

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

compound	mf118b	mf118b	mf118b
empirical formula	C ₃₈ H ₅₄ Fe ₂ N ₁₂ S ₂	C ₃₈ H ₅₄ Fe ₂ N ₁₂ S ₂	C ₃₈ H ₅₄ Fe ₂ N ₁₂ S ₂
moiety formula	C ₂₂ H ₁₄ Fe ₂ N ₁₀ S ₂ ²⁻ , 2(C ₈ H ₂₀ N ⁺)	C ₂₂ H ₁₄ Fe ₂ N ₁₀ S ₂ ²⁻ , 2(C ₈ H ₂₀ N ⁺)	C ₂₂ H ₁₄ Fe ₂ N ₁₀ S ₂ ²⁻ , 2(C ₈ H ₂₀ N ⁺)
formula weight	854.75	854.75	854.75
<i>T</i> /K	133(2)	133(2)	133(2)
crystal size /mm ³	0.500 × 0.500 × 0.360	0.500 × 0.500 × 0.360	0.500 × 0.500 × 0.360
crystal system	monoclinic	monoclinic	monoclinic
space group	<i>P</i> 2 ₁ / <i>c</i> (No. 14)	<i>P</i> 2 ₁ / <i>c</i> (No. 14)	<i>P</i> 2 ₁ / <i>c</i> (No. 14)
<i>a</i> /Å	11.2144(4)	11.2144(4)	11.2144(4)
<i>b</i> /Å	14.4686(4)	14.4686(4)	14.4686(4)
<i>c</i> /Å	13.7454(5)	13.7454(5)	13.7454(5)
α /°	90	90	90
β /°	113.658(3)	113.658(3)	113.658(3)
γ /°	90	90	90
<i>V</i> /Å ³	2042.84(13)	2042.84(13)	2042.84(13)
<i>Z</i>	2	2	2
ρ /g·cm ⁻³	1.390	1.390	1.390
<i>F</i> (000)	900	900	900
μ /mm ⁻¹	0.857	0.857	0.857
<i>T</i> _{min} / <i>T</i> _{max}	0.6373 / 0.7269	0.6373 / 0.7269	0.6373 / 0.7269
θ -range /°	1.983 - 26.942	1.983 - 26.942	1.983 - 26.942
<i>hkl</i> -range	-14 ≤ <i>h</i> ≤ 14 -18 ≤ <i>k</i> ≤ 18 -17 ≤ <i>l</i> ≤ 18	-14 ≤ <i>h</i> ≤ 14 -18 ≤ <i>k</i> ≤ 18 -17 ≤ <i>l</i> ≤ 17	-14 ≤ <i>h</i> ≤ 14 -18 ≤ <i>k</i> ≤ 18 -17 ≤ <i>l</i> ≤ 17
measured refl.	26072	26072	26072
unique refl. [<i>R</i> _{int}]	4445 [0.0317]	4445 [0.0317]	4445 [0.0317]
obs. refl. (<i>I</i> > 2σ(<i>I</i>))	4191	4191	4191
data / restr. / param.	4445 / 0 / 248	4445 / 0 / 248	4445 / 0 / 248
goodness-of-fit (<i>F</i> ²)	1.037	1.037	1.037
<i>R</i> 1, <i>wR</i> 2 (<i>I</i> > 2σ(<i>I</i>))	0.0227 / 0.0599	0.0227 / 0.0599	0.0227 / 0.0599
<i>R</i> 1, <i>wR</i> 2 (all data)	0.0247 / 0.0608	0.0247 / 0.0608	0.0247 / 0.0608
res. el. dens. /e·Å ⁻³	-0.360 / 0.310	-0.360 / 0.310	-0.360 / 0.310