Electronic Supplementary Material (ESI) for CrystEngComm

The 3D Porous Metal-Organic Frameworks Based on Bis(pyrazinyl)-trizole: Structures, Photoluminescence and Gas Adsorption Properties

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1. Selected Bond Lengths (Å) and Angles (deg) for Complexes **1** and **2**.

Table S1. Selected Bond Lengths (Å) and Angles (deg) for Complexes **1** and **2**.

Complex **1**[a]			
Zn1—O1	1.9754 (19)	Zn1—O3^{i}	2.0190 (18)
Zn1—N3	2.0193 (18)	Zn1—N1^{ii}	2.119 (2)
Zn1—O2^{i}	2.403 (2)		
O1—Zn1—O3^{i}	98.28 (9)	O1—Zn1—N3	107.09 (8)
O3^{i}—Zn1—N3	147.57 (9)	O1—Zn1—N1^{ii}	99.67 (10)
O3^{i}—Zn1—N1^{ii}	101.85 (9)	O1—Zn1—O2^{i}	91.33 (8)
O3^{i}—Zn1—O2^{i}	58.06 (7)	N3—Zn1—O2^{i}	100.73 (9)
N1^{ii}—Zn1—O2^{i}	150.65 (8)	O3^{i}—Zn1—N1^{ii}	93.26 (8)
Complex **2**[b]			
Cd1—O1	2.231 (5)	Cd1—O2^{i}	2.313 (5)
Cd1—O5^{ii}	2.335 (5)	Cd1—N1^{iii}	2.357 (5)
Cd1—N7	2.366 (5)	Cd1—O6^{ii}	2.443 (5)
Cd2—O4^{iv}	2.234 (5)	Cd2—O8	2.297 (6)
Cd2—N5	2.341 (5)	Cd2—N4^{v}	2.346 (5)
Cd2—N2^{v}	2.504 (6)	Cd2—N6	2.524 (6)
O1—Cd1—O2^{i}	134.0 (2)	O1—Cd1—O5^{ii}	90.4 (2)
O2^{i}—Cd1—O5^{ii}	135.54 (18)	O1—Cd1—N1^{iii}	93.8 (2)
O2^{i}—Cd1—N1^{iii}	84.17 (19)	O5^{ii}—Cd1—N1^{iii}	94.87 (19)
O1—Cd1—N7	94.38 (19)	O2^{i}—Cd1—N7	86.75 (18)
O5^{ii}—Cd1—N7	89.80 (18)	N1^{iii}—Cd1—N7	170.6 (2)
O1—Cd1—O6^{ii}	145.27 (19)	O2^{i}—Cd1—O6^{ii}	80.68 (18)
O5^{ii}—Cd1—O6^{ii}	54.89 (17)	N1^{iii}—Cd1—O6^{ii}	88.15 (16)
N7—Cd1—O6^{ii}	87.85 (16)	O4^{iv}—Cd2—O8	164.6 (2)
O4^{iv}—Cd2—N5	97.26 (19)	O8—Cd2—N5	93.37 (19)
O4^{iv}—Cd2—N4^{v}	96.36 (19)	O8—Cd2—N4^{v}	95.77 (19)
N5—Cd2—N4^{v}	84.11 (19)	O4^{iv}—Cd2—N2^{v}	95.34 (19)
O8—Cd2—N2^{v}	79.97 (18)	N5—Cd2—N2^{v}	152.37 (17)
N4^{v}—Cd2—N2^{v}	70.09 (18)	O4^{iv}—Cd2—N6	90.09 (19)
O8—Cd2—N6	83.06 (18)	N5—Cd2—N6	70.20 (19)
N4^{v}—Cd2—N6	154.12 (18)	N2^{v}—Cd2—N6	134.34 (19)

[a] Symmetry codes: (i) 1/2+*x*, 1/2-*y*, 1/4-*z*; (ii) -1/2+*x*, 3/2-*y*, 1/4-*z*; (iii) -1/2+*x*, 1/2-*y*, 1/4-*z*; (iv) 1/2+*x*, 3/2-*y*, 1/4-*z*; (v) *y*, *x*, -*z*. [b]Symmetry codes: (i) 1-*x*, *y*, 1/2-*z*; (ii) *x*, 1-*y*, -1/2+*z*; (iii) 1-*x*, 1-*y*, -*z*; (iv) 1/2-*x*, -1/2+*y*, 1/2-*z*; (v) 1-*x*, -*y*, -*z*; (vi) *x*, 1-*y*, 1/2+*z*; (vii) 1/2-*x*, 1/2+*y*, 1/2-*z*.

