Table 1: Crystal data and refinement details for **mf118b**.

empirical formula	$C_{38}H_{54}Fe_2N_{12}S_2$
moiety formula	$C_{22}H_{14}Fe_2N_{10}S_2^{2-}$, $2(C_8H_{20}N^+)$
formula weight	854.75
T [K]	133(2)
crystal size [mm^3]	0.500 × 0.500 × 0.360
crystal system	monoclinic
crystal color	black
space group	$P2_1/c$ (No. 14)
a [Å]	11.2144(4)
b [Å]	14.4686(4)
c [Å]	13.7454(5)
α [°]	90
β [°]	113.658(3)
γ [°]	90
V [Å^3]	2042.84(13)
Z	2
ρ [g·cm^{-3}]	1.390
$F(000)$	900
μ [mm^{-1}]	0.857
T_{min} / T_{max}	0.6373 / 0.7269
θ-range	1.983 - 26.942
hkl-range	$-14 \leq h \leq 14$
	$-18 \leq k \leq 18$
	$-17 \leq l \leq 17$
measured refl.	26072
unique refl. [R_{int}]	4445 [0.0317]
observed refl. ($I > 2\sigma(I)$)	4191
data / restraints / param.	4445 / 0 / 248
goodness-of-fit (F^2)	1.037
$R1$, $wR2$ ($I > 2\sigma(I)$)	0.0227, 0.0599
$R1$, $wR2$ (all data)	0.0247, 0.0608
resid. el. dens. [e·Å^{-3}]	−0.360 / 0.310

Table 2: Selected bond lengths [Å] for **mf118b**.

Atoms	**Bond lengths**
Fe1–N1	2.1142(10)
Fe1–N4	2.1173(10)
Fe1–N3	2.1793(10)
Fe1–S1	2.2138(3)

Fe1–S1′	2.2379(3)
Fe1–Fe1′	2.7913(3)

Symmetry transformation used to generate equivalent atoms: (′) $1-x, 1-y, 1-z$.

Table 3: Selected bond angles [°] for **mf118b**.

Atoms	**Bond angles**
N1–Fe1–N4	141.30(4)
N1–Fe1–N3	73.13(4)
N4–Fe1–N3	72.85(4)
N1–Fe1–S1	102.70(3)
N4–Fe1–S1	106.39(3)
N3–Fe1–S1	111.27(3)
N1–Fe1–S1′	99.78(3)
N4–Fe1–S1′	98.35(3)
N3–Fe1–S1′	146.39(3)
S1–Fe1–S1′	102.343(12)
N1–Fe1–Fe1′	108.09(3)
N4–Fe1–Fe1′	109.89(3)
N3–Fe1–Fe1′	162.82(3)
S1–Fe1–Fe1′	51.557(9)
S1′–Fe1–Fe1′	50.786(9)
Fe1–S1–Fe1′	77.657(11)
C3–N1–Fe1	117.83(8)
C1–N1–Fe1	137.94(9)
C8–N3–Fe1	119.44(8)
C4–N3–Fe1	119.24(8)
C9–N4–Fe1	118.01(8)
C10–N4–Fe1	138.39(9)

Symmetry transformation used to generate equivalent atoms: (′) $1-x, 1-y, 1-z$.

Table 4: Selected bond lengths [Å] for **mf118b**.

Atoms	**Bond lengths**	**Atoms**	**Bond lengths**
Fe1–N1	2.1142(10)	Fe1–S1	2.2138(3)
Fe1–N4	2.1173(10)	Fe1–S1′	2.2379(3)
Fe1–N3	2.1793(10)	Fe1–Fe1′	2.7913(3)

Symmetry transformation used to generate equivalent atoms: (′) $1-x, 1-y, 1-z$.

Table 5: Selected bond angles [°] for **mf118b**.

Atoms	**Bond angles**	**Atoms**	**Bond angles**
N1–Fe1–N4	141.30(4)	N4–Fe1–Fe1′	109.89(3)
N1–Fe1–N3	73.13(4)	N3–Fe1–Fe1′	162.82(3)
N4–Fe1–N3	72.85(4)	S1–Fe1–Fe1′	51.557(9)
N1–Fe1–S1	102.70(3)	S1′–Fe1–Fe1′	50.786(9)
N4–Fe1–S1	106.39(3)	Fe1–S1–Fe1′	77.657(11)
N3–Fe1–S1	111.27(3)	C3–N1–Fe1	117.83(8)
N1–Fe1–S1′	99.78(3)	C1–N1–Fe1	137.94(9)
N4–Fe1–S1′	98.35(3)	C8–N3–Fe1	119.44(8)
N3–Fe1–S1′	146.39(3)	C4–N3–Fe1	119.24(8)
S1–Fe1–S1′	102.343(12)	C9–N4–Fe1	118.01(8)
N1–Fe1–Fe1′	108.09(3)	C10–N4–Fe1	138.39(9)

Symmetry transformation used to generate equivalent atoms: (′) $1-x, 1-y, 1-z$.

Table 6: Selected bond lengths [Å] for **mf118b** (sorted).

Atoms	**Bond lengths**
Fe1–N1	2.1142(10)
Fe1–N4	2.1173(10)
Fe1–N3	2.1793(10)
Fe1–S1	2.2138(3)
Fe1–S1′	2.2379(3)
Fe1–Fe1′	2.7913(3)

Symmetry transformation used to generate equivalent atoms: (′) $1-x, 1-y, 1-z$.

Table 7: Selected bond angles [°] for **mf118b** (sorted).

