

Two novel emissive Pb(II) coordination polymers: Syntheses, structures, properties and WLED application

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Materials and methods

All the reagents and solvents used for the synthesis in this work were of analytical grade, purchased from commercial sources, and did not require further purification. Elemental analysis of C, H and N was carried out using a EuroVector EA3000 elemental analyzer. FT-IR was measured in the range 4000-400 cm^{-1} on a Mattson Alpha-Centauri spectrometer. PXRD patterns were obtained on a PANalytical X-ray diffractometer model X'pert3 with graphite monochromatized Cu $K\alpha$ radiation ($\lambda = 0.15405 \text{ nm}$) at the 2θ region 5-50°. The luminescence properties of the compounds were tested by a Hitachi F-4600 fluorescence spectrometer at ambient temperature. UV-vis absorption spectra were collected from a finely ground sample using a Cary 500 spectrophotometer.

X-ray crystallography

The X-ray diffraction measurement for compounds **1–2** was attained at 293 K on a Bruker D8 Quest diffractometer with graphite monochromated Mo $K\alpha$ radiation ($\lambda = 0.71073 \text{ \AA}$), and absorption corrections were applied by using multi-scan program. All the structures were solved and refined by the SHELXL-2018/3 program within OLEX2.^{1,2} The ordered non-hydrogen atoms in each structure were refined with anisotropic displacement parameters, while the hydrogen atoms were placed in idealized positions and allowed to ride on the relevant carbon atoms. The disordered

atoms of Pb(II) were refined with the PART instructions. Selected bond lengths and bond angles for compounds **1-2** are given in Tables S1–S2.

Bond length deviation (Δd) calculations

$$\Delta d = \frac{1}{n} \sum_{n=1}^n [(d_n - d_0)/d_0]^2 \quad (1)$$

The average bond length of the Pb-X (N or O) bonds is denoted as d_0 , the individual bond lengths are represented by d_n , and n is the number of Pb-X bond.

WLED Device Fabrication

Compound **1** was mixed with commercial phosphor BaMgAl₁₀O₁₇:Eu by pouring sealant, and the mixture was stirred for 15 min. Then the mixture was encapsulated onto a 365 nm UV LED chip. The obtained devices were dried under 40 °C in a vacuum oven. Electroluminescence (EL) spectra of the WLEDs under 60 mA were recorded at room temperature with a SPIC-300BW.

References

- 1 O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, *J. Appl. Cryst.*, 2009, **42**, 339-341.
- 2 G.M. Sheldrick, *Acta Crystallogr. C*, 2015, **71**, 3-8.

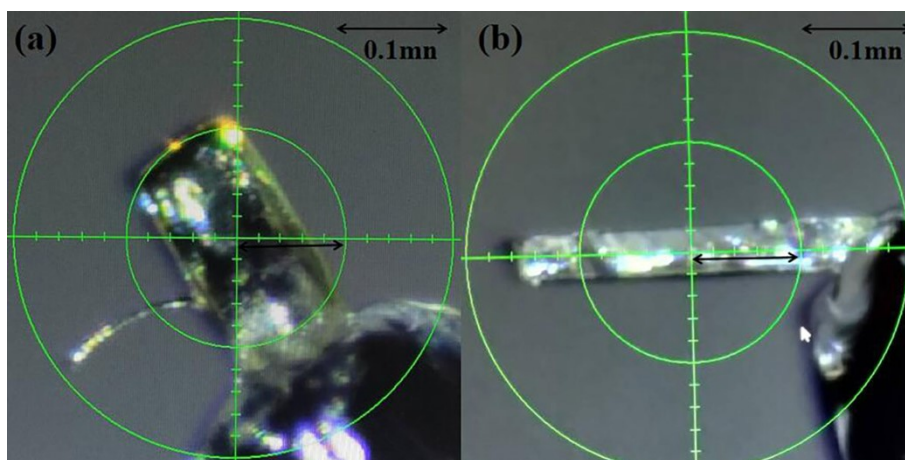


Fig. S1. The photographs of compounds **1-2**.

