
C18A	44(4)	63(4)	74(5)	-6(3)	10(3)	6(3)
C19A	61(4)	61(4)	86(6)	-11(4)	8(4)	-15(3)
C20A	48(4)	84(4)	65(5)	-11(4)	8(3)	2(3)
C1B	53(4)	66(3)	46(4)	17(3)	18(3)	9(3)
C3B	47(3)	66(3)	51(4)	10(3)	14(3)	11(3)
C4B	40(3)	62(3)	46(3)	16(3)	17(3)	5(2)
C5B	39(3)	54(3)	48(4)	10(3)	15(3)	2(2)
C6B	42(3)	42(2)	40(3)	8(2)	17(2)	1(2)
C7B	37(3)	56(3)	57(4)	18(3)	18(3)	2(2)
C8B	44(3)	53(3)	54(4)	15(3)	15(3)	3(2)
C9B	45(3)	44(3)	48(3)	6(2)	23(3)	2(2)
C10B	49(3)	45(3)	51(4)	7(2)	19(3)	-7(2)
C11B	40(3)	46(3)	45(3)	11(2)	12(2)	-2(2)
C12B	45(3)	51(3)	49(4)	13(3)	22(3)	5(2)
C13B	52(3)	48(3)	44(3)	9(2)	20(3)	-1(2)
C14B	53(3)	44(3)	50(4)	7(2)	21(3)	-5(2)
C15B	37(3)	49(3)	52(4)	4(2)	21(3)	5(2)
C16B	46(3)	52(3)	45(3)	11(3)	16(3)	-1(2)
C17B	50(3)	46(3)	50(4)	12(2)	18(3)	-5(2)
C18B	48(3)	48(3)	49(4)	7(3)	19(3)	5(2)
C19B	52(3)	47(3)	46(4)	6(2)	20(3)	6(2)
C20B	51(4)	75(4)	52(4)	10(3)	24(3)	12(3)
C21B	69(5)	71(4)	54(4)	-5(3)	28(4)	3(3)
C1C	51(4)	58(3)	66(5)	18(3)	11(3)	2(3)
C2C	54(4)	49(3)	56(4)	15(3)	14(3)	2(3)
C3C	50(3)	43(3)	50(4)	6(2)	24(3)	1(2)
C4C	45(3)	46(3)	50(4)	10(2)	20(3)	0(2)
C5C	34(3)	42(2)	42(3)	5(2)	14(2)	-6(2)
C6C	55(3)	45(3)	39(3)	6(2)	19(3)	3(2)
C7C	54(3)	52(3)	44(3)	7(3)	17(3)	0(3)
C8C	39(3)	50(3)	45(3)	10(2)	19(2)	-1(2)
C9C	47(3)	50(3)	46(3)	8(2)	21(3)	2(2)
C10C	43(3)	50(3)	46(3)	10(2)	19(3)	5(2)
C11C	40(3)	59(3)	42(3)	11(3)	14(2)	4(2)
C12C	46(3)	58(3)	42(3)	6(3)	13(3)	-5(2)
C13C	33(3)	60(3)	43(3)	4(3)	14(2)	-4(2)

C14C	32(3)	50(3)	41(3)	5(2)	12(2)	7(2)
C15C	42(3)	89(4)	46(4)	10(3)	11(3)	-7(3)
C16C	38(3)	88(4)	56(4)	14(3)	12(3)	-10(3)
C17C	39(3)	53(3)	43(3)	5(2)	15(2)	4(2)
C18C	35(3)	58(3)	44(3)	9(3)	15(2)	4(2)
C19C	54(4)	63(3)	42(3)	13(3)	18(3)	9(3)
C20C	42(3)	77(4)	45(4)	10(3)	17(3)	9(3)
F1	79(6)	169(9)	51(5)	33(5)	47(4)	10(6)
F2	93(7)	92(6)	45(4)	-1(4)	14(4)	28(5)
F4	80(6)	77(6)	73(7)	-7(5)	14(5)	16(5)
F0AA	170(10)	192(10)	67(8)	43(7)	38(8)	99(9)
B9	100(5)	123(6)	67(5)	14(4)	20(4)	37(4)
F006	46(2)	74(2)	75(3)	36(2)	19.1(19)	8.3(17)
F007	92(3)	87(3)	61(3)	37(2)	45(2)	31(2)
F008	46(2)	65(2)	108(4)	18(2)	-8(2)	-3.0(17)
F009	92(3)	90(3)	59(3)	-17(2)	14(2)	17(2)
B02Q	49(4)	53(3)	45(4)	6(3)	20(3)	4(3)
F8	89(8)	131(10)	72(7)	-8(6)	20(6)	25(6)
F10	177(12)	103(7)	115(10)	-30(7)	-61(8)	39(8)
F11	101(8)	156(11)	87(10)	29(7)	28(7)	15(7)
F15	97(7)	100(5)	115(9)	2(5)	68(7)	-5(5)
B9A	100(5)	123(6)	67(5)	14(4)	20(4)	37(4)
F1AA	138(15)	132(9)	270(30)	-3(10)	139(17)	0(8)
F2AA	145(6)	140(4)	252(10)	39(5)	128(6)	17(4)
F5AA	91(8)	189(11)	217(11)	52(7)	66(7)	32(7)
F7AA	67(5)	108(7)	217(13)	109(8)	53(6)	23(4)
F1AB	72(7)	134(8)	131(12)	34(7)	59(8)	10(6)
F0BA	180(12)	92(6)	192(13)	-20(7)	156(12)	-39(7)
B2	172(17)	131(9)	204(16)	24(9)	162(13)	15(8)
B2A	77(8)	117(8)	209(14)	63(7)	69(8)	24(6)
F3AA	162(7)	130(5)	192(9)	30(6)	-59(7)	-28(5)
F4AA	215(9)	160(6)	93(6)	-6(5)	44(6)	52(6)
F6AA	159(7)	348(13)	68(5)	58(7)	52(5)	123(8)
F8AA	127(6)	327(11)	74(5)	62(6)	33(4)	72(7)
B0AA	88(8)	140(10)	61(7)	37(7)	29(6)	47(7)
N01B	76(4)	67(3)	63(4)	14(3)	4(3)	22(3)
C030	153(12)	290(20)	74(7)	60(10)	15(8)	93(13)
C02V	92(6)	101(6)	61(5)	16(5)	4(4)	27(5)
N02E	116(6)	101(5)	54(4)	25(3)	20(4)	39(4)
C02M	100(6)	71(4)	50(4)	16(3)	12(4)	9(4)
C02X	213(14)	104(7)	56(5)	28(5)	32(6)	-10(8)

Table 11 Bond Lengths for **2**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Fe01	N1A	1.959(6)	C13A	C14A	1.409(9)
Fe01	N3A	2.044(5)	C14A	C15A	1.413(9)
Fe01	N1B	1.963(5)	C15A	C16A	1.346(10)
Fe01	N3B	2.025(4)	C17A	C18A	1.455(11)
Fe01	N1C	1.993(4)	C18A	C19A	1.414(10)
Fe01	N3C	2.038(5)	C3B	C4B	1.377(9)
Fe02	N4A	2.192(5)	C4B	C5B	1.440(8)
Fe02	N6A	2.170(6)	C6B	C7B	1.386(8)
Fe02	N4B	2.239(5)	C6B	C11B	1.394(8)
Fe02	N6B	2.141(5)	C7B	C8B	1.405(8)
Fe02	N4C	2.219(5)	C8B	C9B	1.382(8)
Fe02	N6C	2.140(5)	C9B	C10B	1.393(9)
S1A	C8A	1.760(8)	C10B	C11B	1.408(7)
S1A	C11A	1.767(8)	C12B	C13B	1.417(8)
S1B	C9B	1.784(5)	C12B	C17B	1.400(8)
S1B	C12B	1.760(7)	C13B	C14B	1.364(9)
S1C	C8C	1.784(6)	C14B	C15B	1.403(8)
S1C	C11C	1.782(6)	C15B	C16B	1.405(8)
N1A	C1A	1.304(9)	C16B	C17B	1.397(9)
N1A	C3A	1.409(9)	C18B	C19B	1.412(9)
N2A	C1A	1.371(9)	C19B	C20B	1.386(8)
N2A	C2A	1.358(11)	C2C	C3C	1.369(8)
N3A	C4A	1.302(9)	C3C	C4C	1.430(9)
N3A	C5A	1.425(9)	C5C	C6C	1.387(8)
N4A	C14A	1.394(9)	C5C	C10C	1.391(8)
N4A	C17A	1.316(9)	C6C	C7C	1.397(9)
N5A	C19A	1.289(11)	C7C	C8C	1.399(8)
N5A	C20A	1.368(10)	C8C	C9C	1.404(8)
N6A	C18A	1.355(8)	C9C	C10C	1.376(8)
N6A	C20A	1.353(9)	C11C	C12C	1.389(8)
N1B	C1B	1.342(8)	C11C	C16C	1.370(9)
N1B	C4B	1.394(8)	C12C	C13C	1.398(8)
N2B	C1B	1.326(8)	C13C	C14C	1.371(8)
N2B	C3B	1.377(8)	C14C	C15C	1.391(8)
N3B	C5B	1.287(7)	C15C	C16C	1.406(9)
N3B	C6B	1.440(6)	C17C	C18C	1.437(8)
N4B	C15B	1.420(8)	C18C	C19C	1.386(8)

N4B	C18B	1.312(7)	F1	B9	1.470(13)	
N5B	C20B	1.368(9)	F2	B9	1.416(10)	
N5B	C21B	1.357(9)	F4	B9	1.344(11)	
N6B	C19B	1.394(8)	F0AA	B9	1.412(11)	
N6B	C21B	1.333(9)	F006	B02Q	1.408(8)	
N1C	C1C	1.300(8)	F007	B02Q	1.375(7)	
N1C	C3C	1.410(8)	F008	B02Q	1.360(8)	
N2C	C1C	1.368(8)	F009	B02Q	1.383(8)	
N2C	C2C	1.362(9)	F8	B9A	1.426(11)	
N3C	C4C	1.307(6)	F10	B9A	1.385(11)	
N3C	C5C	1.443(7)	F11	B9A	1.369(13)	
N4C	C14C	1.439(7)	F15	B9A	1.403(11)	
N4C	C17C	1.294(7)	F1AA	B2	1.359(11)	
N5C	C19C	1.372(8)	F2AA	B2	1.378(10)	
N5C	C20C	1.351(8)	F2AA	B2A	1.426(16)	
N6C	C18C	1.366(7)	F5AA	B2A	1.420(19)	
N6C	C20C	1.329(8)	F7AA	B2A	1.386(15)	
C2A	C3A	1.370(10)	F1AB	B2A	1.291(16)	
C3A	C4A	1.399(10)	F0BA	B2	1.435(12)	
C5A	C6A	1.409(8)	F3AA	B0AA	1.389(13)	
C5A	C10A	1.358(9)	F4AA	B0AA	1.351(16)	
C6A	C7A	1.375(10)	F6AA	B0AA	1.310(12)	
C7A	C8A	1.407(10)	F8AA	B0AA	1.390(13)	
C8A	C9A	1.391(8)	N01B	C02V	1.151(10)	
C9A	C10A	1.381(9)	C030	C02V	1.476(14)	
C11A	C12A	1.412(10)	N02E	C02M	1.118(10)	
C11A	C16A	1.413(10)	C02M	C02X	1.455(11)	
C12A	C13A	1.393(10)				

