Intense greenish phosphorescence emission at room temperature in a two

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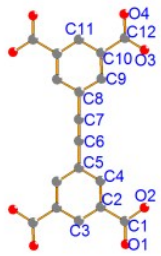
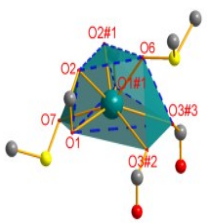
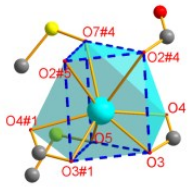
Table S1: Selected bond lengths (Å) and angles (°) in crystal of **1** at 291 K

Bond lengths					
Pb1 –O2	2.0079(14)	Pb1–O6	2.471(14)	Pb1–O7	2.801(16)
Pb2 –O3	2.456(8)	Pb2–O5	2.462(14)	Pb2–O4	2.727(8)
Bond angles					
O2-Pb1-O2#1	78.1 (4)	O2-Pb1-O6	75.6(3)	O2#1-Pb1-O6	75.6(3)
O2-Pb1-O7	80.5(3)	O2#1-Pb1-O7	80.5(3)	O6-Pb1-O7	149.0(5)
O3-Pb2-O3#1	76.5(4)	O3-Pb2-O5	88.1(3)	O3#1-Pb2-O5	88.1(3)
O3- Pb2- O4	50.3(2)	O3-Pb2-O4#1	123.8(3)	O5-Pb2-O4#1	74.8(2)
O3#1-Pb2-O4	50.3(2)	O3#1-Pb2-O4#1	123.8(3)	O5-Pb2-O4	74.9(2)
O4-Pb2-O4#1	149.3(4)				

symmetry code: #1 = x, 2–y, z

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

	Bond lengths			Bond angles		
	C1-O1	1.231	1.225(13)	O1-C1-O2	123.651	123.7(9)
	C1-O2	1.265	1.275(12)	O1-C1-C2	118.542	119.9(9)
	C1-C2	1.511	1.514(12)	C2-C1-O2	117.717	116.3(8)
	C2-C3	1.399	1.402(10)	C4-C2-C3	120.383	120.4(9)
	C2-C4	1.391	1.399(12)	C4-C2-C1	120.053	120.7(8)
	C4-C5	1.398	1.399(12)	C3-C2-C1	119.564	118.9(8)
	C5-C6	1.425	1.440(19)	C2-C4-C5	121.576	120.7(9)
	C6-C7	1.205	1.19(2)	C4-C5-C6	121.314	120.7(6)
	C7-C8	1.437	1.46(2)	C6-C7-C8	172.823	177.0(18)
	C8-C9	1.384	1.381(12)	C8-C9-C10	119.503	119.7(9)
	C9-C10	1.409	1.387(12)	C9-C10-C11	120.567	120.2(9)
	C10-C11	1.410	1.413(11)	C9-C10-C12	121.036	121.4(8)
	C10-C12	1.492	1.508(13)	O3-C12-C10	117.036	117.2(8)
	C12-O3	1.289	1.276(12)	O4-C12-O3	122.307	122.9(9)
	C12-O4	1.256	1.246(13)			
	Bond lengths			Bond angles		
	Pb1-O1	2.7913	2.7900	O2-Pb1-O7	80.5(4)	80.5(3)
	Pb1-O1#1	2.7913	2.7900	O2#1-Pb1-O7	80.5(4)	80.5(3)
	Pb1-O3#2	2.9710	2.456(8)	O2-Pb1-O2#1	78.0(4)	78.1(4)
	Pb1-O3#3	2.9710	2.456(8)	O6-Pb1-O7	148.9(5)	149.0(5)
	Pb1-O2	2.4270	2.432(8)	O2-Pb1-O2#1	78.023	78.1(4)
	Pb1-O2#1	2.4270	2.432(8)	O2-Pb1-O6	75.5(3)	75.6(3)
	Pb1-O6	2.5390	2.471(14)	O2#1-Pb1-O6	75.5(3)	75.6(3)
	Pb1-O7	2.7350	2.801(16)			

	Bond lengths			Bond angles		
	Pb2-O2#4	2.9990	2.9944	O3-Pb2-O3#1	76.714	76.5(4)
	Pb2-O2#5	2.9990	2.9944	O3-Pb2-O5	88.972	88.1(3)
	Pb2-O4	2.7328	2.727(8)	O3#1-Pb2-O5	88.082	88.1(3)
	Pb2-O3	2.4702	2.456(8)	O3-Pb2-O4	50.554	50.3(2)
	Pb2-O5	2.4184	2.462(14)	O3#1-Pb2-O4	123.858	123.8(3)
	Pb2-O3#1	2.4702	2.456(8)	O3-Pb2-O3	76.714	76.5(4)
	Pb2-O4#1	2.7238	2.727(8)	O5-Pb2-O4	74.744	74.8(2)
	Pb2-O7#4	2.9688	2.9674	O5-Pb2-O4#1	74.700	74.9(2)