2. TGA curves of the samples after immerged in methanol and dehydrated.

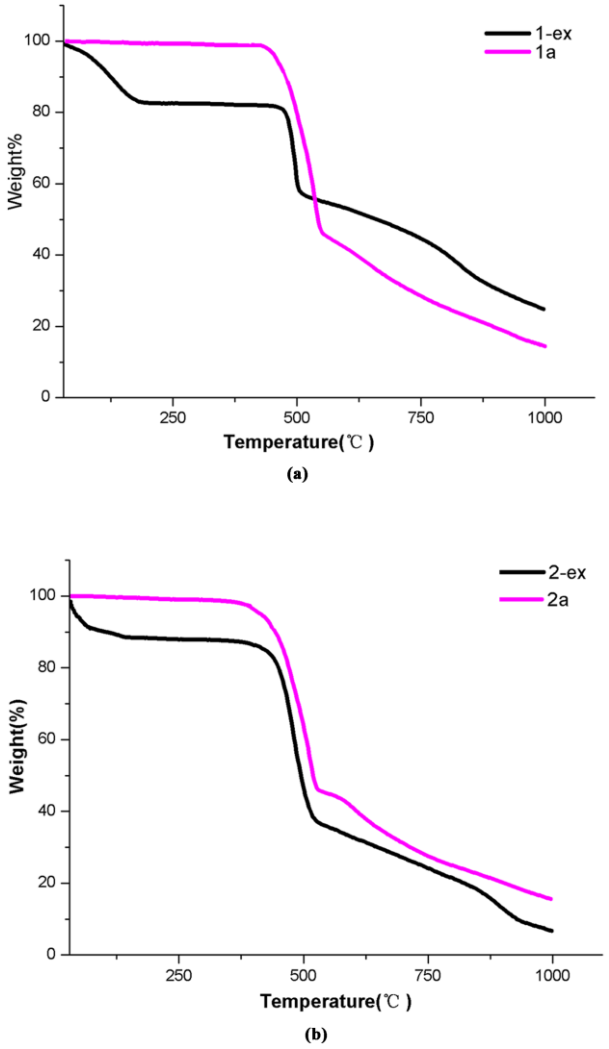
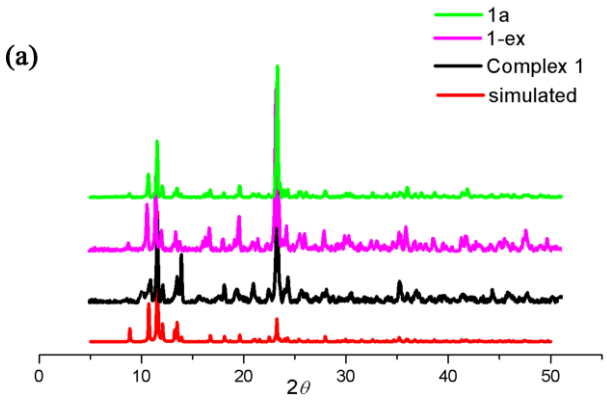


Figure S1. (a) TGA curves of **1**-ex and **1**a; (b) TGA curves of **2**-ex and **2**a.

