

Supplementary Information

Comprehensively understanding the steric hindrance effect on coordination sphere of Pb²⁺ ion and photophysical natures of two luminescent Pb(II)-coordination polymers

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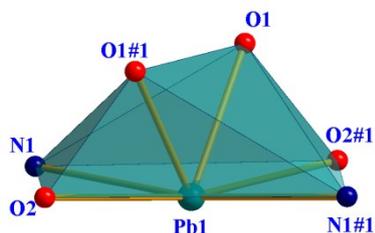
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Fig. S17: (a) Close-up view of several highest occupied band and the lowest unoccupied bands in energy band structure of **2** (b) Plots of DOS and PDOS of Pb, O, N and C atoms in **2**.

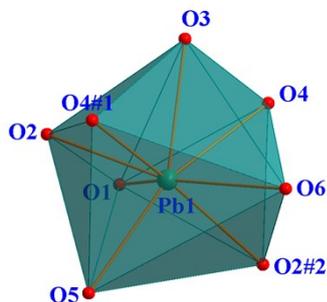
Table S1: Bond lengths (Å) and bond angles (°) in coordination polyhedra of **1**



Pb1-O1	2.515(3)	Pb1-O2	2.662(3)	Pb1-N1	2.716(3)
Pb1-O1#1	2.515(3)	Pb1-O2#1	2.662(3)	Pb1-N1#1	2.716(3)
O1-Pb1-O1#1	73.92(14)	O1-Pb1-O2#1	50.33(10)	O1#1-Pb1-O2#1	118.91(10)
O1-Pb1-O2	118.91(10)	O1#1-Pb1-O2	50.33(10)	O2#1-Pb1-O2	168.87(13)
O1-Pb1-N1	83.38(11)	O1#1-Pb1-N1	89.15(11)	O2#1-Pb1-N1	105.00(10)
O2-Pb1-N1	74.06(10)	O1-Pb1-N1#1	89.15(11)	O1#1-Pb1-N1#1	83.38(11)
O2#1-Pb1-N1#1	74.06(10)	O2-Pb1-N1#1	105.00(10)	N1-Pb1-N1#1	170.67(16)

Symmetry transformations used to generate equivalent atoms: #1 = -x+3/2, -y+1/2, z

Table S2: Bond lengths (Å) and bond angles (°) in coordination polyhedra of **2**



Pb1-O2	2.570(4)	Pb1-O(4)#1	2.596(4)	Pb1-O4	2.610(5)
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Pb1-O1	2.611(4)	Pb1-O3	2.647(5)	Pb1-O2#2	2.649(4)
Pb1-O5	2.669(5)	Pb1-O6	2.716(6)	O2-Pb1-O1	50.20(13)
O2-Pb1-O4#1	71.04(14)	O2-Pb1-O4	105.32(18)	O4#1-Pb1-O4	118.03(17)
O4#1-Pb1-O1	121.23(14)	O4#1-Pb1-O2#2	160.12(17)	O2-Pb1-O2#2	126.52(17)
O1-Pb1-O3	91.21(19)	O4-Pb1-O3	49.2414	O4#1-Pb1-O3	71.53(16)
O4-Pb1-O1	80.94(16)	O2-Pb1-O3	75.88(17)	O1-Pb1-O2#2	77.09(15)
O4-Pb1-O2#2	69.60(14)	O3-Pb1-O2#2	118.83(13)	O2-Pb1-O5	84.11(17)
O4-Pb1-O6	74.24(19)	O4#1-Pb1-O6	91.17(15)	O2-Pb1-O6	159.88(18)
O2#2-Pb1-O5	91.06(14)	O3-Pb1-O5	149.96(14)	O1-Pb1-O5	92.94(17)
O4-Pb1-O5	160.54(15)	O4#1-Pb1-O5	80.96(16)	O1-Pb1-O6	146.04(15)
O3-Pb1-O6	89.9(2)	O2#2-Pb1-O6	72.76(17)	O5-Pb1-O6	102.8(2)

Symmetry transformations used to generate equivalent atoms: #1 = $x, -y+1/2, z-1/2$; #2 = $x, -y+1/2, z+1/2$

