# Two Cu(I) coordination polymers based on a new benzimidazolyl-tetrazolyl heterotopic ligand for visible-light-driven photocatalytic dye degradation

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## Supporting Information

**Table S1** Crystallographic data and structure refinement summary for CPs **1**-**2**

| Complex | CP **1** | CP **2** |
|---|---|---|
| Empirical formula | $C_{21}H_{15}CuN_8O$ | $C_{24}H_{20}CuN_9O$ |
| Formula weight | 458.95 | 514.03 |
| Crystal system | Monoclinic | Monoclinic |
| Space group | *P* 21/c | *P* 21/n |
| a / Å | 15.5585(2) | 10.6532(5) |
| b / Å | 16.1849(3) | 16.4768(8) |
| c / Å | 7.67250(10) | 13.9291(7) |
| α / ° | 90 | 90 |
| β / ° | 100.337(2) | 102.397(2) |
| γ / ° | 90 | 90 |
| V / Å$^3$ | 1900.68(5) | 2388.0(2) |
| Z | 4 | 4 |
| D / g cm$^{-3}$ | 1.604 | 1.430 |
| μ / mm$^{-1}$ | 1.906 | 0.951 |
| T / K | 293(2) | 293(2) |
| $R^a$ / $wR^b$ | 0.0333 / 0.0954 | 0.0627 / 0.1575 |
| Total / unique | 10388 / 3626 | 37660 / 5534 |

[a] $R_1 = \Sigma||F_o| - |F_c||/|F_o|$, [b] $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$, where $w = 1/[\sigma^2(F_o^2) + (aP)_2 + bP]$. $P = (F_o^2 + 2F_c^2)/3$.

**Table S2** Selected bond lengths [Å] and angles [°] for CPs **1**-**2**

| CP **1** | | | |
|---|---|---|---|
| Cu(1)-N(1) | 1.9644(17) | N(1)-Cu(1)-N(8)#1 | 133.67(7) |
| Cu(1)-N(8)#1 | 1.9757(17) | N(1)-Cu(1)-N(2)#2 | 113.22(7) |
| Cu(1)-N(2)#2 | 2.0204(18) | N(8)#1-Cu(1)-N(2)#2 | 112.34(7) |
| C(21)-N(8)-C(20) | 105.20(16) | C(20)-N(8)-Cu(1)#3 | 131.78(13) |
| C(21)-N(8)-Cu(1)#3 | 122.85(14) | | |
| CP **1** | | | |
| Cu(1)-N(5)#1 | 1.983(3) | Cu(1)-N(3) | 2.085(3) |
| Cu(1)-N(1)#2 | 2.021(3) | Cu(1)-N(6)#3 | 2.144(3) |
| N(5)#1-Cu(1)-N(1)#2 | 127.21(12) | N(5)#1-Cu(1)-N(6)#3 | 113.48(11) |
| N(5)#1-Cu(1)-N(3) | 108.73(12) | N(1)#2-Cu(1)-N(6)#3 | 100.64(12) |
| N(1)#2-Cu(1)-N(3) | 108.22(13) | N(3)-Cu(1)-N(6)#3 | 93.12(12) |

Symmetry transformations used to generate equivalent atoms: #1 x, -y + 1/2, z + 1/2, #2 -x + 1, -y + 1, -z + 2, #3 x, -y + 1/2, z-1/2 for CP **1**; #1 -x, -y, -z, #2 x + 1/2, -y + 1/2, z + 1/2, #3 x + 1, y, z, #4 x - 1, y, z, #5 x - 1/2, -y + 1/2, z - 1/2 CP **2**.

