

Electronic Supplementary Information

Blue and White-light emitting 2D Metal-organic frameworks of *cis*-5-Norbornene-endo-2,3-dicarboxylic acid

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X-ray Crystallography

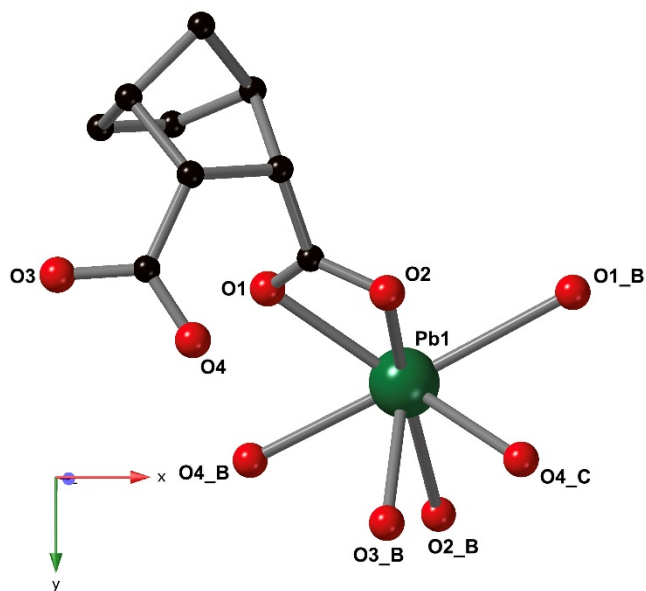


Figure S1. An illustration of coordination environment in **1** along z axis.

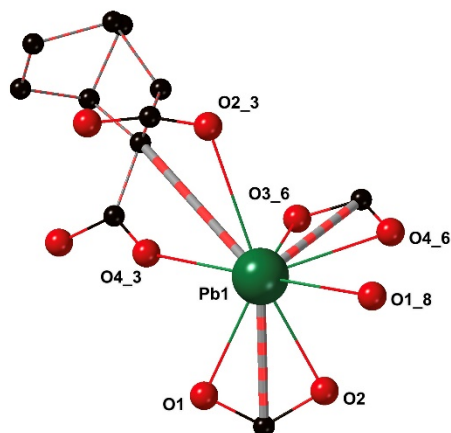


Figure S2. Schematic representation of seven-coordinated geometry in **1** and its reduction to a simple, planar trigonal description using VBV model as described in Miguel A. H et al. *Acta Cryst.* 2006. **B62**, 1038–1042.

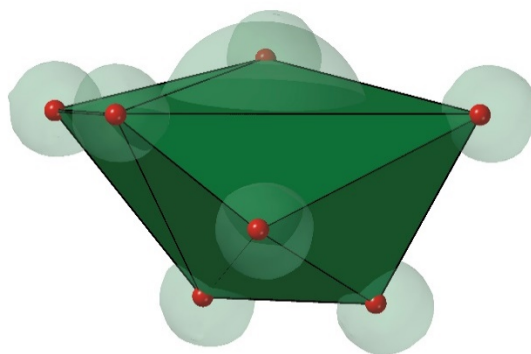


Figure S3. An illustration of mapping of surface space-filling in a polyhedra of Pb(II) in **1**. The surface space-filling clearly shows the hemi-directed coordination geometry.

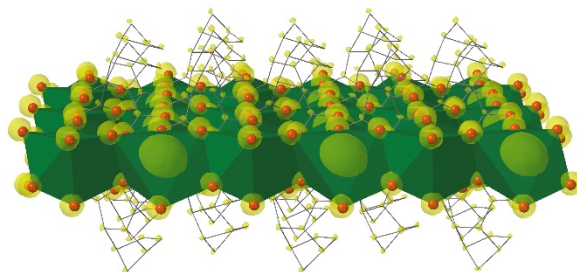


Figure S4. An illustration of mapping of surface space-filling in a 2D layer in **1**.

