

A photoluminescent microporous metal organic anionic framework for nitroaromatic explosive sensing

Yun-Shan Xue,^a Ya-Bing He,^b Lian Zhou,^a Fei-Jian Chen,^a Yan Xu,^c Hong-Bin Du^{a*} Xiao-Zeng You^a, Bang-Lin Chen^b

^a State Key Laboratory of Coordination Chemistry, School of Chemistry and Chemical Engineering, Nanjing University, Nanjing, 210093, China. E-mail: hbdu@nju.edu.cn.

^b Department of Chemistry, University of Texas at San Antonio, Texas 78249-0698, USA. E-mail: banglin.chen@utsa.edu

^c Department of Chemistry, Nanjing University of Technology, Nanjing 210009, China.

Table S1. Selected bond lengths (\AA) 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.

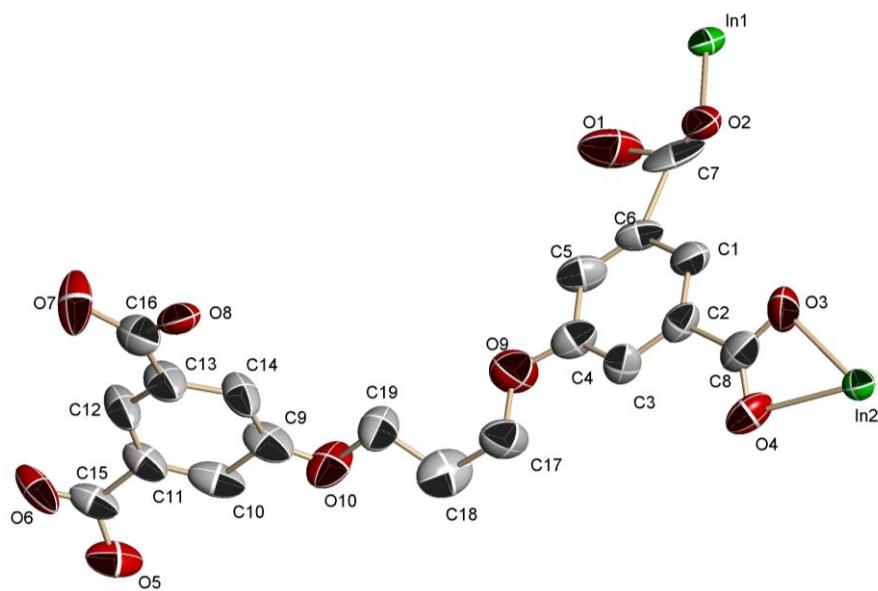


Fig. S1. An ORTEP drawing of the asymmetric unit of **1** (with thermal ellipsoids at 30% probability). The H atoms and guest molecules are omitted for clarity.

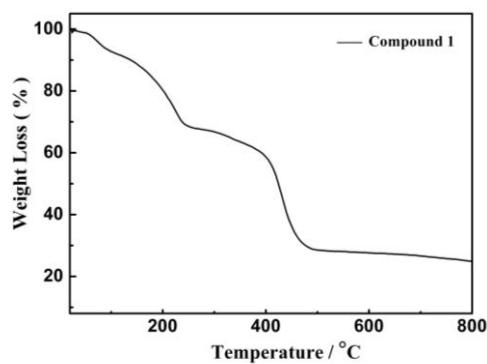


Fig. S2 TGA curve of compound **1**.

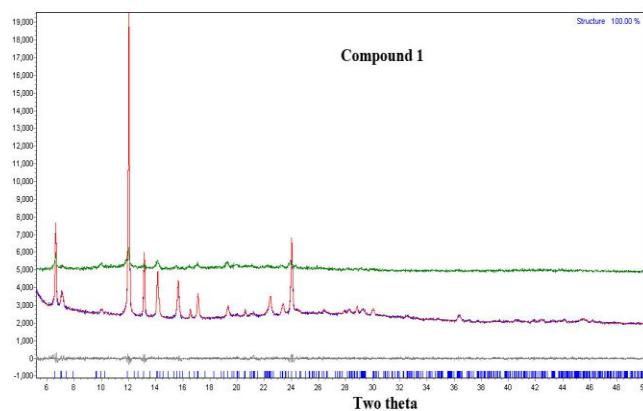


Fig. S3 PXRD patterns of **1**: The red, blue, and gray lines are the calculated, the as-synthesized and the difference between the calculated and the as-synthesized. The blue bars are the calculated brag positions. The best fitting results for **1**: $a = 12.537(9)$, $b = 13.483(5)$, $c = 25.13(2)$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

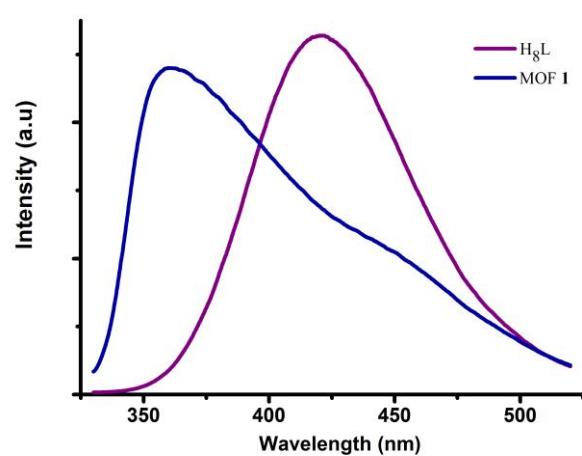


Fig. S4 Solid-state photoluminescent spectra of **1** and ligand H_8L at room temperature.