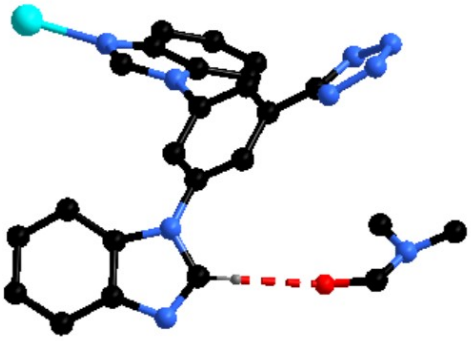

**Fig. S1** The hydrogen bond between DMF and the framework in CP **2**.

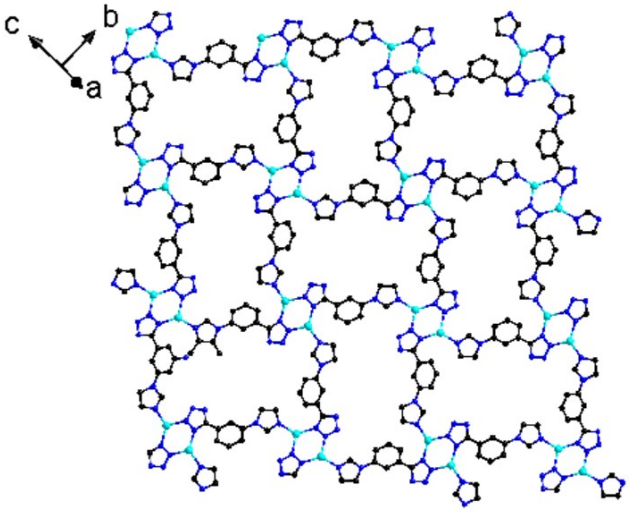


**Fig. S2** The 2D layer in CP **2**.

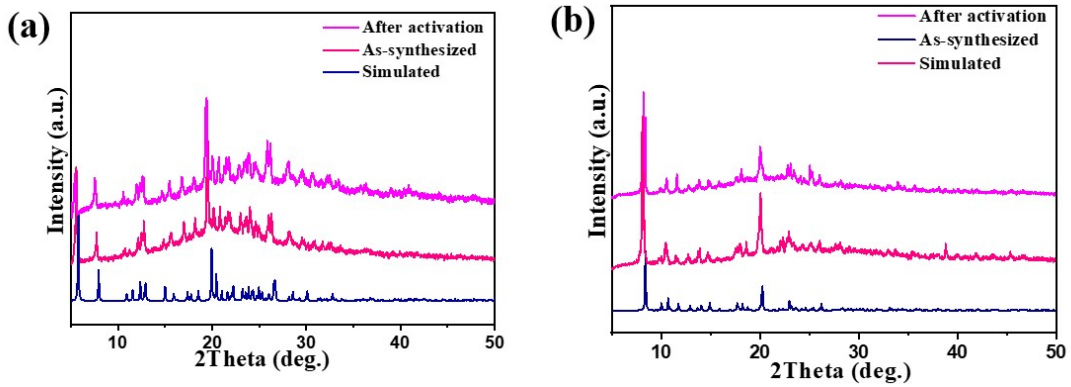


**Fig. S3** PXRD of (a) Simulated and as-synthesized CP **1** and (b) Simulated and as-synthesized CP **2**.

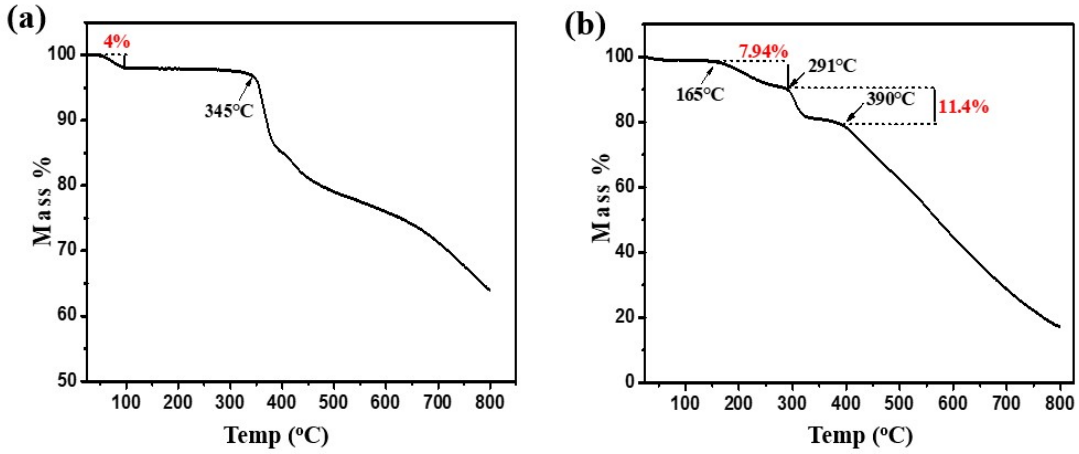


**Fig. S4** TG curve of (a) CP **1** and (b) CP **2**.

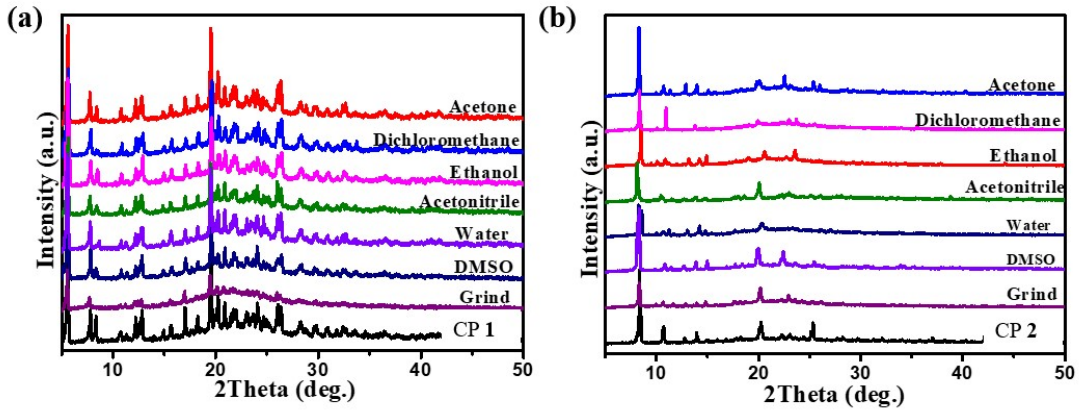