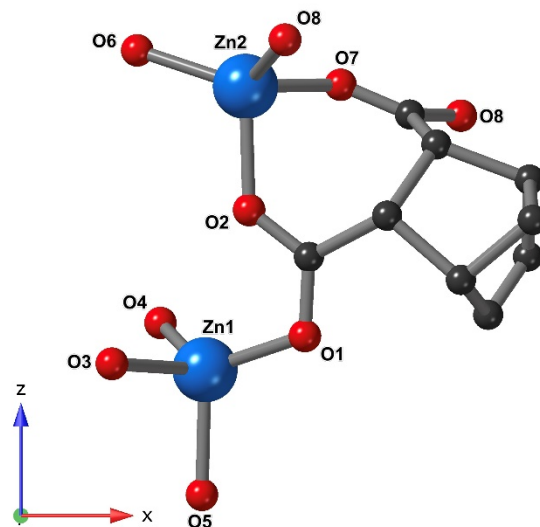


Figure S5. An illustration of coordination environment in **2** along *y* axis.

Table S1. Selected bond length (Å) and bond angles (°) in **1**

| | |
|---------------------|-----------|
| Pb(1)-O(3)#1 | 2.405(8) |
| Pb(1)-O(2) | 2.503(8) |
| Pb(1)-O(1) | 2.551(11) |
| Pb(1)-O(4)#1 | 2.602(10) |
| Pb(1)-O(4)#2 | 2.619(10) |
| Pb(1)-C(4)#1 | 2.849(13) |
| Pb(1)-C(1) | 2.860(14) |
| O(1)-C(1) | 1.231(18) |
| O(2)-C(1) | 1.29(2) |
| O(3)-C(4) | 1.30(3) |
| O(4)-C(4) | 1.247(16) |
| C(1)-C(2) | 1.517(19) |
| C(2)-C(3) | 1.557(18) |
| C(2)-C(8) | 1.574(18) |
| C(3)-C(4) | 1.504(18) |
| C(3)-C(5) | 1.535(18) |
| C(5)-C(6) | 1.50(2) |
| C(5)-C(9) | 1.517(19) |
| C(6)-C(7) | 1.30(2) |
| C(7)-C(8) | 1.53(2) |
| C(8)-C(9) | 1.536(19) |
| O(3)#1-Pb(1)-O(2) | 89.6(3) |
| O(3)#1-Pb(1)-O(1) | 102.4(5) |
| O(2)-Pb(1)-O(1) | 51.8(4) |
| O(3)#1-Pb(1)-O(4)#1 | 52.0(6) |
| O(2)-Pb(1)-O(4)#1 | 75.9(4) |
| O(1)-Pb(1)-O(4)#1 | 123.4(3) |
| O(3)#1-Pb(1)-O(4)#2 | 70.2(6) |
| O(2)-Pb(1)-O(4)#2 | 110.2(4) |

