Electronic Supplementary Material for CrystEngComm

Supporting Information

An eight-connected 3D lead (II) MOF with octanuclear lead(II) as SBU: synthesis, structure and luminescent property

En-Cui Yang, Jian Li, Bin Ding, Qing-Qing Liang, Xiu-Guang Wang, and Xiao-Jun Zhao *

College of Chemistry and Life Science, Key Laboratory of Molecular Structure and Materials Performance, Tianjin Normal University, Tianjin 300387, People's Republic of China.

Experimental details:

All reagents were purchased commercially and used without further purification. Doubly deionized water was used for the conventional synthesis. Elemental analyses of carbon, hydrogen and nitrogen were carried out with a CE-440 (Leeman-Labs) analyzer. Fourier transform (FT) IR spectra (KBr pellets) were taken on an AVATAR-370 (Nicolet) spectrometer in the range 4000 – 400 cm^{-1} region. Thermogravimetric analysis (TGA) experiments were carried out on Shimadzu simultaneous DTG-60A compositional analysis instrument from room temperature to 800^{o}C under N_2 atmosphere at a heating rate of 5^{o}C/min. Fluorescence spectra of the polycrystalline powder samples were performed on a Cary Eclipse fluorescence spectrophotometer (Varian) equipped with a xenon lamp and quartz carrier at room temperature.

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

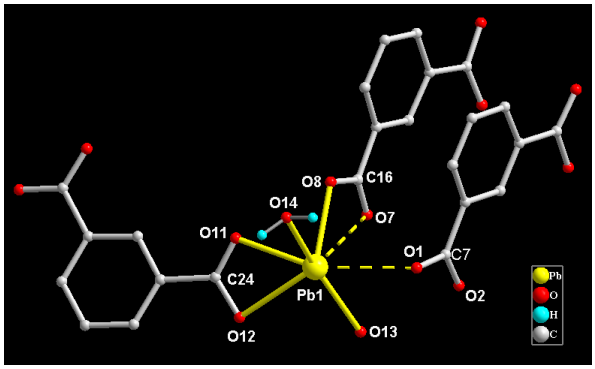
Pb(1)–O(8)#1	2.367(11)	Pb(2)–Pb(3)	3.5687(6)
Pb(1)–O(11)#2	2.475(10)	Pb(3)–O(13)	2.288(7)
Pb(1)–O(13)	2.557(8)	Pb(3)–O(9)	2.407(9)
Pb(1)–O(14)	2.655(12)	Pb(3)–O(2)	2.541(7)
Pb(1)–O(12)#2	2.734(11)	Pb(3)–O(3)#4	2.617(7)
Pb(2)–O(13)	2.255(7)	Pb(3)–O(1)	2.635(9)
Pb(2)–O(5)	2.454(8)	Pb(4)–O(13)	2.261(7)
Pb(2)–O(6)#3	2.537(9)	Pb(4)–O(3)#4	2.397(7)

Pb(2)–O(2)	2.543(8)	Pb(4)–O(10)	2.429(9)
Pb(2)–O(7)#1	2.668(12)	Pb(4)–O(12)#2	2.634(10)
O(8)#1–Pb(1)–O(11)#2	75.9(4)	O(5)–Pb(2)–O(2)	68.5(3)
O(8)#1–Pb(1)–O(13)	115.9(4)	O(6)#3–Pb(2)–O(2)	148.9(3)
O(11)#2–Pb(1)–O(13)	112.5(4)	O(13)–Pb(2)–O(7)#1	82.0(3)
O(8)#1–Pb(1)–O(14)	76.3(4)	O(5)–Pb(2)–O(7)#1	146.0(4)
O(11)#2–Pb(1)–O(14)	86.8(5)	O(6)#3–Pb(2)–O(7)#1	107.7(3)
O(13)–Pb(1)–O(14)	158.7(4)	O(2)–Pb(2)–O(7)#1	78.8(3)
O(8)#1–Pb(1)–O(12)#2	119.7(4)	O(13)–Pb(2)–Pb(3)	38.56(18)
O(11)#2–Pb(1)–O(12)#2	48.0(3)	O(5)–Pb(2)–Pb(3)	51.0(2)
O(13)–Pb(1)–O(12)#2	75.9(3)	O(6)#3–Pb(2)–Pb(3)	103.8(2)
O(14)–Pb(1)–O(12)#2	114.5(4)	O(2)–Pb(2)–Pb(3)	45.40(17)
O(13)–Pb(2)–O(5)	80.5(3)	O(7)#1–Pb(2)–Pb(3)	98.8(3)
O(13)–Pb(2)–O(6)#3	76.3(3)	O(13)–Pb(3)–Pb(2)	37.91(17)
O(5)–Pb(2)–O(6)#3	96.1(3)	O(9)–Pb(3)–Pb(2)	123.0(2)
O(13)–Pb(2)–O(2)	74.6(2)	O(2)–Pb(3)–Pb(2)	45.45(18)
O(13)–Pb(3)–O(9)	87.1(3)	O(3)#4–Pb(3)–Pb(2)	88.98(16)
O(13)–Pb(3)–O(2)	74.2(3)	O(1)–Pb(3)–Pb(2)	78.70(17)
O(9)–Pb(3)–O(2)	124.8(3)	O(13)–Pb(4)–O(3)#4	77.6(3)
O(13)–Pb(3)–O(3)#4	72.7(2)	O(13)–Pb(4)–O(10)	82.8(3)
O(9)–Pb(3)–O(3)#4	85.5(3)	O(3)#4–Pb(4)–O(10)	78.2(3)
O(2)–Pb(3)–O(3)#4	133.1(2)	O(13)–Pb(4)–O(12)#2	83.1(3)
O(13)–Pb(3)–O(1)	78.7(3)	O(3)#4–Pb(4)–O(12)#2	144.5(3)
O(9)–Pb(3)–O(1)	75.7(3)	O(10)–Pb(4)–O(12)#2	70.0(4)
O(2)–Pb(3)–O(1)	50.1(3)	O(3)#4–Pb(3)–O(1)	146.4(2)