Table 12 Bond Angles for **2**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N1A	Fe01	N3A	81.2(2)	N6A	C18A	C19A	107.3(7)
N1A	Fe01	N1B	90.6(2)	C19A	C18A	C17A	134.1(6)
N1A	Fe01	N3B	94.0(2)	N5A	C19A	C18A	107.0(6)
N1A	Fe01	N1C	89.2(2)	N6A	C20A	N5A	107.6(7)
N1A	Fe01	N3C	169.97(19)	N2B	C1B	N1B	110.2(5)
N1B	Fe01	N3A	171.8(2)	N2B	C3B	C4B	104.8(6)
N1B	Fe01	N3B	80.12(19)	N1B	C4B	C5B	113.9(5)
N1B	Fe01	N1C	90.6(2)	C3B	C4B	N1B	109.2(5)

N1B	Fe01	N3C	91.4(2)	C3B	C4B	C5B	136.8(6)
N3B	Fe01	N3A	100.98(18)	N3B	C5B	C4B	115.7(5)
N3B	Fe01	N3C	96.01(19)	C7B	C6B	N3B	121.6(5)
N1C	Fe01	N3A	88.7(2)	C7B	C6B	C11B	120.3(5)
N1C	Fe01	N3B	170.2(2)	C11B	C6B	N3B	118.1(5)
N1C	Fe01	N3C	81.0(2)	C6B	C7B	C8B	120.0(5)
N3C	Fe01	N3A	96.6(2)	C9B	C8B	C7B	120.1(6)
N4A	Fe02	N4B	102.0(2)	C8B	C9B	S1B	123.1(5)
N4A	Fe02	N4C	92.33(18)	C8B	C9B	C10B	120.1(5)
N6A	Fe02	N4A	77.2(2)	C10B	C9B	S1B	116.6(4)
N6A	Fe02	N4B	170.3(2)	C9B	C10B	C11B	120.1(5)
N6A	Fe02	N4C	88.2(2)	C6B	C11B	C10B	119.4(5)
N6B	Fe02	N4A	101.89(19)	C13B	C12B	S1B	125.7(5)
N6B	Fe02	N6A	92.5(2)	C17B	C12B	S1B	117.1(4)
N6B	Fe02	N4B	78.1(2)	C17B	C12B	C13B	116.9(6)
N6B	Fe02	N4C	165.57(18)	C14B	C13B	C12B	122.0(5)
N4C	Fe02	N4B	101.53(18)	C13B	C14B	C15B	120.9(5)
N6C	Fe02	N4A	160.7(2)	C14B	C15B	N4B	120.7(5)
N6C	Fe02	N6A	86.9(2)	C14B	C15B	C16B	118.4(6)
N6C	Fe02	N4B	95.54(18)	C16B	C15B	N4B	120.9(5)
N6C	Fe02	N6B	89.3(2)	C17B	C16B	C15B	120.1(5)
N6C	Fe02	N4C	76.30(18)	C16B	C17B	C12B	121.6(5)
C8A	S1A	C11A	105.5(3)	N4B	C18B	C19B	121.0(5)
C12B	S1B	C9B	105.3(3)	N6B	C19B	C18B	118.8(5)
C11C	S1C	C8C	103.7(3)	C20B	C19B	N6B	108.6(6)
C1A	N1A	Fe01	139.9(5)	C20B	C19B	C18B	132.5(6)
C1A	N1A	C3A	106.2(6)	N5B	C20B	C19B	106.6(6)
C3A	N1A	Fe01	112.3(5)	N6B	C21B	N5B	111.4(7)
C2A	N2A	C1A	107.5(7)	N1C	C1C	N2C	110.1(6)
C4A	N3A	Fe01	112.0(5)	N2C	C2C	C3C	106.7(5)
C4A	N3A	C5A	117.5(5)	N1C	C3C	C4C	115.5(4)
C5A	N3A	Fe01	129.7(4)	C2C	C3C	N1C	107.6(6)
C14A	N4A	Fe02	126.4(4)	C2C	C3C	C4C	136.7(6)
C17A	N4A	Fe02	112.7(5)	N3C	C4C	C3C	116.2(5)
C17A	N4A	C14A	120.9(5)	C6C	C5C	N3C	120.8(5)
C19A	N5A	C20A	110.6(7)	C6C	C5C	C10C	120.2(6)
C18A	N6A	Fe02	112.4(5)	C10C	C5C	N3C	118.9(5)
C20A	N6A	Fe02	140.0(5)	C5C	C6C	C7C	121.2(5)
C20A	N6A	C18A	107.5(6)	C6C	C7C	C8C	118.6(6)
C1B	N1B	Fe01	139.0(4)	C7C	C8C	S1C	121.6(5)
C1B	N1B	C4B	105.8(5)	C7C	C8C	C9C	119.5(6)

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C4B	N1B	Fe01	114.4(3)	C9C	C8C	S1C	118.7(4)
C1B	N2B	C3B	110.0(5)	C10C	C9C	C8C	121.4(6)
C5B	N3B	Fe01	115.7(4)	C9C	C10C	C5C	119.1(6)
C5B	N3B	C6B	118.2(5)	C12C	C11C	S1C	123.2(5)
C6B	N3B	Fe01	126.1(4)	C16C	C11C	S1C	116.5(4)
C15B	N4B	Fe02	132.1(3)	C16C	C11C	C12C	119.9(5)
C18B	N4B	Fe02	108.6(4)	C11C	C12C	C13C	119.3(6)
C18B	N4B	C15B	117.4(5)	C14C	C13C	C12C	121.1(5)
C21B	N5B	C20B	107.6(6)	C13C	C14C	N4C	119.7(5)
C19B	N6B	Fe02	109.4(4)	C13C	C14C	C15C	119.7(5)
C21B	N6B	Fe02	139.3(5)	C15C	C14C	N4C	120.6(5)
C21B	N6B	C19B	105.8(5)	C14C	C15C	C16C	119.2(6)
C1C	N1C	Fe01	139.2(5)	C11C	C16C	C15C	120.8(5)
C1C	N1C	C3C	107.3(5)	N4C	C17C	C18C	118.3(5)
C3C	N1C	Fe01	112.4(4)	N6C	C18C	C17C	118.0(5)
C2C	N2C	C1C	108.2(5)	N6C	C18C	C19C	109.3(5)
C4C	N3C	Fe01	114.6(4)	C19C	C18C	C17C	132.5(6)
C4C	N3C	C5C	114.9(5)	N5C	C19C	C18C	105.6(6)
C5C	N3C	Fe01	130.3(3)	N6C	C20C	N5C	110.9(5)
C14C	N4C	Fe02	129.3(3)	F2	B9	F1	95.6(11)
C17C	N4C	Fe02	111.9(4)	F4	B9	F1	105.2(10)
C17C	N4C	C14C	117.5(5)	F4	B9	F2	116.7(9)
C20C	N5C	C19C	107.7(5)	F4	B9	F0AA	135.6(11)
C18C	N6C	Fe02	111.6(3)	F0AA	B9	F1	91.4(13)
C20C	N6C	Fe02	138.1(4)	F0AA	B9	F2	101.8(9)
C20C	N6C	C18C	106.4(5)	F007	B02Q	F006	108.2(5)
N1A	C1A	N2A	111.1(7)	F007	B02Q	F009	109.4(5)
N2A	C2A	C3A	107.0(7)	F008	B02Q	F006	109.7(5)
C2A	C3A	N1A	108.2(7)	F008	B02Q	F007	111.8(6)
C2A	C3A	C4A	137.2(7)	F008	B02Q	F009	108.5(6)
C4A	C3A	N1A	114.7(6)	F009	B02Q	F006	109.3(6)
N3A	C4A	C3A	118.1(6)	F10	B9A	F8	108.4(11)
C6A	C5A	N3A	118.9(6)	F10	B9A	F15	106.6(10)
C10A	C5A	N3A	122.1(5)	F11	B9A	F8	108.6(12)
C10A	C5A	C6A	119.0(7)	F11	B9A	F10	119.9(13)
C7A	C6A	C5A	119.2(7)	F11	B9A	F15	114.8(12)
C6A	C7A	C8A	122.1(6)	F15	B9A	F8	95.7(9)
C7A	C8A	S1A	116.5(5)	F1AA	B2	F2AA	121.5(14)
C9A	C8A	S1A	126.6(6)	F1AA	B2	F0BA	101.6(14)
C9A	C8A	C7A	116.9(7)	F2AA	B2	F0BA	99.7(9)
C10A	C9A	C8A	120.9(7)	F5AA	B2A	F2AA	81.9(12)

C5A C10A C9A 121.8(6)	F7AA B2A F2AA 116.8(12)
C12A C11A S1A 123.4(6)	F7AA B2A F5AA 90.0(14)
C12A C11A C16A 117.8(7)	F1AB B2A F2AA 118.2(15)
C16A C11A S1A 118.7(5)	F1AB B2A F5AA 88.9(16)
C13A C12A C11A 120.3(6)	F1AB B2A F7AA 124.2(17)
C12A C13A C14A 120.7(6)	F3AA B0AA F8AA 110.1(10)
N4A C14A C13A 123.4(6)	F4AA B0AA F3AA 101.2(9)
N4A C14A C15A 118.6(6)	F4AA B0AA F8AA 103.1(10)
C13A C14A C15A 118.0(7)	F6AA B0AA F3AA 118.5(11)
C16A C15A C14A 121.3(7)	F6AA B0AA F4AA 113.1(12)
C15A C16A C11A 121.8(6)	F6AA B0AA F8AA 109.7(9)
N4A C17A C18A 118.5(6)	N01B C02V C030 179.3(13)
N6A C18A C17A 118.0(6)	N02E C02M C02X 175.6(12)

Table 13 Hydrogen Bonds for **2**.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
N2A	H2A	F2[1]	0.86	2.01	2.816(15)	156.0
N2A	H2A	F10[1]	0.86	1.87	2.726(16)	173.2
N5A	H5A	F3AA[2]	0.86	2.09	2.883(12)	152.8
N5A	H5A	F4AA[2]	0.86	2.28	2.889(11)	128.1
N2B	H2B	F0AA[3]	0.86	1.98	2.824(14)	166.7
N2B	H2B	F15[3]	0.86	2.05	2.878(11)	161.8
N2C	H2C	N01B[4]	0.86	2.04	2.887(8)	168.4

[1] 1+X,+Y,1+Z; [2] -1+X,+Y,-1+Z; [3] +X,+Y,1+Z; [4] 1-X,1-Y,1-Z

Table 14 Hydrogen Atom Coordinates ($Å×10^4$) and Isotropic Displacement Parameters ($Å^2×10^3$) for **2**.

