

Electronic Supplementary Information for CrystEngComm

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Electronic Supplementary Information (ESI)

**Effect of ligand configurations, secondary Pb-O interactions
and auxiliary ligands on Pb(II)-mono/disulfonate complexes:
synthesis, structures, and luminescent properties**

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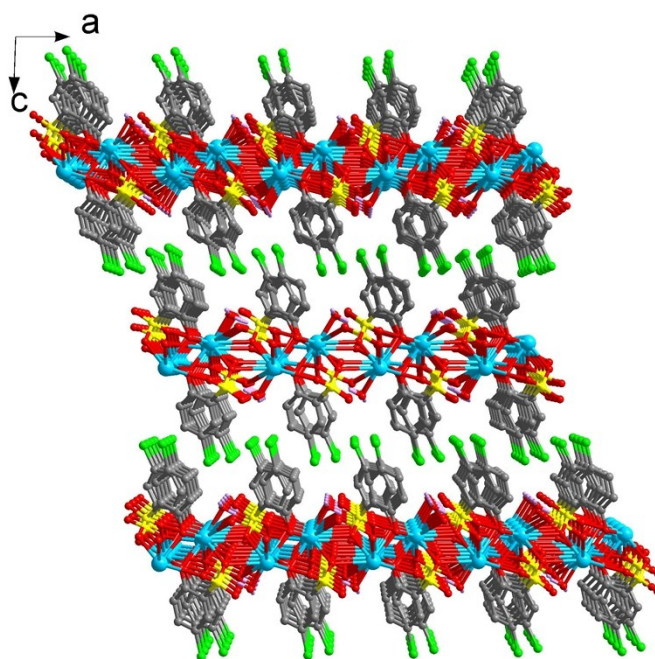


Fig. S1 3-D network of complex 1.

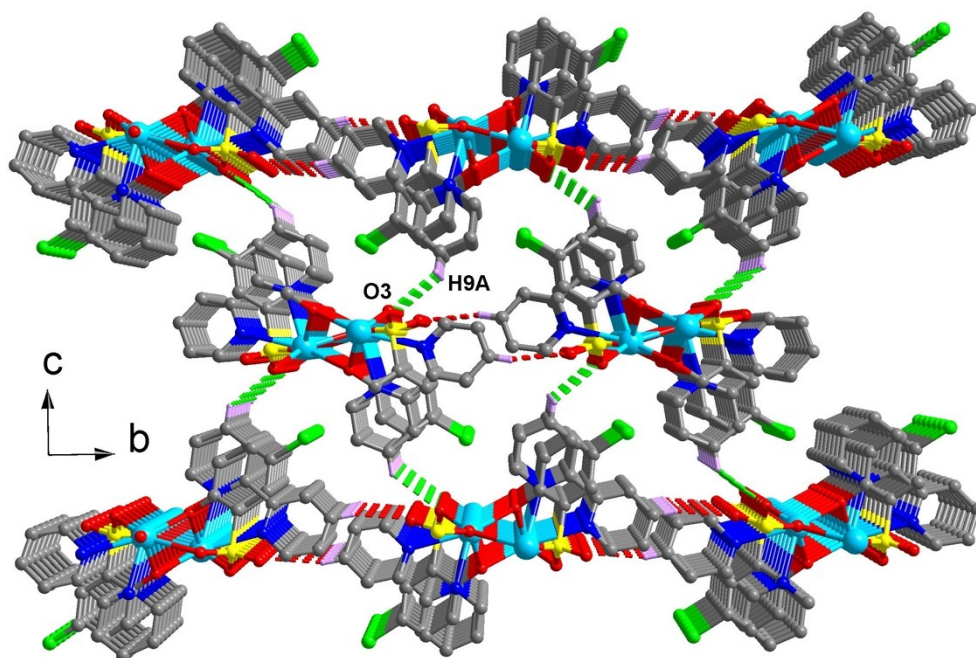


Fig. S2 3-D supramolecular network of complex 2 extended by the C-H...O interactions.