**Fig. S5** PXRD of (a) CP **1** and (b) CP **2** after immersing in different organic solvents for 72 h.

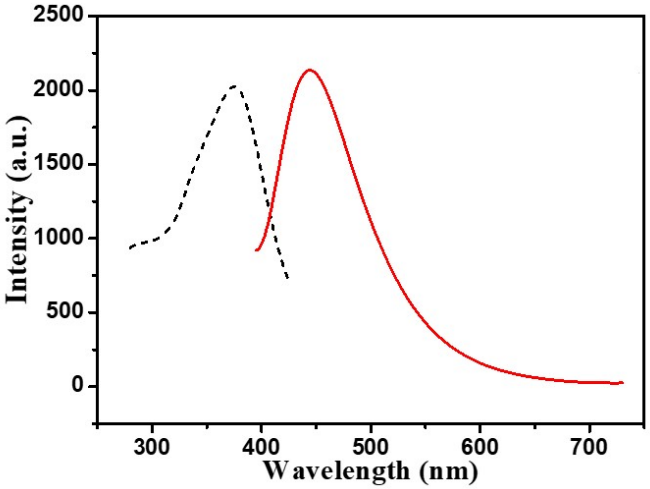


**Fig. S6** Photoluminescence spectrum of HDBPT.

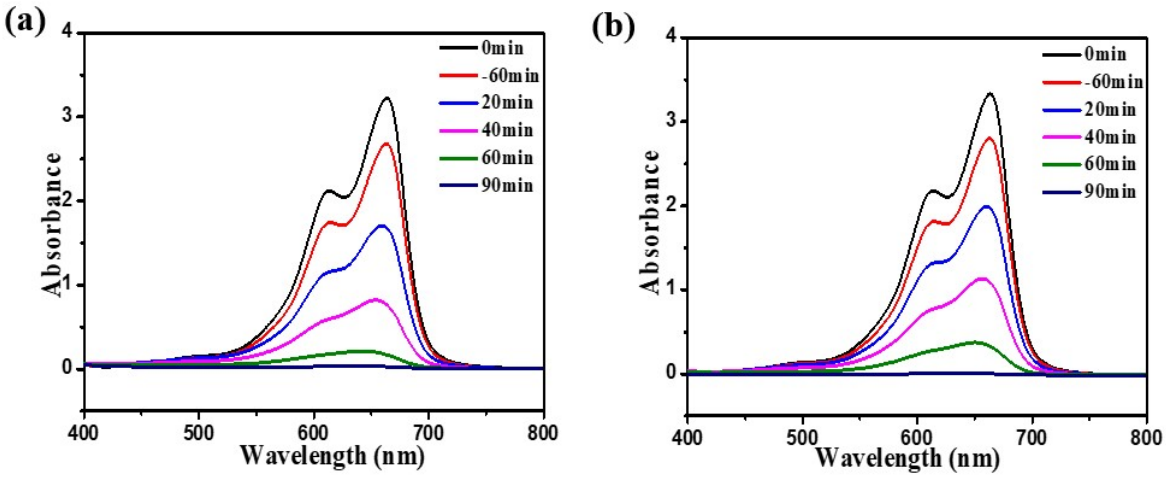


**Fig. S7** UV–vis spectra of MLB solutions which were recorded after photocatalytic degradation had been performed for different lengths of time with (a) CP **1** and (b) CP **2** in the presence of $H_2O_2$.