Atom	x	y	z	U(eq)
H2A	11188	8272	9112	89
H5A	-850	6631	1143	98
H2B	4607	8046	9227	68
H5B	6119	7298	786	76
H2C	7687	4964	8678	67
H5C	2364	9899	1220	64
H1A	8637	8336	8856	71
H2AA	12123	7614	8316	83
H4A	10497	6931	7164	67

H6A	9313	5644	6710	70
H7A	8991	4989	5794	73
H9A	6728	6772	5168	67
H10A	6981	7399	6089	59
H12A	4792	5617	4632	78
H13A	3128	6142	3950	66
H15A	6097	6343	2937	66
H16A	7746	5891	3620	69
H17A	1889	5777	2877	79
H19A	-506	5756	1862	86
H20A	1011	7700	1284	80
H1B	5787	7011	8805	64
H3B	4396	9197	8662	65
H5BA	5442	9343	7525	55
H7B	4966	8944	6393	58
H8B	5714	9500	5617	59
H10B	9809	9280	6334	57
H11B	9068	8741	7122	51
H13B	7148	8287	4930	56
H14B	6184	7660	4040	57
H16B	6917	9700	3321	56
H17B	7817	10347	4233	57
H18B	7727	8465	2743	56
H20B	7856	8065	1548	68
H21B	4059	6856	1151	76
H1C	8830	6240	8561	69
H2CA	5568	4632	7940	62
H4C	4276	5643	7017	54
H6C	4567	6206	5980	54
H7C	2730	6554	5274	59
H9C	1653	8185	6464	56
H10C	3427	7803	7163	53
H12C	3222	8176	5009	58
H13C	3907	8440	4143	54
H15C	-50	7768	3281	70
H16C	-694	7426	4141	72
H17C	1034	9182	3003	53
H19C	840	9989	1949	62
H20C	4175	8987	1456	63
H03A	535	5789	-607	253
H03B	2173	5953	-604	253

H03C	1269	6658	-421	253
H02A	11797	10117	9215	184
H02B	12822	10899	9394	184
H02C	11160	10961	9266	184

Table 14 Atomic Occupancy for **2**.

Atom	*Occupancy*	Atom	*Occupancy*	Atom	*Occupancy*
F1	0.5	F2	0.5	F4	0.5
F0AA	0.5	B9	0.5	F8	0.5
F10	0.5	F11	0.5	F15	0.5
B9A	0.5	F1AA	0.5	F5AA	0.5
F7AA	0.5	F1AB	0.5	F0BA	0.5
B2	0.5	B2A	0.5		

Experimental

Single crystals of $C_{64}H_{54}B_4F_{15.5}Fe_2N_{20}S_3$ **2** were crystallised using a vapour diffusion of diethyl ether into acetonitrile. A suitable crystal was selected and [mounted with parafin oil] on a Bruker APEX-II CCD diffractometer. The crystal was kept at 100 K during data collection. Using Olex2 [1], the structure was solved with the ShelXT [2] structure solution program using Intrinsic Phasing and refined with the ShelXL [3] refinement package using Least Squares minimisation.

1. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.
2. Sheldrick, G.M. (2015). Acta Cryst. A71, 3-8.
3. Sheldrick, G.M. (2015). Acta Cryst. C71, 3-8.

Crystal structure determination of 2

Crystal Data for $C_{64}H_{54}B_4F_{15.5}Fe_2N_{20}S_3$ (M =1648.89 g/mol): triclinic, space group P-1 (no. 2), a = 9.5210(19) Å, b = 16.723(3) Å, c = 23.621(5) Å, α = 95.29(3)°, β = 100.29(3)°, γ = 92.93(3)°, V = 3675.8(13) Å^3, Z = 2, T = 293(2) K, μ(MoKα) = 0.575 mm^{-1}, $Dcalc$ = 1.490 g/cm^3, 45853 reflections measured (1.762° ≤ 2Θ ≤ 52.742°), 13521 unique (R_{int} = 0.0971, R$_{sigma}$ = 0.0898) which were used in all calculations. The final R_1 was 0.1086 (I > 2σ(I)) and wR_2 was 0.3308 (all data).

Refinement model description

Number of restraints - 193, number of constraints - unknown.

Details:

```
1. Fixed Uiso
 At 1.2 times of:
  All C(H) groups, All N(H) groups
```

```
  At 1.5 times of:
   All C(H,H,H) groups
2. Shared sites
{B9, B9A}
3. Restrained distances
 F007-F006
 2.25 with sigma of 0.02
 F7AA-F2AA
 2.25 with sigma of 0.02
 F7AA-F1AA
 2.25 with sigma of 0.02
 F7AA-B2 = F2AA-B2 = F1AA-B2
 1.4 with sigma of 0.02
 B2-F1AA = B2-F2AA = B2-F7AA = B2-F0BA = B2-F1AB = B2-F5AA
 1.4 with sigma of 0.02
 B2A-F2AA = B2A-F7AA = B2A-F1AB = B2A-F5AA
 1.39 with sigma of 0.02
 B2-F1AA = B2-F2AA = B2-F0BA
 1.39 with sigma of 0.02
 F2AA-F1AA
 2.25 with sigma of 0.04
 F2AA-F7AA
 2.25 with sigma of 0.04
 F1AA-F0BA
 2.25 with sigma of 0.04
 F7AA-F0BA
 2.25 with sigma of 0.04
 F2AA-F0BA
 2.25 with sigma of 0.04
 F8-F10 ≈ F8-F11 ≈ F8-F15 ≈ F10-F11 ≈ F10-F15 ≈ F11-F15
 with sigma of 0.04
 B9-F8 ≈ B9-F10 ≈ B9-F11 ≈ B9-F15
 with sigma of 0.02
 F15-B9 ≈ F0AA-B9 ≈ F11-B9 ≈ F1-B9 ≈ F2-B9 ≈ F10-B9 ≈
F4-B9 ≈ F8-B9
 with sigma of 0.02
 B9-F4 ≈ B9-F10 ≈ B9-F11 ≈ B9-F15 ≈ B9-F8 ≈ B9-F0AA ≈
B9-F2 ≈ B9-F1
 with sigma of 0.02
4. Uiso/Uaniso restraints and constraints
Uanis(C030) ≈ Ueq: with sigma of 0.1 and sigma for terminal atoms of 0.2
Uanis(B9) = Uanis(B9A)
5. Rigid body (RIGU) restrains
 N02E, C02M, C02X
 with sigma for 1-2 distances of 0.004 and sigma for 1-3 distances of 0.004
 C030
 with sigma for 1-2 distances of 0.004 and sigma for 1-3 distances of 0.004
 C030, C02V
 with sigma for 1-2 distances of 0.004 and sigma for 1-3 distances of 0.004
 F3AA, F4AA, F6AA, F8AA
 with sigma for 1-2 distances of 0.004 and sigma for 1-3 distances of 0.004
 F1, F2, F4, F0AA, B9, F8, F10, F11, F15
 with sigma for 1-2 distances of 0.004 and sigma for 1-3 distances of 0.004
 F1AA, F2AA, F7AA, F0BA, B2
 with sigma for 1-2 distances of 0.004 and sigma for 1-3 distances of 0.004
 F1AA, F2AA, F5AA, F7AA, F1AB, F0BA, B2, B2A
 with sigma for 1-2 distances of 0.004 and sigma for 1-3 distances of 0.004
 F1, F2, F4, F0AA, B9, F8, F10, F11, F15, B9A
 with sigma for 1-2 distances of 0.004 and sigma for 1-3 distances of 0.004
 F8, F10, F11, F15, B9A
 with sigma for 1-2 distances of 0.004 and sigma for 1-3 distances of 0.004
```

```
 F1, F2, F4, F0AA, B9
 with sigma for 1-2 distances of 0.004 and sigma for 1-3 distances of 0.004
6. Others
 Fixed Sof: F1(0.5) F2(0.5) F4(0.5) F0AA(0.5) B9(0.5) F8(0.5) F10(0.5)
 F11(0.5) F15(0.5) B9A(0.5) F1AA(0.5) F5AA(0.5) F7AA(0.5) F1AB(0.5)
F0BA(0.5)
 B2(0.5) B2A(0.5)
7.a Aromatic/amide H refined with riding coordinates:
 N2A(H2A), N5A(H5A), N2B(H2B), N5B(H5B), N2C(H2C), N5C(H5C), C1A(H1A),
 C2A(H2AA), 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), C3B(H3B), C5B(H5BA), C7B(H7B), C8B(H8B), C10B(H10B), C11B(H11B),
 C13B(H13B), C14B(H14B), C16B(H16B), C17B(H17B), C18B(H18B), C20B(H20B),
 C21B(H21B), C1C(H1C), C2C(H2CA), C4C(H4C), C6C(H6C), C7C(H7C), C9C(H9C),
 C10C(H10C), C12C(H12C), C13C(H13C), C15C(H15C), C16C(H16C), C17C(H17C),
 C19C(H19C), C20C(H20C)
7.b Idealised Me refined as rotating group:
 C030(H03A,H03B,H03C), C02X(H02A,H02B,H02C)
```

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

Identification code	FL204_a
Empirical formula	$C_{64}H_{54}B_4F_{16}Fe_2N_{20}O_3$
Formula weight	1610.21
Temperature/K	100
Crystal system	triclinic
Space group	P-1
a/Å	13.837(3)
b/Å	13.855(3)
c/Å	20.684(4)
α/°	77.43(3)
β/°	77.58(3)
γ/°	86.73(3)
Volume/Å^3	3779.5(15)
Z	2
ρ_{calc}g/cm^3	1.415
μ/mm^{-1}	0.481
F(000)	1636.0
Crystal size/mm^3	0.02 × 0.01 × 0.01
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	2.062 to 53.998
Index ranges	-17 ≤ h ≤ 17, -17 ≤ k ≤ 17, -26 ≤ l ≤ 26
Reflections collected	57096
Independent reflections	14860 [R_{int} = 0.0446, R_{sigma} = 0.0360]
Data/restraints/parameters	14860/33/1095
Goodness-of-fit on F^2	1.071
Final R indexes [I>=2σ (I)]	R_1 = 0.0691, wR_2 = 0.1966
Final R indexes [all data]	R_1 = 0.0873, wR_2 = 0.2111
Largest diff. peak/hole / e Å^{-3}	1.21/-0.79

