

***Electronic Supplementary Information for***

**Structural Analyses and Luminescent Properties of  
a Series of Lead(II) Metal-Organic Frameworks Based on  
2-Sulfoterephthalate**

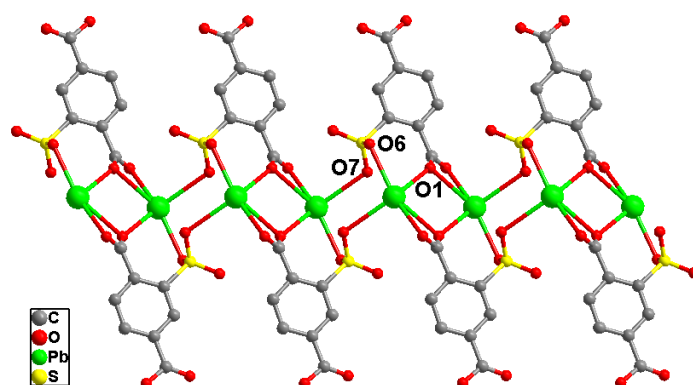
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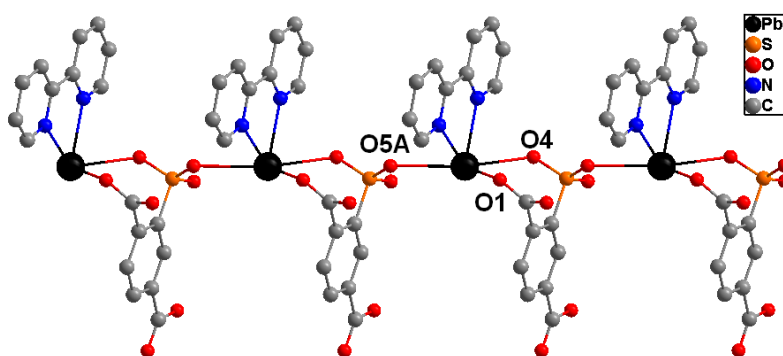
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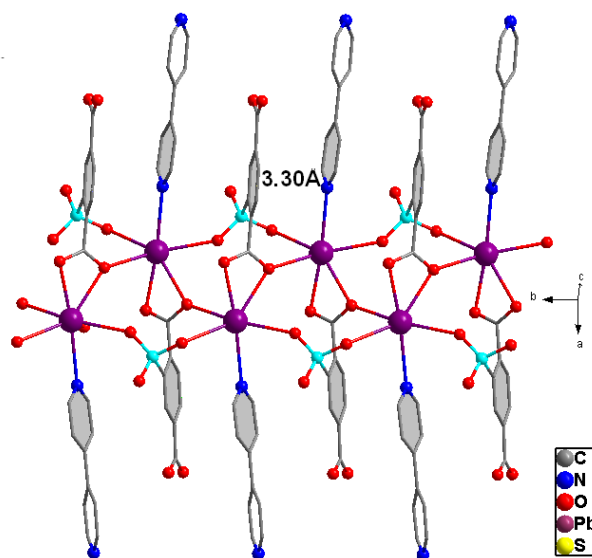
***CrystEngComm***



**Fig. S1** 1D chain-like structure in complex **1** along *a* axis.  
(The *o*-phen molecules on the two sides of chain are deleted for clarity)