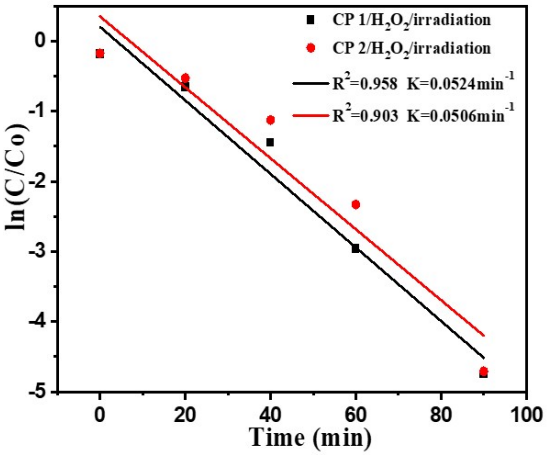


**Fig. S8** Pseudo-first-order plot with respect to time for CP **1** and CP **2** in an aqueous MLB solution.

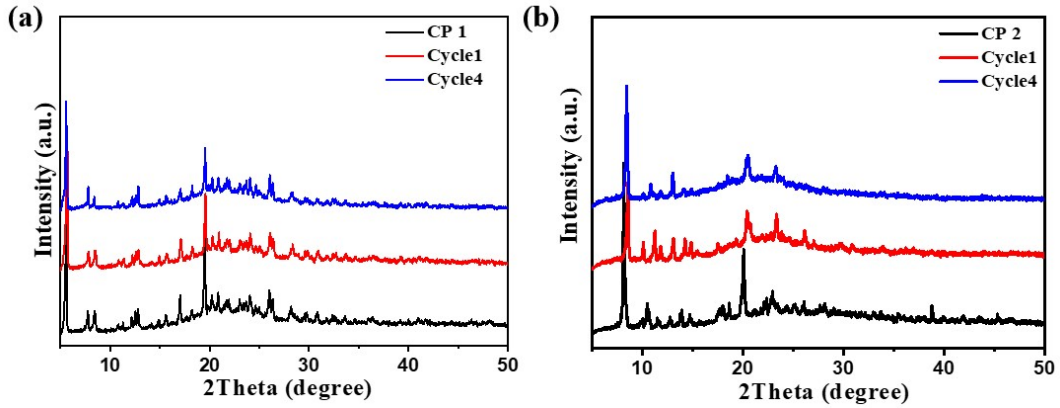


**Fig. S9** The PXRD patterns of (a) CP **1** and (b) CP **2** before and after recycling test for MLB.

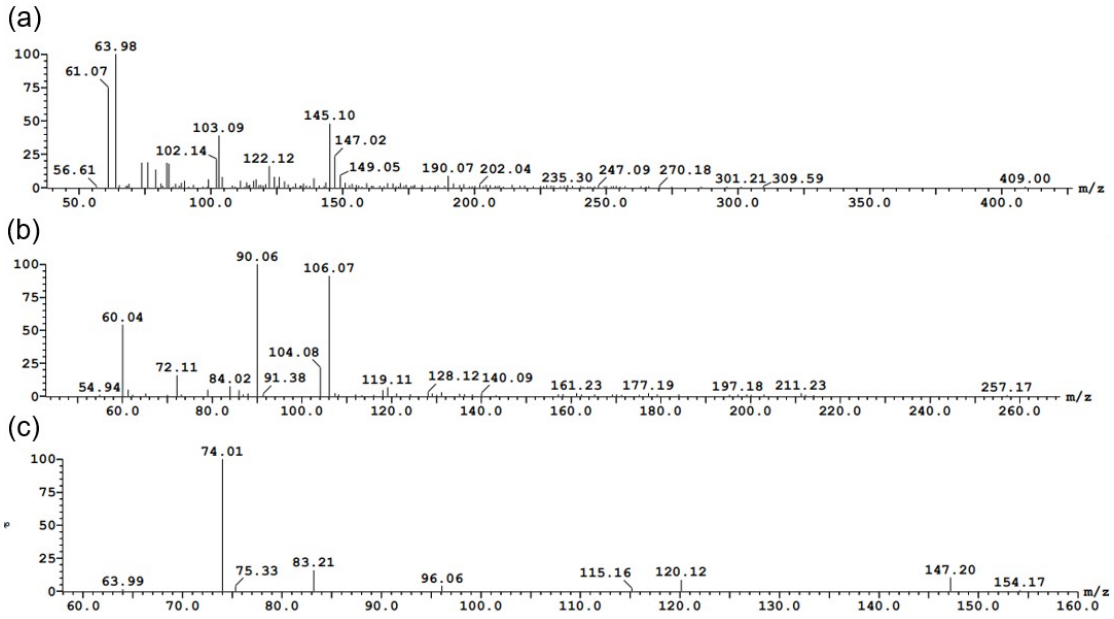


