

Annex

Table 3.

The crystallographic data and the details of X-ray analysis of compound **2**.

Empirical formula	2(C ₆₀ H ₄₀ N ₁₆ O ₁₂ S ₄), 3(CH ₂ Cl ₂)	
Formula weight	2865.42	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 11.6227(2) Å	α = 95.7220(10)°
	b = 15.2675(3) Å	β = 104.3480(10)°
	c = 19.0555(4) Å	γ = 100.4700(10)°
Volume	3183.98(11) Å ³	
Z	1	
d _{calc}	1.494 Mg/m ³	
Absorption coefficient	0.352 mm ⁻¹	
F(000)	1470	
Crystal size	0.07×0.04×0.04 mm ³	
Theta range for data collection	1.88 to 28.53°	
Index ranges	-12≤h≤15, -20≤k≤20, -25≤l≤25	
Reflections collected	46325	
Independent reflections	15511 [R(int) = 0.0308]	
Completeness to theta = 29.55°	95.2 %	
Max. and min. transmission	0.9861 and 0.9758	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	15511 / 2 / 883	
Goodness-of-fit on F ²	1.043	
Final R indices [I>2σ(I)]	R1 = 0.0574, wR2 = 0.1565	
R indices (all data)	R1 = 0.0965, wR2 = 0.1818	
Largest diff. peak and hole	1.108 and -1.163 e.Å ⁻³	

Table 4.

The crystallographic data and the details of X-ray analysis of complex **2**₂-(AgNO₃)₆.

Empirical formula	C ₁₂₂ H ₈₈ Ag ₆ N ₃₆ O ₃₆ S ₈ , 2(NO ₃), 3(CH ₂ Cl ₂), 2(CH ₃ OH), 2(H ₂ O)'	
Formula weight	4016.90	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 14.1046(3) Å	α = 84.3470(10)°
	b = 16.7385(4) Å	β = 69.7820(10)°
	c = 18.6546(5) Å	γ = 81.3740(10)°
Volume	4080.88(17) Å ³	
Z	1	
d _{calc}	1.635 Mg/m ³	
Absorption coefficient	0.996 mm ⁻¹	
F(000)	2014	
Crystal size	0.09×0.08×0.07 mm ³	

Theta range for data collection	1.60 to 30.15°
Index ranges	-19<=h<=19, -23<=k<=21, -26<=l<=26
Reflections collected	79844
Independent reflections	21867 [R(int) = 0.0472]
Completeness to theta = 29.55°	99.6 %
Max. and min. transmission	0.9335 and 0.9157
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	21867 / 3 / 1086
Goodness-of-fit on F ²	1.010
Final R indices [I>2sigma(I)]	R1 = 0.0864, wR2 = 0.2651
R indices (all data)	R1 = 0.1306, wR2 = 0.3010
Largest diff. peak and hole	1.755 and -1.464 e.Å ⁻³