Table 15 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **3**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Fe01	6322.1(4)	2436.6(4)	10428.6(3)	27.99(14)
Fe02	7602.8(4)	3648.4(4)	4569.3(3)	28.78(15)

O1A	6035(2)	186(2)	7692.9(15)	40.5(7)
O1B	4740(2)	5195(2)	7461.2(18)	50.3(9)
O1C	9843(2)	3910(3)	7292.3(15)	48.2(9)
N1A	4952(3)	2648(2)	11084.0(19)	37.7(8)
N2A	3577(3)	2906(3)	11784(2)	54.6(11)
N3A	5238(2)	1887(2)	9967.4(17)	30.2(7)
N4A	8062(2)	2354(2)	5213.4(17)	29.5(7)
N5A	10417(3)	3177(3)	3384(2)	50.4(10)
N6A	8971(2)	3370(3)	4016.8(18)	35.5(7)
N1B	7258(3)	3258(3)	10810(2)	43.2(9)
N2B	8331(3)	4005(4)	11160(3)	58.6(12)
N3B	6396(2)	3908(2)	9744(2)	36.1(8)
N4B	6147(3)	3574(2)	5188(2)	39.3(8)
N5B	6594(12)	1694(8)	3598(6)	50(2)
N6B	6703(9)	2730(11)	4184(8)	29(3)
N1C	6640(3)	1050(2)	11005.6(18)	33.7(7)
N2C	6849(3)	-396(3)	11642(2)	48(1)
N3C	7662(2)	1940(2)	9777.6(16)	28.6(6)
N4C	8119(2)	4701(2)	5024.1(17)	30.7(7)
N5C	7169(3)	6317(4)	3176(2)	63.5(13)
N6C	7398(3)	4972(3)	3913.6(19)	42.1(9)
C1A	4574(4)	2911(3)	11659(3)	48.8(11)
C2A	3287(3)	2629(3)	11267(3)	46.0(11)
C3A	4147(3)	2457(3)	10830(2)	36.3(9)
C4A	4332(3)	2058(3)	10232(2)	33.7(8)
C5A	5417(3)	1461(3)	9383(2)	31.3(8)
C6A	6022(3)	619(3)	9375(2)	30.1(8)
C7A	6231(3)	202(3)	8810(2)	33.2(8)
C8A	5837(3)	627(3)	8255(2)	35.6(9)
C9A	5229(4)	1451(3)	8255(2)	42.8(10)
C10A	5015(3)	1871(3)	8825(2)	38.0(9)
C11A	6519(3)	770(3)	7085(2)	35.2(9)
C12A	6385(3)	547(3)	6501(2)	33.5(8)
C13A	6892(3)	1080(3)	5881(2)	34.1(8)
C14A	7536(3)	1814(3)	5856(2)	30.5(8)
C15A	7638(5)	2054(4)	6448(3)	60.8(16)
C16A	7129(5)	1534(4)	7061(2)	63.7(17)
C17A	8916(3)	2019(3)	4974(2)	34.4(8)
C18A	9440(3)	2549(3)	4338(2)	35.0(9)
C19A	10354(3)	2439(4)	3941(3)	46.5(11)
C20A	9581(3)	3721(4)	3447(2)	45.3(11)

C1B	7803(4)	3184(4)	11276(3)	53.6(12)
C2B	8164(4)	4643(4)	10611(3)	52.0(12)
C3B	7488(3)	4178(3)	10403(3)	41.1(10)
C4B	7027(3)	4491(3)	9838(3)	40.9(10)
C5B	5981(3)	4235(3)	9155(2)	35.5(9)
C6B	4959(3)	4320(3)	9223(2)	34.9(9)
C7B	4546(3)	4628(3)	8658(2)	35.8(9)
C8B	5160(3)	4841(3)	8025(3)	43.3(11)
C9B	6179(3)	4759(4)	7951(3)	57.8(15)
C10B	6587(3)	4452(4)	8521(3)	52.7(13)
C11B	5119(3)	4785(3)	6901(3)	43.1(11)
C12B	5169(4)	3771(3)	6962(3)	58.5(15)
C13B	5498(4)	3369(3)	6402(3)	52.8(13)
C14B	5782(3)	3992(3)	5768(2)	37.9(10)
C15B	5719(3)	5009(3)	5713(2)	37.4(9)
C16B	5384(3)	5414(3)	6276(2)	36.8(9)
C17B	5574(4)	2956(3)	5064(3)	49.9(13)
C18B	5791(11)	2501(11)	4602(9)	25(3)
C19B	5774(12)	1833(10)	4092(9)	40(4)
C20B	7366(11)	2243(7)	3637(5)	40(2)
C1C	6308(3)	444(3)	11586(2)	41(1)
C2C	7558(4)	-339(3)	11075(2)	46.0(11)
C3C	7439(3)	572(3)	10680(2)	35.2(9)
C4C	7964(3)	1075(3)	10030(2)	33.5(8)
C8C	9269(3)	3419(4)	7901(2)	41.3(10)
C4AA	8760(9)	2522(9)	7922(6)	47(3)
C3AA	8211(8)	2064(9)	8551(6)	39(2)
C5E	8211(3)	2440(3)	9135(2)	31.0(8)
C9C	8413(8)	2922(9)	7931(5)	42(3)
C10C	7881(8)	2416(9)	8552(5)	40(2)
C11C	9394(3)	4097(4)	6734(2)	39.7(10)
C12C	8562(3)	4686(4)	6740(2)	49.1(12)
C13C	8133(3)	4903(4)	6172(2)	45.7(11)
C14C	8551(3)	4515(3)	5612(2)	32.2(8)
C15C	9401(3)	3937(3)	5605(2)	31.4(8)
C16C	9820(3)	3722(3)	6179(2)	35.2(9)
C17C	7966(3)	5612(3)	4753(2)	34.2(8)
C18C	7577(3)	5793(3)	4147(2)	38.1(9)
C19C	7426(3)	6634(4)	3693(3)	50.4(12)
C20C	7153(4)	5320(5)	3322(3)	57.0(14)
C1	8497(8)	-770(8)	7338(6)	57(3)

C1AA	9021(9)	-326(8)	6732(9)	74(3)
N3	9470(9)	0(9)	6180(8)	96(4)
N031	8045(7)	-1067(6)	9395(5)	54(2)
C02S	9601(5)	-2038(6)	9629(4)	33.1(17)
C02W	8752(6)	-1464(5)	9482(4)	32.1(17)
N02Y	11143(6)	2034(6)	5548(5)	50(2)
C02X	12022(7)	442(6)	5341(5)	41(2)
C02Z	11498(6)	1300(6)	5483(5)	38(2)
F003	3058(2)	2667(2)	8124.0(14)	51.4(7)
F00D	2701(3)	2997(2)	9183.9(16)	62.2(8)
F00G	1491(2)	2503(2)	8752(2)	72.2(10)
F00H	2127(3)	4024(2)	8324.2(17)	69.1(9)
B02R	2333(4)	3054(4)	8609(3)	45.9(12)
F004	10153.1(19)	5980(2)	8119.2(14)	46.7(6)
F006	8555.2(19)	6091(2)	7992.7(14)	55.3(7)
F00A	8901(2)	5863(3)	9041.5(15)	62.6(8)
F00L	9207(3)	7316(2)	8308(2)	74.4(10)
B02N	9198(4)	6309(4)	8374(3)	41.3(11)
F008	3875(3)	1480.8(19)	7005.0(14)	56.4(8)
F009	4012(2)	-99(2)	6847.1(15)	50.9(7)
F00F	4151(3)	1193(3)	5943.4(16)	70.4(9)
F00T	2680(2)	861(3)	6642(2)	86.8(12)
B02P	3685(4)	864(4)	6600(3)	46.0(12)
F005	7360(2)	6883(2)	6899.1(15)	53.5(7)
F00C	6993(3)	7213(3)	5850.5(16)	68.6(9)
F00M	7448(2)	8447(2)	6269(2)	76.7(11)
F00P	5955(2)	7741(3)	6720(2)	83.0(12)
B02Q	6933(4)	7573(5)	6424(3)	50.0(13)
C2	10751(13)	1486(13)	7679(9)	39(4)
N4	10054(14)	531(14)	8835(10)	61(5)
C5	10357(15)	959(15)	8298(11)	49(4)
N0AA	11693(10)	-1148(10)	7611(7)	37(3)
C0AA	11206(12)	-385(11)	7676(9)	34(3)
C2AA	10714(12)	595(12)	7715(9)	38(3)
N1AA	7088(8)	2740(12)	4121(9)	31(3)
C5AA	6826(9)	2182(9)	3709(5)	37(2)
N2AA	6021(10)	1627(9)	3830(7)	36(2)
C6AA	5350(9)	1816(8)	4382(7)	36(3)
C7AA	6112(11)	2502(11)	4407(10)	27(3)
C7D	9443(3)	3621(3)	8479(2)	32.3(6)
C6D	8901(3)	3133(3)	9100(2)	32.3(6)