**Fig. S10** The ESI positive mass spectra of MLB after reacting for 90 min by using CP **1** as catalyst.

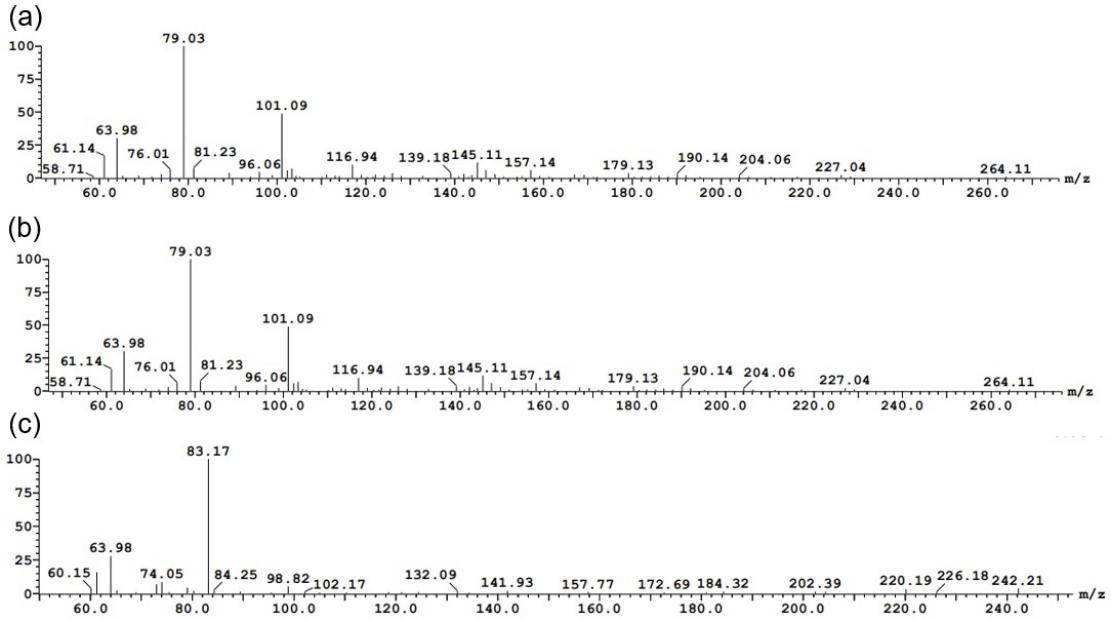


**Fig. S11** The ESI positive mass spectra of MLB after reacting for 90 min by using CP **2** as catalyst.