3. PXRD patterns of the samples after immerged in methanol and dehydrated.



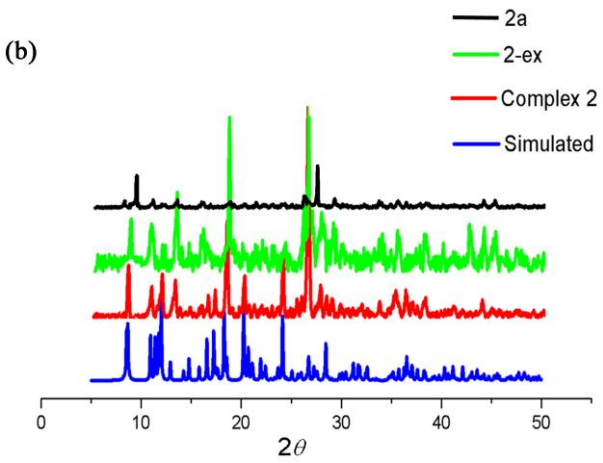


Figure S2. (a) PXRD patterns of simulated one and complex **1**, **1**-ex and **1**a;
(b) PXRD patterns of simulated one and complex **2**, **2**-ex and **2**a.

4. Coverage dependency of the isosteric heat of adsorption for CO_2 and CH_4 in **1**a.

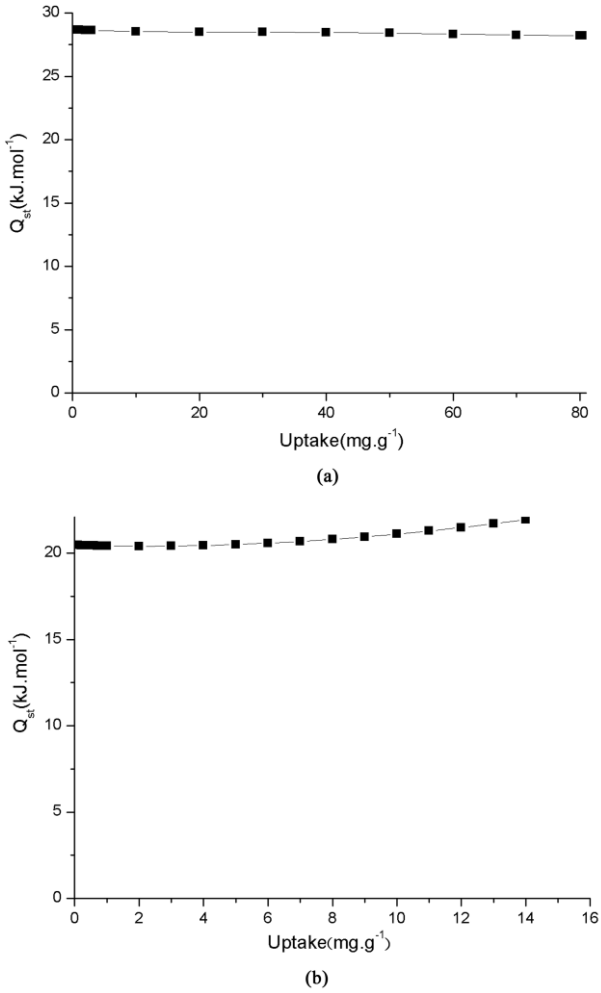


Figure S3. (a) Coverage dependency of the isosteric heat of adsorption for CO_2 in **1**a; (b) Coverage dependency of the isosteric heat of adsorption for CH_4 in **1**a.

5. Crystal photographs of **1** under UV irradiation at room temperature.

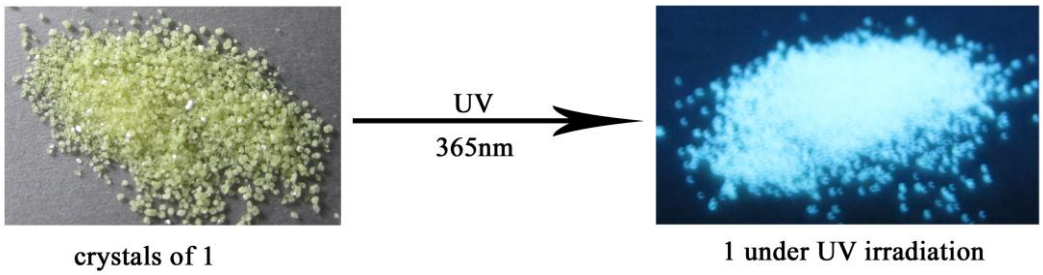


Figure S4. Crystal photographs of **1** under UV irradiation at room temperature.