Supporting Information

A magnesium MOF as highly selective fluorescence sensor for CS_2 and nitroaromatic compounds

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Table S1. Selected bond lengths (Å) and angles (°) for compound **1**[a].

Mg(1)-O(9)	2.0195(15)	Mg(2)-O(9)	2.0859(15)
Mg(1)-O(10)	2.0352(18)	Mg(2)-O(11)	2.1033(17)
Mg(1)-O(1)	2.0400(16)	Mg(2)-O(5)	2.1310(15)
Mg(1)-O(6)#1	2.0543(16)	Mg(2)-Mg(3)	3.1523(7)
Mg(1)-O(7)#2	2.1678(15)	Mg(3)-O(3)#3	2.0501(14)
Mg(1)-O(8)#2	2.2604(15)	Mg(3)-O(3)#5	2.0501(14)
Mg(1)-C(10)#2	2.550(2)	Mg(3)-O(9)	2.0812(13)
Mg(1)-Mg(3)	3.5147(7)	Mg(3)-O(9)#1	2.0812(13)
Mg(1)-Mg(2)	3.5275(10)	Mg(3)-O(5)	2.1302(13)
Mg(2)-O(4)#3	2.0423(16)	Mg(3)-O(5)#1	2.1302(13)
Mg(2)-O(8)#4	2.0617(15)	Mg(3)-Mg(2)#1	3.1523(7)
Mg(2)-O(2)	2.0635(16)	Mg(3)-Mg(1)#1	3.5147(7)
O(9)-Mg(1)-O(10)	113.54(7)	O(2)-Mg(2)-O(11)	89.32(7)
O(9)-Mg(1)-O(1)	97.70(6)	O(9)-Mg(2)-O(11)	170.92(7)
O(10)-Mg(1)-O(1)	86.19(7)	O(4)#3-Mg(2)-O(5)	90.77(6)
O(9)-Mg(1)-O(6)#1	96.60(6)	O(8)#4-Mg(2)-O(5)	83.80(6)
O(10)-Mg(1)-O(6)#1	85.15(8)	O(2)-Mg(2)-O(5)	173.30(7)
O(1)-Mg(1)-O(6)#1	165.33(7)	O(9)-Mg(2)-O(5)	79.63(5)
O(9)-Mg(1)-O(7)#2	151.19(7)	O(11)-Mg(2)-O(5)	95.46(7)
O(10)-Mg(1)-O(7)#2	95.21(7)	O(3)#3-Mg(3)-O(3)#5	180.00(9)
O(1)-Mg(1)-O(7)#2	85.54(6)	O(3)#3-Mg(3)-O(9)	90.46(5)
O(6)#1-Mg(1)-O(7)#2	83.49(6)	O(3)#5-Mg(3)-O(9)	89.54(5)
O(9)-Mg(1)-O(8)#2	92.30(6)	O(3)#3-Mg(3)-O(9)#1	89.54(5)
O(10)-Mg(1)-O(8)#2	154.14(7)	O(3)#5-Mg(3)-O(9)#1	90.46(5)
O(1)-Mg(1)-O(8)#2	89.52(6)	O(9)-Mg(3)-O(9)#1	180.0
O(6)#1-Mg(1)-O(8)#2	93.13(6)	O(3)#3-Mg(3)-O(5)	88.52(6)
O(7)#2-Mg(1)-O(8)#2	59.01(5)	O(3)#5-Mg(3)-O(5)	91.48(6)
O(4)#3-Mg(2)-O(8)#4	170.08(7)	O(9)-Mg(3)-O(5)	79.76(5)
O(4)#3-Mg(2)-O(2)	94.54(7)	O(9)#1-Mg(3)-O(5)	100.24(5)
O(8)#4-Mg(2)-O(2)	91.52(6)	O(3)#3-Mg(3)-O(5)#1	91.48(6)
O(4)#3-Mg(2)-O(9)	90.20(6)	O(3)#5-Mg(3)-O(5)#1	88.52(6)
O(8)#4-Mg(2)-O(9)	96.96(6)	O(9)-Mg(3)-O(5)#1	100.24(5)
O(2)-Mg(2)-O(9)	96.24(6)	O(9)#1-Mg(3)-O(5)#1	79.76(5)
O(4)#3-Mg(2)-O(11)	82.19(7)	O(5)-Mg(3)-O(5)#1	180.0

O(8)#4-Mg(2)-O(11)	90.04(7)

Symmetry transformations used to generate equivalent atoms: #1 -*x*+1,-*y*,-*z*+1; #2 *x*-1, *y*, *z*+1; #3 *x*+1, *y*, *z*; #4 -*x*+1,-*y*,-*z*; #5 -*x*,-*y*,-*z*+1; #6 x-1,*y*,*z*; #7 *x*+1, *y*, *z*-1; #8 -*x*-1,-*y*+1,-*z*+1; #9 -*x*,-*y*+1,-*z*+2.