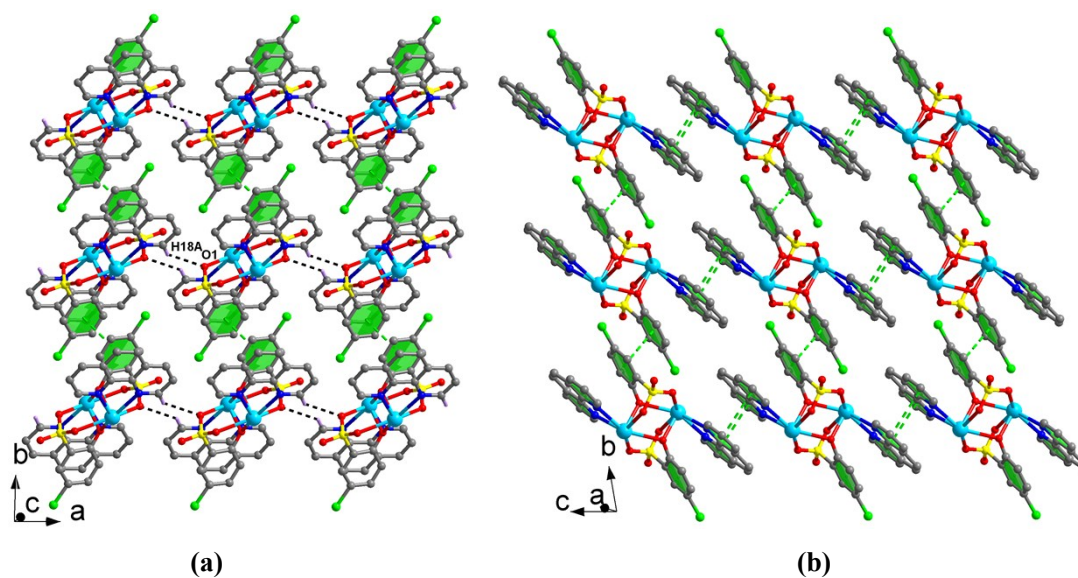


Fig. S3 Two types of layers in complex **3** extended by the C-H $\cdots$ O and $\pi\cdots\pi$ stacking interactions.

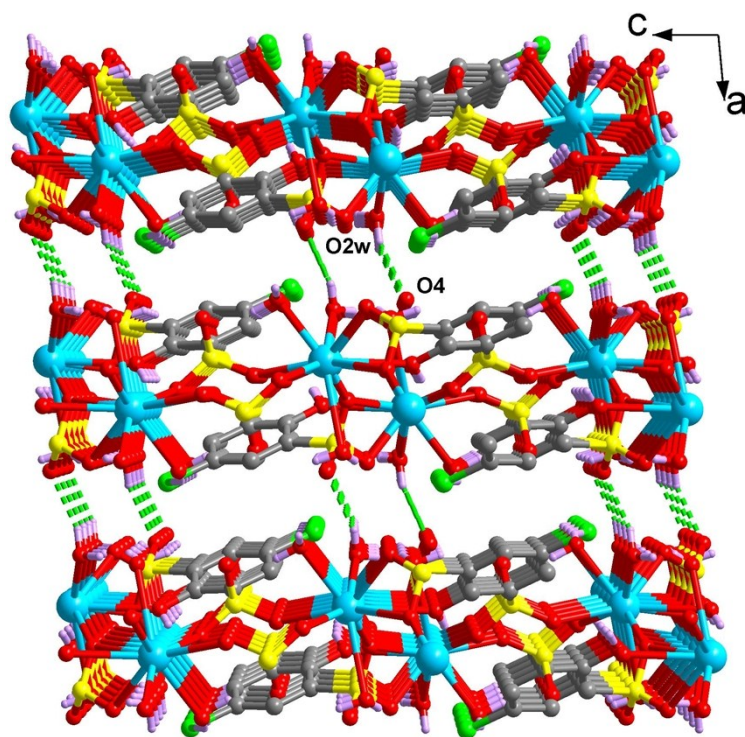


Fig. S4 3-D supramolecular network of complex **5** extended by the O-H $\cdots$ O interactions.

