A photoluminescent microporous metal organic anionic framework for nitroaromatic explosive sensing

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Table S1. Selected bond lengths (Å) and angles (deg) for **1**

In1—O2	2.112(6)	In2—O3	2.140(7)	In2—O5^{v}	2.434(7)
In1—O7^{ii}	2.175(6)	In2—O6^{v}	2.152(7)		
In1—O8^{ii}	2.278(5)	In2—O4	2.381(6)		
O2^{i}—In1—O2	117.2(3)	O3—In2—O3^{iv}	80.5(5)	O3—In2—O5^{v}	90.9(3)
O2—In1—O7^{ii}	112.7(3)	O3—In2—O6^{v}	138.0(3)	O6^{v}—In2—O5^{v}	53.9(2)
O2—In1—O7^{iii}	81.5(3)	O3—In2—O6^{vi}	110.0(3)	O6^{vi}—In2—O5^{v}	138.3(2)
O7^{ii}—In1—O7^{iii}	153.4(3)	O6^{v}—In2—O6^{vi}	89.4(4)	O4—In2—O5^{v}	78.4(2)
O2^{i}—In1—O8^{ii}	145.1(3)	O3—In2—O4	55.3(3)	O3—In2—O5^{vi}	79.4(2)
O2—In1—O8^{ii}	87.4(2)	O6^{v}—In2—O4	91.8(2)	O4—In2—O5^{vi}	102.22(19)
O7^{ii}—In1—O8^{ii}	65.5(3)	O6^{vi}—In2—O4	84.6(2)	O5^{v}—In2—O5^{vi}	167.3(3)
O2^{i}—In1—O8^{iii}	87.4(2)	O3—In2—O4^{iv}	129.5(3)		
O7^{ii}—In1—O8^{iii}	94.2(3)	O4—In2—O4^{iv}	174.9(3)		
O8^{ii}—In1—O8^{iii}	84.1(3)				

Symmetry transformations: (i) 1-x, y, 1.5-z; (ii) x, 1+y, z; (iii) 1-x, 1+y, 1.5-z; (iv) x, 2-y, 2-z; (v) 2-x, 1-y, 0.5+z; (vi) 2-x, 1+y, 1.5-z; (vii) 2-x, 1-y, -0.5+z; (viii) x, -1+y, z; (ix) 2-x, y, 1.5-z.

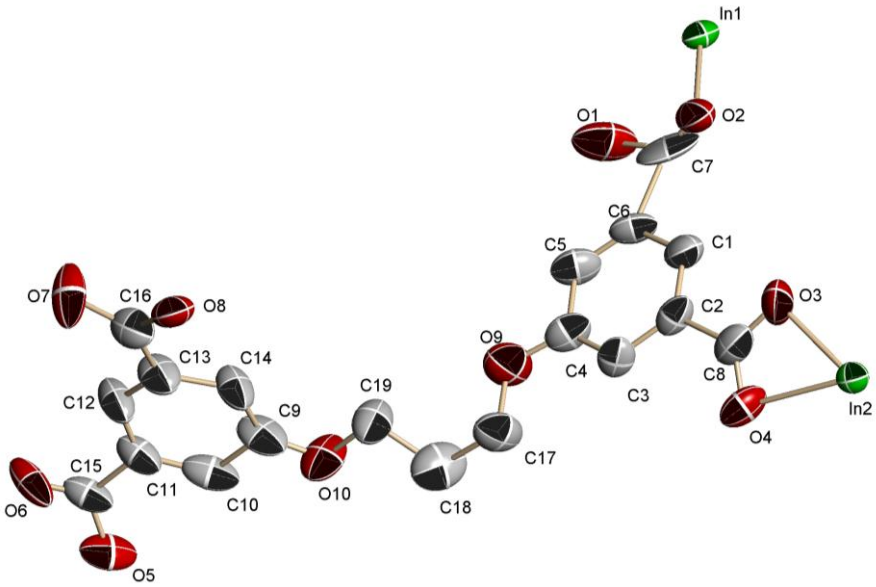

Fig. S1. An ORTEP drawing of the asymmetric unit of **1** (with thermal ellipsoids at 30% probability). The H atoms and guest molecules are omitted for clarity.

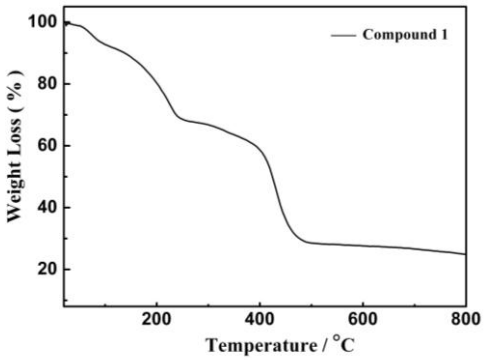

Fig. S2 TGA curve of compound **1**.

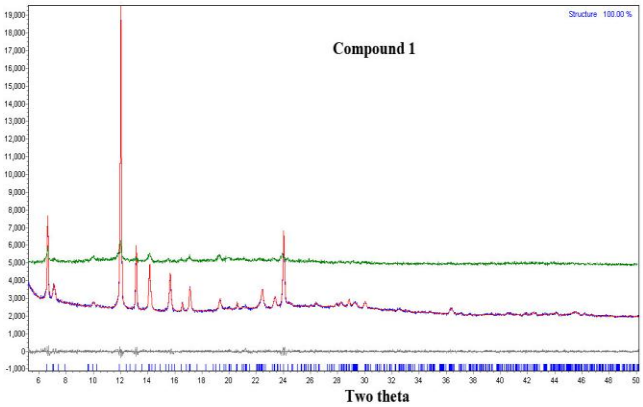

Fig. S3 PXRD patterns of **1**: The red, blue, and gray lines are the calculated, the as-synthesized and the difference between the calculated and the as-synthesized. The blue bars are the calculated brag positions. The best fitting results for **1**: a = 12.537(9), b = 13.483(5), c = 25.13(2) Å. The green line is that of the activated sample after gas adsorption measurements.

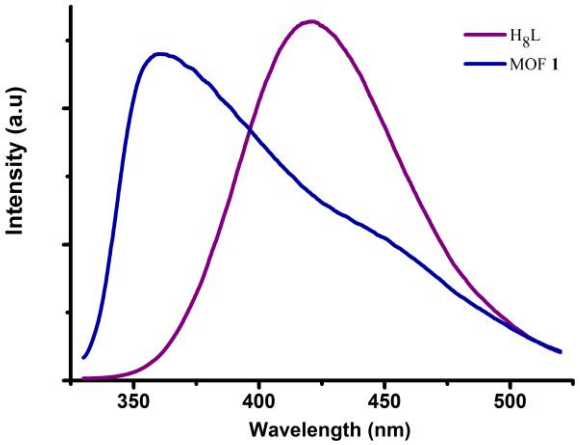

Fig. S4 Solid-state photoluminescent spectra of **1** and ligand H_8L at room temperature.