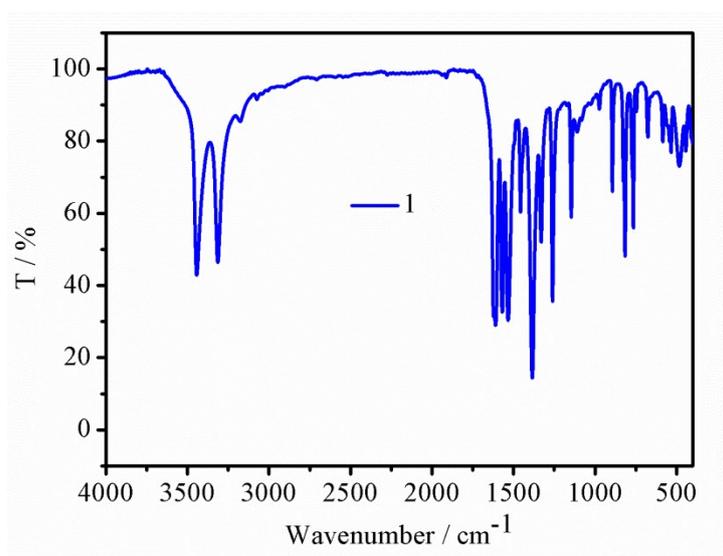


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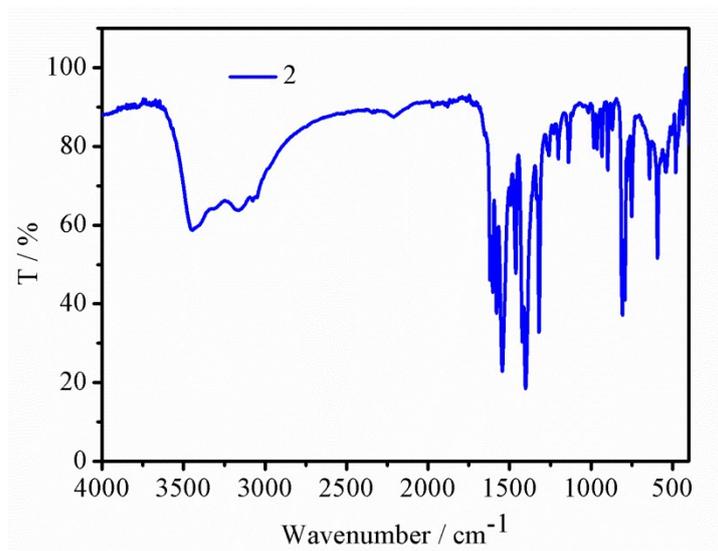


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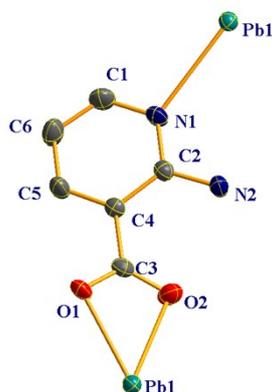


Fig. S3: Connection fashion of 2-anc ligands in **1**.

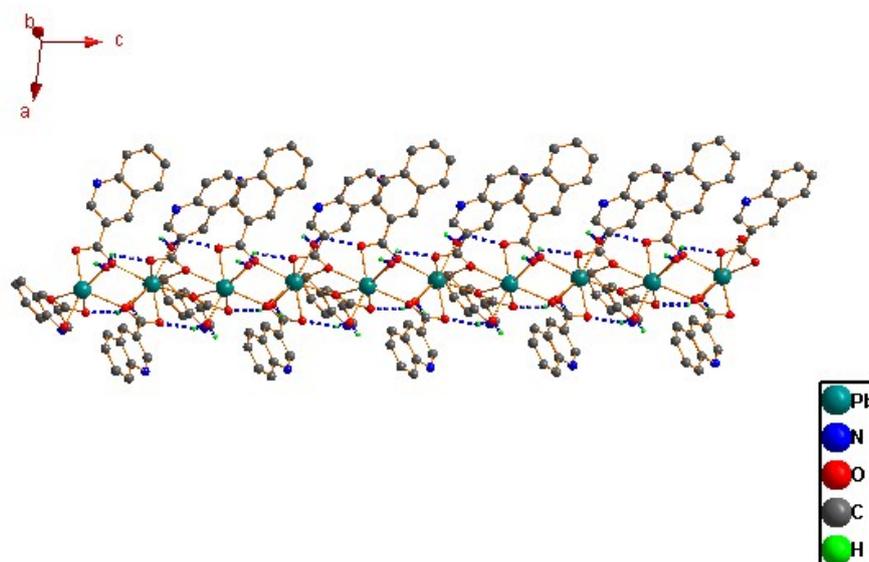


Fig. S4: Intramolecular hydrogen bonding interactions in **2**.