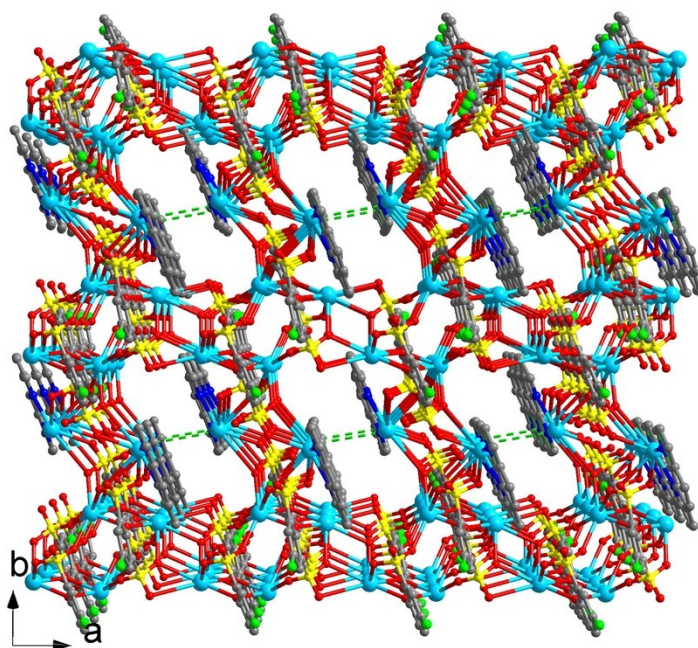


Fig. S5 3-D supramolecular network of complex **7** extended by $\pi \cdots \pi$ stacking interactions.

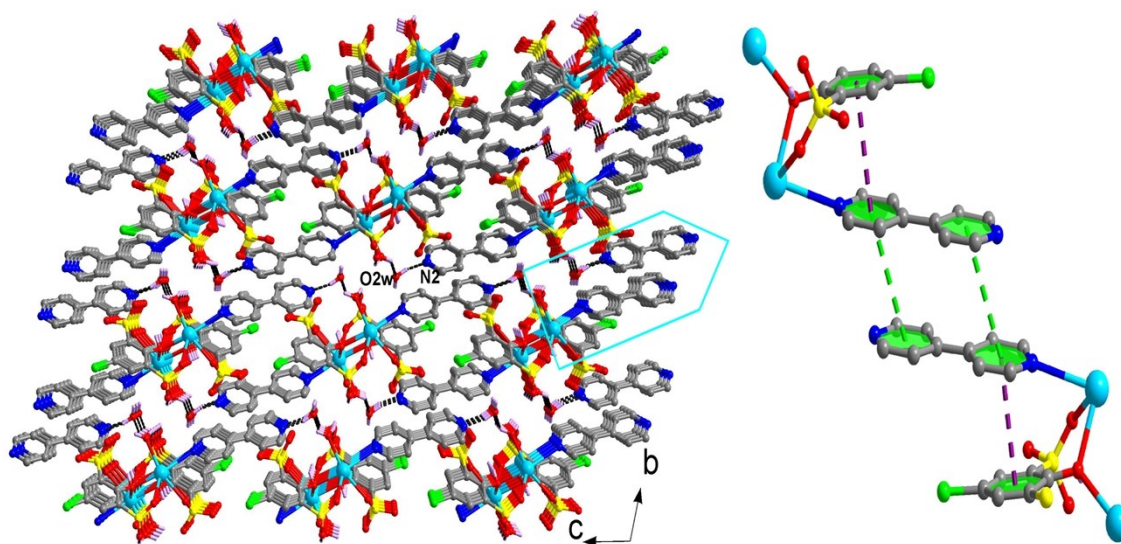


Fig. S6 3-D supramolecular network of complex **8** extended by the $\text{O}-\text{H} \cdots \text{N}$ and $\pi \cdots \pi$ stacking interactions. The different $\pi \cdots \pi$ stacking interactions between two pyridyl rings, phenyl and pyridyl rings were denoted as different color.

