

**Synthesis, structure and hydrogen adsorption of a novel porous metal-organic framework, Mn₉(btt)₂(HCOO)₁₂·0.7DMF·0.9H₂O, where
btt = 1,3,5-benzenetristetrazolate**

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Supporting Information

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- Figure S1. (a) Simulated X-ray powder diffraction pattern (in blue) of **1**, based on single-crystal data. (b) Experimental XRPD of the as-synthesized product (in red).
- Figure S2. (a) Experimental X-ray powder diffraction pattern (in green) of **1** annealed at 120°C. (b) Experimental XRPD of the as-synthesized product (in red).
- Figure S3. Thermogravimetric analysis of **1**.
- Figure S4. Solid-state photoluminescence spectrum of H₃btt·2HCl with $\lambda_{\text{ex}} = 300$ nm.
- Figure S5. Infrared spectrum of **1**.

Figure 1S

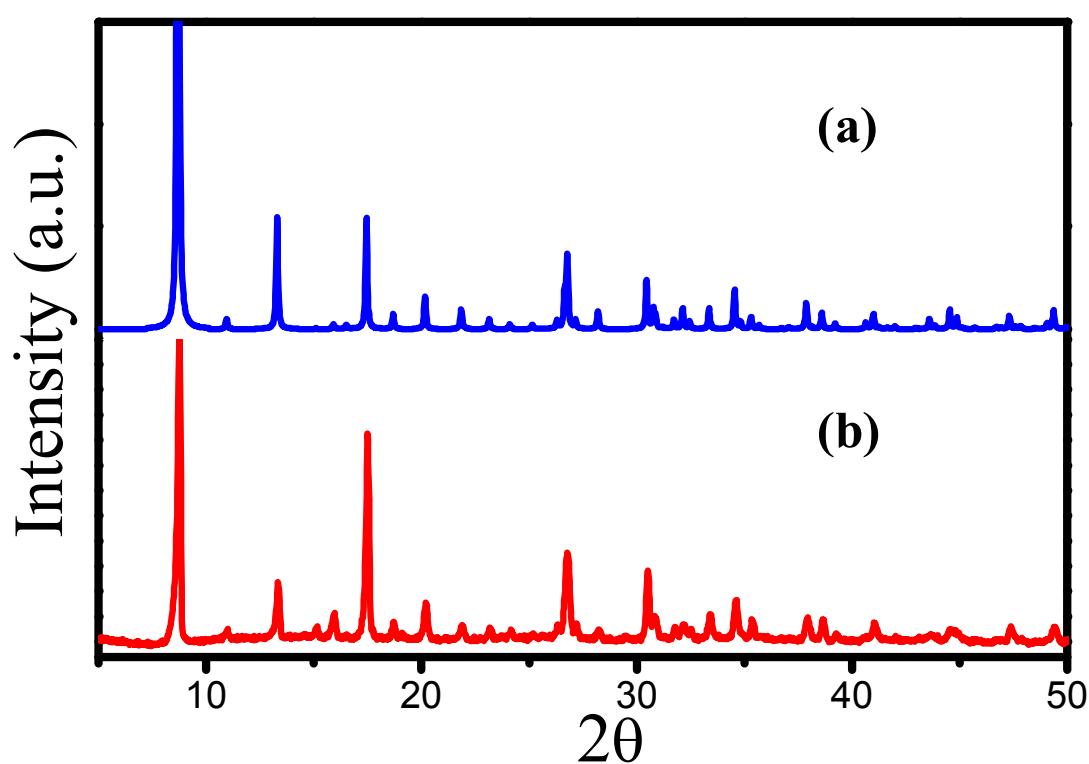


Figure 2S.