**Fig. S2** 1D chain-like structure along *a* axis in complex **2**  
(symmetry code: (A)  $1+x, y, z$ )



**Fig. S3** 1D bimetallic chain along *b* axis in complex **3**

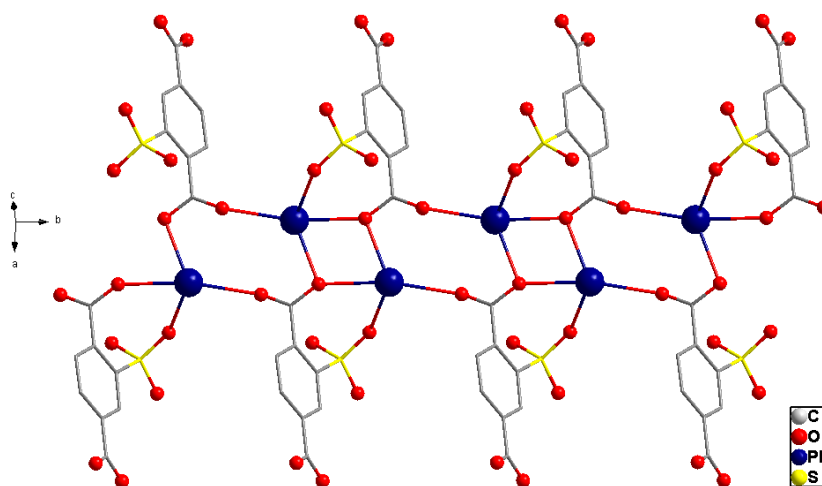


Fig. S4 1D bimetallic chain along *b* axis in complex 4

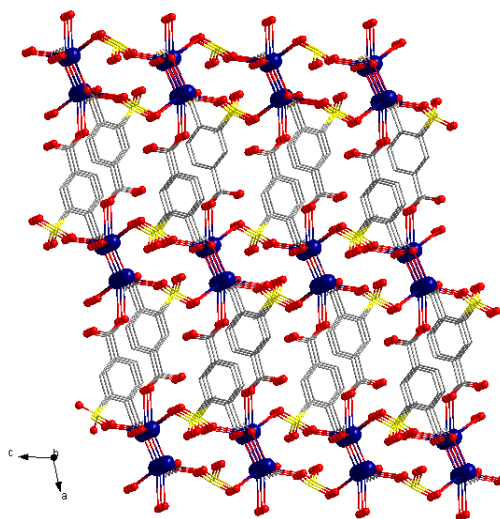


Fig. S5 3D structure in complex 4

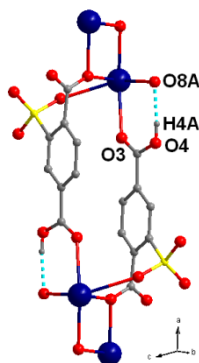


Fig. S6 The H-bonds existing in 2D layer of complex 4.

(O4-H4A $\cdots$ O8A = 2.661 Å,  $\angle$ O4-H4A $\cdots$ O8A = 172.45°, symmetry code: (A) 2-x, -y, 2-z)

