Supporting Information

Phosphorescence emission and fine structure observed respectively at ambient condition and *ca.* 55 K in a coordination polymer of lead(II)-thiophenedicarboxylate

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Table S1. Selected Bond Lengths (Å) and Bond Angles (°) for CP**1**.

Pb1-O1	2.660(13)	O1-Pb1-1i	85.6(4)
Pb1-O1i	2.527(15)	O1-Pb1-O2ii	108.3(5)
Pb1-O1iv	2.527(15)	O1-Pb1-O2iii	71.8(5)
Pb1-O1v	2.660(13)	O1-Pb1-O1iv	94.4(4)
Pb1-O2ii	2.660(16)	O1-Pb1-O1v	180.00
Pb1-O2iii	2.660(16)	O1i-Pb1-O2ii	91.0(5)
Pb1-O2vi	3.050(10)	O1v-Pb1-O2iii	89.0(5)

Symmetry transformations used to generate equivalent atoms:

i= x,-y,-1/2+z; *ii*= x,1-y,-1/2+z; *iii*= 1/2-x,-1/2+y,1/2-z; *iv*= 1/2-x,1/2+y,1/2-z; *v* = 1/2-x,1/2-y,-z ; *vi*= x, −y, 1/2+z

Table S2: Comparison of bond lengths (Å) and angles (°) in the geometry optimization and single crystal structures of CP**1**.

MOF-**1**		OPT-**1**	
Pb1-O1	2.660(13)	Pb1-O1	2.6171
Pb1-O1i	2.527(15)	Pb1-O1i	2.5608
Pb1-O2ii	2.660(16)	Pb1-O2ii	2.6118
Pb1-O2iii	2.660(16)	Pb1-O2iii	2.6118
Pb1-O1iv	2.527(15)	Pb1-O1iv	2.5608
Pb1-O1v	2.660(13)	Pb1-O1v	2.6171
S1-C2	1.666(16)	S1-C2	1.7059
O1-Pb1-O1i	85.6(4)	O1-Pb1-1i	86.00
O1-Pb1-O2ii	108.3(5)	O1-Pb1-O2ii	107.24
O1-Pb1-O2iii	71.8(5)	O1-Pb1-O2iii	72.76
O1-Pb1-O1iv	94.4(4)	O1-Pb1-O1iv	94.00
O1-Pb1-O1v	180.00	O1-Pb1-O1v	180.00
O1i-Pb1-O2ii	91.0(5)	O1i-Pb1-O2ii	89.37
O1i-Pb1-O2iii	89.0(5)	O1i-Pb1-O2iii	90.63

Symmetry transformations used to generate equivalent atoms:

i= x,-y,-1/2+z; *ii*= x,1-y,-1/2+z; *iii*= 1/2-x,-1/2+y,1/2-z; *iv*= 1/2-x,1/2+y,1/2-z; *v* = 1/2-x,1/2-y,-z ; *vi*= x, −y, 1/2+z

[1] G. M. Sheldrick, SHELXTL, Structure Determination Software Suite, Bruker AXS, Madison, WI, 2003.

[2] A. L. Spek, PLATON, A multipurpose crystallographic tool, Utrecht University, The Netherlands, 2001.

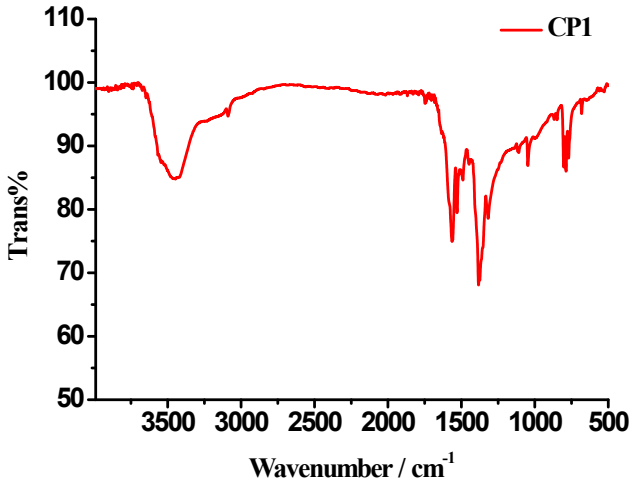

Fig. S1: IR spectrum of CP**1** recorded from a KBr pellet.

