

Electronic Supplementary Information

**Template-directed synthesis of a luminescent Tb-MOF material for highly selective
Fe³⁺ and Al³⁺ ions detection and VOC vapor sensing**

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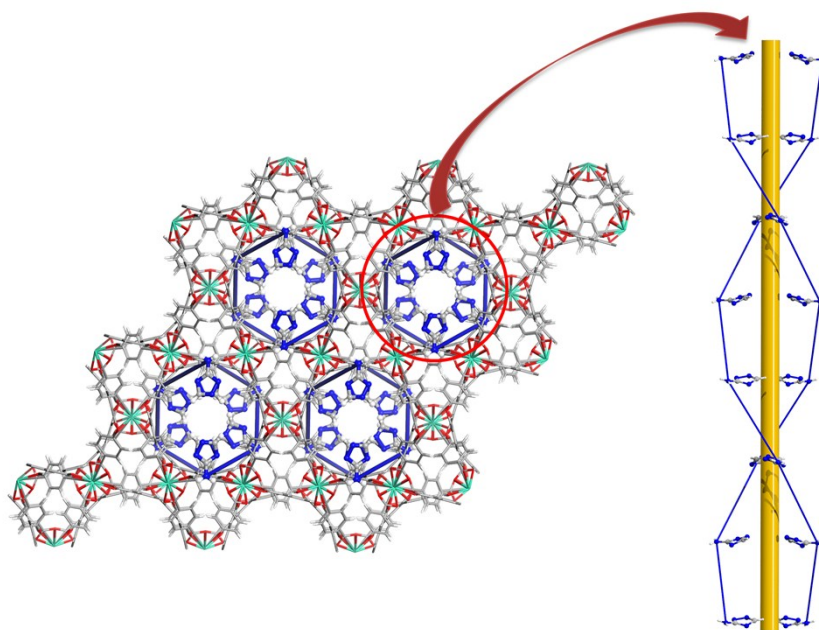


Fig. S1 View of the double-stranded helical chains formed by the Hatz ligands.

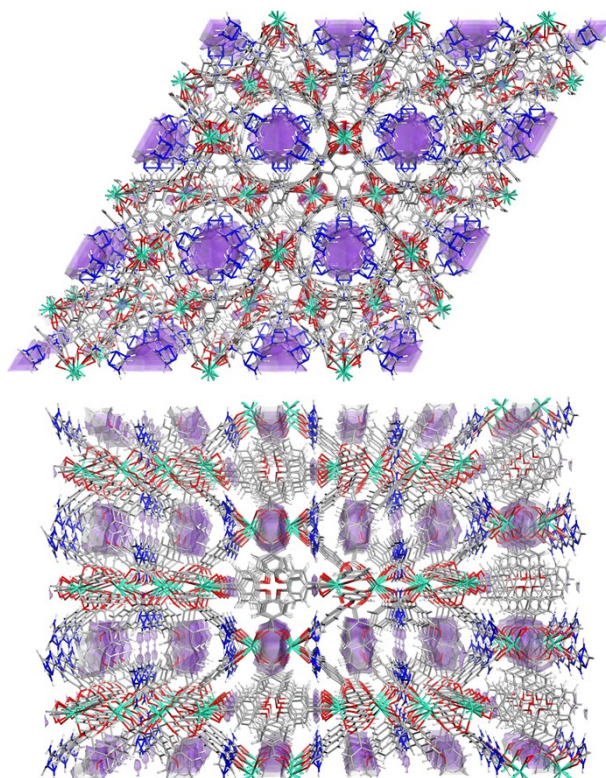


Fig. S2 View of the finite spaces partitioned by the Hatz ligands.

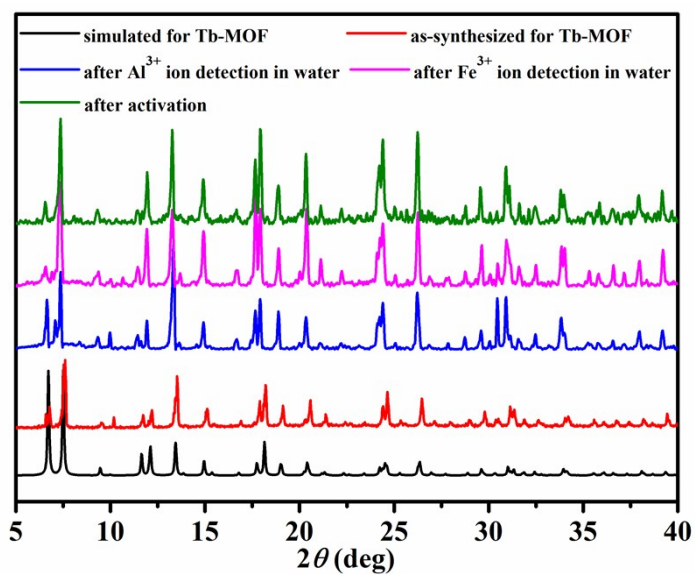


Fig. S3 PXR D patterns for the Tb-MOF and its derivatives.

