

X-ray crystallographic data of H₃L₁ (data up to 50°)

Parameters	H ₃ L ₁ 50 deg
Molecular formula	C ₆₃ H ₈₉ N ₃ O ₁₀
Formula weight	1048.37
Temperature (K)	298(2)
Crystal system	monoclinic
Space group	P2 ₁
Crystal colour	Colourless
a (Å)	10.9618(8)
b (Å)	21.0542(14)
c (Å)	14.0676(9)
α (°)	90
β (°)	111.390(2)
γ (°)	90
Volume (Å ³)	3023.1(4)
Z	2
Density (g/cm ³)	1.152
μ mm ⁻¹	0.077
F(000)	1136
Crystal size (mm ³)	0.34 × 0.18 × 0.05
2θ range for data collection	3.87 to 50
Reflections collected	53139
Independent reflections	10608
R _{int}	0.0870
R _{sigma}	0.0665
Data/restraints/parameters	10608/2/720
Goodness of fit on F ²	1.056
R1(F ₀), wR2(F ₀) (I ≥ 2 σ(I))	0.0512 0.1119
R1(F ₀ ²), wR2(F ₀ ²) (all data)	0.0926 0.1356
Largest diffraction peak/hole / e Å ⁻³	0.20/-0.23
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