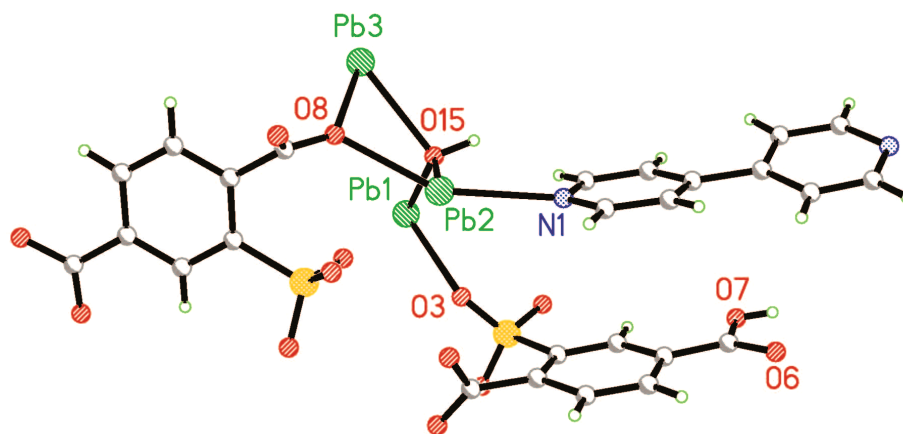


Fig. S7 The asymmetric unit of complex 5

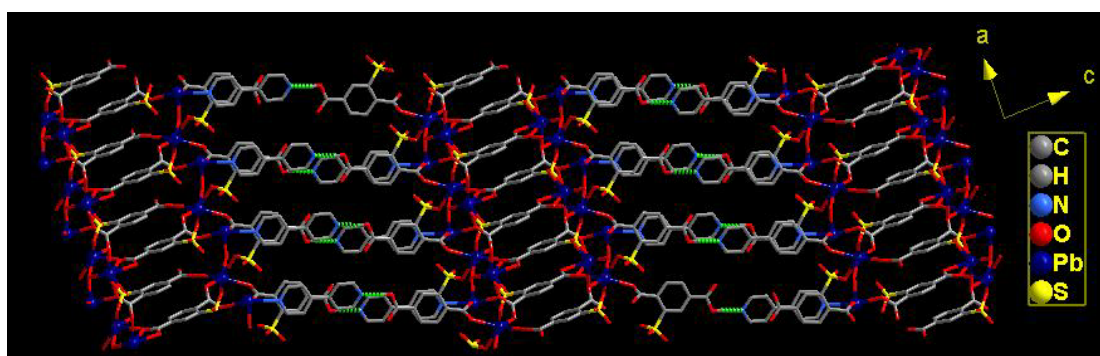
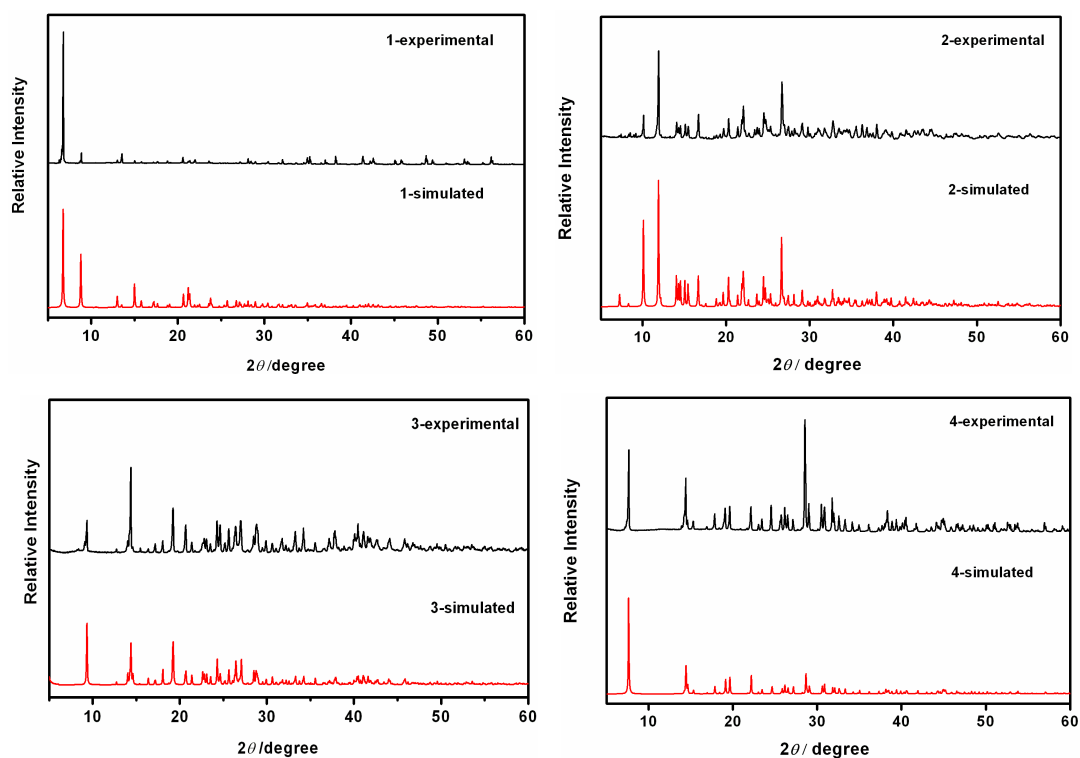


Fig. S8 The 3D supramolecular structure by H-bonds between O7A-H7A...N2 in complex 5. (H-bonds in green dotted line : O7A-H7A...N2 = 2.626 Å,  $\angle$  O7A-H7A...N2 = 172.84°, symmetry code: (A)  $-x, 1-y, 1-z$ )



