Electronic Supplementary Information (ESI)

Exploring thiophene-2-acetate and thiophene-3-acetate binding modes towards the molecular, supramolecular structures and photoluminescence properties of Pb(II) polymers

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

Bond lengths (Å)							
Pb1–O2	2.451(5)	Pb1–O3	2.528(4)	Pb1–O1	2.658(5)	Pb1–O5	2.732(5)
Pb1–O4	2.482(4)	Pb1–O4^{ii}	2.579(5)	Pb1–O3^{i}	2.660(4)		
Bond angles (°)							
O1–Pb1–O3^{i}	77.6(1)	O3^{i}–Pb1–O3	69.3(1)	O5–Pb1–O2	146.0(1)		
O1–Pb1–O5	150.8(1)	O3^{i}–Pb1–O4	117.8(1)	O3–Pb1–O4	51.7(1)		
O1–Pb1–O3	79.7(1)	O3^{i}–Pb1–O4^{ii}	153.3(1)	O3–Pb1–O4^{ii}	115.1(1)		
O1–Pb1–O4	106.4(1)	O3^{i}–Pb1–O2	127.5(1)	O3–Pb1–O2	89.9(1)		
O1–Pb1–O4^{ii}	128.7(1)	O5–Pb1–O3	77.5(1)	O4–Pb1–O4^{ii}	63.8(1)		
O1–Pb1–O2	50.8(1)	O5–Pb1–O4	72.6(1)	O4–Pb1–O2	74.8(1)		
O3^{i}–Pb1–O5	77.5(1)	O5–Pb1–O4^{ii}	78.1(1)	O4^{ii}–Pb1–O2	79.1(1)		

Symmetry codes: (i) 2-x, 1-y, 1-z; (ii) 1-x, 1-y, 1-z.

Table S2. Selected bond lengths (Å) and angles (°) for complex **2**.

Bond lengths (Å)					
Pb1–O1	2.405(5)	Pb1–O2	2.562(5)	Pb1–O1^{ii}	2.657(6)
Pb1–O1^{i}	2.405(5)	Pb1–O2^{i}	2.562(5)	Pb1–O1^{iii}	2.657(6)
Bond angles (°)					
O1–Pb1–O2	52.6(2)	O2–Pb1–O1^{ii}	76.5(2)	O1^{ii}–Pb1–O2^{i}	108.7(2)
O1–Pb1–O1^{ii}	122.0(2)	O2–Pb1–O1^{iii}	168.4(2)	O1^{ii}–Pb1–O1^{i}	67.8(2)
O1–Pb1–O1^{iii}	67.8(2)	O2–Pb1–O2^{i}	108.7(2)	O1^{iii}–Pb1–O2^{i}	76.5(2)
O1–Pb1–O2^{i}	85.5(2)	O2–Pb1–O1^{i}	86.5(2)	O1^{iii}–Pb1–O1^{i}	122.0(2)
O1–Pb1–O1^{i}	81.7(2)	O1^{ii}–Pb1–O1^{iii}	168.4(2)	O2^{i}–Pb1–O1^{i}	52.6(2)

Symmetry codes (i) 0,5-x, y, 1-z; (ii) x, 0,5-y, -0,5+z; (iii) 0,5-x, 0,5-y, 1,5-z.

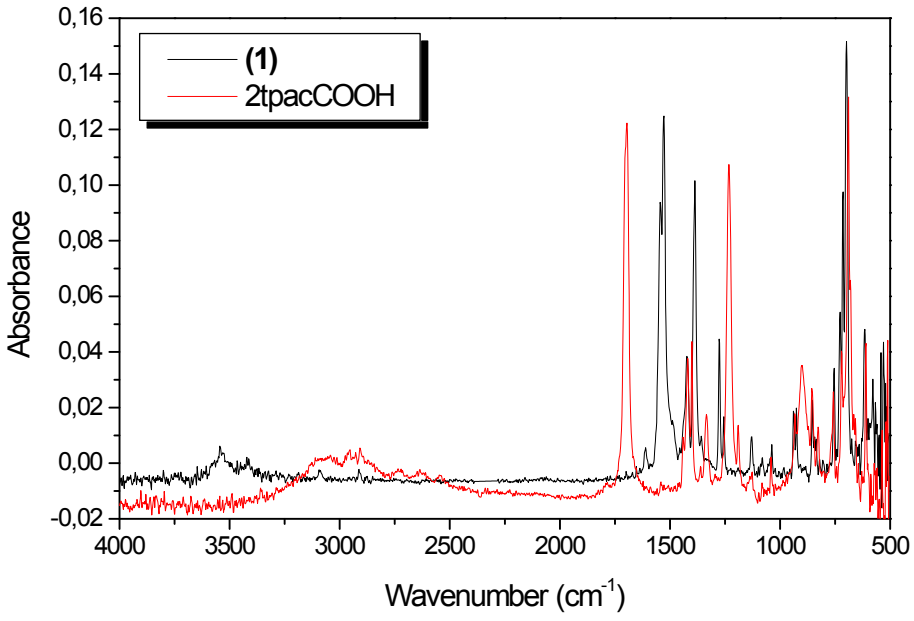

Fig. S1 The FT-IR spectra for the starting ligand and the complex **1**.

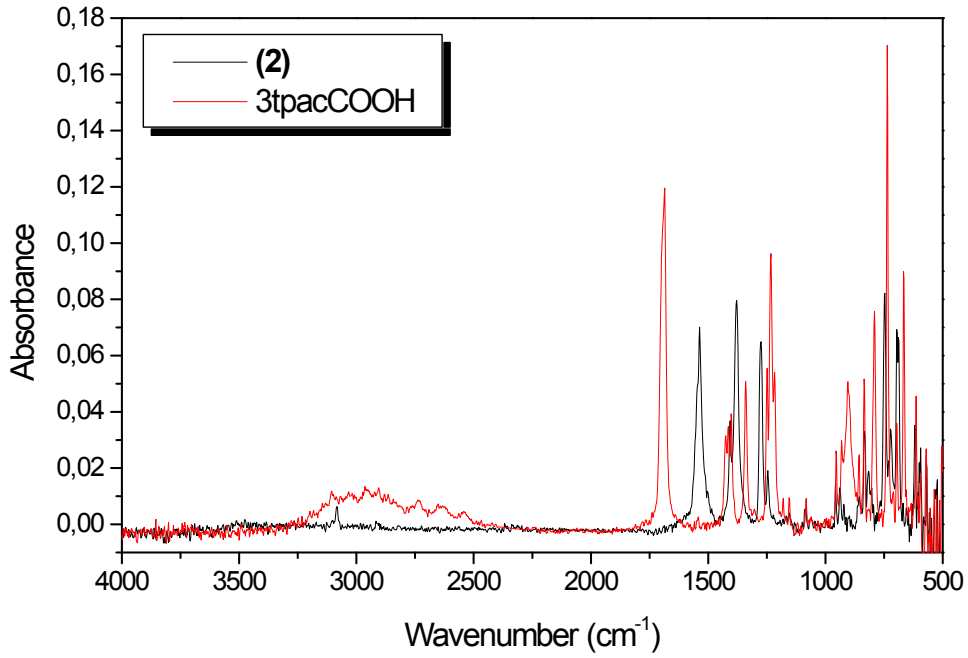

Fig. S2 The FT-IR spectra for the starting ligand and the complex **2**.