

A new Zn(II) MOF assembled from metal–organic cubes (MOCs) as an ultimate adsorbent for cationic dyes

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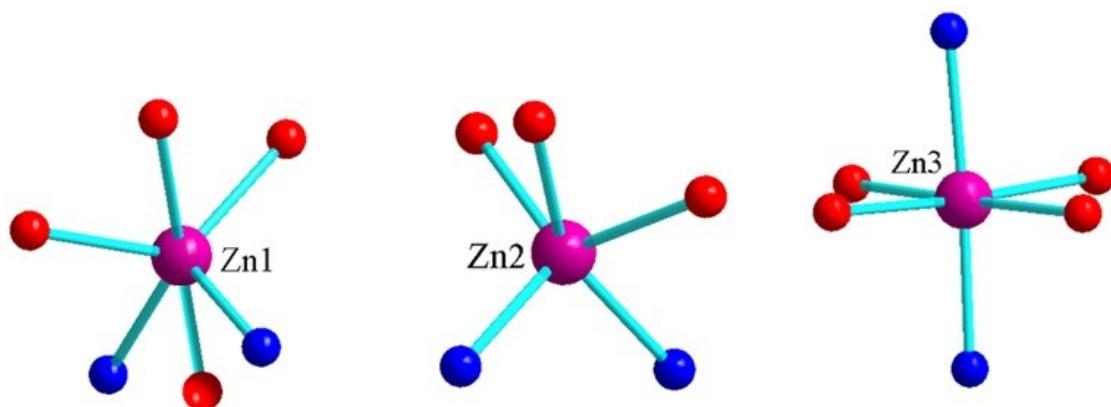


Fig. S1 Various coordination modes of Zn metal atom present in **1**.