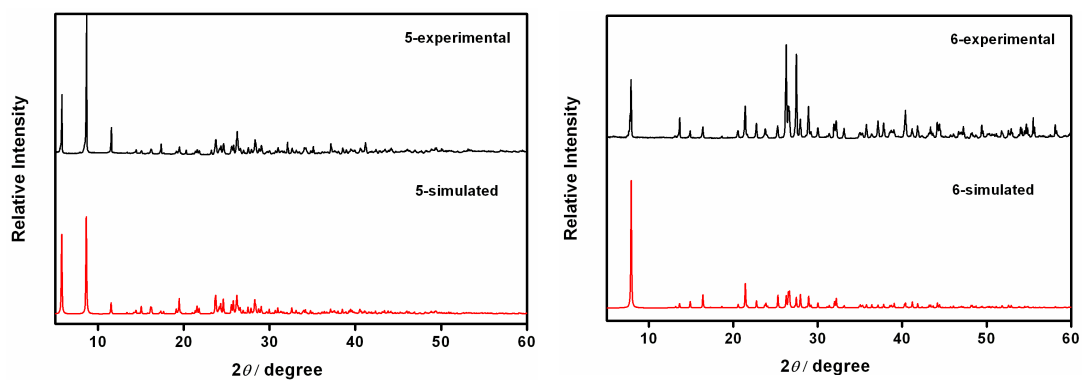


Fig. S9 The PXRD patterns for complexes 1-6. Red line-simulated and black line-experimental.

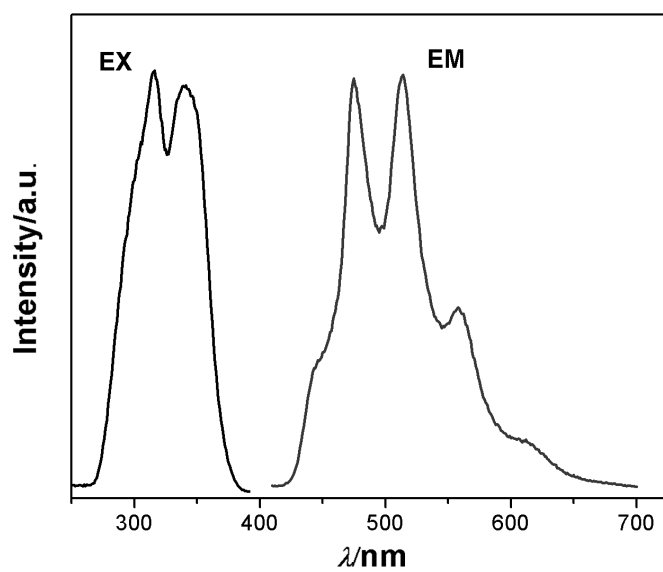


Fig. S10 The excited and emission curves of 2-NaH<sub>2</sub>stp in solid state.

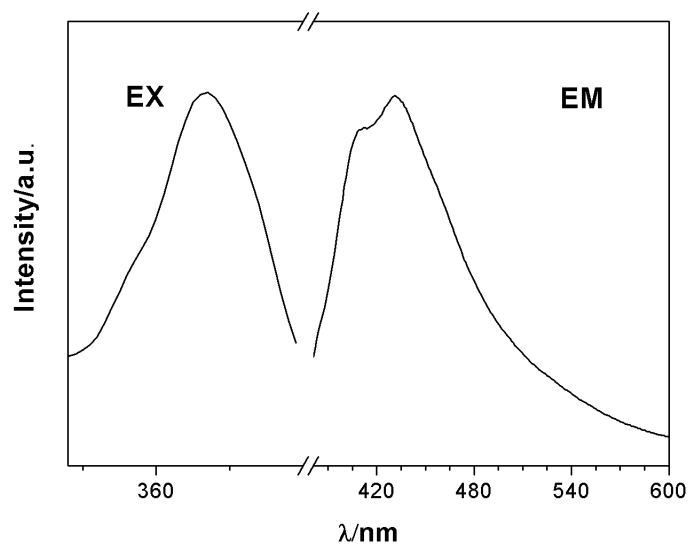


Fig. S11 The excited and emission curves of *o*-phen molecule in solid state.