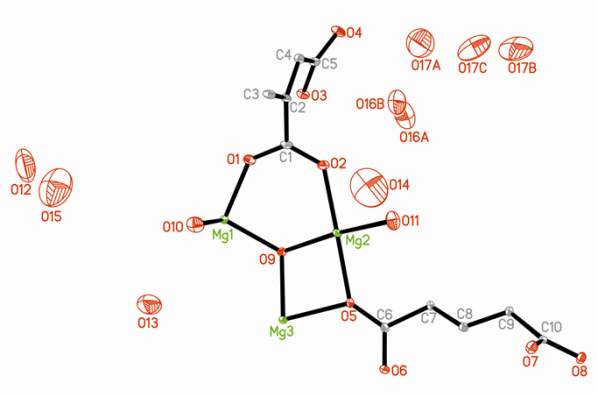

Fig. S1 *ORTEP* of the asymmetric unit of **1** (30% probability level).

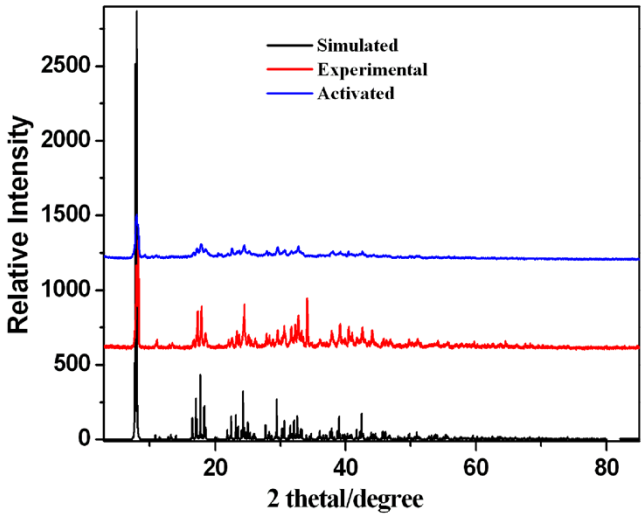

Fig. S2 The PXRD pattern of compound **1** is comparable to the simulated from the single crystal X-ray data and after activated at 100℃ for 5h, respectively.

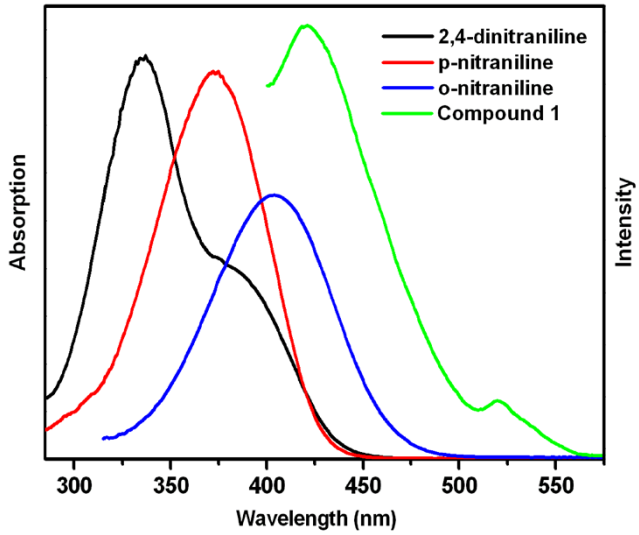

Fig. S3 PL emission spectrum of **1** and absorption spectra of 2,4-dinitraniline, O- and p-nitraniline in CH_3CH_2OH (1×10^{-5} M).

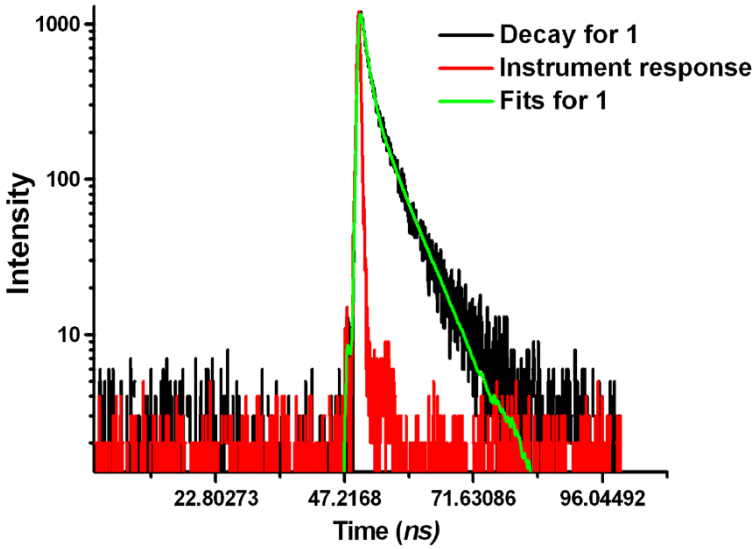

Fig. S4 The decay curve of compound **1**.