Fig. S5: Connection fashion of 3-qlc ligands in **2**.

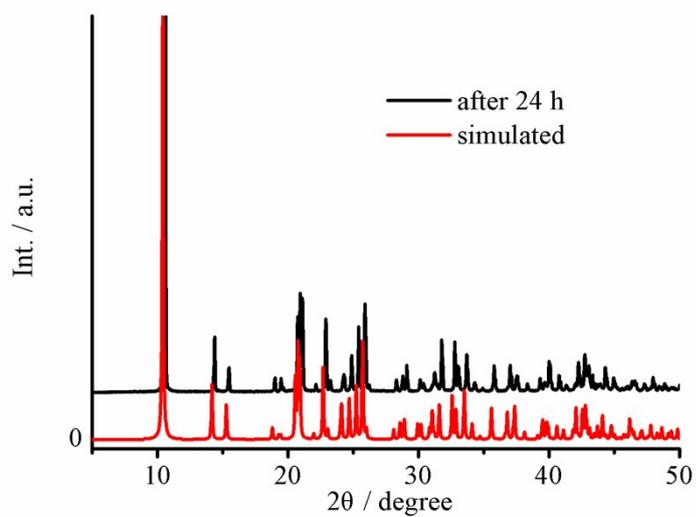


Fig. S6: PXRD patterns of **1** immersed in water for 24 hours.

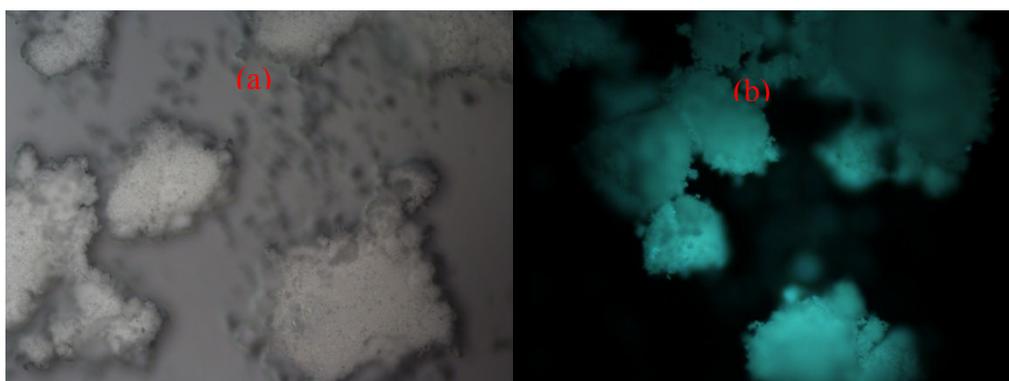


Fig. S7: Images of 2-aminonicotinic acid under (a) daylight and (b) UV light.



Fig. S8: Images of crystals of **1** under (a) daylight and (b) UV light.

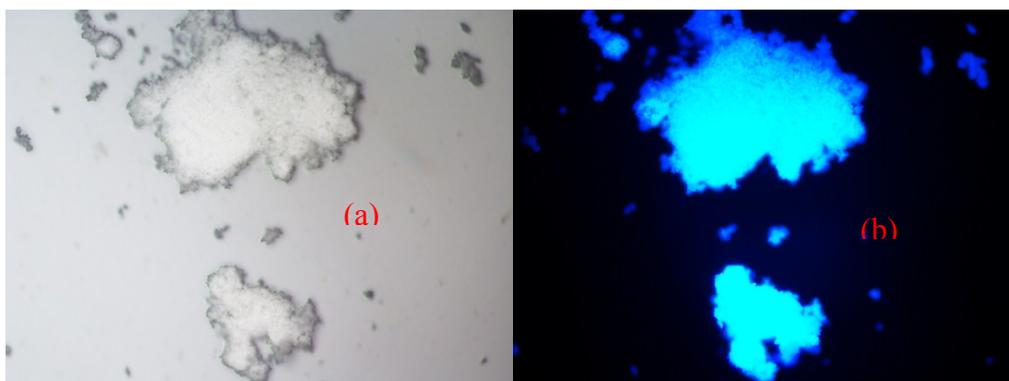


Fig. S9: Images of 3-quinolinecarboxylic acid under (a) daylight and (b) UV light.