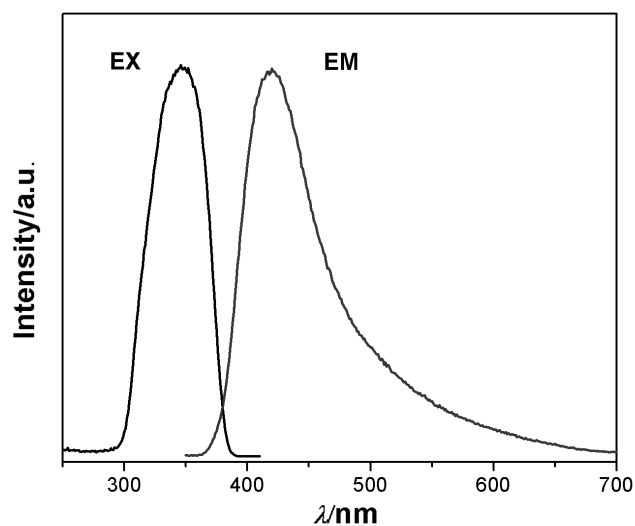


Fig. S12 The excited and emission curves of 2-Na<sub>3</sub>stp·H<sub>2</sub>O in solid state.

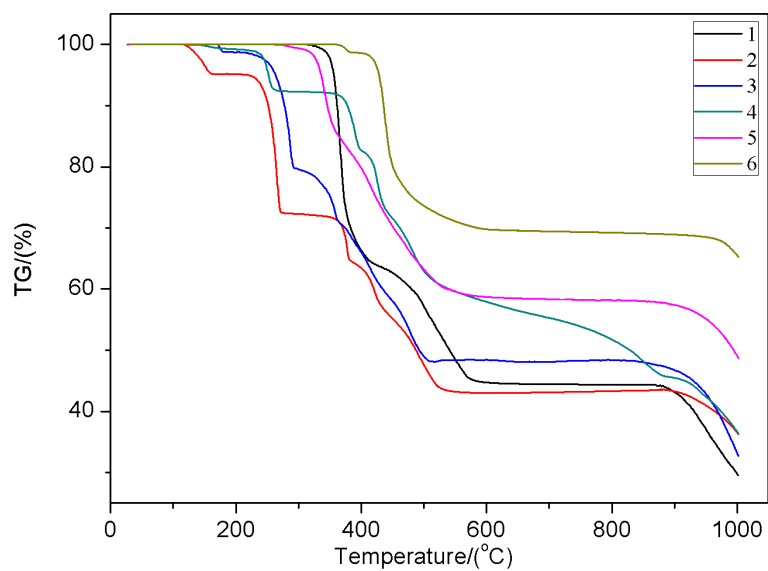


Fig. S13 TG curves of complexes 1-6.

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

|                     |            |                     |            |
|---------------------|------------|---------------------|------------|
| Pb(1)-O(1)          | 2.586(4)   | Pb(1)-O(2)#1        | 2.563(4)   |
| Pb(1)-O(6)          | 2.658(4)   | Pb(1)-N(1)          | 2.509(5)   |
| Pb(1)-O(1)#1        | 2.750(4)   | Pb(1)-N(2)          | 2.528(5)   |
| Pb(1)-O(7)#2        | 2.799(4)   | N(1)-Pb(1)-N(2)     | 66.15(16)  |
| N(1)-Pb(1)-O(2)#1   | 75.03(15)  | N(1)-Pb(1)-O(6)     | 83.37(15)  |
| N(2)-Pb(1)-O(2)#1   | 75.30(15)  | N(2)-Pb(1)-O(6)     | 88.21(15)  |
| N(1)-Pb(1)-O(1)     | 78.15(15)  | O(2)#1-Pb(1)-O(6)   | 156.72(14) |
| N(2)-Pb(1)-O(1)     | 141.13(16) | O(1)-Pb(1)-O(6)     | 72.35(13)  |
| O(2)#1-Pb(1)-O(1)   | 110.70(14) | N(1)-Pb(1)-O(1)#1   | 96.54(15)  |
| N(2)-Pb(1)-O(1)#1   | 124.07(15) | O(2)#1-Pb(1)-O(1)#1 | 48.80(13)  |
| O(1)-Pb(1)-O(1)#1   | 73.21(15)  | O(6)-Pb(1)-O(1)#1   | 144.80(12) |
| O(1)-Pb(1)-O(7)#2   | 134.59(13) | O(2)#1-Pb(1)-O(7)#2 | 95.17(14)  |
| O(6)-Pb(1)-O(7)#2   | 98.12(13)  | N(1)-Pb(1)-O(7)#2   | 146.28(15) |
| O(1)#1-Pb(1)-O(7)#2 | 100.79(13) | N(2)-Pb(1)-O(7)#2   | 80.18(14)  |

Symmetry codes: #1: 1-x, 1-y, 1-z; #2: -x, 1-y, 1-z.