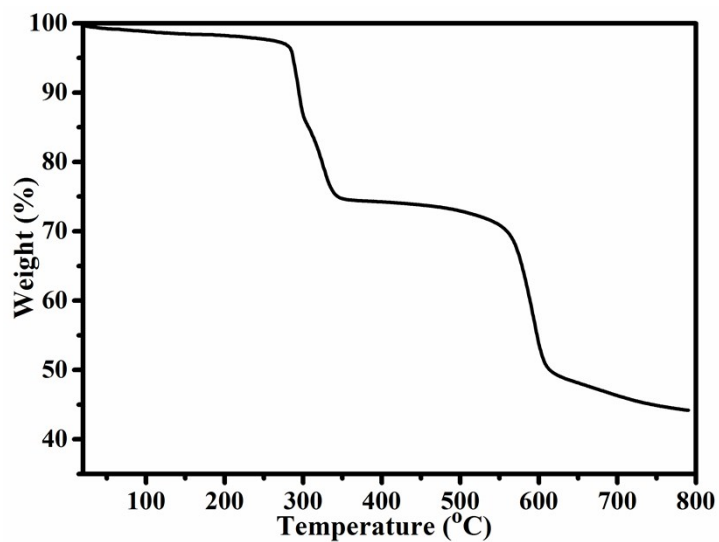


Fig. S4 TGA curve for the Tb-MOF.

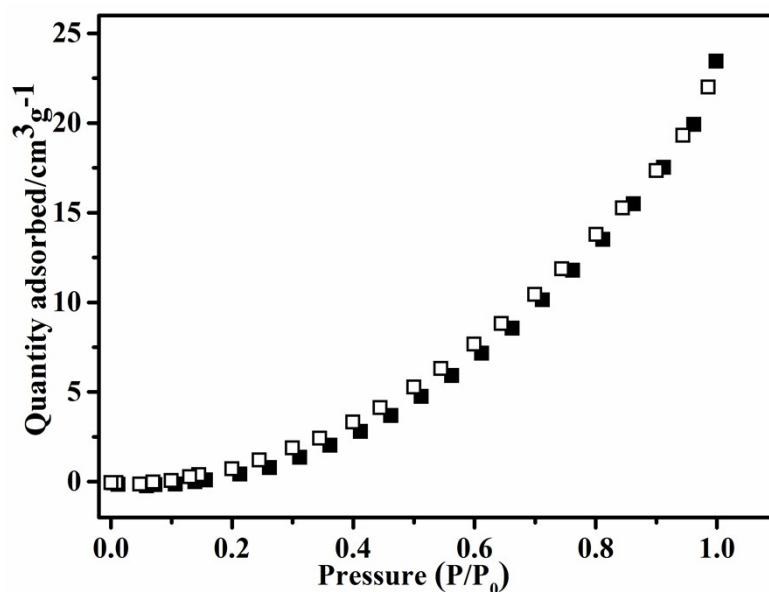


Fig. S5 N₂ sorption isotherm for the activated Tb-MOF at 77 K.

Calculation of sorption heat for CO₂ and C₂H₂ uptake using Virial fitting

$$\ln P = \ln N + 1/T \sum_{i=0}^m a_i N^i + \sum_{i=0}^n b_i N^i \quad Q_{\text{st}} = -R \sum_{i=0}^m a_i N^i$$

The above virial expression was used to fit the combined isotherm data for **1a** at 273 and 298 K, where P is the pressure, N is the adsorbed amount, T is the temperature, a_i and b_i are virial coefficients, and m and n are the number of coefficients used to describe the isotherms. Q_{st} is the coverage-dependent enthalpy of sorption and R is the universal gas constant.

