**Synthesis, crystal structure and desulfurization properties of** **zig-zag 1D coordination polymer of copper(II)** **containing 4-methoxybenzoic acid ligand**

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**Supplementary Information**



**Fig. S1.** Nitrogen adsorption-desorption isotherm of [Cu(4-mba)2(H2O)3].



A



B

**Fig. S2** ORTEP diagram showing (A) zigzag 1D unit of [Cu(4-mba)2(H2O)3] held by strong hydrogen bonds and (b) crystal packing of zigzag 1D unit of [Cu(4-mba)2(H2O)3].

**Table S1** Crystal data and structure refinement for [Cu(4-mba)2(H2O)2]

|  |  |
| --- | --- |
| Empirical formula  | C16H18CuO8  |
| Shape and Colour | Plate and Blue |
| Formula weight  | 401.85  |
| Temperature/K  | 193.0  |
| Crystal system  | monoclinic  |
| Space group  | P 21  |
| Hall group | P 2yb |
| a/Å  | 7.3339(1)  |
| b/Å  | 5.7970(9)  |
| c/Å  | 19.6400(3)  |
| α/°  | 90.00  |
| β/°  | 93.30  |
| γ/°  | 90.00 |
| Volume/Å3  | 833.60(4)  |
| Z  | 2 |
| ρcalcmg/mm3  | 1.572 |
| m/mm‑1  | 0.89  |
| F(000)  | 414.0  |
| µ/mm-1  | 1.352  |
| θ range for data collection  | 3.8 to 28°  |
| Index ranges  | -8 ≤ h ≤ 8, -9 ≤ k ≤ 9, -8 ≤ l ≤ 13  |
| Reflections collected  | 1902  |
| Independent reflections  | 1966[R(int) = 0.0857]  |
| Data/restraints/parameters  | 2137/0/181  |
| Goodness-of-fit on F2  | 1.07 |
| Final R indexes [I>=2σ (I)]  | R1 = 0.042, wR2 = 0.094  |
| Final R indexes [all data]  | R1 = 0.0605, wR2 = 0.1337  |
| Largest diff. peak/hole / e Å-3  | 0.32/-0.45  |

**Fig. S3.** Effect of concentrations over [Cu(4-mba)2(H2O)3].

**Fig. S4.** Effect of contact time on desulfurization over adsorbent, [Cu(4-mba)2(H2O)3].

**Fig. S5.** Effect of temperature on the desulfurization over [Cu(4-mba)2(H2O)3].

**Fig. S6.** Effect of adsorbent dosage on the desulfurization over [Cu(4-mba)2(H2O)3] at initial concentrations of 100 mg/L.

**Fig. S7** Plots of the adsorption kinetics of the desulfurization over [Cu(4-mba)2(H2O)3] (a) pseudo-first-order kinetics (b) pseudo-second-order kinetics.

**Fig S8**(a). Langmuir isotherm plot of the desulphurization over [Cu(4-mba)2(H2O)3]

**Fig S8** (b). Freundlich isotherm plot of the desulphurization over [Cu(4-mba)2(H2O)3]



**Fig. S9.** GC-FIDchromatograms of model fuel, dibenzothiophene in hexane (A) before adsorption, and (B) after adsorption.