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

|                   |           |                 |           |
|-------------------|-----------|-----------------|-----------|
| Pb(1)-O(1)        | 2.479(6)  | Pb(1)-O(4)      | 2.598(5)  |
| Pb(1)-N(2)        | 2.530(6)  | Pb(1)-N(1)      | 2.549(6)  |
| Pb(1)-O(5)#1      | 2.802(6)  | Pb(1)-O(8)      | 2.807(6)  |
| O(1)-Pb(1)-N(2)   | 100.6(2)  | O(1)-Pb(1)-O(4) | 74.4(2)   |
| O(1)-Pb(1)-N(1)   | 72.64(19) | N(2)-Pb(1)-O(4) | 70.89(18) |
| N(2)-Pb(1)-N(1)   | 64.4(2)   | N(1)-Pb(1)-O(4) | 116.8(2)  |
| O(1)-Pb(1)-O(5)#1 | 136.02(5) | O(1)-Pb(1)-O(8) | 150.67(6) |
| O(4)-Pb(1)-O(5)#1 | 149.61(5) | O(4)-Pb(1)-O(8) | 77.05(4)  |
| O(8)-Pb(1)-O(5)#1 | 72.74(4)  | N(1)-Pb(1)-O(8) | 127.68(5) |
| N(1)-Pb(1)-O(5)#1 | 80.47(4)  | N(2)-Pb(1)-O(8) | 75.81(5)  |
| N(2)-Pb(1)-O(5)#1 | 98.16(6)  |                 |           |

Symmetry codes: #1: 1+x, y, z.

**Table S3** Selected bond lengths (Å) and angles (°) for complex **3**

|                   |            |                     |            |
|-------------------|------------|---------------------|------------|
| Pb(1)-O(1)        | 2.596(5)   | Pb(1)-O(2)#1        | 2.564(4)   |
| Pb(1)-O(6)        | 2.739(5)   | Pb(1)-O(7)#2        | 2.634(4)   |
| Pb(1)-O(8)        | 2.497(6)   | Pb(1)-O(1) #1       | 2.706(4)   |
| Pb(1)-N(1)        | 2.802(4)   | O(2)-Pb(1)-O(1)#1   | 49.68(14)  |
| O(8)-Pb(1)-O(2)#1 | 108.77(17) | O(7)#2-Pb(1)-O(1)#1 | 74.44(14)  |
| O(8)-Pb(1)-O(1)   | 70.92(16)  | O(8)-Pb(1)-O(6)     | 125.35(15) |
| O(2)-Pb(1)-O(1)   | 71.65(15)  | O(2)#1-Pb(1)-O(6)   | 95.21(14)  |

|                   |            |                    |            |
|-------------------|------------|--------------------|------------|
| O(8)-Pb(1)-O(7)#2 | 90.32(16)  | O(1)-Pb(1)-O(6)    | 71.55(15)  |
| O(2)-Pb(1)-O(7)#2 | 108.87(14) | O(7)#2-Pb(1)-O(6)  | 127.68(15) |
| O(1)-Pb(1)-O(7)#2 | 159.70(16) | O(1)#1-Pb(1)-O(6)  | 144.87(14) |
| O(8)-Pb(1)-O(1)#1 | 74.32(17)  | O(1)-Pb(1)-O(1)#1  | 92.52(7)   |
| O(1)-Pb(1)-N(1)   | 104.92(17) | O(1) #1-Pb(1)-N(1) | 135.88(17) |
| O(6)-Pb(1)-N(1)   | 79.19(17)  | O(7)#2-Pb(1)-N(1)  | 75.99(17)  |
| O(8)-Pb(1)-N(1)   | 73.82(19)  | O(2)#1-Pb(1)-N(1)  | 174.22(15) |

Symmetry codes: #1: 1-x, 1+y, 0.5-z; #2: x, 1+y, z.