Table 16 Anisotropic Displacement Parameters ($\text{Å}^2 \times 10^3$) for **3**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\dots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe01	26.7(3)	27.5(3)	28.7(3)	-7.8(2)	-0.9(2)	-3.17(19)
Fe02	30.1(3)	28.2(3)	27.4(3)	-4.5(2)	-5.0(2)	-4.5(2)
O1A	62.2(19)	29.0(14)	28.5(17)	-10.5(11)	3.0(14)	-15.7(13)
O1B	38.7(16)	45.9(17)	51(2)	6.5(14)	3.1(15)	17.3(13)
O1C	32.8(15)	83(2)	25.4(16)	4.2(15)	-8.1(13)	-25.4(15)
N1A	45.6(19)	31.0(17)	37(2)	-12.8(14)	-2.2(17)	-6.9(14)
N2A	56(2)	60(3)	45(3)	-31(2)	17(2)	-12.6(19)
N3A	37.5(17)	22.4(14)	29.4(19)	-7.0(12)	-2.3(14)	-2.6(12)
N4A	28.0(15)	31.9(16)	28.1(18)	-6.3(12)	-5.5(13)	0.8(12)
N5A	34.4(19)	76(3)	33(2)	-6.7(19)	6.8(17)	-6.0(18)
N6A	29.2(16)	39.8(18)	33(2)	-0.1(14)	-5.0(15)	-2.4(13)
N1B	28.3(16)	70(3)	35(2)	-22.3(18)	-3.6(16)	2.9(16)
N2B	43(2)	77(3)	63(3)	-40(3)	1(2)	-13(2)
N3B	26.6(15)	33.6(17)	49(2)	-19.4(15)	2.6(15)	-2.4(12)
N4B	45.1(19)	25.5(15)	51(2)	1.5(14)	-27.1(18)	-5.3(13)
N5B	77(8)	44(5)	35(6)	-18(4)	-18(6)	-1(6)
N6B	28(8)	25(4)	33(7)	-5(4)	-9(8)	5(6)
N1C	39.8(17)	29.4(16)	29(2)	-7.2(13)	-0.2(15)	-2.8(13)
N2C	70(3)	33.9(18)	34(2)	3.0(15)	-7(2)	-6.3(17)
N3C	32.7(15)	28.4(15)	24.6(18)	-8.9(12)	-2.5(14)	0.3(12)
N4C	22.4(14)	40.8(17)	28.2(18)	-5.4(13)	-5.3(13)	-1.6(12)
N5C	54(3)	81(3)	52(3)	13(2)	-29(2)	-13(2)
N6C	31.5(17)	59(2)	38(2)	-7.7(17)	-10.8(16)	-7.5(15)
C1A	65(3)	41(2)	42(3)	-20(2)	-2(2)	-10(2)
C2A	42(2)	42(2)	52(3)	-21(2)	7(2)	-5.9(18)
C3A	36(2)	28.0(18)	43(3)	-12.6(16)	1.9(18)	-4.4(15)
C4A	34.0(19)	27.5(18)	39(2)	-10.7(15)	-3.0(18)	-3.5(14)
C5A	37.3(19)	23.5(17)	31(2)	-8.1(14)	-0.3(17)	-4.8(14)
C6A	31.6(18)	27.5(17)	28(2)	-4.8(14)	-0.4(16)	-4.7(14)
C7A	37(2)	25.4(17)	34(2)	-7.9(15)	2.3(17)	-5.0(14)
C8A	52(2)	25.1(17)	28(2)	-7.1(15)	0.3(19)	-11.7(16)
C9A	67(3)	26.6(19)	38(3)	-6.8(16)	-19(2)	-1.6(18)
C10A	54(2)	24.8(18)	36(2)	-7.9(15)	-10(2)	0.7(16)
C11A	45(2)	29.6(18)	30(2)	-9.4(15)	-0.7(18)	-7.1(16)
C12A	39(2)	28.2(18)	34(2)	-10.0(15)	-5.0(18)	-3.2(15)
C13A	40(2)	31.8(19)	33(2)	-11.5(16)	-7.8(18)	-2.3(15)

C14A	30.4(18)	32.1(18)	29(2)	-7.4(15)	-4.8(16)	0.7(14)
C15A	88(4)	64(3)	32(3)	-7(2)	-8(3)	-46(3)
C16A	97(4)	70(3)	26(3)	-11(2)	-4(3)	-50(3)
C17A	37(2)	36(2)	30(2)	-7.8(16)	-6.4(17)	6.1(16)
C18A	33.4(19)	40(2)	30(2)	-6.3(16)	-5.3(17)	5.5(16)
C19A	37(2)	60(3)	41(3)	-13(2)	-3(2)	10(2)
C20A	37(2)	56(3)	35(3)	6(2)	-3.1(19)	-9.7(19)
C1B	47(3)	71(3)	39(3)	-16(2)	4(2)	4(2)
C2B	44(2)	60(3)	57(3)	-26(2)	-5(2)	-6(2)
C3B	31.9(19)	42(2)	52(3)	-27(2)	2(2)	-5.0(16)
C4B	28.1(18)	32(2)	65(3)	-22.8(19)	-1(2)	-1.2(15)
C5B	29.5(18)	27.6(18)	47(3)	-10.0(16)	-1.1(18)	0.8(14)
C6B	27.9(18)	32.2(19)	41(3)	-15.3(16)	7.3(17)	0.1(14)
C7B	25.2(17)	28.7(18)	49(3)	-11.3(17)	3.6(17)	2.2(14)
C8B	35(2)	33(2)	51(3)	2.6(18)	2(2)	7.7(16)
C9B	30(2)	68(3)	53(3)	16(2)	8(2)	12(2)
C10B	25.1(19)	58(3)	59(3)	3(2)	8(2)	1.5(18)
C11B	27.4(19)	39(2)	53(3)	0.5(19)	0.4(19)	9.5(16)
C12B	55(3)	35(2)	62(4)	13(2)	13(3)	9(2)
C13B	47(3)	27(2)	68(4)	9(2)	3(2)	2.6(18)
C14B	30.3(19)	29.2(19)	53(3)	1.6(17)	-15.4(19)	-1.7(15)
C15B	31.8(19)	28.7(18)	49(3)	5.5(17)	-15.9(19)	-1.5(15)
C16B	26.7(18)	30.3(19)	49(3)	3.6(17)	-11.0(18)	0.4(14)
C17B	43(2)	28(2)	87(4)	-5(2)	-38(3)	-0.3(17)
C18B	18(7)	23(4)	30(10)	-3(5)	0(5)	-2(5)
C19B	44(9)	46(6)	41(14)	-27(7)	-16(9)	12(6)
C20B	52(6)	39(5)	35(6)	-14(4)	-13(5)	-3(5)
C1C	50(2)	36(2)	33(3)	-7.4(17)	4(2)	-8.4(18)
C2C	60(3)	35(2)	40(3)	-5.0(18)	-10(2)	9.8(19)
C3C	39(2)	31.1(19)	34(2)	-6.1(16)	-5.9(18)	4.2(15)
C4C	33.7(19)	36(2)	30(2)	-9.3(16)	-2.1(17)	5.5(15)
C8C	35(2)	61(3)	26(2)	-3.0(18)	-5.4(18)	-16.4(18)
C4AA	45(6)	64(6)	32(5)	-12(4)	-1(4)	-12(4)
C3AA	36(5)	47(6)	34(4)	-15(4)	-2(4)	-7(4)
C5E	32.2(18)	32.7(18)	27(2)	-8.1(14)	-2.8(16)	-1.7(14)
C9C	39(5)	67(7)	24(4)	-13(4)	-4(4)	-26(5)
C10C	29(5)	59(7)	29(4)	-9(4)	1(3)	-17(4)
C11C	28.1(18)	64(3)	25(2)	0.8(18)	-7.3(17)	-16.5(18)
C12C	25.7(19)	92(4)	33(3)	-23(2)	-2.0(19)	-8(2)
C13C	25.7(19)	73(3)	40(3)	-18(2)	-7.2(19)	2.5(19)
C14C	25.1(17)	43(2)	27(2)	-2.5(16)	-6.7(16)	-7.3(15)

C15C	28.4(17)	36.6(19)	27(2)	-2.5(15)	-4.3(16)	-6.7(14)
C16C	29.1(18)	42(2)	31(2)	3.6(16)	-10.0(17)	-7.4(15)
C17C	29.4(18)	40(2)	33(2)	-5.4(16)	-7.5(17)	-4.7(15)
C18C	31.8(19)	42(2)	39(3)	-1.1(17)	-12.2(18)	-4.9(16)
C19C	39(2)	55(3)	54(3)	7(2)	-20(2)	-7(2)
C20C	39(2)	96(4)	41(3)	-14(3)	-15(2)	-11(2)
C1	60(6)	46(5)	67(7)	-4(5)	-30(6)	16(5)
C1AA	56(6)	44(6)	120(10)	4(6)	-35(6)	-1(5)
N3	71(7)	67(7)	133(10)	19(6)	-27(6)	-1(5)
N031	64(5)	49(4)	71(6)	-39(4)	-45(5)	29(4)
C02S	27(3)	42(4)	36(5)	-13(3)	-19(3)	14(3)
C02W	43(4)	26(3)	42(5)	-21(3)	-28(4)	7(3)
N02Y	59(5)	42(4)	65(6)	-32(4)	-33(4)	21(4)
C02X	56(5)	33(4)	38(5)	-20(3)	-10(4)	16(4)
C02Z	30(4)	50(5)	49(6)	-35(4)	-25(4)	19(3)
F003	64.1(17)	48.2(15)	43.3(17)	-10.2(12)	-17.3(14)	12.3(13)
F00D	77(2)	67.9(19)	45.9(19)	-17.6(14)	-19.4(16)	6.9(16)
F00G	49.9(17)	48.3(17)	118(3)	-8.8(17)	-26.4(18)	5.0(13)
F00H	113(3)	31.9(14)	69(2)	-16.5(13)	-32(2)	15.5(15)
B02R	59(3)	33(2)	50(3)	-14(2)	-16(3)	7(2)
F004	39.0(13)	59.0(16)	45.6(17)	-15.0(12)	-12.6(12)	2.0(11)
F006	34.6(13)	93(2)	37.7(16)	-13.0(14)	-6.8(12)	-6.7(13)
F00A	73(2)	80(2)	31.3(16)	-6.9(14)	-5.6(15)	-10.3(16)
F00L	88(2)	44.2(17)	89(3)	-14.5(16)	-15(2)	4.0(16)
B02N	45(3)	44(3)	35(3)	-9(2)	-7(2)	-1(2)
F008	94(2)	36.2(13)	39.2(16)	-8.1(11)	-13.5(16)	-6.4(14)
F009	60.4(16)	44.8(14)	50.2(18)	-16.8(12)	-10.6(14)	-0.7(12)
F00F	90(2)	81(2)	36.3(18)	-9.5(15)	-9.1(17)	-2.7(18)
F00T	46.9(18)	103(3)	113(3)	-31(2)	-14(2)	-3.5(18)
B02P	48(3)	53(3)	39(3)	-13(2)	-7(2)	-3(2)
F005	45.4(14)	73.4(19)	43.4(17)	-20.0(14)	-8.3(13)	11.3(13)
F00C	81(2)	84(2)	49(2)	-23.3(16)	-19.8(18)	-3.5(18)
F00M	59.0(19)	55.1(18)	121(3)	-36.8(19)	-14(2)	13.1(15)
F00P	33.3(15)	144(4)	78(3)	-36(2)	-19.1(16)	19.9(18)
B02Q	34(2)	70(4)	53(4)	-26(3)	-14(3)	7(2)
N1AA	30(7)	34(4)	28(5)	-6(3)	-4(7)	3(6)
C5AA	35(5)	41(6)	30(6)	1(4)	-4(5)	-2(5)
N2AA	38(6)	39(6)	29(8)	-7(4)	0(5)	-8(5)
C6AA	37(6)	41(5)	32(8)	-13(4)	-6(5)	1(4)
C7AA	19(9)	33(5)	29(11)	-12(6)	0(6)	2(6)
C7D	28.2(12)	38.0(14)	31.6(16)	-8.6(11)	-6.3(12)	-2.1(10)