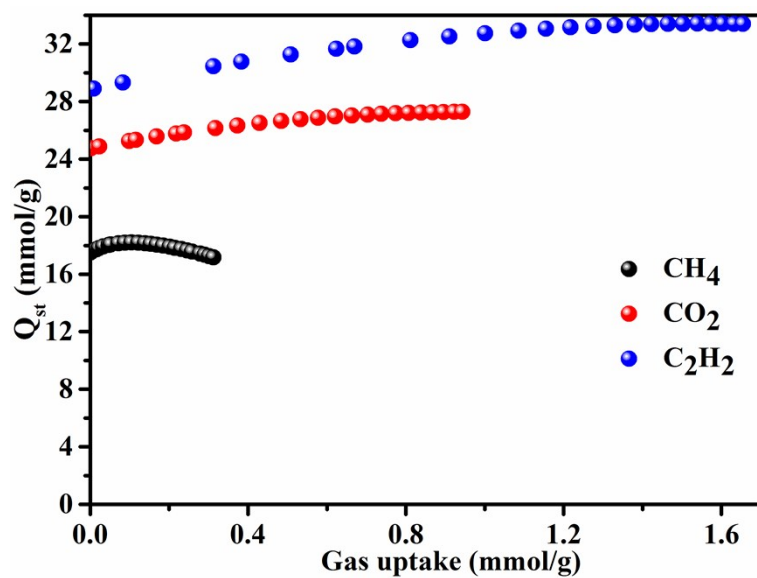


Fig. S6 Gas adsorption heats for the activated Tb-MOF.

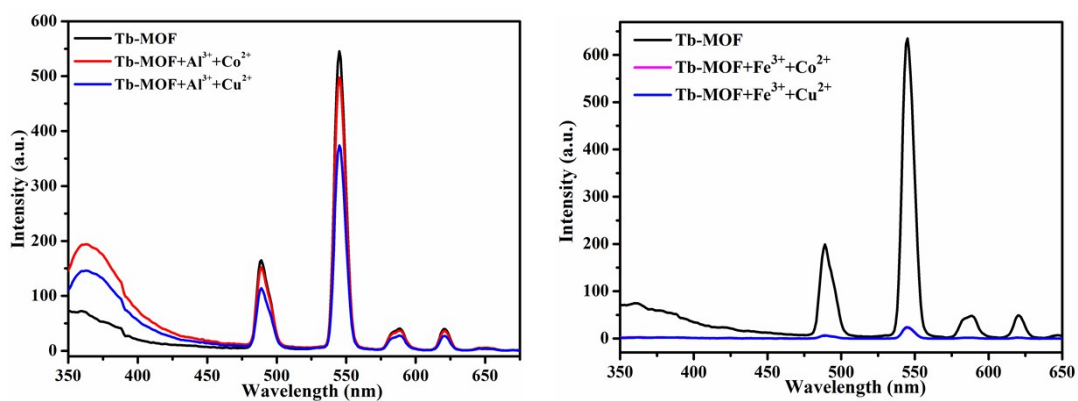


Fig. S7 The competition experiments for the detection of Fe^{3+} and Al^{3+} ions in the presence of Cu^{2+} or Co^{2+} ion.

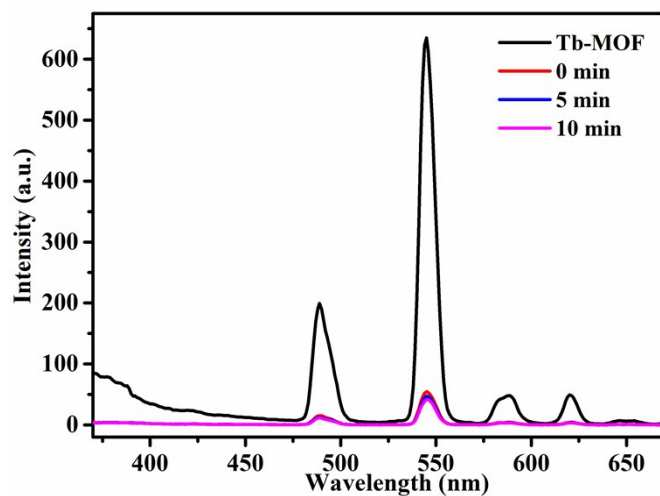


Fig. S8 Time-dependent emission spectra for the Tb-MOF in water containing 10^{-3} M Fe^{3+} ion.