**Table S4** Selected bond lengths (Å) and angles (°) for complex 4

|                     |            |                     |            |
|---------------------|------------|---------------------|------------|
| Pb(1)-O(1)          | 2.557(4)   | Pb(1)-O(3)#3        | 2.606(5)   |
| Pb(1)-O(5)          | 2.672(4)   | Pb(1)-O(2) #2       | 2.656(4)   |
| Pb(1)-O(1)#1        | 2.520(4)   | Pb(1)-O(6) #4       | 2.708(4)   |
| Pb(1)-O(8)          | 2.789(4)   | O(5)-Pb(1)-O(6)#4   | 137.63(14) |
| O(1)#1-Pb(1)-O(1)   | 69.35(17)  | O(1)-Pb(1)-O(5)     | 67.66(14)  |
| O(1)#1-Pb(1)-O(3)#3 | 143.16(16) | O(3)#3-Pb(1)-O(5)   | 78.05(15)  |
| O(1)-Pb(1)-O(3)#3   | 81.82(15)  | O(2)#2-Pb(1)-O(5)   | 92.90(13)  |
| O(1)#1-Pb(1)-O(2)#2 | 116.19(15) | O(1)#1-Pb(1)-O(6)#4 | 112.68(14) |
| O(1)-Pb(1)-O(2)#2   | 160.11(15) | O(1)-Pb(1)-O(6)#4   | 127.52(15) |
| O(3)#3-Pb(1)-O(2)#2 | 98.77(15)  | O(3)#3-Pb(1)-O(6)#4 | 67.56(14)  |
| O(1)#1-Pb(1)-O(5)   | 109.67(15) | O(2)#2-Pb(1)-O(6)#4 | 69.66(14)  |
| O(1)-Pb(1)-O(8)     | 65.86(14)  | O(3)#3-Pb(1)-O(8)   | 73.79(15)  |
| O(5)-Pb(1)-O(8)     | 128.08(15) | O(2)#2-Pb(1)-O(8)   | 133.58(14) |
| O(1)#1-Pb(1)-O(8)   | 73.74(15)  | O(6) #4-Pb(1)-O(8)  | 65.17(13)  |

Symmetry codes: #1: 1-x, -y, 2+z; #2: x, -1+y, z; #3: 2-x, -y, 2-z; #4 : x, -0.5-y, 0.5+z.

**Table S5** Selected bond lengths (Å) and angles (°) for complex 5

|                      |           |                  |           |
|----------------------|-----------|------------------|-----------|
| Pb(1)-O(3)           | 2.697(10) | Pb(3)-O(13)#1    | 2.427(11) |
| Pb(1)-O(15)          | 2.323(8)  | Pb(3)-O(14)#1    | 2.515(9)  |
| Pb(1)-O(5)#2         | 2.581(10) | Pb(3)-O(15)      | 2.643(10) |
| Pb(1)-O(10)#3        | 2.740(9)  | Pb(3)-O(12)#4    | 2.672(10) |
| Pb(1)-O(14) #1       | 2.764(9)  | Pb(3)-O(9)#3     | 2.749(9)  |
| Pb(1)-O(9) #2        | 2.784(9)  | Pb(3)-O(8)       | 2.533(9)  |
| Pb(2)-O(15)          | 2.271(9)  | Pb(2)-N(1)       | 2.678(13) |
| Pb(2)-O(8)           | 2.526(10) | Pb(2)-O(4)       | 2.480(9)  |
| O(15)-Pb(1)-O(5)#2   | 80.8(3)   | O(15)-Pb(2)-O(4) | 74.2(3)   |
| O(15)-Pb(1)-O(3)     | 79.2(4)   | O(15)-Pb(2)-O(8) | 75.0(3)   |
| O(5)#2-Pb(1)-O(3)    | 88.0(4)   | O(4)-Pb(2)-O(8)  | 70.6(3)   |
| O(15)-Pb(1)-O(10)#3  | 79.0(3)   | O(15)-Pb(2)-N(1) | 86.3(4)   |
| O(5)#2-Pb(1)-O(10)#3 | 69.1(3)   | O(4)-Pb(2)-N(1)  | 85.4(4)   |
| O(3)-Pb(1)-O(10)#3   | 150.5(4)  | O(8)-Pb(2)-N(1)  | 152.7(4)  |