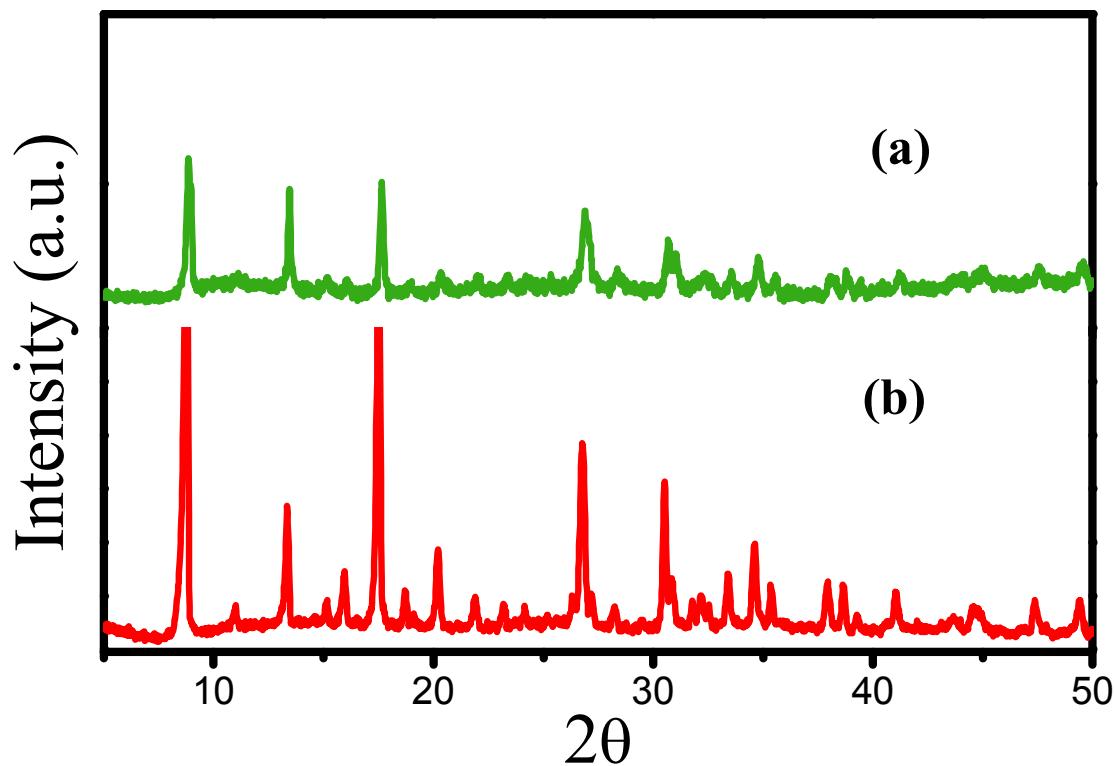


Figure 3S.

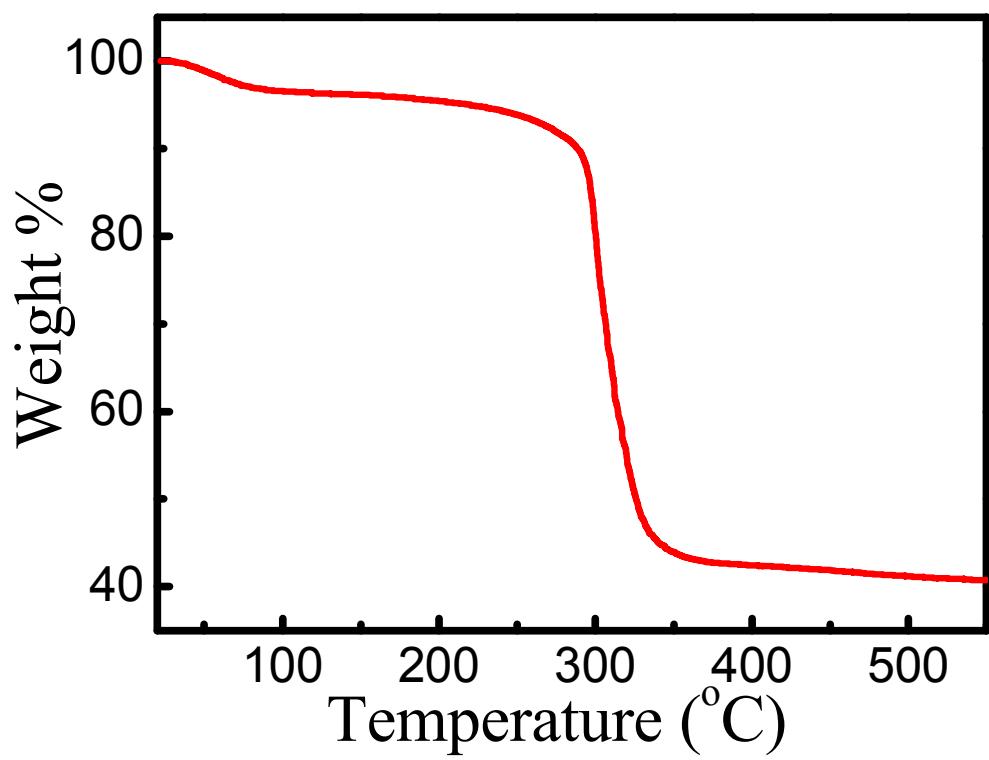


Figure 4S.