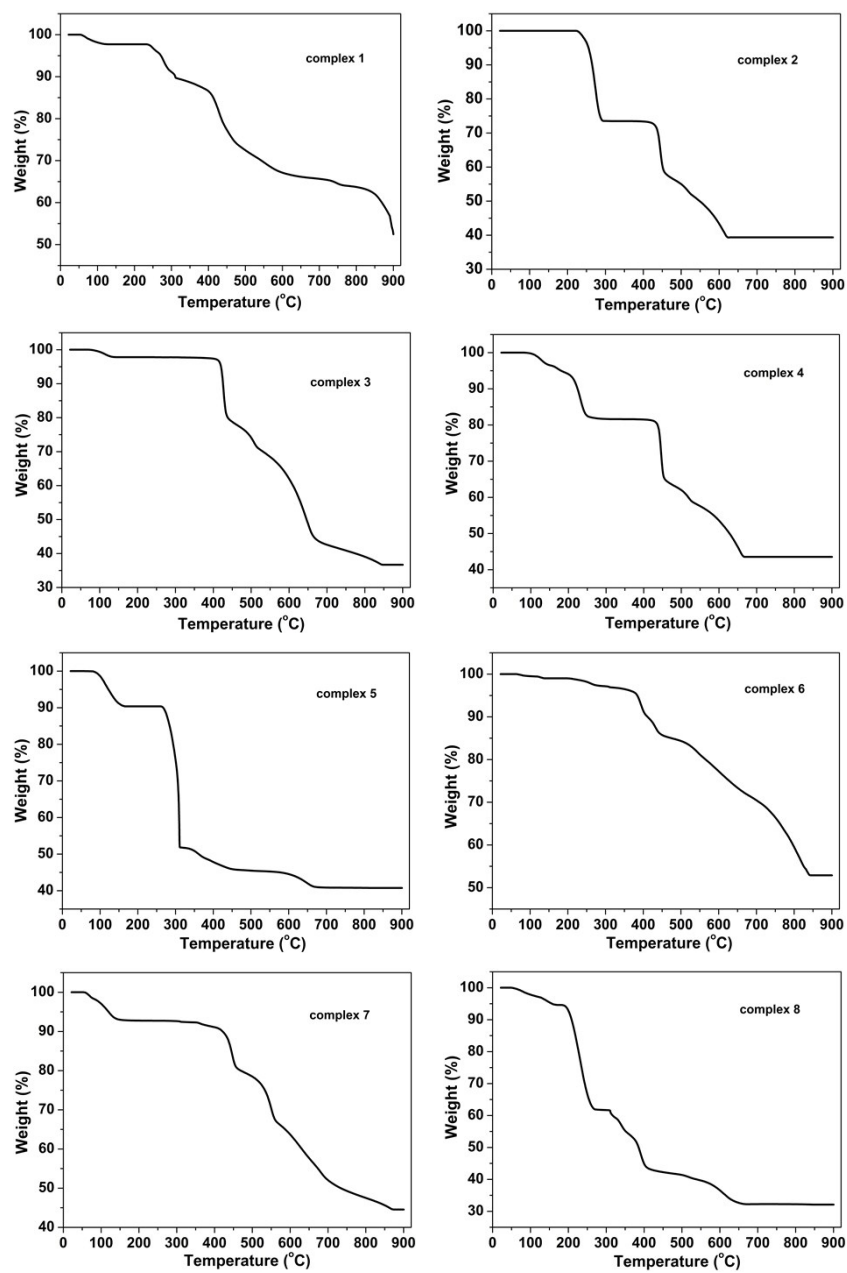


Fig. S7 TG curves of complexes **1-8** at N_2 atmosphere.