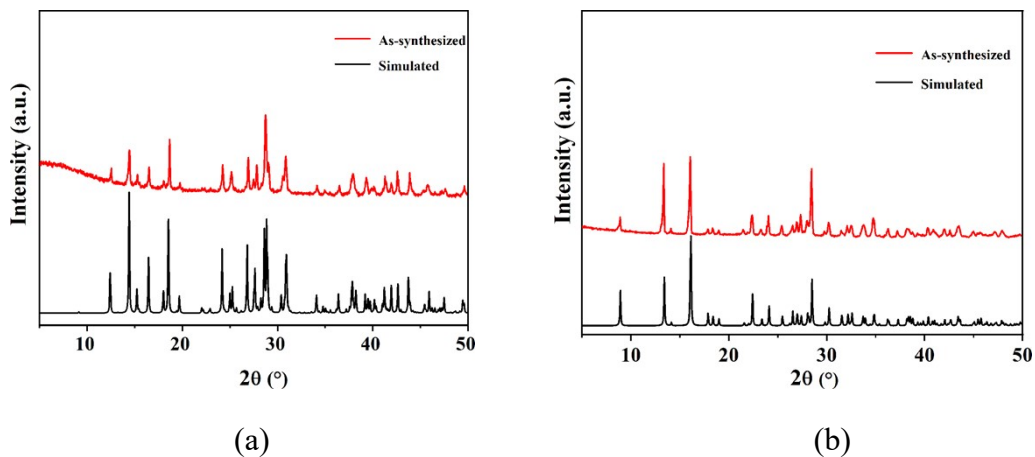


Fig. S2 (a) PXRD patterns of compound 1. (b) PXRD patterns of compound 2.

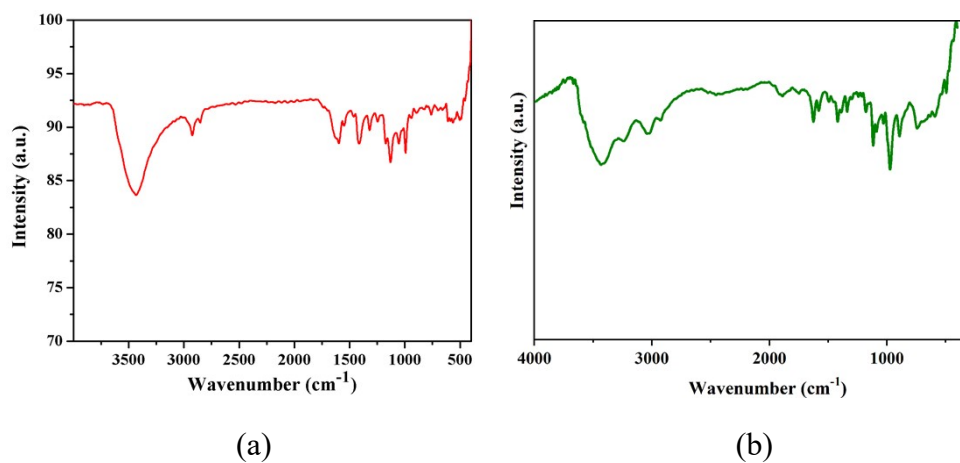
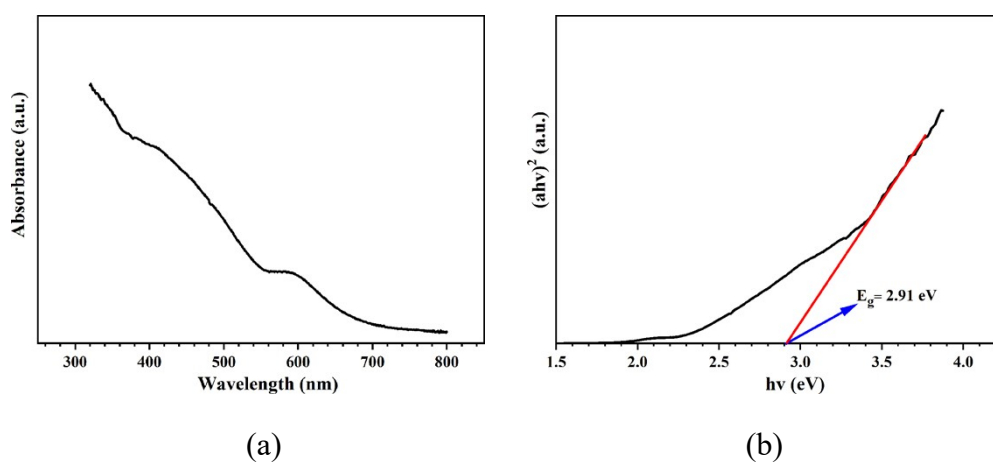


Fig. S3 (a) IR spectrum of compound 1. (b) IR spectrum of compound 2.