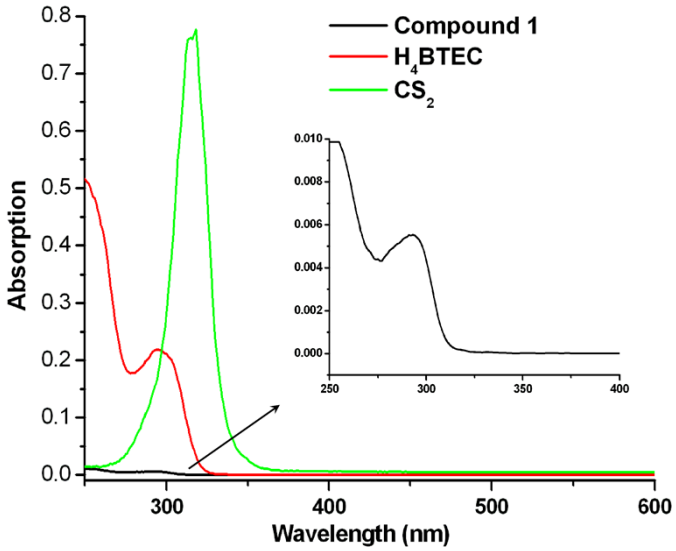

Fig. S5 Absorption spectra of compound **1**, H_4BTEC ligand and CS_2 in CH_3CH_2OH (1×10^{-5} M).

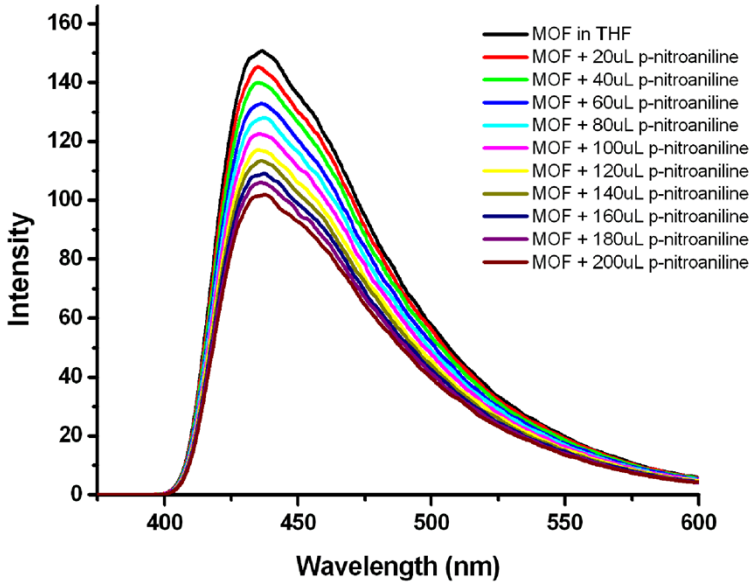

Fig. S6 PL spectra of compound **1** dispersed in THF by gradual addition of 10^{-3} M solution of p-nitraniline in ethanol.

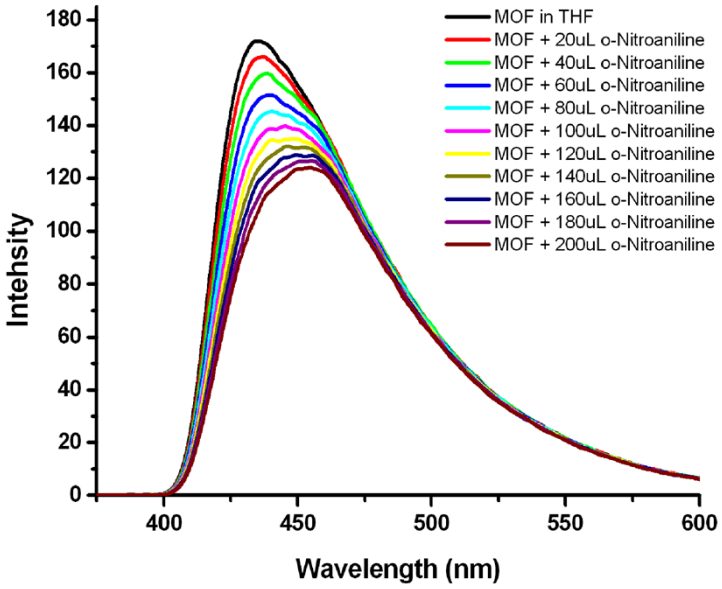

Fig. S7 PL spectra of compound **1** dispersed in THF by gradual addition of 10^{-3} M solution of o-nitraniline in ethanol.