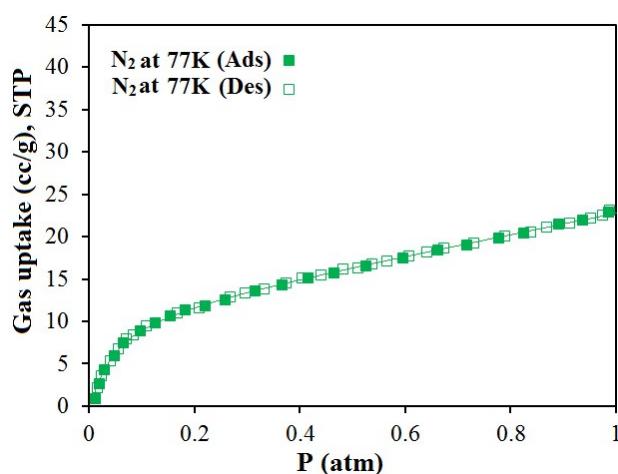


Fig. S2 Adsorption isotherms of **1** at 77 K up to 1 bar pressure for N₂

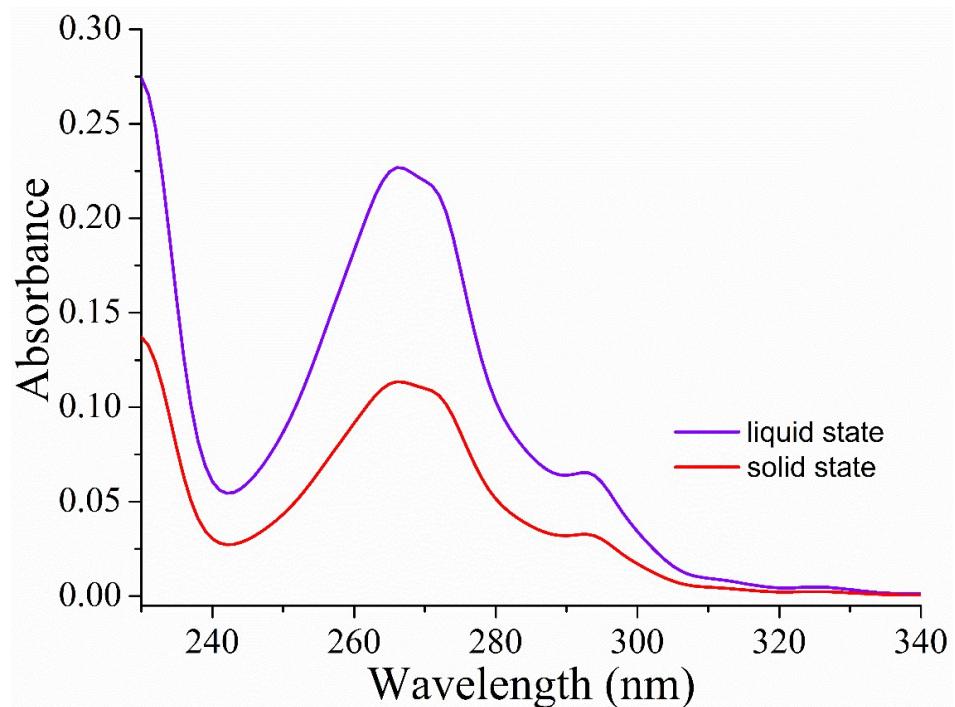


Fig. S3: UV-vis spectra of **1** in liquid and solid state.

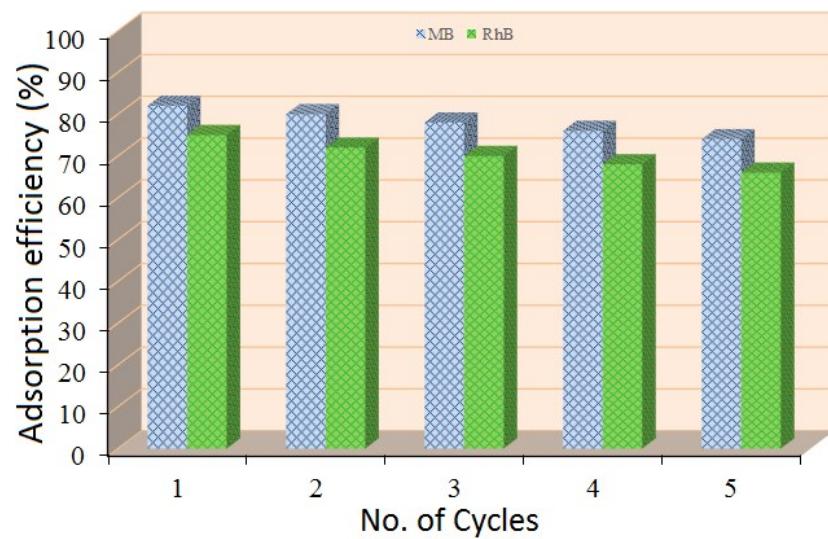


Fig. S4 Recyclability plot of **1**.

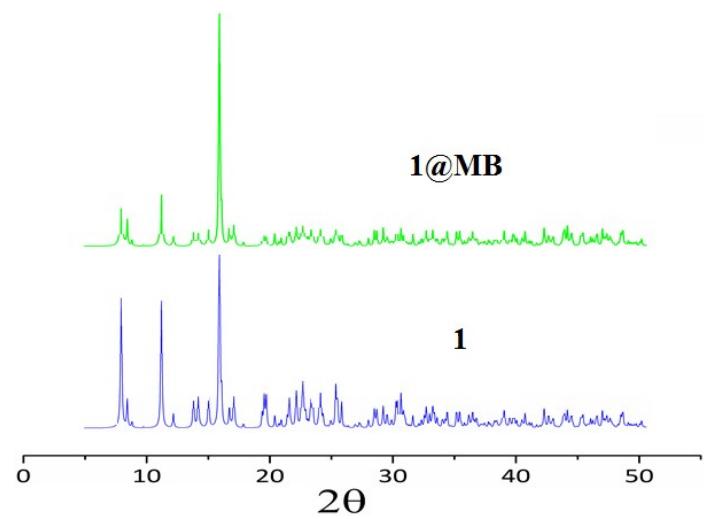


Fig. S5 PXRD patterns of **1** before and after adsorption of MB.

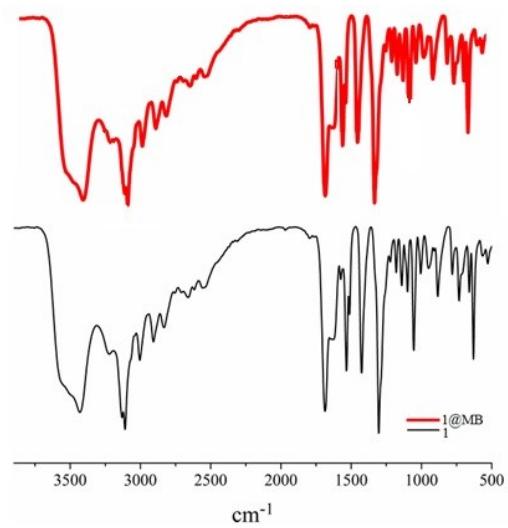


Fig. S6 FTIR spectra of **1** before and after adsorption of MB.