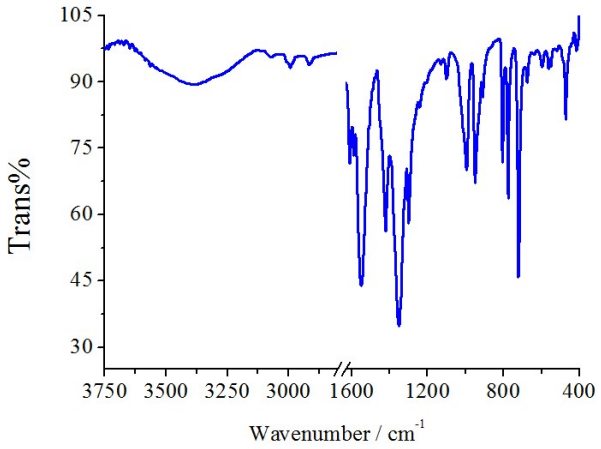


Fig. S1: IR spectrum of **1** recorded from a KBr pellet and the selected vibration bands: 3075w, 2997w, 2915w, 1610m, 1589m, 1551s, 1421s, 1350vs, 1230s, 1103w, 993s, 949s, 908w, 806s, 775s, 721vs, 675w, 596w, 563w, 472m.

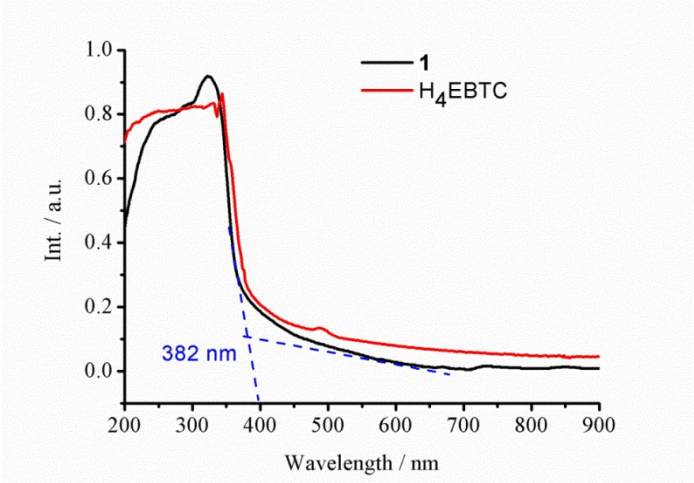


Fig. S2: UV–visible spectra of **1** and the H_4EBTC in the solid state at room temperature.

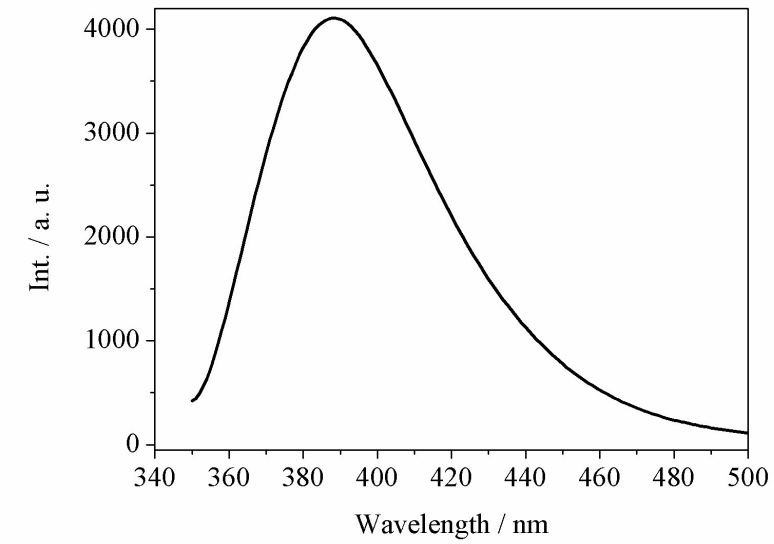


Fig. S3: The solid–state PL spectra of H_4EBTC (λ_{ex}= 278 nm) at room temperature.