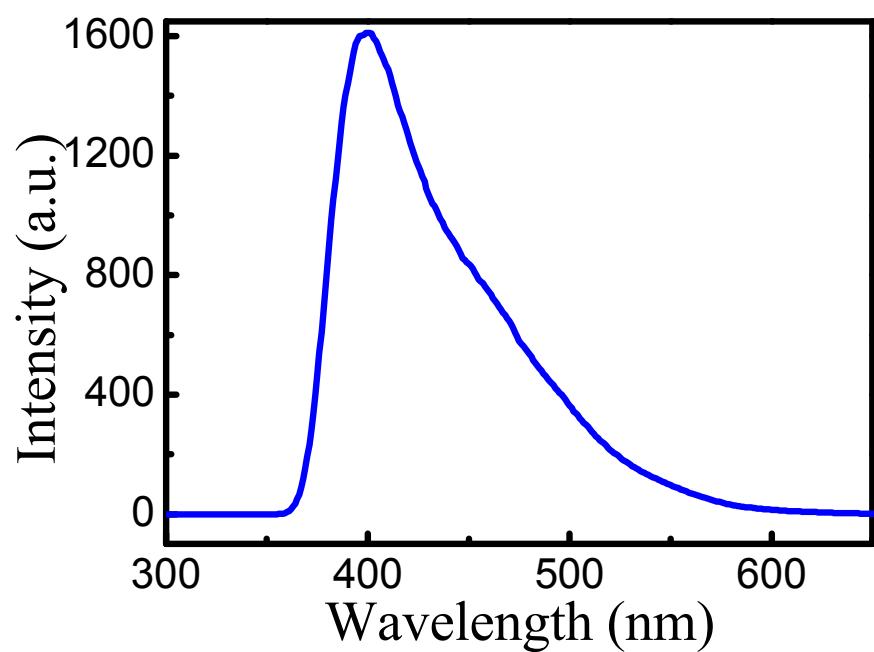
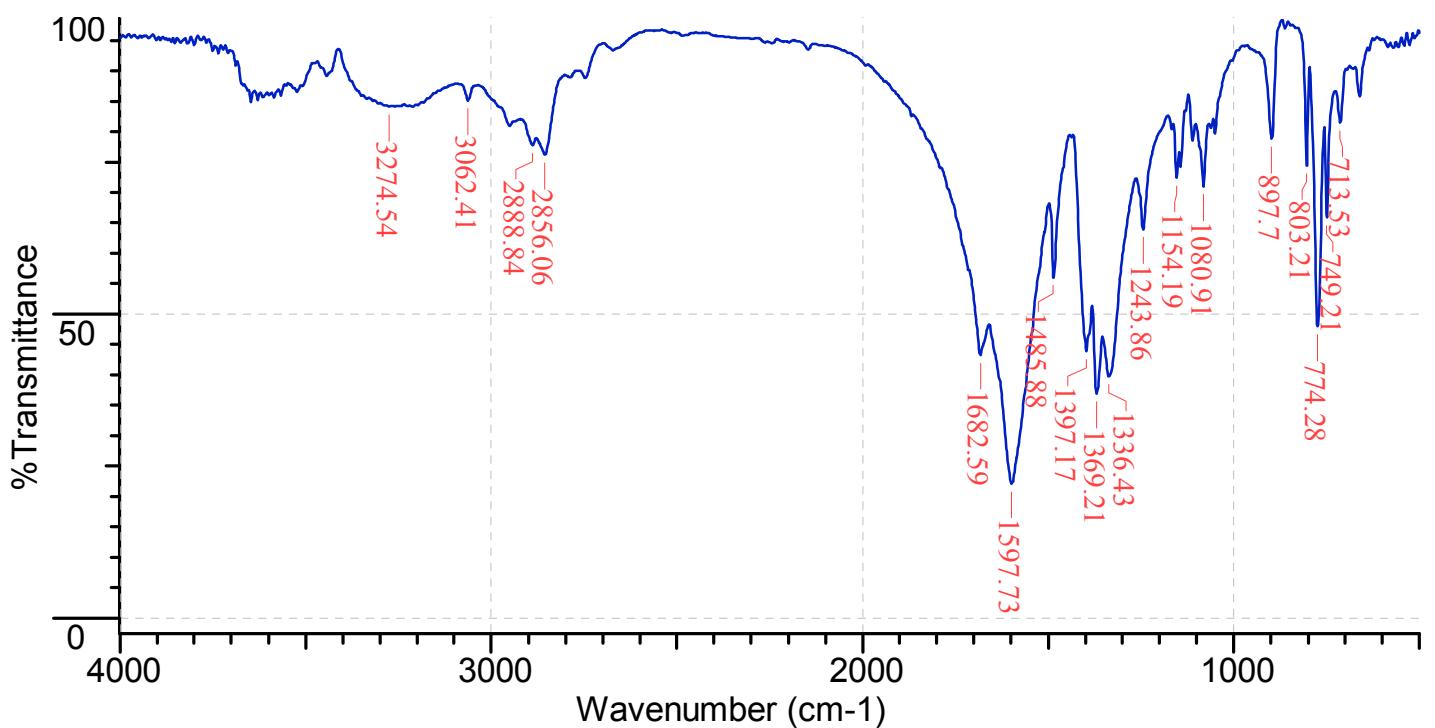


Figure 5S



No	cm-1	%T	Intensity
1	713.53	81.536	W
2	749.21	65.858	M
3	774.28	47.940	S
4	803.21	74.421	M
5	897.70	78.822	W
6	1080.91	71.020	M

No	cm-1	%T	Intensity
7	1154.19	72.462	M
8	1243.86	63.981	M
9	1336.43	39.734	S
10	1369.21	36.899	S
11	1397.17	43.863	S
12	1485.88	56.010	M

No	cm-1	%T	Intensity
13	1597.73	22.086	VS
14	1682.59	43.288	S
15	2856.06	76.221	W
16	2888.84	77.829	W
17	3062.41	85.124	W
18	3274.54	84.088	W