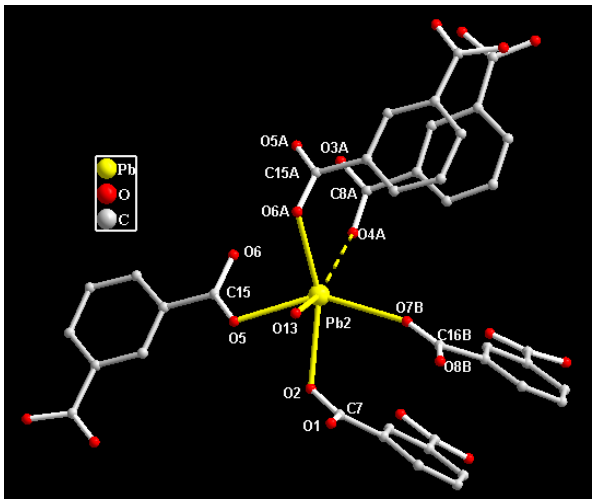
Symmetry codes: #1 $-x + 1, y + 1/2, -z + 3/2$; #2 $-x + 2, y + 1/2, -z + 3/2$; #3 $-x + 1, -y + 1, -z + 1$; #4 $-x + 1, y - 1/2, -z + 3/2$.

Table S2 Hydrogen–Bonding Geometry (Å, °) for **1.**

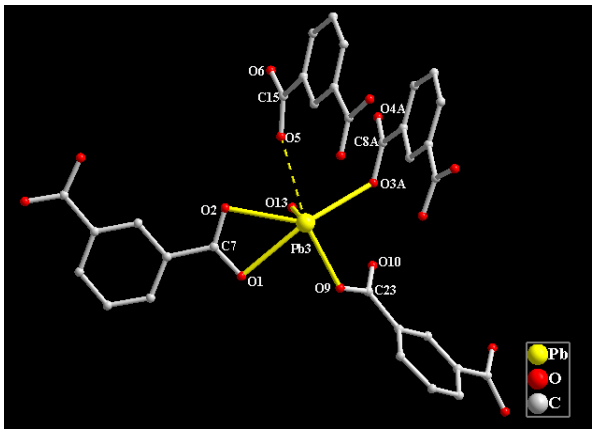
D–H···A	D–H	H···A	D···A	D–H···A
1				
C(2)–H(2)···O(3)	0.93	2.43	2.758(8)	100.0(1)
C(12)–H(12)···O(8)	0.93	2.43	2.745(1)	100.0(1)