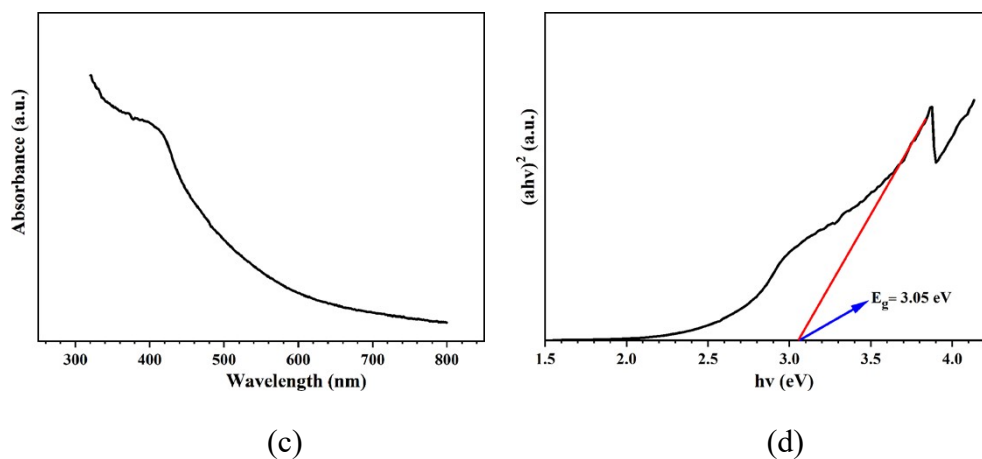


Fig. S4 (a) and (b) Solid-state UV-visible absorption spectra of compound **1**. (c) and (d) Solid-state UV-visible absorption spectra of compound **2**.

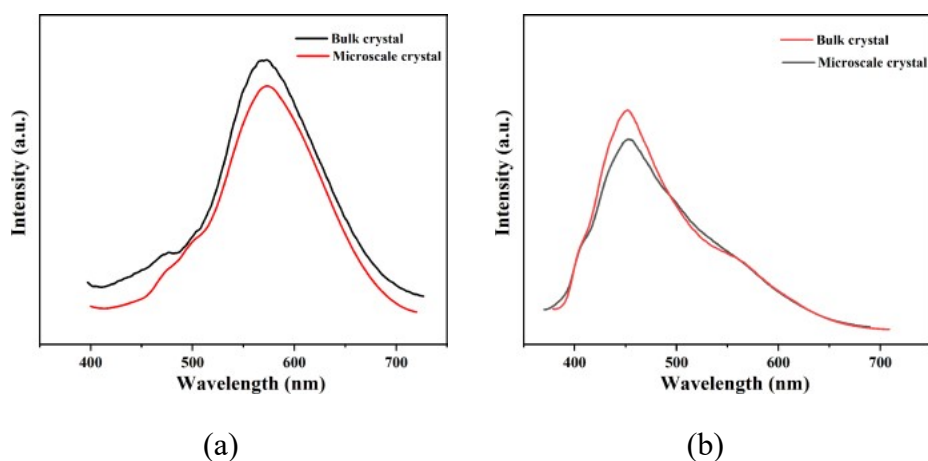


Fig. S5 (a) PL emission spectra of the respective bulk crystals and crystal powders of compound **1**. (b) PL emission spectra of the respective bulk crystals and crystal powders of compound **2**.

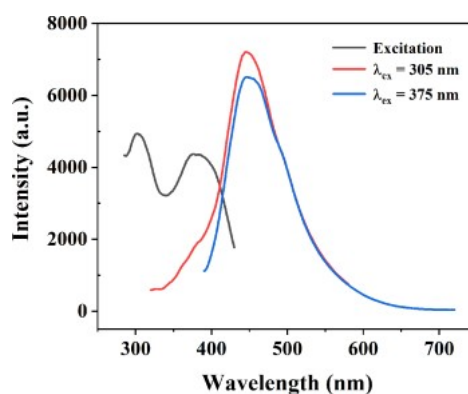


Fig. S6 Excitation and emission spectra of H₃L ligand.

