Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

A Non-interpenetrating Lead-Organic Framework with Large Channels Based on 1D Tube-Shaped SBUs

Fangna Dai,* Weidong Fan, Xue Yuan, Zhaodi Huang, Yutong Wang, Xuelian Xin, Huan Lin, Liangliang Zhang, Rongming Wang, Daofeng Sun*

State Key Laboratory of Heavy Oil Processing, College of Science, China University of Petroleum (East China), Qingdao, Shandong, 266580, People's Republic of China. Email: fndai@upc.edu.cn; dfsun@upc.edu.cn .

Synthesis of [$Pb_{1.5}$Cl L (H_2O)] •($EtOH)_2$• DMF (UPC-10):

H_2L (6.6 mg, 0.02 mmol) and $PbCl_2$ (11.0 mg, 0.04 mmol) were dissolved in 1.0 mL of mixed solvents of DMF and EtOH (2:1, v/v) in a beaker. After 1 drops of perchloric acid was added, the resulting light green solution was sealed in a glass tube, heated to 130 ℃ at a rate of 15 ℃/h, kept at 130 ℃ for 90 h, and then cooled to room temperature at a rate of 15 ℃/h. The resulting light green needle-shaped crystals of UPC-10 were collected by filtration, washed several times with EtOH, and dried in the air. (Yield: 55%.). Elemental analysis calcd (%) for **UPC-10**: C, 37.24 H, 5.09 N, 3.22; found: C: 37.05; H: 4.83; N: 3.39.

Table S1 Crystal data and structure refinement for UPC-10.

Empirical formula	$C_{20}H_{25}ClNO_5Pb_{1.5}$
Formula weight	705.65
Temperature/K	293(2)
Space group	I4/m
a/Å	33.2401(4)
b/Å	33.2401(4)
c/Å	5.88940(10)
α/°	90.00
β/°	90.00
γ/°	90.00
Volume/$Å^3$	6507.22(16)
Z	8
$\rho_{calc}g/cm^3$	1.441
μ/mm^{-1}	15.914
F(000)	2656.0
Crystal size/mm^3	0.1 × 0.1 × 0.1
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	7.52 to 134.06
Index ranges	$-39 \le h \le 39$, $-38 \le k \le 26$, $-5 \le l \le 7$
Reflections collected	9614
Data/restraints/parameters	3199/20/185
Goodness-of-fit on F^2	1.130
Final R indexes [I>=2σ (I)]	$R_1 = 0.0899$, $wR_2 = 0.2504$
Final R indexes [all data]	$R_1 = 0.0949$, $wR_2 = 0.2537$
Largest diff. peak/hole / e $Å^{-3}$	3.17/-4.19

Table S2. Selected bond lengths (Å) for **UPC-10.**

Atom	Atom	Length/Å
Pb1	O1	2.554(7)
Pb1	O1[1]	2.554(7)
Pb1	O2	2.585(6)
Pb1	O2[1]	2.585(6)
Pb1	Cl1[2]	3.0117(6)
Pb1	Cl1	3.0117(6)
Pb1	Cl1[3]	3.012(3)
Pb2	O2	2.406(7)
Pb2	O2[4]	2.406(7)
Pb2	O1[4]	2.499(8)
Pb2	O1	2.499(8)
Pb2	O3	2.70(3)
Pb2	Cl1[2]	2.910(3)

[1]+X,+Y,-Z; [2]+X,+Y,1+Z; [3]1/2+Y,1/2-X,-1/2-Z; [4]+X,+Y,1-Z.

Table S3. Selected bond angles (º) for **UPC-10**.