C6D	28.2(12)	38.0(14)	31.6(16)	-8.6(11)	-6.3(12)	-2.1(10)

Table 17 Bond Lengths for **3**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Fe01	N1A	2.127(4)	C17A	C18A	1.424(6)
Fe01	N3A	2.191(3)	C18A	C19A	1.371(6)
Fe01	N1B	2.144(4)	C2B	C3B	1.356(6)
Fe01	N3B	2.209(4)	C3B	C4B	1.424(7)
Fe01	N1C	2.107(3)	C5B	C6B	1.391(5)
Fe01	N3C	2.215(3)	C5B	C10B	1.377(7)
Fe02	N4A	2.142(3)	C6B	C7B	1.386(6)
Fe02	N6A	2.053(4)	C7B	C8B	1.380(6)
Fe02	N4B	2.137(4)	C8B	C9B	1.387(6)
Fe02	N6B	2.202(15)	C9B	C10B	1.390(8)
Fe02	N4C	2.128(3)	C11B	C12B	1.382(6)
Fe02	N6C	2.075(4)	C11B	C16B	1.382(6)
Fe02	N1AA	1.961(17)	C12B	C13B	1.373(8)
O1A	C8A	1.398(5)	C13B	C14B	1.393(6)
O1A	C11A	1.394(5)	C14B	C15B	1.388(6)
O1B	C8B	1.396(6)	C15B	C16B	1.380(7)
O1B	C11B	1.390(6)	C17B	C18B	1.232(18)
O1C	C8C	1.392(5)	C17B	C7AA	1.637(18)
O1C	C11C	1.395(5)	C18B	C6AA	1.36(2)
N1A	C1A	1.313(6)	C19B	C7AA	1.39(2)
N1A	C3A	1.390(5)	C20B	N1AA	1.31(2)
N2A	C1A	1.348(7)	C2C	C3C	1.368(6)
N2A	C2A	1.352(7)	C3C	C4C	1.432(6)
N3A	C4A	1.287(5)	C8C	C4AA	1.450(13)
N3A	C5A	1.428(5)	C8C	C9C	1.386(10)
N4A	C14A	1.439(5)	C8C	C7D	1.358(6)
N4A	C17A	1.282(5)	C4AA	C3AA	1.393(15)
N5A	C19A	1.354(6)	C3AA	C5E	1.415(12)
N5A	C20A	1.343(6)	C5E	C10C	1.385(12)
N6A	C18A	1.389(5)	C5E	C6D	1.373(5)
N6A	C20A	1.307(6)	C9C	C10C	1.394(14)
N1B	C1B	1.329(6)	C11C	C12C	1.372(7)
N1B	C3B	1.378(6)	C11C	C16C	1.367(7)
N2B	C1B	1.337(7)	C12C	C13C	1.395(6)
N2B	C2B	1.334(7)	C13C	C14C	1.383(6)

N3B	C4B	1.293(5)		C14C	C15C	1.385(6)
N3B	C5B	1.433(6)		C15C	C16C	1.398(5)
N4B	C14B	1.427(6)		C17C	C18C	1.435(6)
N4B	C17B	1.300(5)		C18C	C19C	1.366(6)
N5B	C19B	1.390(19)		C1	C1AA	1.341(18)
N5B	C20B	1.372(15)		C1AA	N3	1.182(19)
N6B	C18B	1.378(13)		N031	C02W	1.124(10)
N6B	C5AA	1.35(2)		C02S	C02W	1.430(9)
N1C	C1C	1.314(5)		N02Y	C02Z	1.126(10)
N1C	C3C	1.381(5)		C02X	C02Z	1.410(10)
N2C	C1C	1.343(6)		F003	B02R	1.427(6)
N2C	C2C	1.348(6)		F00D	B02R	1.377(6)
N3C	C4C	1.284(5)		F00G	B02R	1.372(7)
N3C	C5E	1.432(5)		F00H	B02R	1.385(6)
N4C	C14C	1.435(5)		F004	B02N	1.404(6)
N4C	C17C	1.290(5)		F006	B02N	1.393(6)
N5C	C19C	1.359(7)		F00A	B02N	1.368(6)
N5C	C20C	1.349(8)		F00L	B02N	1.372(6)
N6C	C18C	1.382(6)		F008	B02P	1.390(6)
N6C	C20C	1.321(6)		F009	B02P	1.407(6)
C2A	C3A	1.374(6)		F00F	B02P	1.363(7)
C3A	C4A	1.431(6)		F00T	B02P	1.376(6)
C5A	C6A	1.398(5)		F005	B02Q	1.416(7)
C5A	C10A	1.385(6)		F00C	B02Q	1.370(7)
C6A	C7A	1.384(6)		F00M	B02Q	1.381(7)
C7A	C8A	1.378(6)		F00P	B02Q	1.389(6)
C8A	C9A	1.378(6)		C2	C5	1.35(3)
C9A	C10A	1.395(6)		N4	C5	1.14(3)
C11A	C12A	1.361(6)		N0AA	C0AA	1.24(2)
C11A	C16A	1.377(6)		C0AA	C2AA	1.49(2)
C12A	C13A	1.394(6)		N1AA	C7AA	1.380(13)
C13A	C14A	1.375(5)		C5AA	N2AA	1.338(17)
C14A	C15A	1.374(6)		N2AA	C6AA	1.371(16)
C15A	C16A	1.378(7)		C7D	C6D	1.390(6)

Table 18 Bond Angles for **3**.

Atom	Atom	Atom	Angle/°		Atom	Atom	Atom	Angle/°
N1A	Fe01	N3A	76.95(13)		N5A	C19A	C18A	105.7(4)
N1A	Fe01	N1B	98.98(14)		N6A	C20A	N5A	110.8(4)

N1A	Fe01	N3B	97.54(13)	N1B	C1B	N2B	109.9(5)
N1A	Fe01	N3C	169.74(12)	N2B	C2B	C3B	103.5(5)
N3A	Fe01	N3B	93.40(12)	N1B	C3B	C4B	118.3(4)
N3A	Fe01	N3C	96.79(12)	C2B	C3B	N1B	111.9(5)
N1B	Fe01	N3A	168.52(14)	C2B	C3B	C4B	129.8(5)
N1B	Fe01	N3B	76.36(15)	N3B	C4B	C3B	118.3(4)
N1B	Fe01	N3C	88.66(13)	C6B	C5B	N3B	119.7(4)
N3B	Fe01	N3C	90.87(12)	C10B	C5B	N3B	120.3(4)
N1C	Fe01	N1A	95.28(14)	C10B	C5B	C6B	119.9(4)
N1C	Fe01	N3A	95.78(12)	C7B	C6B	C5B	120.4(4)
N1C	Fe01	N1B	95.29(15)	C8B	C7B	C6B	119.2(4)
N1C	Fe01	N3B	165.64(13)	C7B	C8B	O1B	118.8(4)
N1C	Fe01	N3C	77.10(13)	C7B	C8B	C9B	120.9(5)
N4A	Fe02	N6B	90.2(4)	C9B	C8B	O1B	120.3(4)
N6A	Fe02	N4A	78.41(13)	C8B	C9B	C10B	119.5(5)
N6A	Fe02	N4B	166.71(13)	C5B	C10B	C9B	120.1(4)
N6A	Fe02	N6B	98.9(4)	C12B	C11B	O1B	120.6(4)
N6A	Fe02	N4C	94.98(14)	C16B	C11B	O1B	118.4(4)
N6A	Fe02	N6C	94.23(14)	C16B	C11B	C12B	120.9(5)
N4B	Fe02	N4A	91.49(13)	C13B	C12B	C11B	120.4(5)
N4B	Fe02	N6B	72.2(4)	C12B	C13B	C14B	119.6(4)
N4C	Fe02	N4A	96.81(12)	C13B	C14B	N4B	119.5(4)
N4C	Fe02	N4B	94.79(13)	C15B	C14B	N4B	121.1(4)
N4C	Fe02	N6B	165.5(4)	C15B	C14B	C13B	119.4(5)
N6C	Fe02	N4A	170.64(13)	C16B	C15B	C14B	121.2(4)
N6C	Fe02	N4B	96.62(14)	C15B	C16B	C11B	118.6(4)
N6C	Fe02	N6B	96.8(4)	N4B	C17B	C7AA	111.2(7)
N6C	Fe02	N4C	77.89(14)	C18B	C17B	N4B	125.2(8)
N1AA	Fe02	N4A	86.4(5)	C17B	C18B	N6B	114.4(14)
N1AA	Fe02	N6A	86.2(4)	C17B	C18B	C6AA	136.3(12)
N1AA	Fe02	N4B	84.5(4)	C6AA	C18B	N6B	109.3(13)
N1AA	Fe02	N4C	176.7(5)	N5B	C19B	C7AA	103.0(12)
N1AA	Fe02	N6C	99.0(5)	N1AA	C20B	N5B	110.1(12)
C11A	O1A	C8A	116.2(3)	N1C	C1C	N2C	110.7(4)
C11B	O1B	C8B	115.5(3)	N2C	C2C	C3C	105.7(4)
C8C	O1C	C11C	116.0(3)	N1C	C3C	C4C	118.0(3)
C1A	N1A	Fe01	142.3(3)	C2C	C3C	N1C	109.1(4)
C1A	N1A	C3A	105.6(4)	C2C	C3C	C4C	132.8(4)
C3A	N1A	Fe01	112.1(3)	N3C	C4C	C3C	118.5(4)
C1A	N2A	C2A	108.8(4)	O1C	C8C	C4AA	119.7(6)
C4A	N3A	Fe01	114.2(3)	C9C	C8C	O1C	122.5(5)