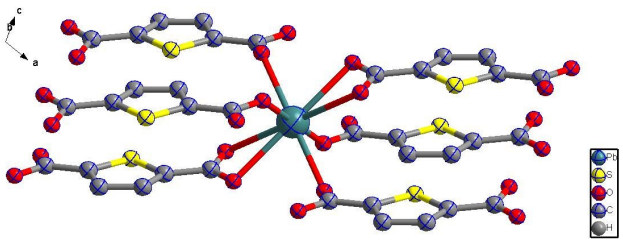

Fig. S2: Coordination mode of Pb^{II} in CP**1**.

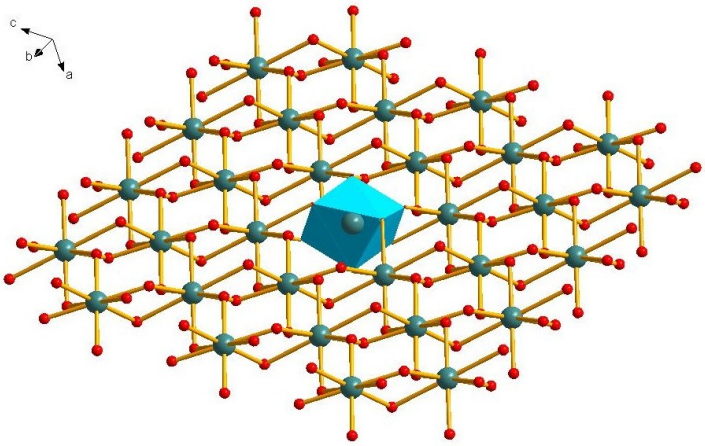

Fig. S3: 2D layer structure constructed by PbO_8 unit.

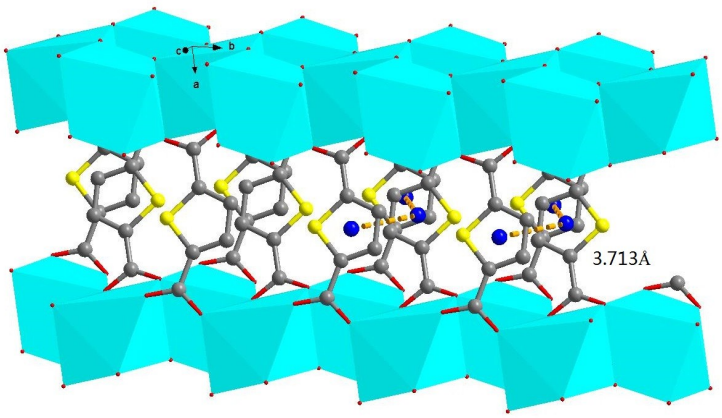

Fig. S4: The relationship of adjacent thiophene ring in CP**1**

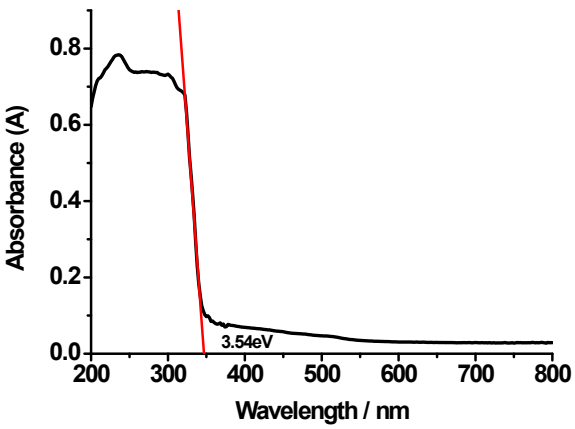

Fig. S5: UV–visible spectra of CP**1** in the solid state at room temperature.