| | |
|----------------------|-----------|
| O(1)-Pb(1)-O(4)#2 | 68.2(3) |
| O(4)#1-Pb(1)-O(4)#2 | 122.0(4) |
| O(3)#1-Pb(1)-C(4)#1 | 26.9(6) |
| O(2)-Pb(1)-C(4)#1 | 86.8(4) |
| O(1)-Pb(1)-C(4)#1 | 120.0(4) |
| O(4)#1-Pb(1)-C(4)#1 | 26.0(3) |
| O(4)#2-Pb(1)-C(4)#1 | 96.2(3) |
| O(3)#1-Pb(1)-C(1) | 99.9(4) |
| O(2)-Pb(1)-C(1) | 26.7(4) |
| O(1)-Pb(1)-C(1) | 25.5(4) |
| O(4)#1-Pb(1)-C(1) | 101.7(4) |
| O(4)#2-Pb(1)-C(1) | 90.5(4) |
| C(4)#1-Pb(1)-C(1) | 107.2(4) |
| C(1)-O(1)-Pb(1) | 91.4(9) |
| C(1)-O(2)-Pb(1) | 92.3(9) |
| C(4)-O(3)-Pb(1)#3 | 96.0(10) |
| C(4)-O(4)-Pb(1)#3 | 88.1(8) |
| C(4)-O(4)-Pb(1)#4 | 150.6(9) |
| Pb(1)#3-O(4)-Pb(1)#4 | 116.0(4) |
| O(1)-C(1)-O(2) | 122.6(13) |
| O(1)-C(1)-C(2) | 120.2(13) |
| O(2)-C(1)-C(2) | 116.9(12) |
| O(1)-C(1)-Pb(1) | 63.1(8) |
| O(2)-C(1)-Pb(1) | 61.0(7) |
| C(2)-C(1)-Pb(1) | 161.5(9) |
| C(1)-C(2)-C(3) | 116.5(11) |
| C(1)-C(2)-C(8) | 114.8(10) |
| C(3)-C(2)-C(8) | 100.6(10) |
| C(4)-C(3)-C(5) | 116.0(11) |
| C(4)-C(3)-C(2) | 115.6(11) |
| C(5)-C(3)-C(2) | 104.2(10) |
| O(4)-C(4)-O(3) | 119.7(12) |
| O(4)-C(4)-C(3) | 122.1(12) |
| O(3)-C(4)-C(3) | 118.1(11) |
| O(4)-C(4)-Pb(1)#3 | 65.9(7) |
| O(3)-C(4)-Pb(1)#3 | 57.1(6) |
| C(3)-C(4)-Pb(1)#3 | 157.2(8) |
| C(6)-C(5)-C(9) | 100.8(12) |
| C(6)-C(5)-C(3) | 107.0(11) |
| C(9)-C(5)-C(3) | 100.1(11) |
| C(7)-C(6)-C(5) | 107.9(16) |
| C(6)-C(7)-C(8) | 107.6(13) |
| C(7)-C(8)-C(9) | 99.6(12) |
| C(7)-C(8)-C(2) | 107.9(10) |
| C(9)-C(8)-C(2) | 99.3(11) |
| C(5)-C(9)-C(8) | 93.6(10) |

Symmetry transformations used to generate equivalent atoms:

#1 $-x+3/2, -y+1/2, z-1/2$ #2 $x-1/2, -y+1/2, z$ #3 $-x+3/2, -y+1/2, z+1/2$
#4 $x+1/2, -y+1/2, z$