Atom	Atom	Atom	Angle/°		Atom	Atom	Atom	Angle/°
O1	Pb1	O1[1]	50.1(4)		O2[4]	Pb2	O1	155.7(2)
O1	Pb1	O2	72.1(2)		O1[4]	Pb2	O1	96.4(4)
O1[1]	Pb1	O2	92.7(2)		O2	Pb2	O3	99.2(3)
O1	Pb1	O2[1]	92.7(2)		O2[4]	Pb2	O3	99.2(3)
O1[1]	Pb1	O2[1]	72.1(2)		O1[4]	Pb2	O3	105.1(3)
O2	Pb1	O2[1]	49.7(3)		O1	Pb2	O3	105.1(3)
O1	Pb1	Cl1[2]	72.4(2)		O2	Pb2	Cl1[2]	80.77(16)
O1[1]	Pb1	Cl1[2]	121.70(19)		O2[4]	Pb2	Cl1[2]	80.77(16)
O2	Pb1	Cl1[2]	76.08(16)		O1[4]	Pb2	Cl1[2]	74.95(16)
O2[1]	Pb1	Cl1[2]	125.49(16)		O1	Pb2	Cl1[2]	74.95(16)
O1	Pb1	Cl1	121.70(19)		O3	Pb2	Cl1[2]	179.9(5)
O1[1]	Pb1	Cl1	72.4(2)		Pb2[5]	Cl1	Pb1	78.05(5)
O2	Pb1	Cl1	125.49(16)		Pb2[5]	Cl1	Pb1[5]	78.05(5)
O2[1]	Pb1	Cl1	76.08(16)		Pb1	Cl1	Pb1[5]	155.78(10)
Cl1[2]	Pb1	Cl1	155.78(10)		Pb2[5]	Cl1	Pb1[6]	152.36(10)
O1	Pb1	Cl1[3]	74.35(16)		Pb1	Cl1	Pb1[6]	99.67(5)
O1[1]	Pb1	Cl1[3]	74.35(16)		Pb1[5]	Cl1	Pb1[6]	99.67(5)
O2	Pb1	Cl1[3]	144.35(16)		C1	O1	Pb2	140.4(7)
O2[1]	Pb1	Cl1[3]	144.35(16)		C1	O1	Pb1	94.1(6)
Cl1[2]	Pb1	Cl1[3]	82.78(6)		Pb2	O1	Pb1	95.1(2)
Cl1	Pb1	Cl1[3]	82.78(6)		C7	O2	Pb2	145.8(7)
O2	Pb2	O2[4]	101.2(3)		C7	O2	Pb1	94.6(6)
O2	Pb2	O1[4]	155.7(2)		Pb2	O2	Pb1	96.6(2)
O2[4]	Pb2	O1[4]	76.1(2)		O2[4]	Pb2	O1	155.7(2)
O2	Pb2	O1	76.1(2)		O1[4]	Pb2	O1	96.4(4)

[1]+X,+Y,-Z; [2]+X,+Y,1+Z; [3]1/2+Y,1/2-X,-1/2-Z; [4]+X,+Y,1-Z; [5]+X,+Y,-1+Z; [6]1/2-Y,-1/2+X,-1/2+Z.

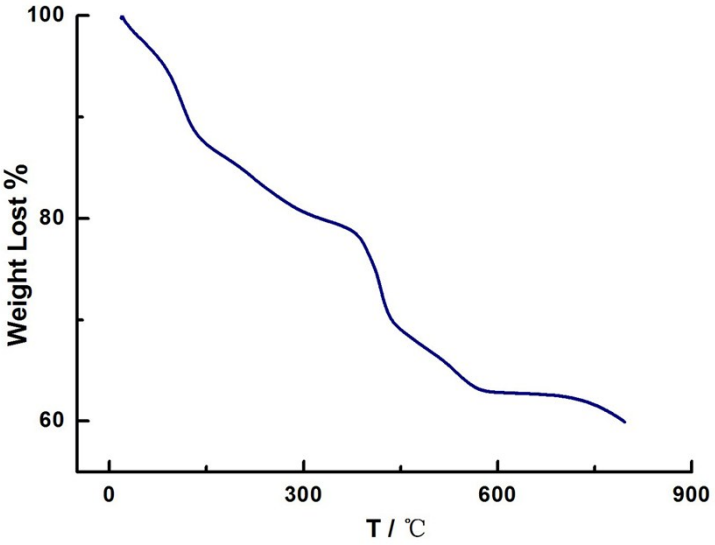

Fig S1. The TGA curve of **UPC-10**.