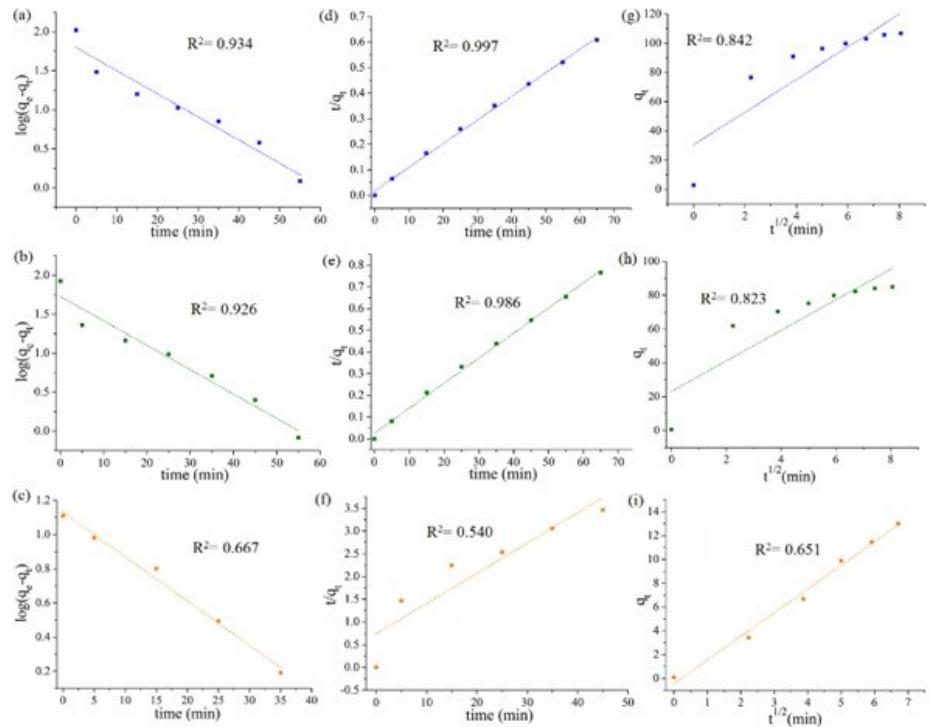


Fig. S7 The adsorption kinetics of dye pollutants MB, RB and MO by **1** are represented by (a), (b) and (c), respectively as pseudo-first order kinetics and by (d), (e) and (f), respectively as pseudo-second order kinetics and by (g), (h) and (i), respectively, as intraparticle diffusion.

Table S1: Bond length and bond angle for **1.**

Cu-btc-1

	Bond Angle(°)	Bond distance(Å)	
O3 Zn1 O2	130.5(5)	Zn1 O2	2.238(12)
N3 Zn1 O2	113.5(4)	Zn1 O3	2.339(11)
N3 Zn1 O3	92.8(4)	Zn1 N3	2.258(12)
N5 Zn1 O2	113.7(4)	Zn1 N5	2.274(12)
N5 Zn1 O3	95.2(4)	Zn2 O5	2.198(12)
N5 Zn1 N3	107.6(5)	Zn2 O8	2.343(10)
O8 Zn2 O5	122.7(5)	Zn2 N2	2.320(13)
N2 Zn2 O5	119.9(5)	Zn2 N4	2.236(12)
N2 Zn2 O8	99.1(4)	Zn3 O9	2.312(12)
N4 Zn2 O5	111.6(4)	Zn3 O10	2.293(10)
N4 Zn2 O8	94.2(4)	Zn3 O11	2.309(14)
N4 Zn2 N2	105.5(4)	Zn3 O13	2.358(12)
O10 Zn3 O9	90.8(6)	Zn3 N1	2.252(11)
O11 Zn3 O9	92.3(6)	Zn3 N6	2.249(13)
O11 Zn3 O10	176.9(4)		
O13 Zn3 O9	176.3(4)		
O13 Zn3 O10	88.7(5)		
O13 Zn3 O11	88.2(5)		
N1 Zn3 O9	85.1(4)		
N1 Zn3 O10	87.6(4)		
N1 Zn3 O11	92.1(4)		
N1 Zn3 O13	91.2(4)		
N6 Zn3 O9	92.8(4)		
N6 Zn3 O10	90.6(4)		
N6 Zn3 O11	89.9(4)		
N6 Zn3 O13	90.9(4)		
N6 Zn3 N1	177.2(4)		