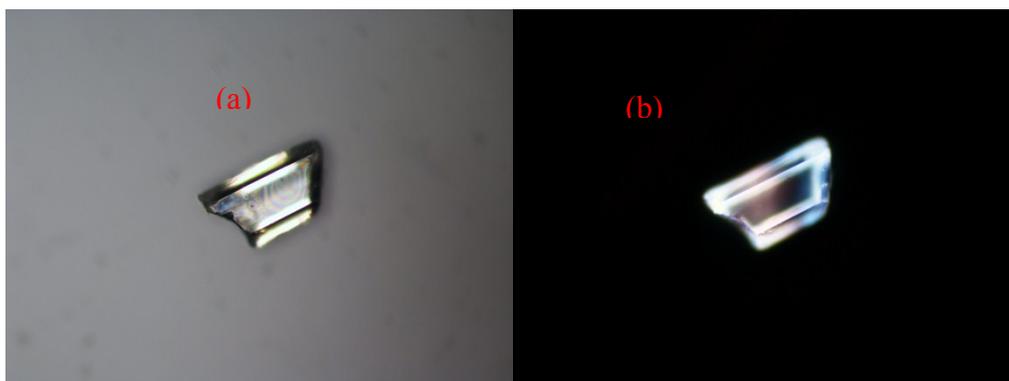


Fig. S10: Images of crystals of **2** under (a) daylight and (b) UV light.

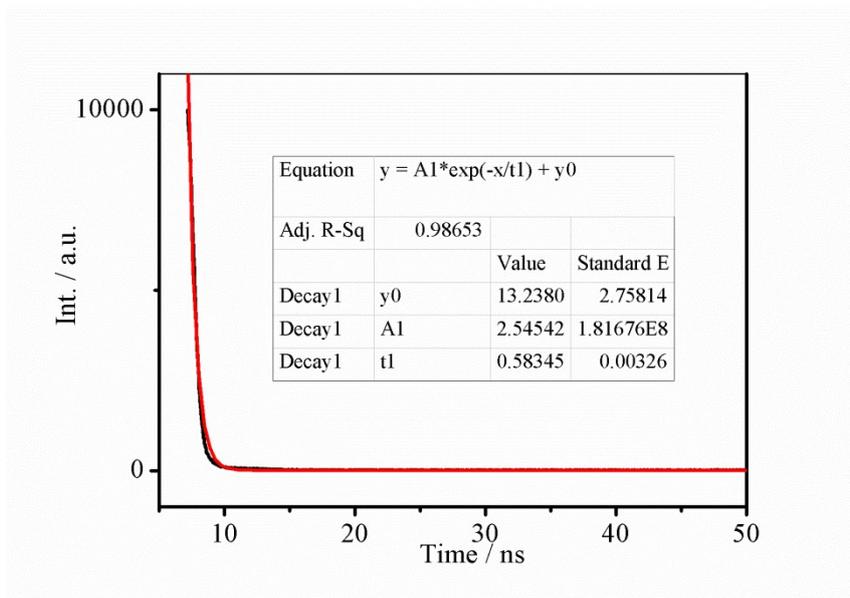


Fig. S11: Emission decay curves at room temperature upon pulsed excitation at 360 nm and the main emission peak at 410 nm of **1**.

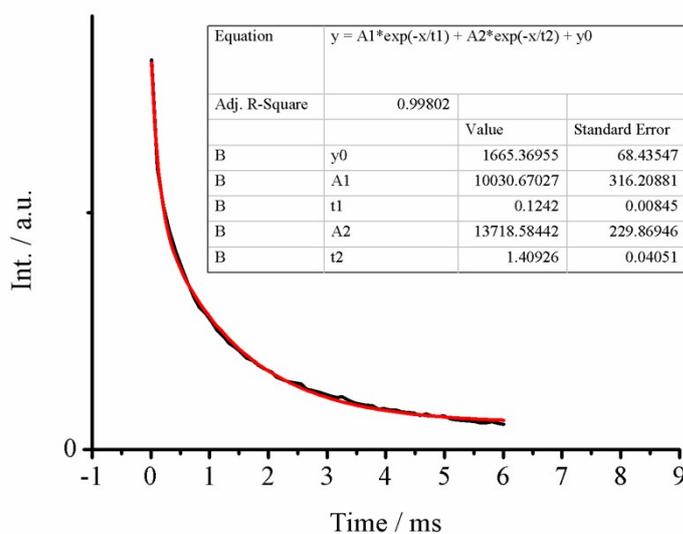


Fig. S12: Emission decay curves at room temperature upon pulsed excitation at 370 nm and the main emission peak at 548 nm of **1**.