Atoms	**Bond angles**
S1′–Fe1–Fe1′	50.786(9)
S1–Fe1–Fe1′	51.557(9)
N4–Fe1–N3	72.85(4)
N1–Fe1–N3	73.13(4)
Fe1–S1–Fe1′	77.657(11)
N4–Fe1–S1′	98.35(3)
N1–Fe1–S1′	99.78(3)
S1–Fe1–S1′	102.343(12)
N1–Fe1–S1	102.70(3)
N4–Fe1–S1	106.39(3)
N1–Fe1–Fe1′	108.09(3)

N4–Fe1–Fe1′	109.89(3)
N3–Fe1–S1	111.27(3)
C3–N1–Fe1	117.83(8)
C9–N4–Fe1	118.01(8)
C4–N3–Fe1	119.24(8)
C8–N3–Fe1	119.44(8)
C1–N1–Fe1	137.94(9)
C10–N4–Fe1	138.39(9)
N1–Fe1–N4	141.30(4)
N3–Fe1–S1′	146.39(3)
N3–Fe1–Fe1′	162.82(3)

Symmetry transformation used to generate equivalent atoms: (′) $1-x, 1-y, 1-z$.

Table 8: Selected bond lengths [Å] for **mf118b** (sorted).

Atoms	**Bond lengths**	**Atoms**	**Bond lengths**
Fe1–N1	2.1142(10)	Fe1–S1	2.2138(3)
Fe1–N4	2.1173(10)	Fe1–S1′	2.2379(3)
Fe1–N3	2.1793(10)	Fe1–Fe1′	2.7913(3)

Symmetry transformation used to generate equivalent atoms: (′) $1-x, 1-y, 1-z$.

Table 9: Selected bond angles [°] for **mf118b** (sorted).

Atoms	**Bond angles**	**Atoms**	**Bond angles**
S1′–Fe1–Fe1′	50.786(9)	N4–Fe1–Fe1′	109.89(3)
S1–Fe1–Fe1′	51.557(9)	N3–Fe1–S1	111.27(3)
N4–Fe1–N3	72.85(4)	C3–N1–Fe1	117.83(8)
N1–Fe1–N3	73.13(4)	C9–N4–Fe1	118.01(8)
Fe1–S1–Fe1′	77.657(11)	C4–N3–Fe1	119.24(8)
N4–Fe1–S1′	98.35(3)	C8–N3–Fe1	119.44(8)
N1–Fe1–S1′	99.78(3)	C1–N1–Fe1	137.94(9)
S1–Fe1–S1′	102.343(12)	C10–N4–Fe1	138.39(9)
N1–Fe1–S1	102.70(3)	N1–Fe1–N4	141.30(4)
N4–Fe1–S1	106.39(3)	N3–Fe1–S1′	146.39(3)
N1–Fe1–Fe1′	108.09(3)	N3–Fe1–Fe1′	162.82(3)

Symmetry transformation used to generate equivalent atoms: (′) $1-x, 1-y, 1-z$.

Figure 1: Selected bond lengths [Å] and angles [°] for **mf118b**: Fe1–N1 2.1142(10), Fe1–N4 2.1173(10), Fe1–N3 2.1793(10), Fe1–S1 2.2138(3), Fe1–S1′ 2.2379(3), Fe1–Fe1′ 2.7913(3); N1–Fe1–N4 141.30(4), N1–Fe1–N3 73.13(4), N4–Fe1–N3 72.85(4), N1–Fe1–S1 102.70(3), N4–Fe1–S1 106.39(3), N3–Fe1–S1 111.27(3), N1–Fe1–S1′ 99.78(3), N4–Fe1–S1′ 98.35(3), N3–Fe1–S1′ 146.39(3), S1–Fe1–S1′ 102.343(12), N1–Fe1–Fe1′ 108.09(3), N4–Fe1–Fe1′ 109.89(3), N3–Fe1–Fe1′ 162.82(3), S1–Fe1–Fe1′ 51.557(9), S1′–Fe1–Fe1′ 50.786(9), Fe1–S1–Fe1′ 77.657(11), C3–N1–Fe1 117.83(8), C1–N1–Fe1 137.94(9), C8–N3–Fe1 119.44(8), C4–N3–Fe1 119.24(8), C9–N4–Fe1 118.01(8), C10–N4–Fe1 138.39(9). Symmetry transformation used to generate equivalent atoms: (′) $1-x, 1-y, 1-z$.

Figure 2: Selected bond lengths [Å] and angles [°] for **mf118b** (sorted): Fe1–N1 2.1142(10), Fe1–N4 2.1173(10), Fe1–N3 2.1793(10), Fe1–S1 2.2138(3), Fe1–S1′ 2.2379(3), Fe1–Fe1′ 2.7913(3); S1′–Fe1–Fe1′ 50.786(9), S1–Fe1–Fe1′ 51.557(9), N4–Fe1–N3 72.85(4), N1–Fe1–N3 73.13(4), Fe1–S1–Fe1′ 77.657(11), N4–Fe1–S1′ 98.35(3), N1–Fe1–S1′ 99.78(3), S1–Fe1–S1′ 102.343(12), N1–Fe1–S1 102.70(3), N4–Fe1–S1 106.39(3), N1–Fe1–Fe1′ 108.09(3), N4–Fe1–Fe1′ 109.89(3), N3–Fe1–S1 111.27(3), C3–N1–Fe1 117.83(8), C9–N4–Fe1 118.01(8), C4–N3–Fe1 119.24(8), C8–N3–Fe1 119.44(8), C1–N1–Fe1 137.94(9), C10–N4–Fe1 138.39(9), N1–Fe1–N4 141.30(4), N3–Fe1–S1′ 146.39(3), N3–Fe1–Fe1′ 162.82(3). Symmetry transformation used to generate equivalent atoms: (′) $1-x, 1-y, 1-z$.