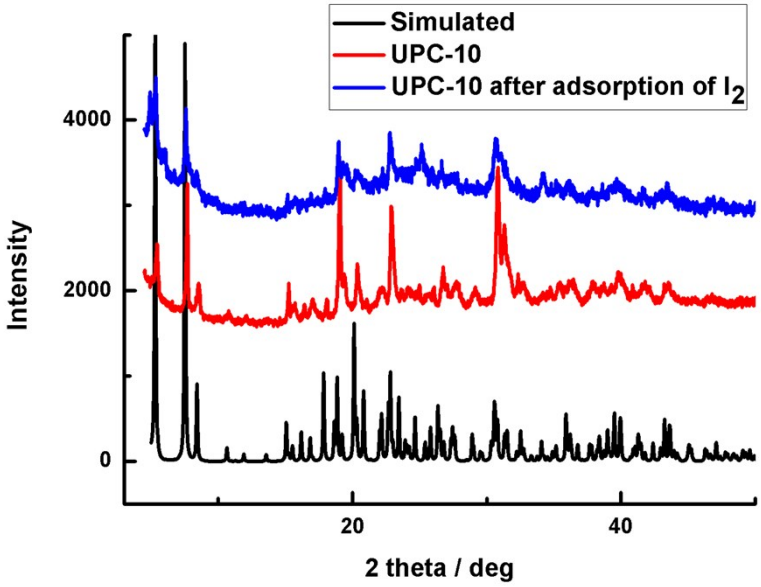

Fig S2. The XRD pattern of **UPC-10** before and after adsorption of I_2.

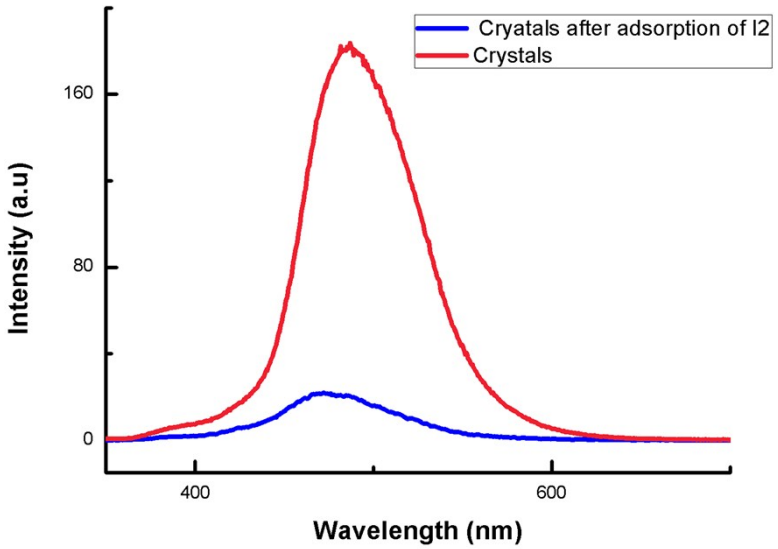

Fig S3. Fluorescence of **UPC-10** before and after adsorption of I_2.

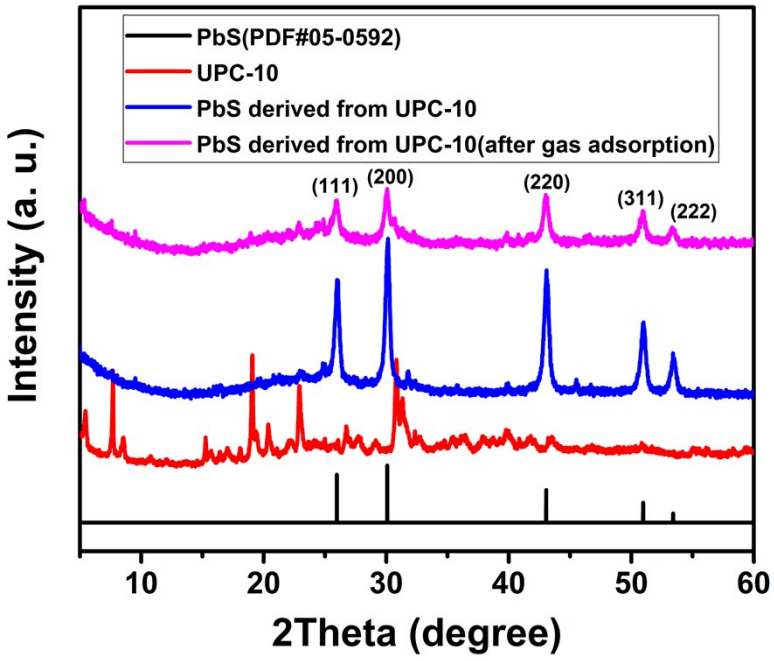

Fig S4. The XRD pattern of **UPC-10** and the derived PbS.

