

Table S1: Details of data collection and structure refinement for the crystal analysis of the Cu(II)-[H(56)NH₂Cl]H₁ complex.

Compound	Cu(II)-[H(56)NH ₂ Cl] (CuLH ₁)
Formula	Cu C ₉ H ₁₂ N ₃ OCl, 2(H ₂ O)
Molecular weight (g mol ⁻¹)	313.25
Temperature (K)	173(2)
Crystal system	Monoclinic
Space group	<i>P2₁/c</i>
a (Å)	7.3116(2)
b (Å)	22.4070(9)
c (Å)	7.3570(2)
α (°)	90
β (°)	90.080(2)
γ (°)	90
Volume of unit cell (Å ³)	1205.30(7)
Z	4
No. of reflections collected	5280
No. unique reflections	2860
Calculated density (g cm ⁻³)	1.726
Absorption coefficient (mm ⁻¹)	2.034
F(000)	644
Crystal Size (mm)	0.05 x 0.07 x 0.10
Radiation	Mo Kα (λ= 0.71073 Å)
theta range for data collection (°)	3.3 - 27.9
Reflections measured	2860
R, R _w , goodness-of-fit	0.0267, 0.0668, 1.07
Min and max residual density (e Å ⁻³)	-0.65, 0.43