Table S2. Selected bond length (Å) and bond angles (°) in **2**

| | |
|---------------------|------------|
| Zn(1)-O(2) | 1.9394(19) |
| Zn(1)-O(4)#1 | 1.9610(18) |
| Zn(1)-O(3)#2 | 1.967(2) |
| Zn(1)-O(1)#2 | 1.980(2) |
| O(1)-C(1) | 1.258(3) |
| O(2)-C(1) | 1.266(3) |
| O(3)-C(9) | 1.261(3) |
| O(4)-C(9) | 1.254(3) |
| C(1)-C(2) | 1.516(3) |
| C(2)-C(3) | 1.563(3) |
| C(2)-C(6) | 1.585(3) |
| C(9)-C(6) | 1.520(3) |
| C(3)-C(7) | 1.511(4) |
| C(3)-C(4) | 1.533(4) |
| C(6)-C(5) | 1.555(4) |
| C(8)-C(7) | 1.331(4) |
| C(8)-C(5) | 1.504(4) |
| C(5)-C(4) | 1.533(4) |
| <hr/> | |
| O(2)-Zn(1)-O(4)#1 | 122.92(8) |
| O(2)-Zn(1)-O(3)#2 | 112.41(9) |
| O(4)#1-Zn(1)-O(3)#2 | 105.92(9) |
| O(2)-Zn(1)-O(1)#2 | 110.02(8) |
| O(4)#1-Zn(1)-O(1)#2 | 108.96(9) |
| O(3)#2-Zn(1)-O(1)#2 | 92.26(9) |
| C(1)-O(1)-Zn(1)#3 | 126.02(17) |
| C(1)-O(2)-Zn(1) | 111.17(17) |
| C(9)-O(3)-Zn(1)#3 | 125.84(18) |
| C(9)-O(4)-Zn(1)#1 | 113.13(17) |
| O(1)-C(1)-O(2) | 120.4(2) |
| O(1)-C(1)-C(2) | 121.5(2) |
| O(2)-C(1)-C(2) | 117.9(2) |
| C(1)-C(2)-C(3) | 113.8(2) |
| C(1)-C(2)-C(6) | 120.39(19) |
| C(3)-C(2)-C(6) | 101.93(18) |
| O(4)-C(9)-O(3) | 120.5(2) |
| O(4)-C(9)-C(6) | 117.8(2) |
| O(3)-C(9)-C(6) | 121.5(2) |
| C(7)-C(3)-C(4) | 100.6(2) |
| C(7)-C(3)-C(2) | 106.7(2) |
| C(4)-C(3)-C(2) | 100.2(2) |
| C(9)-C(6)-C(5) | 113.1(2) |
| C(9)-C(6)-C(2) | 120.4(2) |
| C(5)-C(6)-C(2) | 102.23(19) |
| C(7)-C(8)-C(5) | 107.8(3) |
| C(8)-C(7)-C(3) | 107.2(3) |
| C(8)-C(5)-C(4) | 100.5(2) |
| C(8)-C(5)-C(6) | 106.8(2) |
| C(4)-C(5)-C(6) | 100.4(2) |
| C(5)-C(4)-C(3) | 93.8(2) |

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1 #2 -x+1,y-1/2,-z+3/2 #3 -x+1,y+1/2,-z+3/2

X-ray Powder Pattern

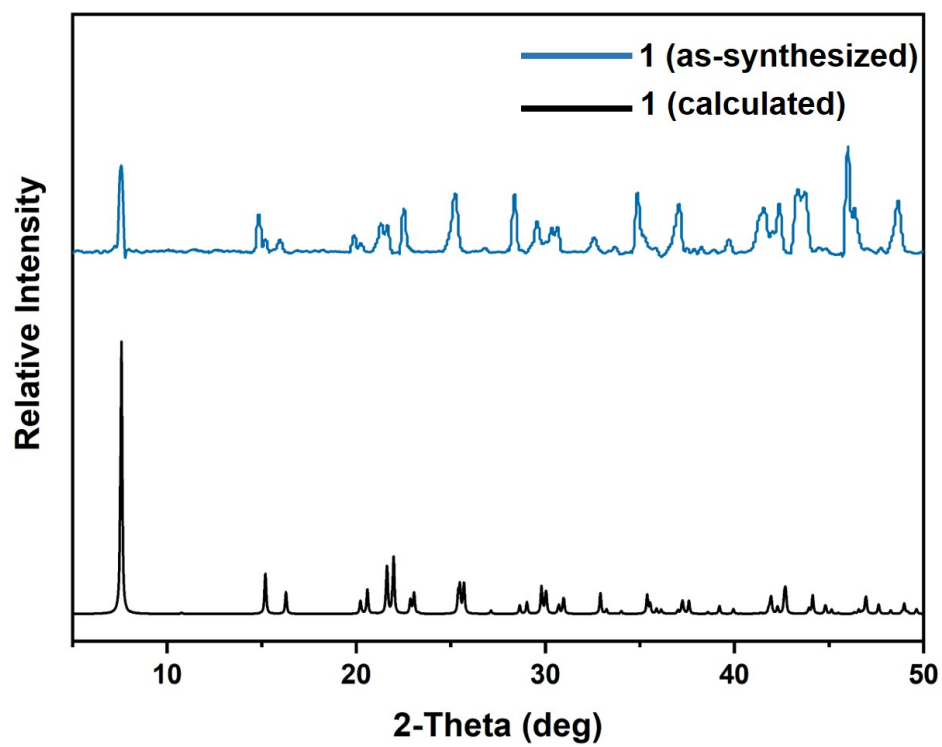


Figure S6. X-ray powder patterns of compounds 1.