O8
C16
O14
O7
O11
O1
C7
C24
Pb1
O2
O12
O13
Pb
O
H
C

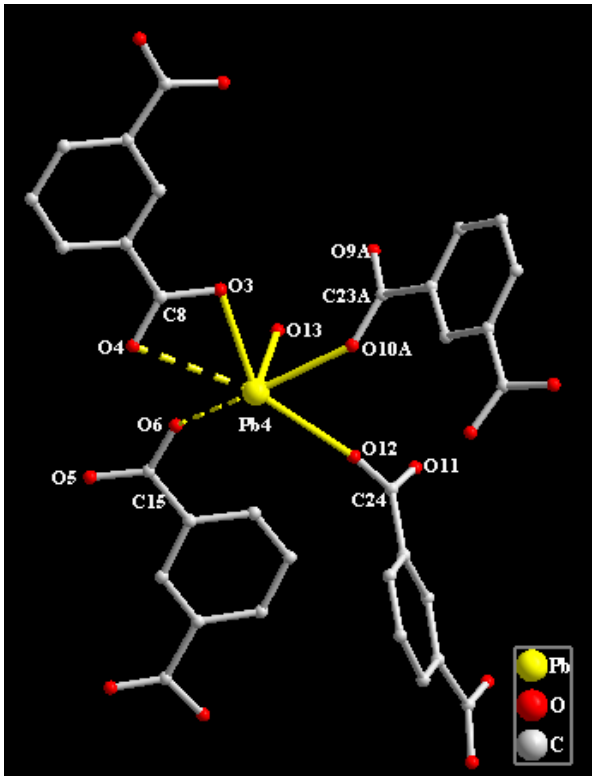
（a）


O5A
O3A
C15A
C8A
O6A
O4A
O6
C15
O7B
O13
Pb2
C16B
O5
O8B
O2
C7
O1
Pb
O
C

（b）


O6
C15
O4A
O5
C8A
O3A
O13
O2
C7
Pb3
O10
O1
O9
C23
Pb
O
C

(c)



(d)

Figure S1 Coordination geometry of (a) Pb1 (b) Pb2 (c) Pb3 and (d) Pb4 with Pb···O weak interactions (yellow dash line).

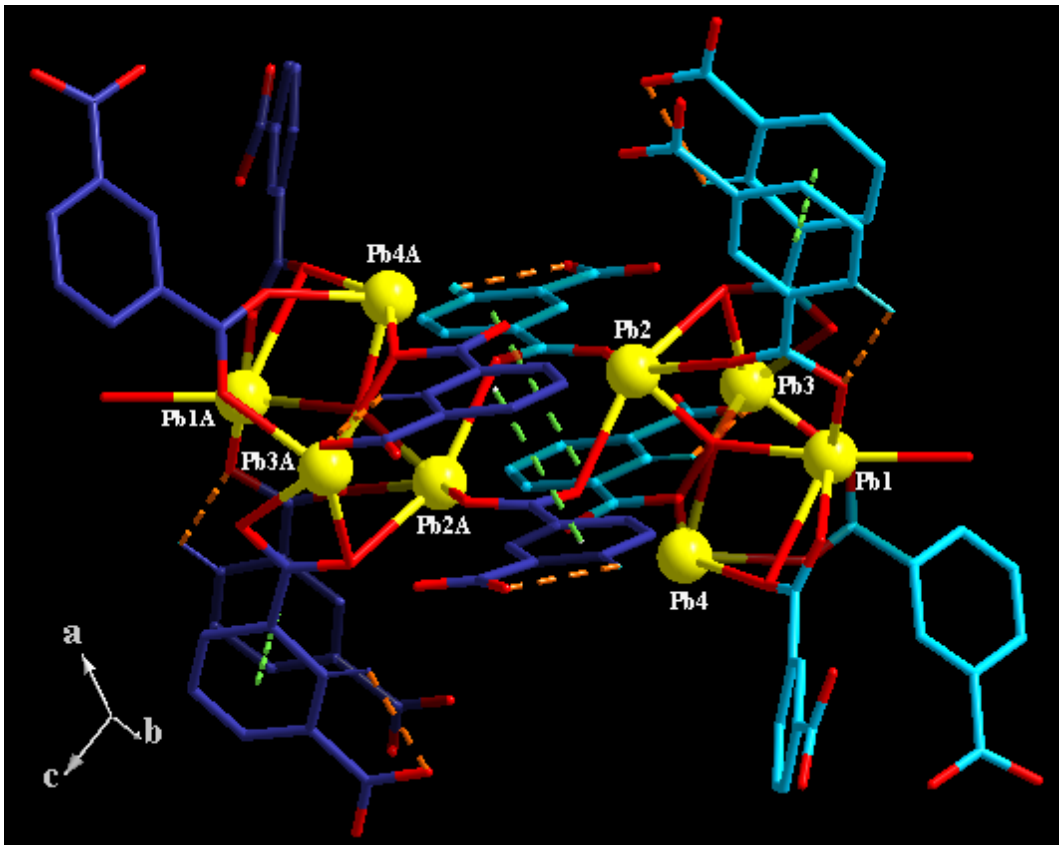


Figure S2 Octanuclear lead(II) SBU with intramolecular π···π stack (green dash line) and C–H···O(orange dash line) weak interactions.