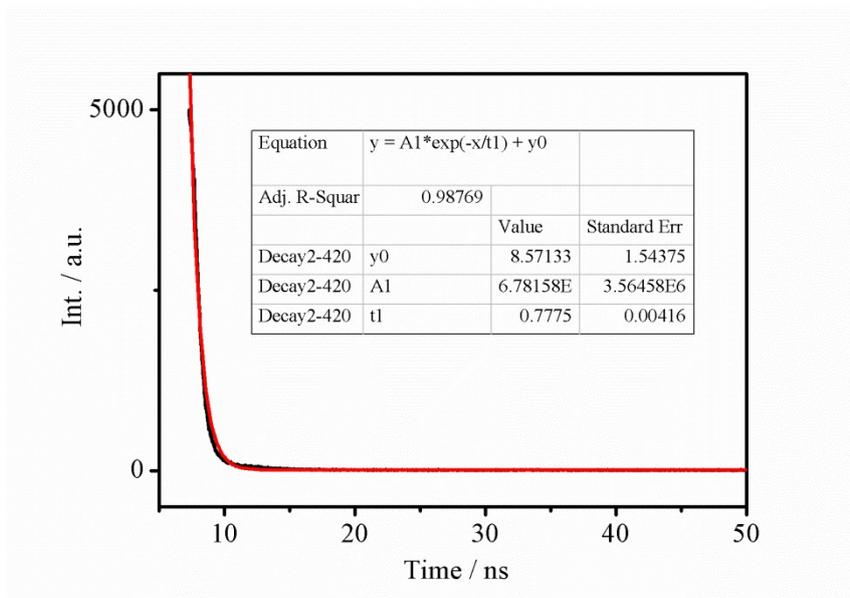


Fig. S13: Emission decay curves at room temperature upon pulsed excitation at 360 nm and the main emission peak at 430 nm of **2**.

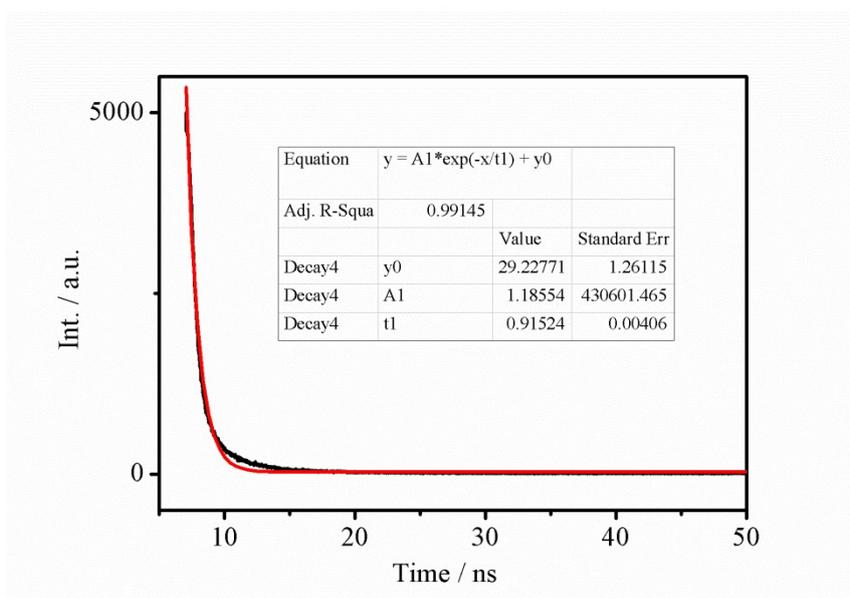


Fig. S14: Emission decay curves at room temperature upon pulsed excitation at 360 nm and the main emission peak at 460 nm of 2-aminonicotinic acid.