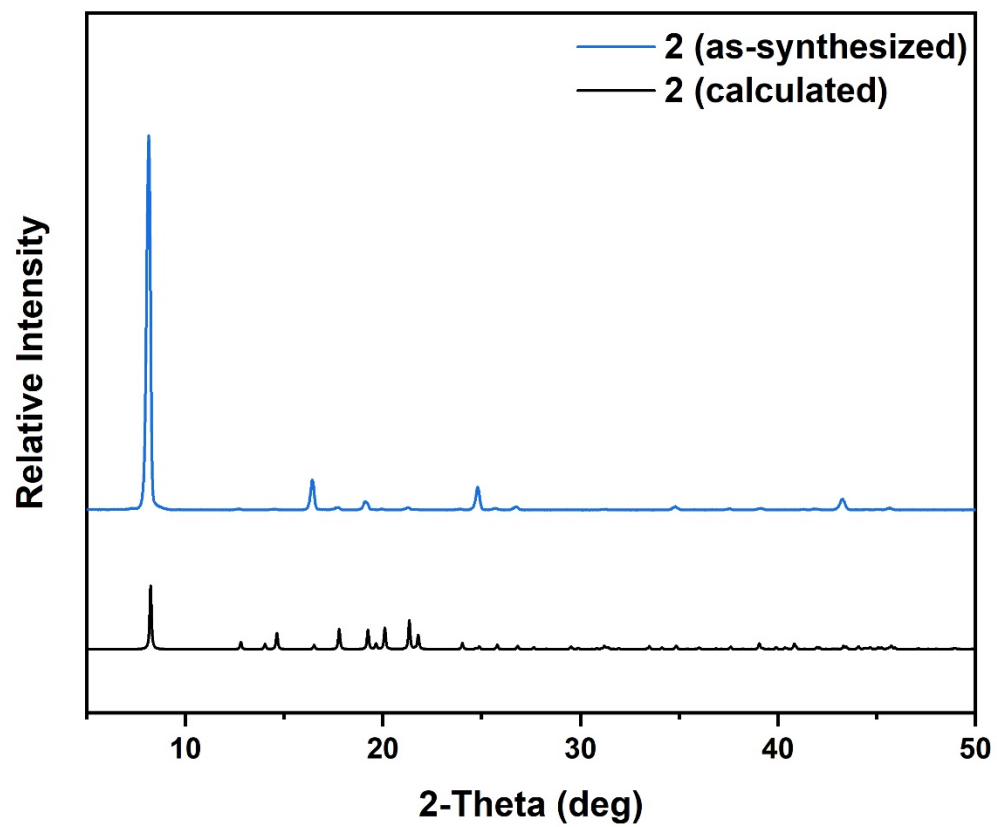


Figure S7. X-ray powder patterns of compounds 2.