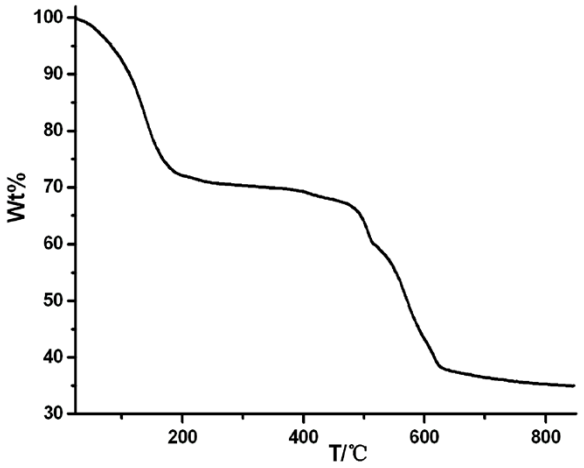

Fig. S8 TGA curves of compound **1**.

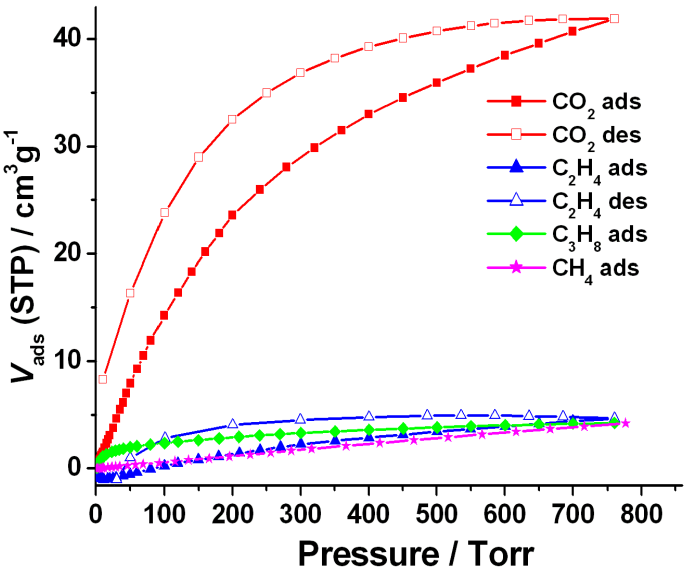

Fig. S9 The CO_2, CH_4, C_2H_4 and C_3H_8 adsorption isotherms of **1'** at room temperature.

Gas adsorption

As a good candidate for gas storage, the Mg-MOFs could provide a boost in reaching the mass percentage (wt%) of gas storage targets because of the lower density compared to the MOFs based on transition-metals.[1] Hence we investigated the gas adsorption behaviour of compound **1**. In the TG curve of **1** (Fig. S8), the first weight loss of 28.5% at about 220 °C corresponds to the loss of guest water molecules (calcd: 28.5%, corresponding to the solvent water molecules) and the BTEC ligand decomposes after 500 °C. In order to remove the guest water molecules, compound **1** was activated at 100 ºC under vacuum. The activated one (**1'**) has a high degree of crystallinity evidenced by the PXRD characterization (Fig. S2), which indicates the rigid framework of compound **1** still maintained. Gas adsorption measurements show that the CO_2 adsorption of **1'** exhibits the adsorption of 41.9 $cm^3 \cdot g^{-1}$ at 298.15 K and 1 atm (Fig. S9). In the same measurement conditions, while for other energy gases such as CH_4, C_2H_4 and C_3H_8, **1'** shows almost no adsorption behaviour. Compared to the former reported Mg-MOFs for CO_2 adsorption at lower 77K or 87K,[2] **1'** could selectively separate CO_2 from the energy gases at room temperature which may have the purification effects.

references

1 (a) D. Britt, H. Furukawa, B.Wang, T. G. Glover and O. M. Yaghi, *PNAS*, 2009, **106**, 20637; (b) M. Dinca and J. R. Long, *J. Am. Chem. Soc.*, 2005, 127, 9376; c) Y. P. He, Y. X. Tan and J. Zhang, *Cryst. Growth Des.* 2013, 13, 6.

2 Y. E. Cheon, J. Park and M. P. Suh, *Chem. Commun.* 2009, 5436.