C4A	N3A	C5A	117.3(3)	C7D	C8C	O1C	117.1(4)
C5A	N3A	Fe01	128.2(3)	C7D	C8C	C9C	118.8(6)
C14A	N4A	Fe02	128.9(2)	C3AA	C4AA	C8C	116.4(10)
C17A	N4A	Fe02	114.0(3)	C4AA	C3AA	C5E	120.5(10)
C17A	N4A	C14A	117.1(3)	C3AA	C5E	N3C	119.4(6)
C20A	N5A	C19A	108.7(4)	C10C	C5E	N3C	119.4(5)
C18A	N6A	Fe02	112.9(3)	C6D	C5E	N3C	120.4(3)
C20A	N6A	Fe02	140.9(3)	C6D	C5E	C10C	118.2(6)
C20A	N6A	C18A	106.2(4)	C8C	C9C	C10C	120.2(9)
C1B	N1B	Fe01	143.1(4)	C5E	C10C	C9C	118.8(9)
C1B	N1B	C3B	103.8(4)	C12C	C11C	O1C	119.7(4)
C3B	N1B	Fe01	112.7(3)	C16C	C11C	O1C	119.0(4)
C2B	N2B	C1B	110.9(5)	C16C	C11C	C12C	121.3(4)
C4B	N3B	Fe01	113.6(3)	C11C	C12C	C13C	119.7(5)
C4B	N3B	C5B	116.4(4)	C14C	C13C	C12C	119.4(4)
C5B	N3B	Fe01	129.0(2)	C13C	C14C	N4C	121.1(4)
C14B	N4B	Fe02	128.7(2)	C13C	C14C	C15C	120.5(4)
C17B	N4B	Fe02	113.7(4)	C15C	C14C	N4C	118.4(4)
C17B	N4B	C14B	116.9(4)	C14C	C15C	C16C	119.4(4)
C20B	N5B	C19B	109.4(10)	C11C	C16C	C15C	119.6(4)
C18B	N6B	Fe02	113.3(12)	N4C	C17C	C18C	116.9(4)
C5AA	N6B	Fe02	138.4(11)	N6C	C18C	C17C	116.7(4)
C5AA	N6B	C18B	107.2(12)	C19C	C18C	N6C	109.9(4)
C1C	N1C	Fe01	141.0(3)	C19C	C18C	C17C	133.1(4)
C1C	N1C	C3C	105.8(3)	N5C	C19C	C18C	105.2(5)
C3C	N1C	Fe01	113.2(3)	N6C	C20C	N5C	110.3(5)
C1C	N2C	C2C	108.7(4)	N3	C1AA	C1	174.8(16)
C4C	N3C	Fe01	113.1(3)	N031	C02W	C02S	175.0(10)
C4C	N3C	C5E	117.6(3)	N02Y	C02Z	C02X	173.5(12)
C5E	N3C	Fe01	129.4(2)	F00D	B02R	F003	108.9(4)
C14C	N4C	Fe02	127.9(3)	F00D	B02R	F00H	111.2(4)
C17C	N4C	Fe02	114.7(3)	F00G	B02R	F003	108.4(4)
C17C	N4C	C14C	117.3(3)	F00G	B02R	F00D	110.6(5)
C20C	N5C	C19C	109.0(4)	F00G	B02R	F00H	109.4(4)
C18C	N6C	Fe02	113.0(3)	F00H	B02R	F003	108.3(4)
C20C	N6C	Fe02	141.3(4)	F006	B02N	F004	108.8(4)
C20C	N6C	C18C	105.7(4)	F00A	B02N	F004	109.8(4)
N1A	C1A	N2A	110.9(4)	F00A	B02N	F006	110.8(4)
N2A	C2A	C3A	105.5(4)	F00A	B02N	F00L	109.8(4)
N1A	C3A	C4A	118.3(4)	F00L	B02N	F004	109.1(4)
C2A	C3A	N1A	109.2(4)	F00L	B02N	F006	108.4(4)

C2A	C3A	C4A	132.2(4)	F008	B02P	F009	108.8(4)
N3A	C4A	C3A	117.5(4)	F00F	B02P	F008	110.7(4)
C6A	C5A	N3A	118.8(4)	F00F	B02P	F009	110.3(4)
C10A	C5A	N3A	121.5(3)	F00F	B02P	F00T	109.4(5)
C10A	C5A	C6A	119.8(4)	F00T	B02P	F008	108.1(5)
C7A	C6A	C5A	120.3(4)	F00T	B02P	F009	109.4(4)
C8A	C7A	C6A	119.3(4)	F00C	B02Q	F005	109.7(4)
C7A	C8A	O1A	118.7(4)	F00C	B02Q	F00M	110.0(5)
C7A	C8A	C9A	121.4(4)	F00C	B02Q	F00P	111.1(4)
C9A	C8A	O1A	119.9(4)	F00M	B02Q	F005	108.3(4)
C8A	C9A	C10A	119.5(4)	F00M	B02Q	F00P	109.2(5)
C5A	C10A	C9A	119.8(4)	F00P	B02Q	F005	108.5(5)
C12A	C11A	O1A	117.3(3)	N4	C5	C2	177(2)
C12A	C11A	C16A	120.3(4)	N0AA	C0AA	C2AA	173.9(17)
C16A	C11A	O1A	122.4(4)	C20B	N1AA	Fe02	141.3(10)
C11A	C12A	C13A	119.4(4)	C20B	N1AA	C7AA	106.5(14)
C14A	C13A	C12A	120.6(4)	C7AA	N1AA	Fe02	112.2(13)
C13A	C14A	N4A	120.1(3)	N2AA	C5AA	N6B	108.0(11)
C15A	C14A	N4A	120.5(4)	C5AA	N2AA	C6AA	110.5(12)
C15A	C14A	C13A	119.4(4)	C18B	C6AA	N2AA	105.0(10)
C14A	C15A	C16A	120.1(4)	C19B	C7AA	C17B	130.9(14)
C11A	C16A	C15A	120.3(4)	N1AA	C7AA	C17B	118.0(15)
N4A	C17A	C18A	117.4(4)	N1AA	C7AA	C19B	111.0(16)
N6A	C18A	C17A	117.3(3)	C8C	C7D	C6D	119.2(4)
C19A	C18A	N6A	108.7(4)	C5E	C6D	C7D	121.0(4)
C19A	C18A	C17A	134.1(4)				

Table 19 Hydrogen Bonds for **3**.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
N2A	H2A	F005[1]	0.86	2.00	2.823(5)	159.9
N5A	H5A	F006[2]	0.86	2.12	2.885(5)	147.9
N2B	H2B	F004[3]	0.86	1.99	2.826(5)	163.5
N5B	H5B	F009[4]	0.86	2.07	2.805(13)	143.6
N2C	H2C	F008[5]	0.86	2.09	2.870(5)	150.1
N5C	H5C	F003[6]	0.86	1.98	2.825(5)	166.5
N2AA	H2AB	F009[4]	0.86	1.94	2.788(14)	166.7

[1]1-X,1-Y,2-Z; [2]2-X,1-Y,1-Z; [3]2-X,1-Y,2-Z; [4]1-X,-Y,1-Z; [5]1-X,-Y,2-Z; [6]1-X,1-Y,1-Z

Table 20 Hydrogen Atom Coordinates ($\text{Å}\times10^4$) and Isotropic Displacement Parameters ($\text{Å}^2\times10^3$) for **3**.

Atom	x	y	z	U(eq)
H2A	3189	3055	12133	66
H5A	10912	3280	3046	60
H2B	8726	4108	11407	70
H5B	6615	1322	3312	60
H2C	6758	-888	11982	58
H5C	7037	6692	2815	76
H1A	4944	3079	11944	59
H2AA	2642	2568	11219	55
H4A	3816	1927	10041	40
H6A	6284	337	9752	36
H7A	6634	-358	8804	40
H9A	4965	1725	7878	51
H10A	4603	2425	8830	46
H12A	5958	44	6516	40
H13A	6794	937	5481	41
H15A	8050	2568	6435	73
H16A	7197	1700	7461	76
H17A	9184	1453	5208	41
H19A	10830	1958	4035	56
H20A	9454	4273	3128	54
H1B	7815	2641	11630	64
H2BA	8445	5260	10416	62
H4B	7176	5099	9543	49
H6B	4550	4169	9652	42
H7B	3863	4690	8704	43
H9B	6588	4909	7522	69
H10B	7270	4393	8475	63
H12B	4979	3357	7386	70
H13B	5531	2687	6445	63
H15B	5906	5425	5290	45
H16B	5337	6096	6234	44
H17C	4952	2847	5347	60
H17B	4941	2792	5316	60
H19B	5152	1549	4189	49
H20B	7994	2261	3362	48
H1C	5773	577	11914	49
H2CA	8030	-819	10974	55
H4C	8511	782	9796	40

H4AA	8797	2267	7537	57
H3AA	7843	1507	8588	47
H9C	8193	2927	7536	51
H10C	7315	2068	8575	48
H12C	8285	4939	7120	59
H13C	7572	5306	6170	55
H15C	9692	3694	5223	38
H16C	10385	3326	6183	42
H17D	8102	6127	4941	41
H19C	7486	7285	3729	60
H20C	6992	4932	3046	68
H1D	8531	-387	7667	86
H1E	8767	-1419	7472	86
H1F	7820	-823	7309	86
H02A	9547	-2218	10110	50
H02B	10188	-1656	9425	50
H02C	9637	-2626	9450	50
H02D	11655	-133	5599	61
H02E	12657	426	5460	61
H02F	12110	449	4867	61
H2D	11200	1963	7718	59
H2E	10232	1821	7472	59
H2F	11101	1049	7404	59
H2AC	10139	509	8076	57
H2AD	10519	875	7294	57
H2AE	11166	1030	7798	57
H5AA	7375	2187	3358	44
H2AB	5936	1210	3595	43
H6AA	4729	1538	4565	43
H7D	9918	4081	8460	39
H6D	9009	3278	9497	39

Table 21 Atomic Occupancy for **3**.

Atom	*Occupancy*	Atom	*Occupancy*	Atom	*Occupancy*
N5B	0.5	H5B	0.5	N6B	0.5
H17C	0.5	H17B	0.5	C18B	0.5
C19B	0.5	H19B	0.5	C20B	0.5
H20B	0.5	C4AA	0.5	H4AA	0.5
C3AA	0.5	H3AA	0.5	C9C	0.5

H9C	0.5	C10C	0.5	H10C	0.5
C1	0.5	H1D	0.5	H1E	0.5
H1F	0.5	C1AA	0.5	N3	0.5
N031	0.5	C02S	0.5	H02A	0.5
H02B	0.5	H02C	0.5	C02W	0.5
N02Y	0.5	C02X	0.5	H02D	0.5
H02E	0.5	H02F	0.5	C02Z	0.5
C2	0.25	H2D	0.25	H2E	0.25
H2F	0.25	N4	0.25	C5	0.25
N0AA	0.25	C0AA	0.25	C2AA	0.25
H2AC	0.25	H2AD	0.25	H2AE	0.25
N1AA	0.5	C5AA	0.5	H5AA	0.5
N2AA	0.5	H2AB	0.5	C6AA	0.5
H6AA	0.5	C7AA	0.5		

Experimental

Single crystals of $C_{64}H_{54}B_4F_{16}Fe_2N_{20}O_3$ **3** were crystallised by a Diethyl ether diffusion into acetonitrile. A suitable crystal was selected and [room temperature in parafin oil]. The crystal was kept at 100 K during data collection. Using Olex2 [1], the structure was solved with the ShelXT [2] structure solution program using Intrinsic Phasing and refined with the ShelXL [3] refinement package using Least Squares minimisation.

1. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.
2. Sheldrick, G.M. (2015). Acta Cryst. A71, 3-8.
3. Sheldrick, G.M. (2015). Acta Cryst. C71, 3-8.