|                        |           |                        |           |
|------------------------|-----------|------------------------|-----------|
| O(14)#1-Pb(3)-O(8)     | 77.5(3)   | O(13)#1-Pb(3)-O(14)#1  | 52.6(3)   |
| O(13)#1-Pb(3)-O(15)    | 123.2(3)  | O(13)#1-Pb(3)-O(8)     | 85.4(3)   |
| O(14)#1-Pb(3)-O(15)    | 72.3(3)   | O(8)-Pb(3)-O(15)       | 68.9(3)   |
| O(14)#1-Pb(3)-O(12)#4  | 122.1(3)  | O(13)#1-Pb(3)-O(12)#4  | 77.4(3)   |
| O(8)-Pb(3)-O(12)#4     | 70.4(3)   | O(14)#1-Pb(3)-O(9)#2   | 98.1(3)   |
| O(15)-Pb(3)-O(12)#4    | 131.7(3)  | O(8)-Pb(3)-O(9)#2      | 165.3(3)  |
| O(13)#1-Pb(3)-O(9)#2   | 80.9(3)   | O(15)-Pb(3)-O(9)#2     | 123.6(3)  |
| O(12)#4-Pb(3)-O(9)#2   | 101.1(3)  | O(9) #2-Pb(1)-O(14) #1 | 93.57(3)  |
| O(3)-Pb(1)-O(14) #1    | 126.88(3) | O(3)-Pb(1)-O(9) #2     | 82.93(4)  |
| O(15)-Pb(1)-O(14) #1   | 72.99(3)  | O(15)-Pb(1)-O(9) #2    | 143.54(3) |
| O(5)#2-Pb(1)-O(14) #1  | 129.23(3) | O(5)#2-Pb(1)-O(9) #2   | 130.16(3) |
| O(10)#3-Pb(1)-O(14) #1 | 67.77(3)  | O(10)#3-Pb(1)-O(9) #2  | 125.90(3) |

Symmetry codes: #1: 1-x, 2-y, -z ; #2 : 1+x, y, z; #3: 1+x, 1+y, z ; #4: x, 1+y, z.

**Table S6 Selected bond lengths (Å) and angles (°) for complex 6**

|                     |          |                     |           |
|---------------------|----------|---------------------|-----------|
| Pb(1)-O(2)#1        | 2.722(8) | Pb(2)-O(1)          | 2.419(9)  |
| Pb(1)-O(4)          | 2.813(8) | Pb(2)-O(2)          | 2.569(9)  |
| Pb(1)-O(6)#3        | 2.480(8) | Pb(2)-O(4)#3        | 2.611(9)  |
| Pb(1)-O(8)#1        | 2.322(8) | Pb(2)-O(6)#3        | 2.474(10) |
| Pb(1)-O(8)          | 2.367(8) | Pb(2)-O(8)          | 2.576(8)  |
| O(8)#1-Pb(1)-O(8)   | 71.3(3)  | O(6)#3-Pb(2)-O(2)   | 73.3(3)   |
| O(8)#1-Pb(1)-O(6)#3 | 83.7(3)  | O(1)-Pb(2)-O(8)     | 128.1(3)  |
| O(8)-Pb(1)-O(6)#3   | 69.7(3)  | O(6)#3-Pb(2)-O(8)   | 66.6(3)   |
| O(8)#1-Pb(1)-O(2)#1 | 77.9(3)  | O(2)-Pb(2)-O(8)     | 76.5(3)   |
| O(8)-Pb(1)-O(2)#1   | 97.5(3)  | O(1)-Pb(2)-O(4)#3   | 81.3(3)   |
| O(6)#3-Pb(1)-O(2)#1 | 160.3(3) | O(6)#3-Pb(2)-O(4)#3 | 67.9(3)   |
| O(1)-Pb(2)-O(6)#3   | 95.0(3)  | O(2)-Pb(2)-O(4)#3   | 114.3(3)  |
| O(1)-Pb(2)-O(2)     | 51.6(3)  | O(8)-Pb(2)-O(4)#3   | 126.8(3)  |

Symmetry codes: #1: 1-x, 2-y, 1-z ; #2: x, 1.5-y, -0.5+z; #3: x, 3-y, 0.5+z .