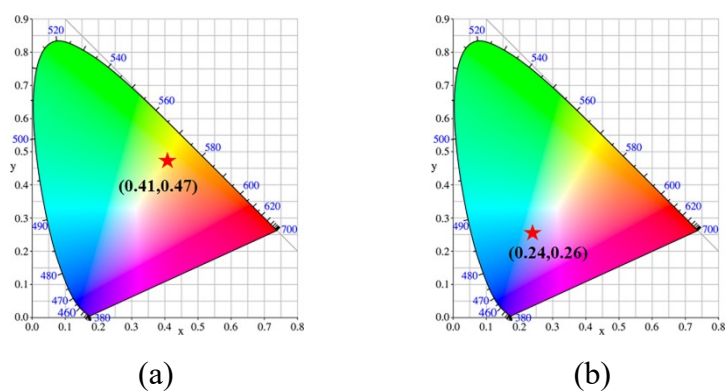


Fig. S7 (a) the CIE chromaticity diagrams for compound **1**. (b) the CIE chromaticity diagrams for compound **2**.

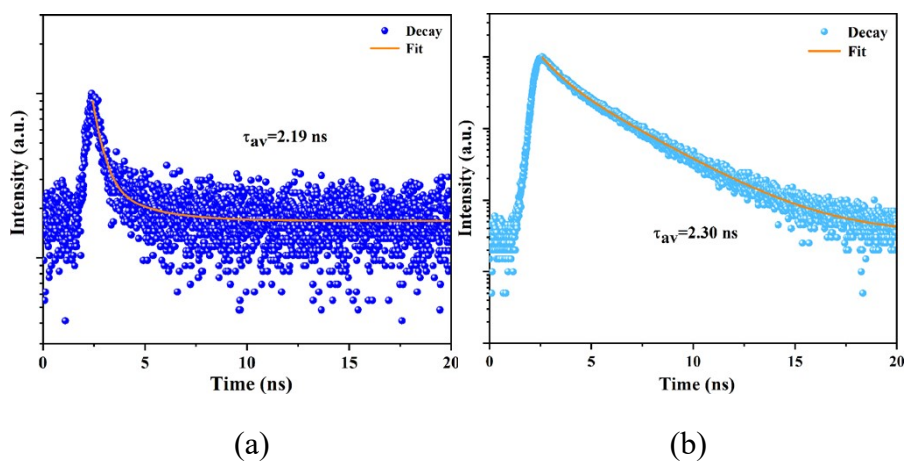


Fig. S8 (a) Time-resolved PL decay curves for compound **1** (at room temperature). (b) Time-resolved PL decay curves for compound **2** (at room temperature).

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

Atom	Dist	Atom	Dist
Pb1-N4	2.592(15)	Pb1-N10 ^{#4}	2.789(18)
Pb1-N5	2.652(17)	Pb2-N8	2.620(17)
Pb1-N1 ^{#1}	2.617(16)	Pb2-N9	2.601(16)
Pb1-N11 ^{#1}	2.656(15)		
Angle	(°)	Angle	(°)
N1 ^{#1} -Pb1-N5	91.0(5)	N1 ^{#1} -Pb1-N10 ^{#2}	147.1(5)

N5-Pb1-N10 ^{#2}	75.6(5)	N1 ^{#1} -Pb1-N11 ^{#1}	64.9(4)
N4-Pb1-N5	72.3(5)	N11 ^{#1} -Pb1-N10 ^{#2}	107.1(5)
N4-Pb1-N10 ^{#2}	71.9(5)	N4-Pb1-N11 ^{#1}	71.1(5)

Symmetry transformations used to generate equivalent atoms: ^{#1}-1/2+X,1/2-Y,1-Z; ^{#2}-X,1-Y,1-Z; ^{#3}1/2-X,1/2+Y,+Z; ^{#4}1/2+X,1/2-Y,1-Z; ^{#5}1/2-X,-1/2+Y,+Z.

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

Atom	Dist	Atom	Dist
Pb1-N1 ^{#1}	2.547(8)	Pb1-N3	2.746(8)
Pb1-N1 ^{#2}	2.547(8)	Pb1-N3 ^{#3}	2.746(8)
Angle	(°)	Angle	(°)
N1 ^{#1} -Pb1-N1 ^{#2}	80.7(4)	N1 ^{#2} -Pb1-N3 ^{#3}	127.6(3)
N3-Pb1-N3 ^{#3}	146.1(4)	N1 ^{#1} -Pb1-N3	127.6(3)
N1 ^{#1} -Pb1-N3 ^{#3}	80.5(3)		

Symmetry transformations used to generate equivalent atoms: ^{#1}1-X,+Y,1/2-Z; ^{#2}1/2+X,1/2+Y,+Z; ^{#3}1/2-X,1/2+Y,1/2-Z; ^{#4}-1/2+X,-1/2+Y,+Z.