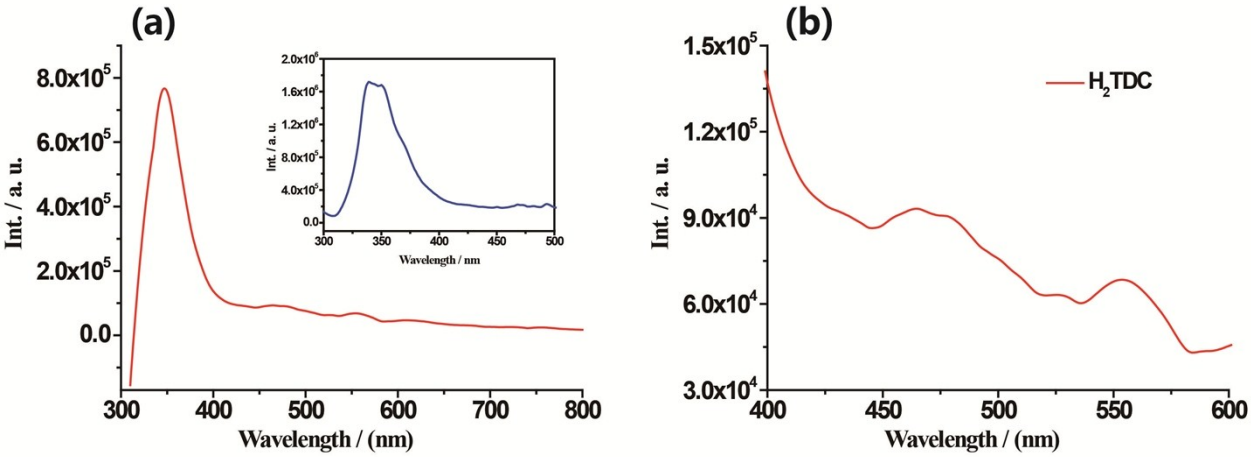

Fig. S6: The solid state photoluminescence emission spectra of H_2TDC at room temperature with excite spectra as insert.

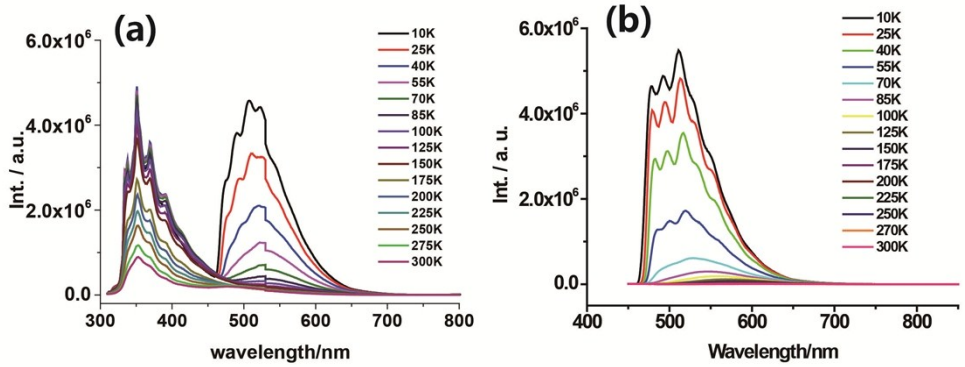

Fig. S7 Temperature-dependent (10–300 K) solid-state emission spectra of H_2TDC excited under UV light with λ_{ex} = 292 nm (a) and CP**1** excited under UV light with λ_{ex} = 250 nm(b).

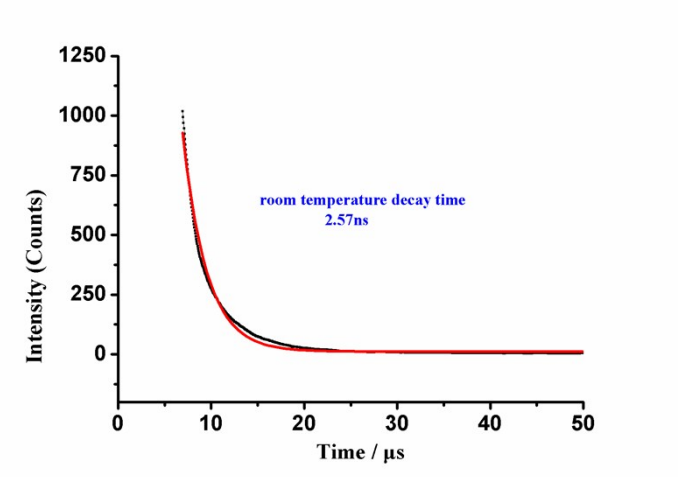

Fig. S8 Emission decay of H_2TDC (around 555nm) obtained at room temperature upon pulsed excitation at 292 nm, where the red lines and the black squares represent the fitting curves and the experimental data.

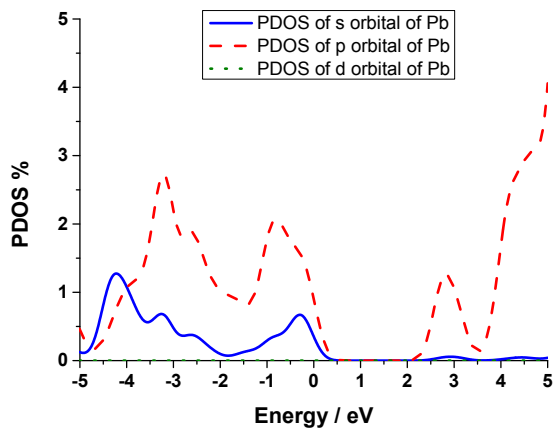

Fig. S9: PDOS of Pb^{2+} ions near the Fermi level in CP**1**.