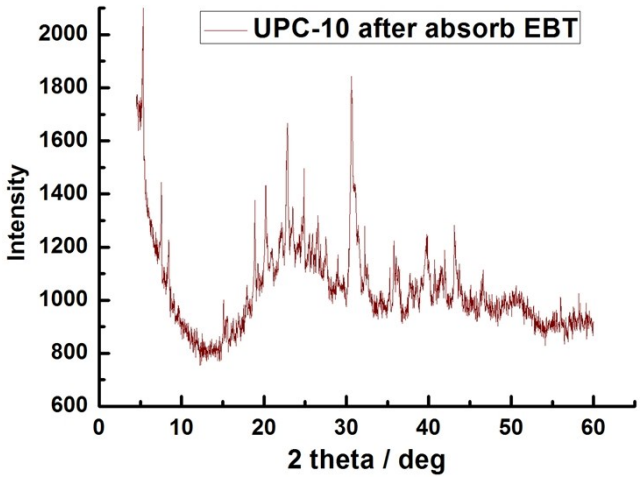

Fig S5. The XRD pattern of **UPC-10** after absorb EBT.

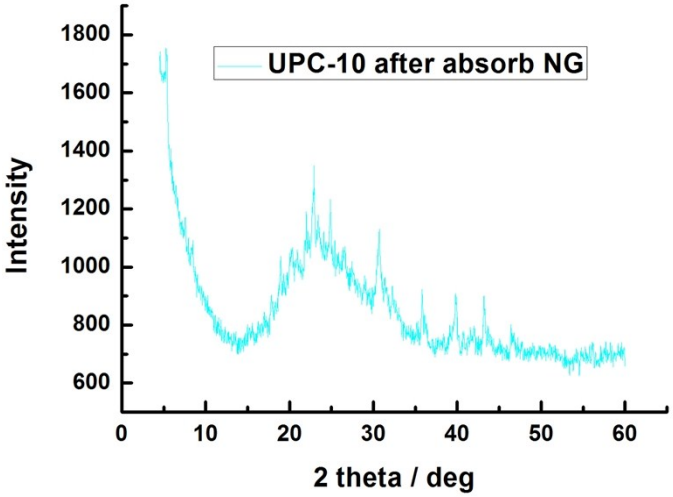

Fig S6. The XRD pattern of **UPC-10** after absorb the NG.

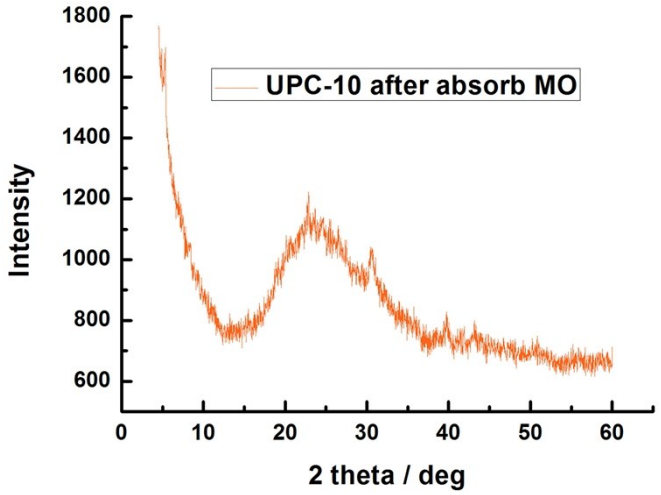

Fig S7. The XRD pattern of **UPC-10** after absorb the MO.