FT-IR Spectra

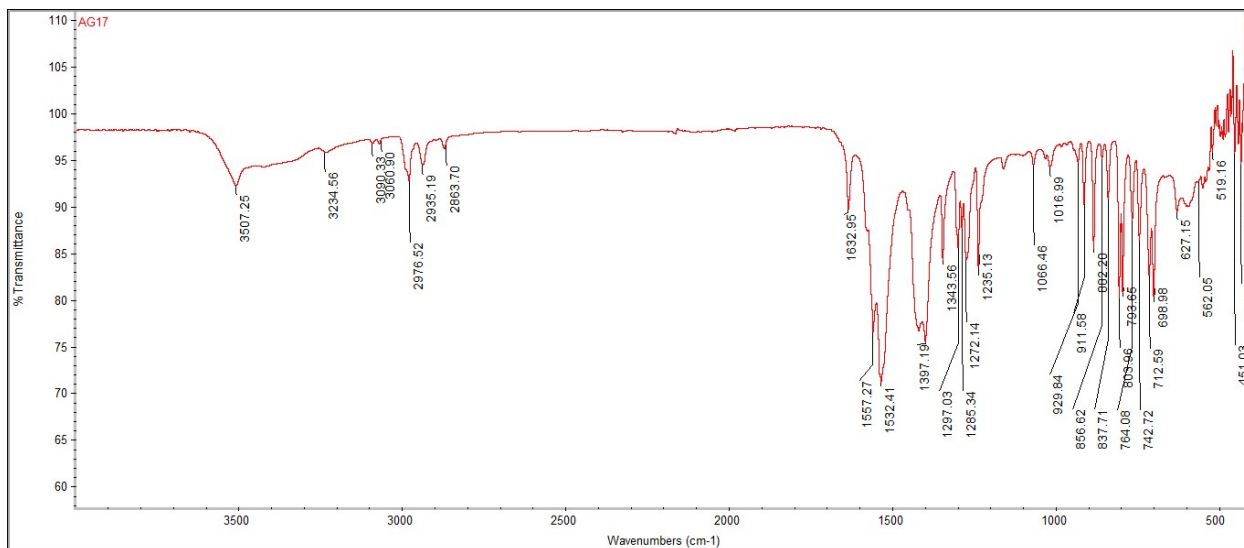


Figure S8. FT-IR Spectra of 1.

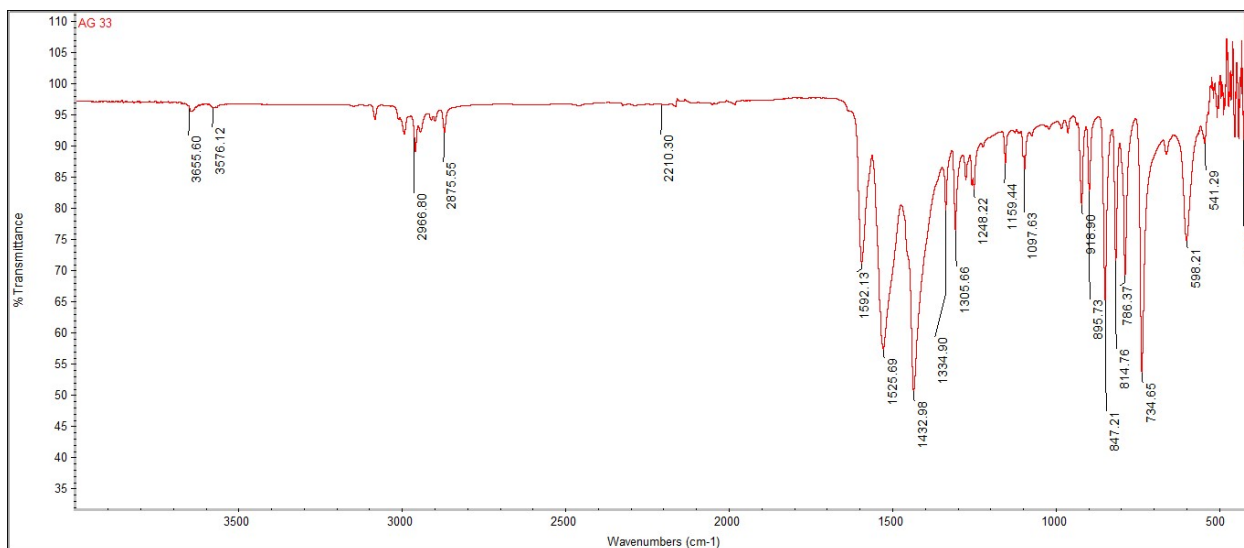


Figure S9. FT-IR Spectra of 2.