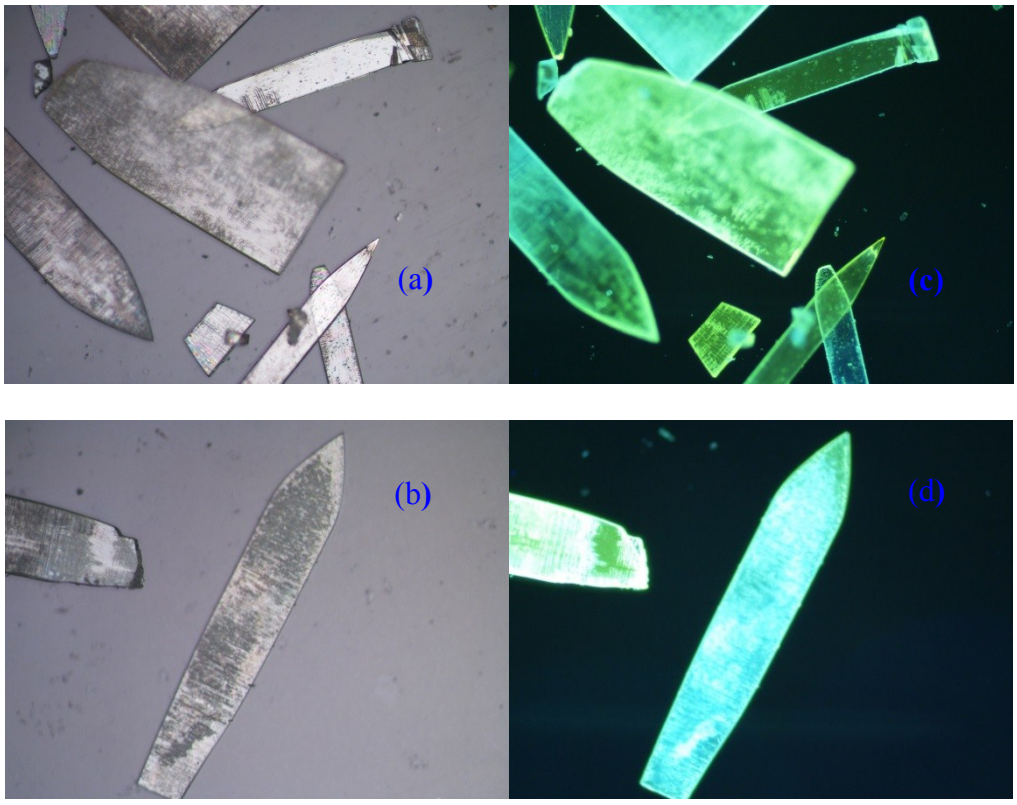


Fig. S4: Photographs of crystals of **1** under (a, b) daylight and (c, d) 330–380 nm ultraviolet irradiation at room temperature.

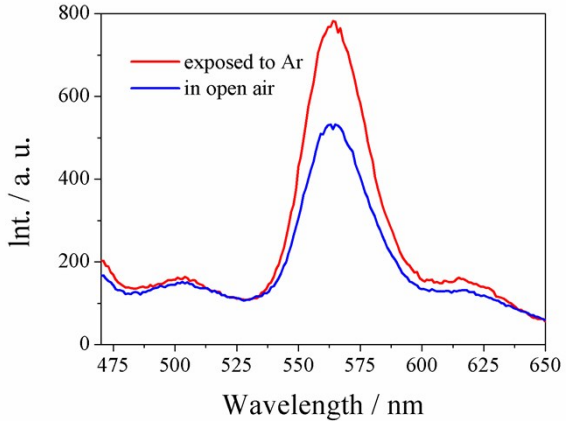


Fig. S5: Emission spectra of **1** in (a) open air and (b) after exposure to argon atmosphere for 5 minutes at ambient temperature.

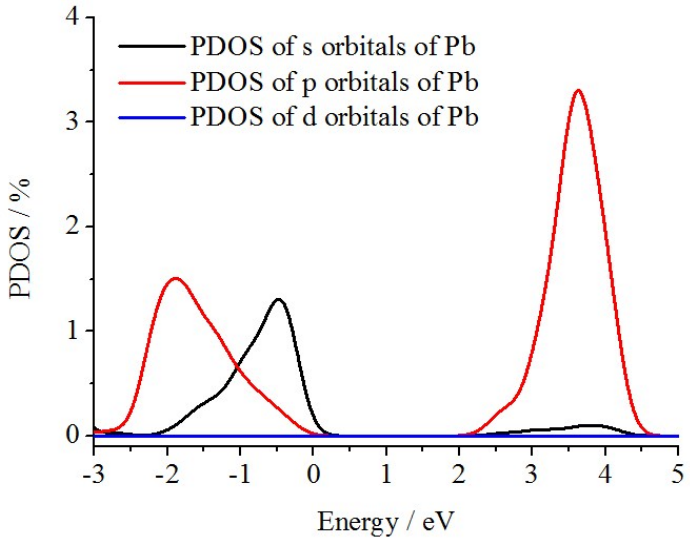


Fig. S6: PDOS of Pb^{2+} ions near the Fermi level in **1**.