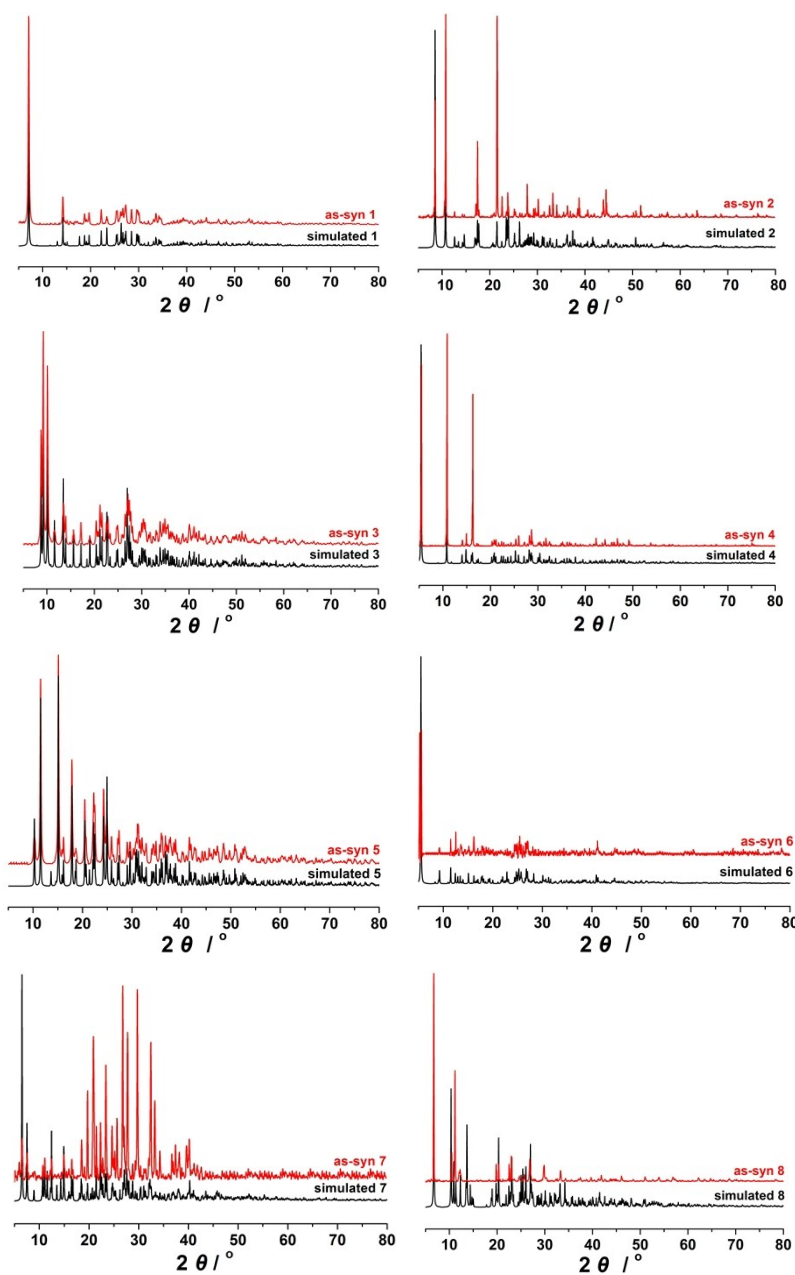


Fig. S8 PXRD patterns of complexes 1-8.