TGA analysis

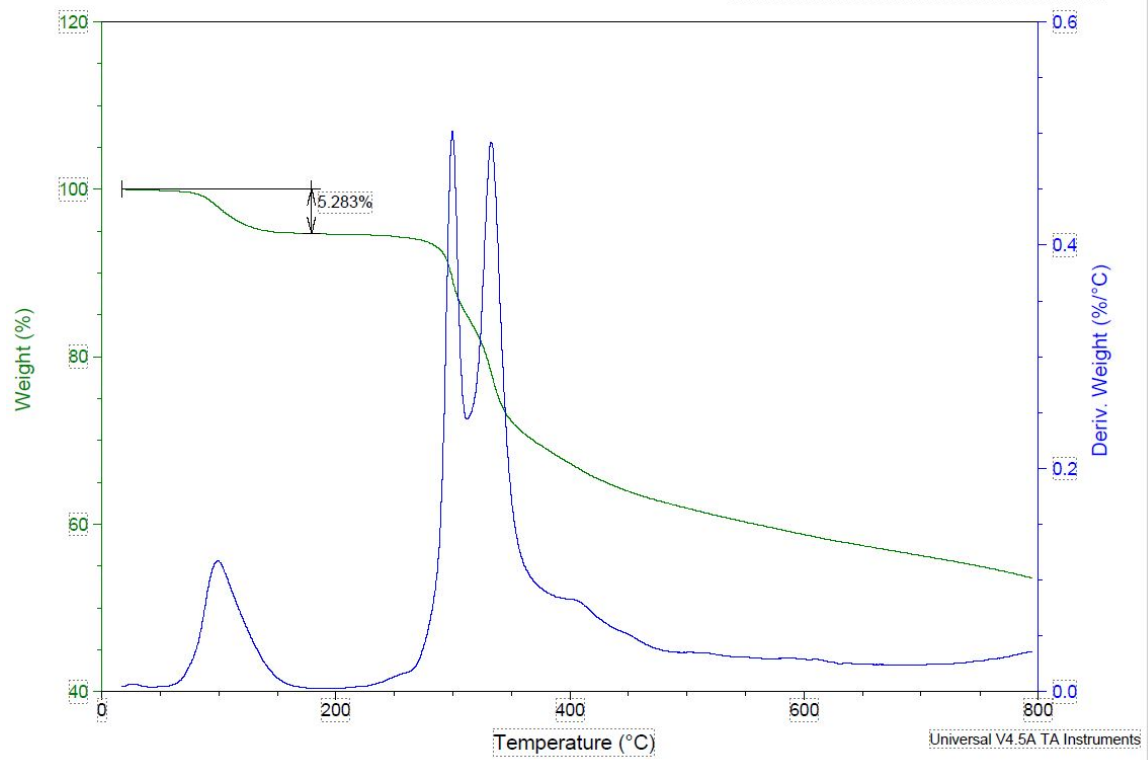


Figure S10. TGA Analysis of 1.