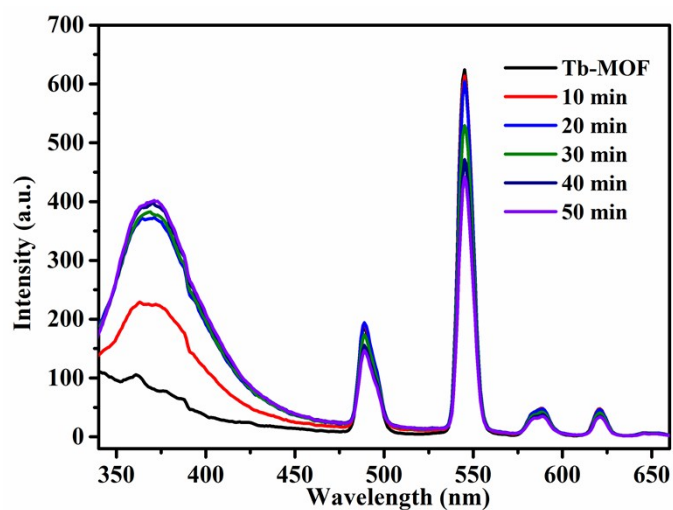


Fig. S9 Time-dependent emission spectra for the Tb-MOF in water containing 10^{-3} M Al^{3+} ion.

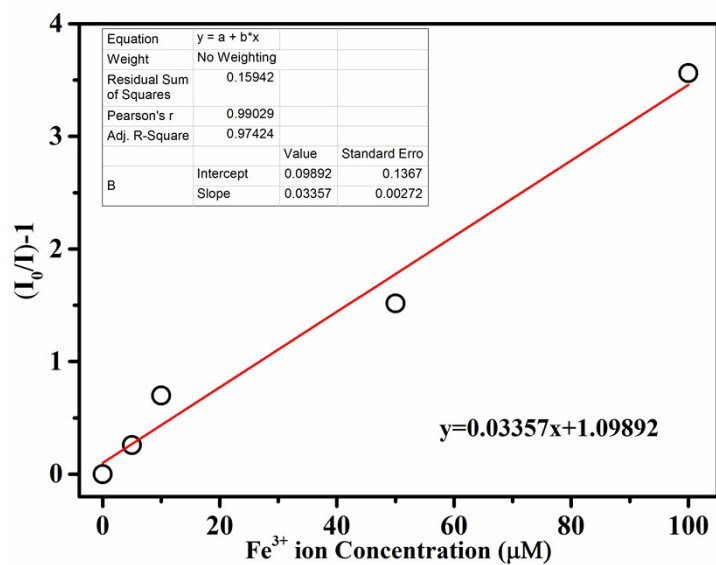


Fig. S10 K_{sv} curve of Tb-MOF in aqueous solutions in the presence of various concentrations of Fe^{3+} ion.

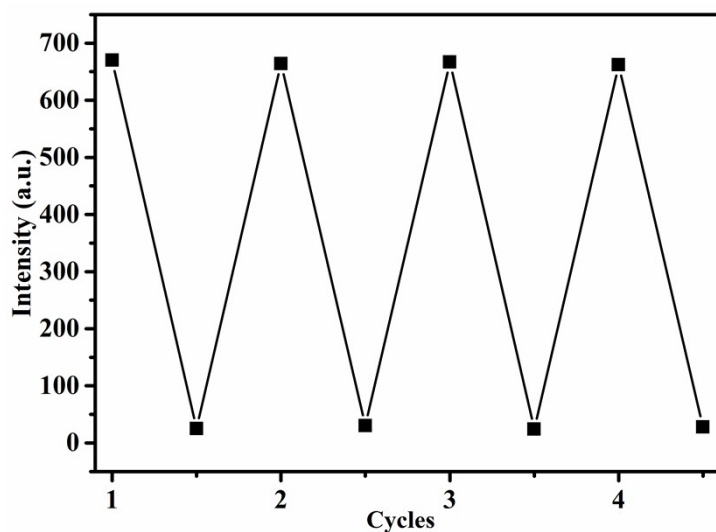


Fig. S11 The quenching and recovery tests of **1**.