Table S1 Selected Hydrogen Bond Parameters for Complexes **1-8**^a

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
Complex 1				
O(1W)-H(1W1)...O(5) ⁱⁱⁱ	0.85	2.09	2.754(11)	134.8
Complex 3				
O(1W)-H(1W1)...O(2)	0.85	2.38	3.057(11)	137.1
Complex 4				
O(1W)-H(1W1)...O(2) ^{vii}	0.85(9)	2.14(9)	2.889(13)	146(15)
O(1W)-H(1W2)...N(1)	0.85(9)	2.01(11)	2.750(19)	145(18)
Complex 5				
O(1W)-H(1W1)...O(1) ⁱ	0.85(5)	1.99(5)	2.763(9)	151(10)
O(1W)-H(1W1)...O(2) ⁱ	0.85(5)	2.59(8)	3.104(9)	120(8)
O(1W)-H(1W2)...Cl(1) ^v	0.85(5)	2.73(5)	3.527(8)	155(10)
O(2W)-H(2W1)...O(3W) ⁱⁱ	0.85(5)	1.858(16)	2.706(10)	174(9)
O(2W)-H(2W2)...O(4) ^{vi}	0.85(5)	2.01(5)	2.798(9)	154(11)
O(3W)-H(3W1)...O(4) ⁱⁱ	0.85(5)	2.22(9)	2.838(9)	130(9)
O(3W)-H(3W2)...O(1) ^{iv}	0.85(5)	2.08(5)	2.846(11)	150(10)
O(7)-H(7O)...O(3)	0.85(5)	1.83(4)	2.623(9)	155(10)
Complex 6				
O(1W)-H(1W1)...O(13) ⁱⁱ	0.85(4)	1.93(4)	2.773(13)	168(17)
O(1W)-H(1W2)...O(3)	0.85(4)	2.31(11)	3.069(16)	149(20)
Complex 7				
O(1W)-H(1W1)...O(6W) ⁱⁱ	0.85	2.27	2.814(13)	121.4
O(1W)-H(1W2)...O(3) ⁱⁱⁱ	0.85	2.22	2.899(11)	136.0
O(2W)-H(2W1)...O(5)	0.85	1.94	2.794(10)	179.8
O(2W)-H(2W2)...O(11)	0.85	1.91	2.762(10)	179.8
O(3W)-H(3W1)...O(2W) ^{iv}	0.85	2.24	3.093(15)	177.3
O(4W)-H(4W1)...O(9) ⁱ	0.85	1.90	2.749(12)	172.2
O(4W)-H(4W2)...O(6W)	0.85	2.48	3.328(18)	172.3
O(5W)-H(5W1)...O(13) ⁱ	0.85	2.26	3.101(15)	173.4
O(5W)-H(5W2)...O(2)	0.85	1.90	2.721(17)	162.7
O(6W)-H(6W1)...O(5W) ⁱ	0.85	2.14	2.93(2)	155.2
O(6W)-H(6W1)...O(13)	0.85	2.84	3.268(13)	112.8
O(7W)-H(7W2)...O(5)	0.85	2.36	2.91(2)	123.4

Complex 8

O(1W)-H(1W1)...O(4)	0.85	2.19	2.899(12)	140.3
O(1W)-H(1W1)...O(2W)	0.85	2.30	2.873(14)	125.0
O(1W)-H(1W2)...O(1) ⁱ	0.85	2.25	2.831(11)	125.3
O(1W)-H(1W2)...O(1) ⁱⁱ	0.85	2.39	3.097(13)	141.6
O(2W)-H(2W2)...N(2) ⁱⁱⁱ	0.85	1.82	2.638(15)	159.8
O(7)-H(7O)...O(6)	0.85	2.43	2.944(9)	120.0

^a Symmetry transformations used to generate equivalent atoms: iii -x,-y,-z+2 for **1**; (vii) x,y,z+1 for **4**; i x,-y+3/2,z-1/2, ii -x+1,y-1/2,-z+1/2, iii -x+1,y+1/2,-z+1/2, v x,-y+5/2,z-1/2, vi -x+2,y-1/2,-z+1/2 for **5**; ii x-1,y,z for **6**; i -x+1,-y,-z+1, ii x+1,y,z, iii -x+2,-y,-z+1, iv x-1,y,z for **7**; i -x+2,-y,-z+1, ii x,y-1,z, iii x-1,y,z-1 for **8**.