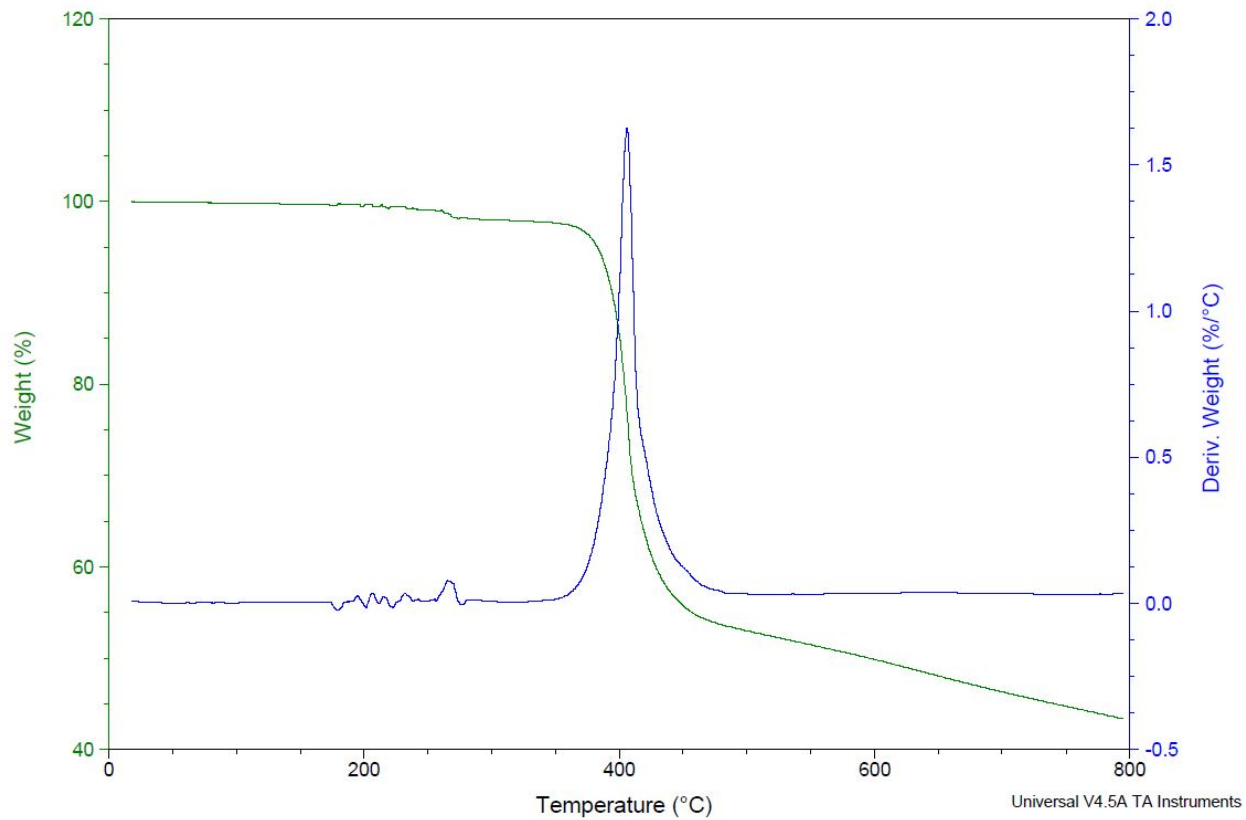


Figure S11. TGA Analysis of **2**.

Solid-state UV-vis spectra

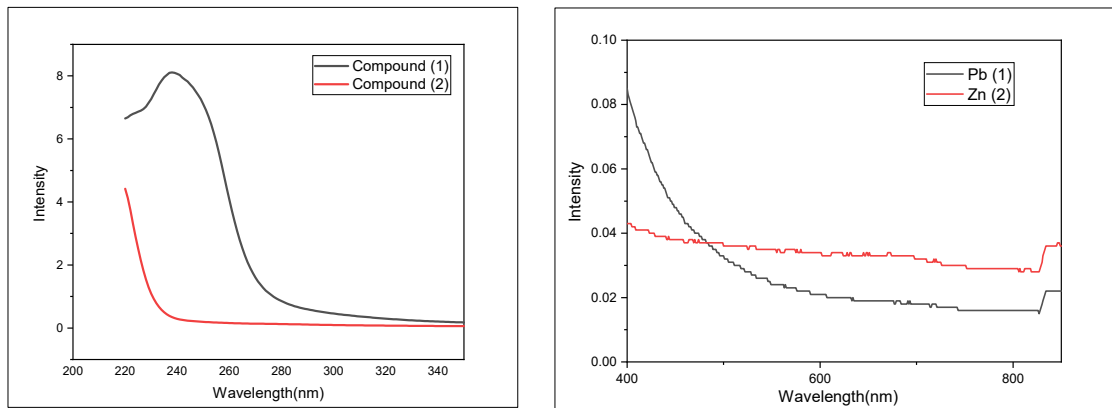


Figure S12. Solid-state UV-vis spectra of compounds **1-2**.