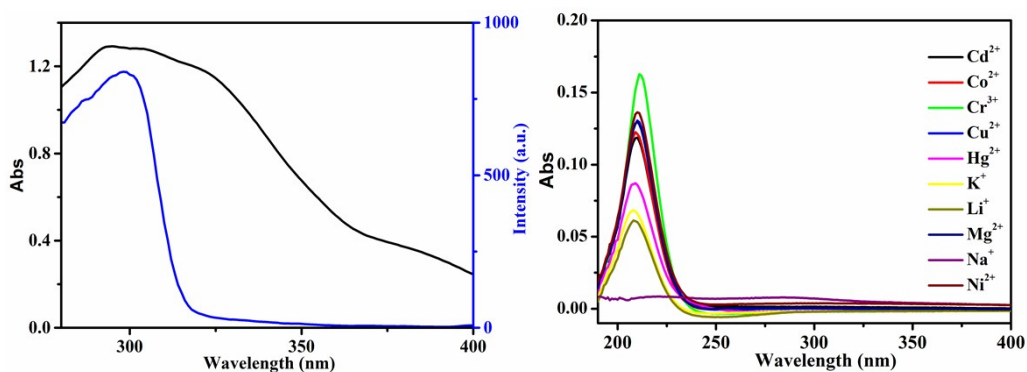


Fig. S12 Views for the UV adsorption spectrum of Fe^{3+} ion in water and extraction spectrum for the Tb-MOF (left) and the UV adsorption spectra of other metal ions used in the luminescent detection (right).

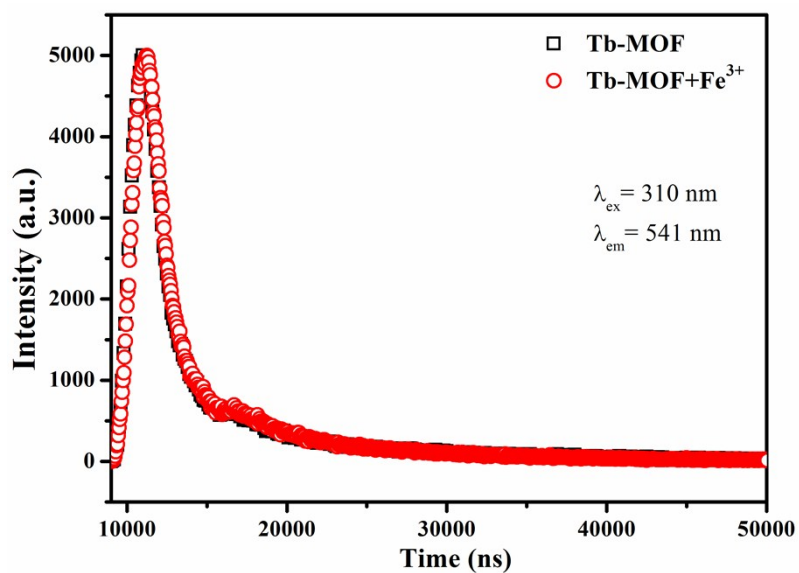


Fig. S13 Fluorescence decay profiles of Tb-MOF in the presence or absence of Fe^{3+} ion.

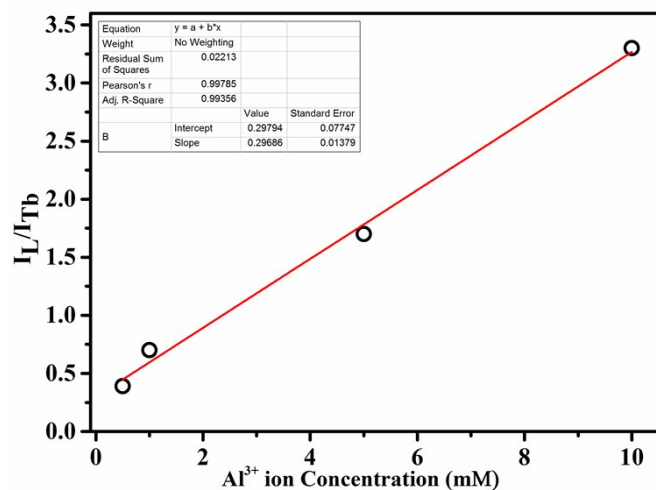


Fig. S14 Linear relationship of ratio for the ligand-based and metal-based emission intensity vs. the concentration of Al^{3+} ion.