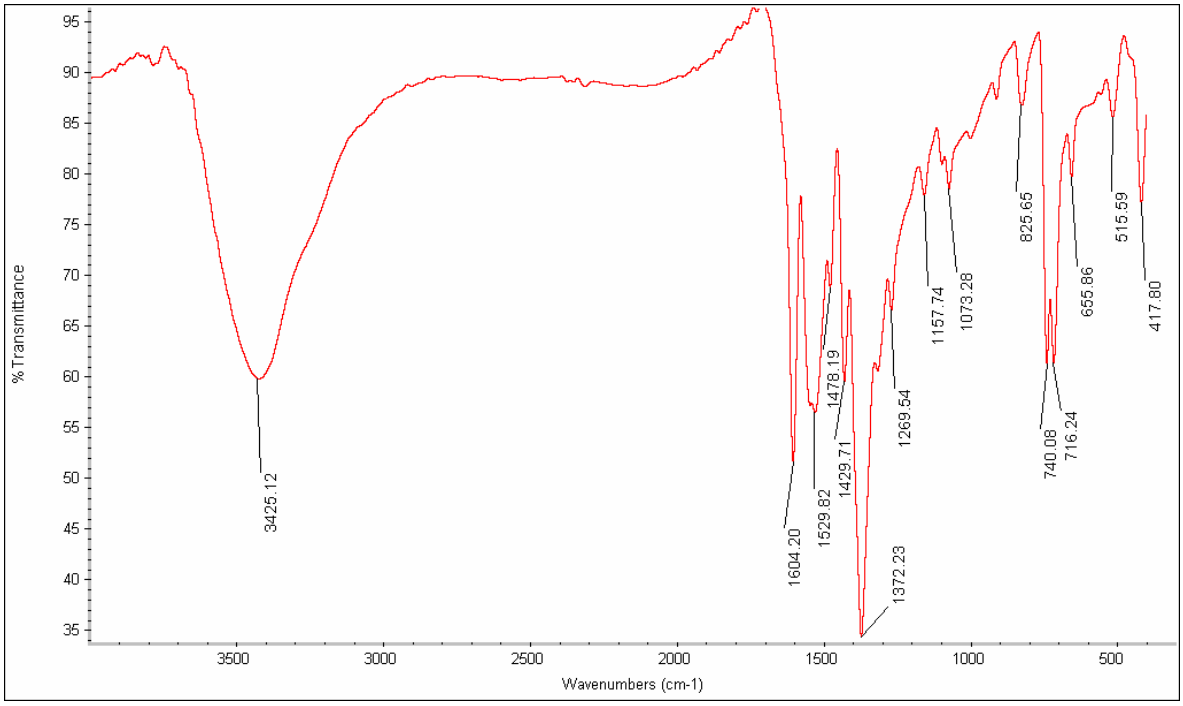


Figure S3 IR spectrum of **1**.

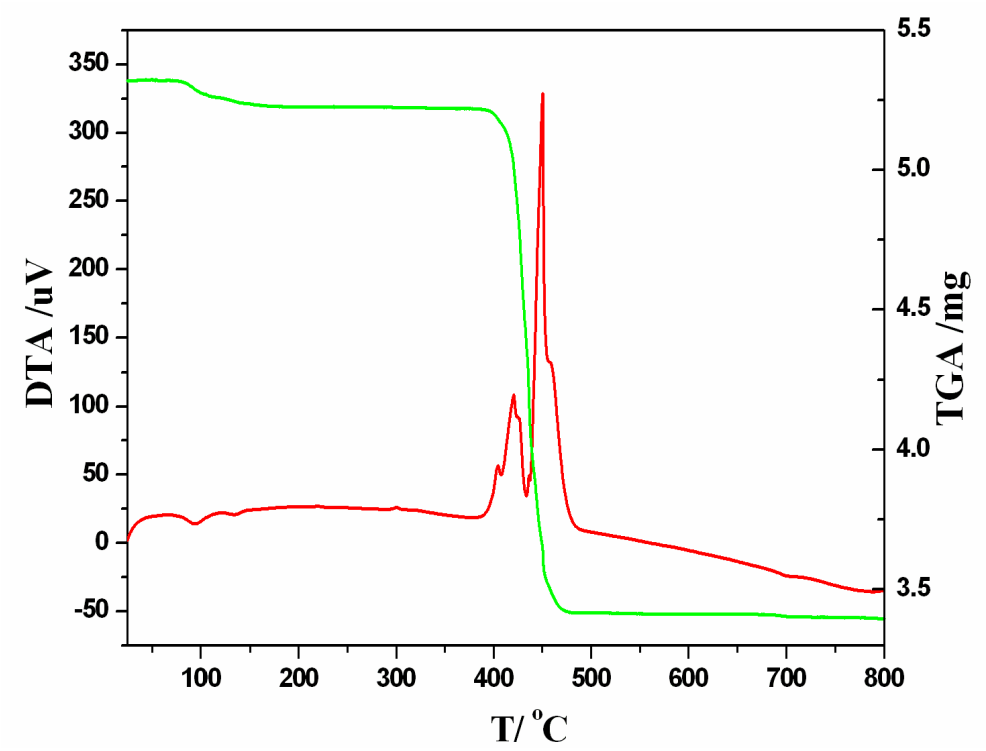


Figure S4. TG-DTA plot of **1**.