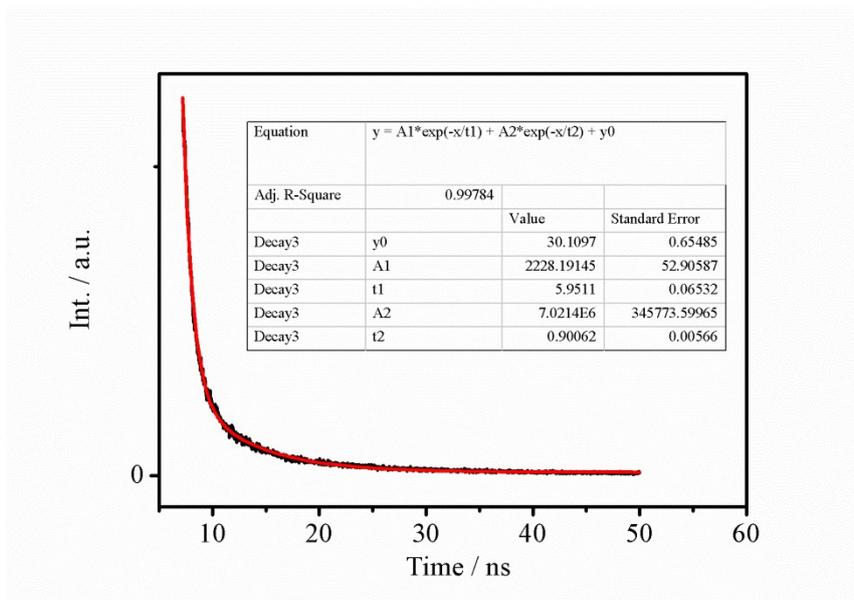


Fig. S15: Emission decay curves at room temperature upon pulsed excitation at 360 nm and the main emission peak at 430 nm of 3-quinolinecarboxylic acid.

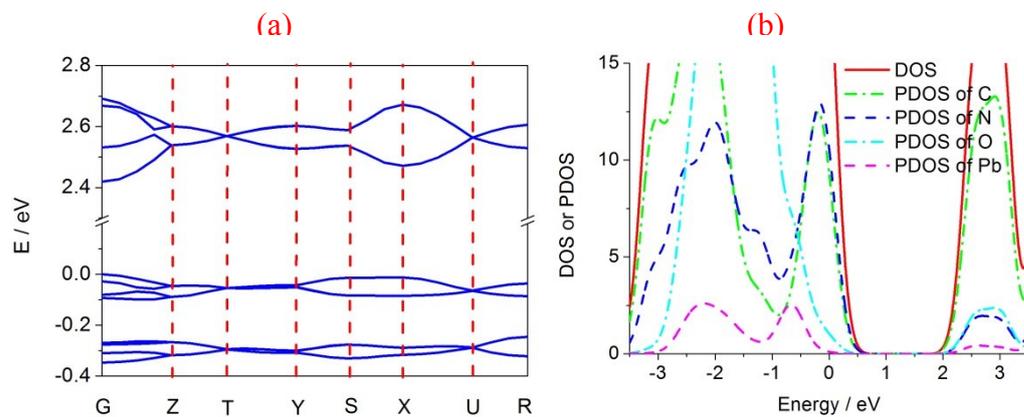


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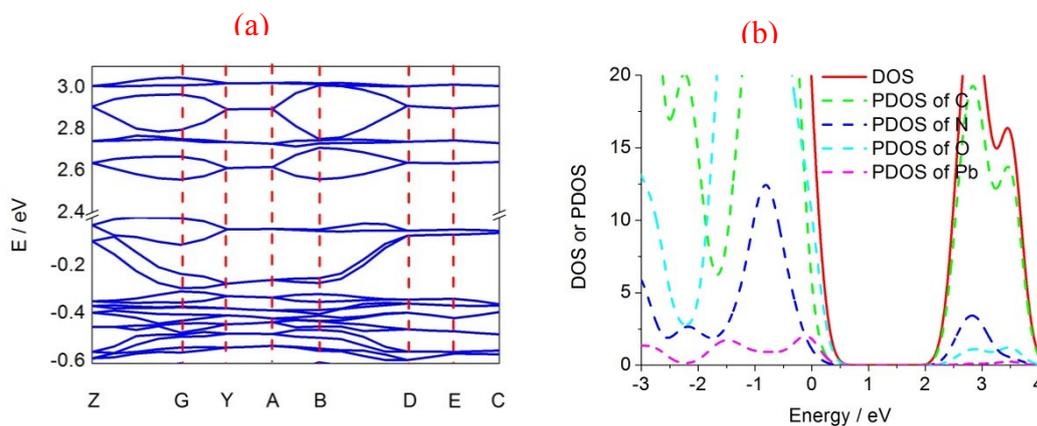


Fig. S17: (a) Close-up view of several highest occupied band and the lowest unoccupied bands in energy band structure of **2**. (b) Plots of DOS and PDOS of Pb, O, N and C atoms in **2**.