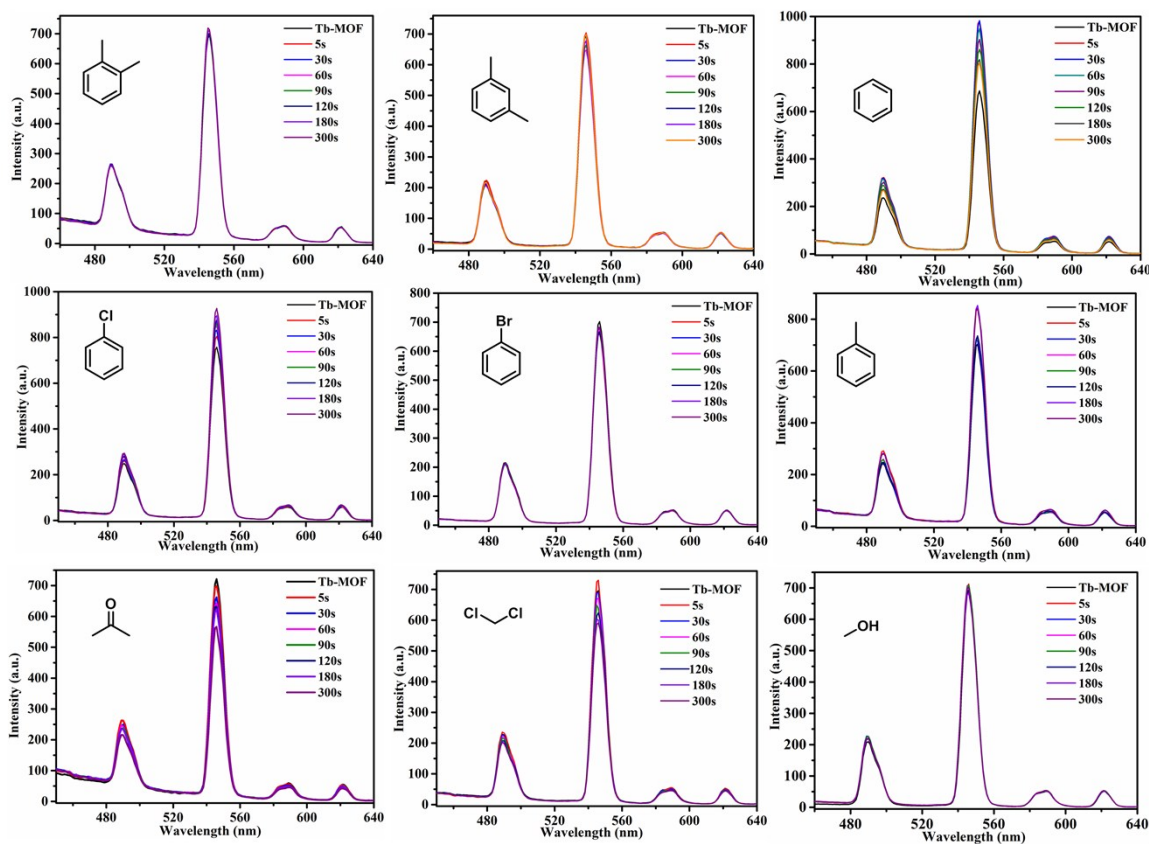


Fig. S15 Time-dependent emission spectra for the Tb-MOF in various VOC vapors.

Table S1 Crystal data and structure refinement details for Tb-MOF.

Empirical formula	C ₃₂ H ₂₈ N ₅ O ₁₀ Tb
Formula weight	801.51
Temperature / K	293(2)
Crystal system	hexagonal
Space group	<i>P</i> 6 ₄ 22
<i>a</i> / Å	15.1834(4)
<i>b</i> / Å	15.1834(4)
<i>c</i> / Å	26.5282(9)
α / °	90
β / °	90
γ / °	120
Volume / Å ³	5296.3(3)
<i>Z</i>	6
ρ_{calc} / g cm ⁻³	1.508
μ / mm ⁻¹	2.063
<i>F</i> (000)	2400.0
Radiation	Mo K α (λ = 0.7107)
Reflections collected	14753
Independent reflections	3121 [R_{int} = 0.0275, R_{sigma} = 0.0205]
Data/restraints/parameters	3121/46/242
Goodness-of-fit on <i>F</i> ²	1.124
Final <i>R</i> indexes [$I \geq 2\sigma(I)$]	$R_1 = 0.0381$, $wR_2 = 0.1045$
Final <i>R</i> indexes [all data]	$R_1 = 0.0456$, $wR_2 = 0.1120$
Largest diff. peak and hole / e Å ⁻³	1.03 and -0.62
Flack parameter	-0.003(8)