Crystal structure determination of [FL204_a]

Crystal Data for $C_{64}H_{54}B_4F_{16}Fe_2N_{20}O_3$ (M =1610.21 g/mol): triclinic, space group P-1 (no. 2), a = 13.837(3) Å, b = 13.855(3) Å, c = 20.684(4) Å, α = 77.43(3)°, β = 77.58(3)°, γ = 86.73(3)°, V = 3779.5(15) Å^3, Z = 2, T = ? K, μ(MoKα) = 0.481 mm^{-1}, $Dcalc$ = 1.415 g/cm^3, 57096 reflections measured (2.062° ≤ 2Θ ≤ 53.998°), 14860 unique (R_{int} = 0.0446, R_{sigma} = 0.0360) which were used in all calculations. The final R_1 was 0.0691 (I > 2σ(I)) and wR_2 was 0.2111 (all data).

Refinement model description

Number of restraints - 33, number of constraints - unknown.

Details:

```
1. Fixed Uiso
 At 1.2 times of:
  All C(H) groups, All C(H,H) groups, All N(H) groups
 At 1.5 times of:
  All C(H,H,H) groups
```

2. Rigid bond restraints
 C5E
 with sigma for 1-2 distances of 0.01 and sigma for 1-3 distances of 0.01
3. Uiso/Uaniso restraints and constraints
Uanis(C7D) = Uanis(C6D)
4. Rigid body (RIGU) restrains
 N3, C1AA
 with sigma for 1-2 distances of 0.004 and sigma for 1-3 distances of 0.004
 N031
 with sigma for 1-2 distances of 0.004 and sigma for 1-3 distances of 0.004
 N02Y
 with sigma for 1-2 distances of 0.004 and sigma for 1-3 distances of 0.004
 C2AA, C0AA, N0AA
 with sigma for 1-2 distances of 0.004 and sigma for 1-3 distances of 0.004
 N4, C2, C5
 with sigma for 1-2 distances of 0.004 and sigma for 1-3 distances of 0.004
 C2, C5, N4
 with sigma for 1-2 distances of 0.004 and sigma for 1-3 distances of 0.004
 N0AA, C0AA, C2AA
 with sigma for 1-2 distances of 0.004 and sigma for 1-3 distances of 0.004
 N0AA
 with sigma for 1-2 distances of 0.004 and sigma for 1-3 distances of 0.004
 C8C, C9C, C4AA, C3AA, C10C, C5E
 with sigma for 1-2 distances of 0.004 and sigma for 1-3 distances of 0.004
 C5E
 with sigma for 1-2 distances of 0.004 and sigma for 1-3 distances of 0.004
5. Others
 Fixed Sof: N5B(0.5) H5B(0.5) N6B(0.5) H17C(0.5) H17B(0.5) C18B(0.5)
C19B(0.5)
 H19B(0.5) C20B(0.5) H20B(0.5) C4AA(0.5) H4AA(0.5) C3AA(0.5) H3AA(0.5)
C9C(0.5)
 H9C(0.5) C10C(0.5) H10C(0.5) C1(0.5) H1D(0.5) H1E(0.5) H1F(0.5) C1AA(0.5)
 N3(0.5) N031(0.5) C02S(0.5) H02A(0.5) H02B(0.5) H02C(0.5) C02W(0.5)
N02Y(0.5)
 C02X(0.5) H02D(0.5) H02E(0.5) H02F(0.5) C02Z(0.5) C2(0.25) H2D(0.25)
H2E(0.25)
 H2F(0.25) N4(0.25) C5(0.25) N0AA(0.25) C0AA(0.25) C2AA(0.25) H2AC(0.25)
 H2AD(0.25) H2AE(0.25) N1AA(0.5) C5AA(0.5) H5AA(0.5) N2AA(0.5) H2AB(0.5)
 C6AA(0.5) H6AA(0.5) C7AA(0.5)
6.a Aromatic/amide H refined with riding coordinates:
 N2A(H2A), N5A(H5A), N2B(H2B), N5B(H5B), N2C(H2C), N5C(H5C), C1A(H1A),
 C2A(H2AA), 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(H2BA), C4B(H4B), C6B(H6B), C7B(H7B), C9B(H9B), C10B(H10B),
 C12B(H12B), C13B(H13B), C15B(H15B), C16B(H16B), C17B(H17C), C17B(H17B),
 C19B(H19B), C20B(H20B), C1C(H1C), C2C(H2CA), C4C(H4C), C4AA(H4AA),
C3AA(H3AA),
 C9C(H9C), C10C(H10C), C12C(H12C), C13C(H13C), C15C(H15C), C16C(H16C),
 C17C(H17D), C19C(H19C), C20C(H20C), C5AA(H5AA), N2AA(H2AB), C6AA(H6AA),
 C7D(H7D), C6D(H6D)
6.b Idealised Me refined as rotating group:
 C1(H1D,H1E,H1F), C02S(H02A,H02B,H02C), C02X(H02D,H02E,H02F),
C2(H2D,H2E,H2F),
 C2AA(H2AC,H2AD,H2AE)
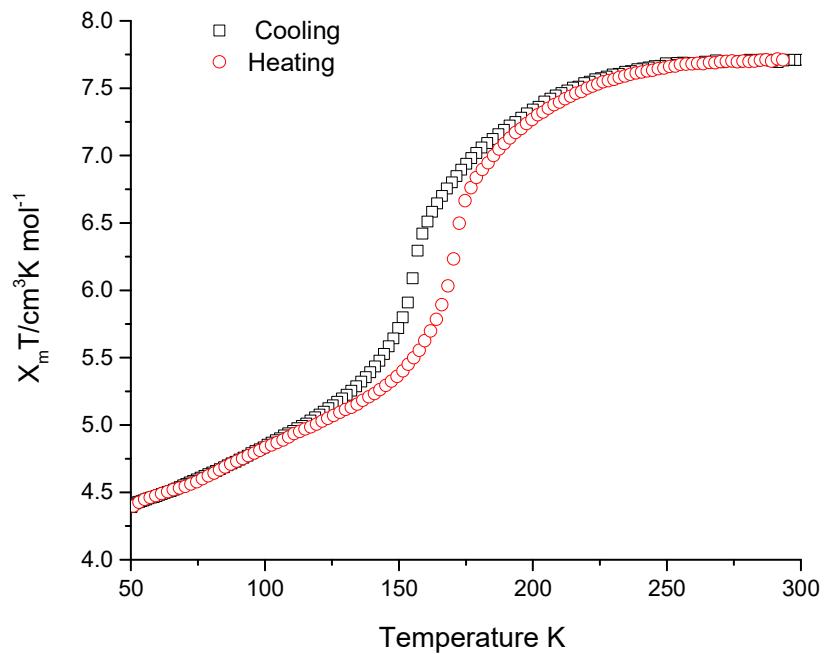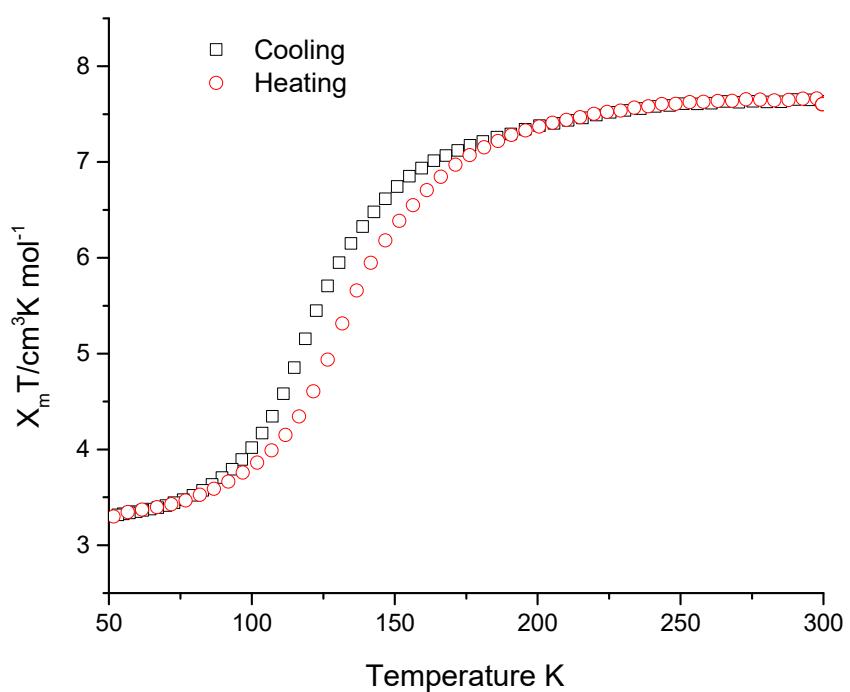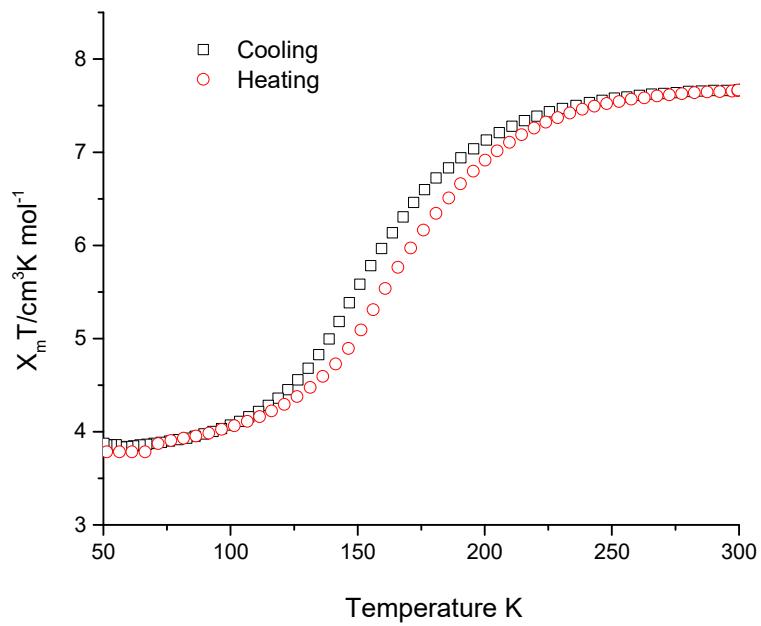
Magnetic susceptibility:

Figure S19. Cooling and heating modes of **1**, cycling from 300-50-300 K, show a thermal hysteresis of 15 K.

Figure S20. Cooling and heating modes of **2**, cycling from 300-50-300 K, showing a Thermal hysteresis of 15 K.

Figure S21. Cooling and heating modes of **3**, cycling from 300-50-300 K, with a thermal hysteresis of 15 K.