Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting Information

Two Ligand-Functionalized Pb(II) Metal-Organic Frameworks: Structures and Catalytic Performance

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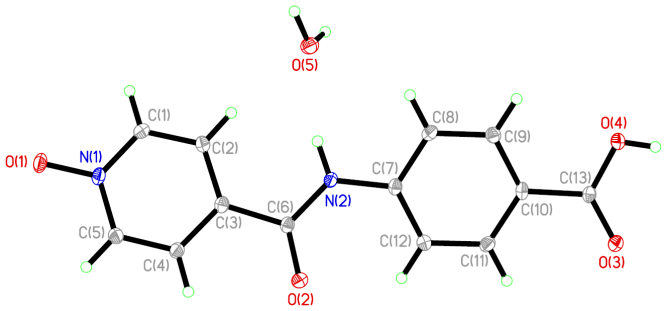

Figure S1. The molecule structure of ligand.

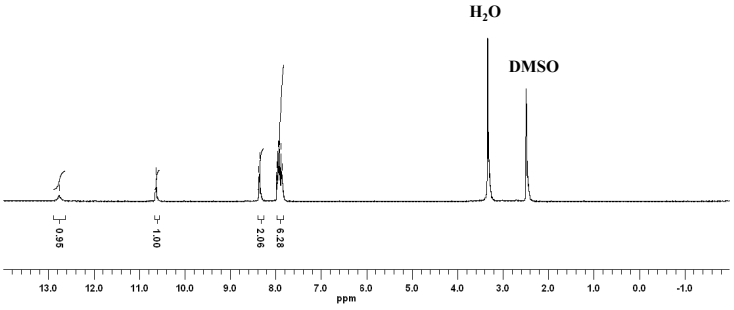

Figure S2. ^{1}H NMR (300 MHz, DMSO-d_6) spectrum of the ligand.

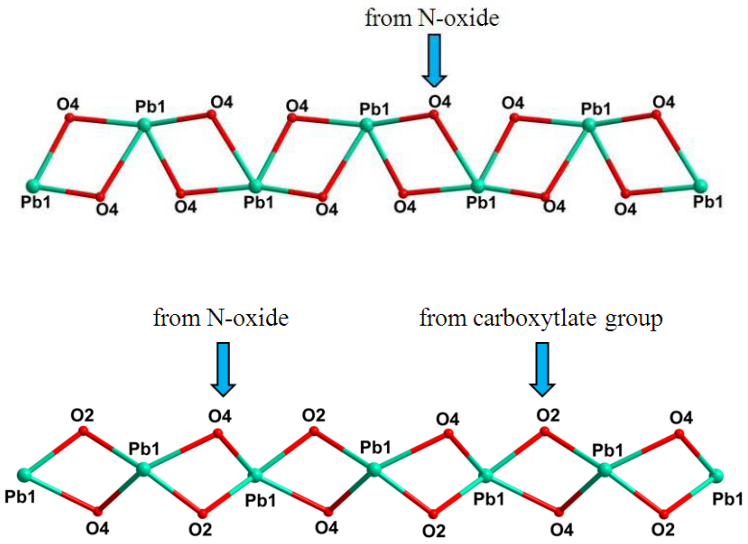

Figure S3. $[PbO_2]_\infty$ chain connected by Pb atom and μ_2-O atoms, showing the difference of the bridging O atoms of Pb_2O_2 rings in **1** (top) and **2** (bottom), respectively.

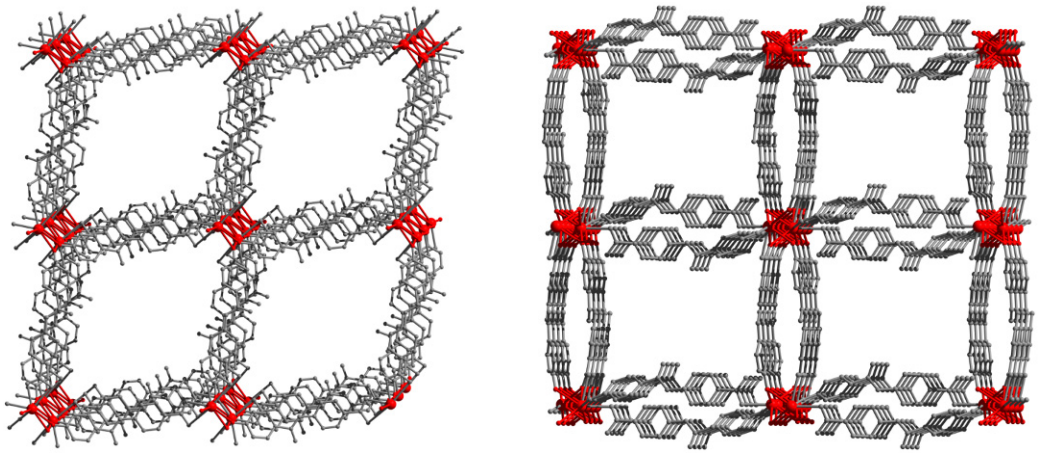

Figure S4. Illustration of the connection of $[PbO_2]_\infty$ chains in **1** (left) and **2** (right) by the ligands. H atoms and solvent molecules are omitted for clarity. $[PbO_2]_\infty$ chains and ligands are highlighted in red and gray colors, respectively.

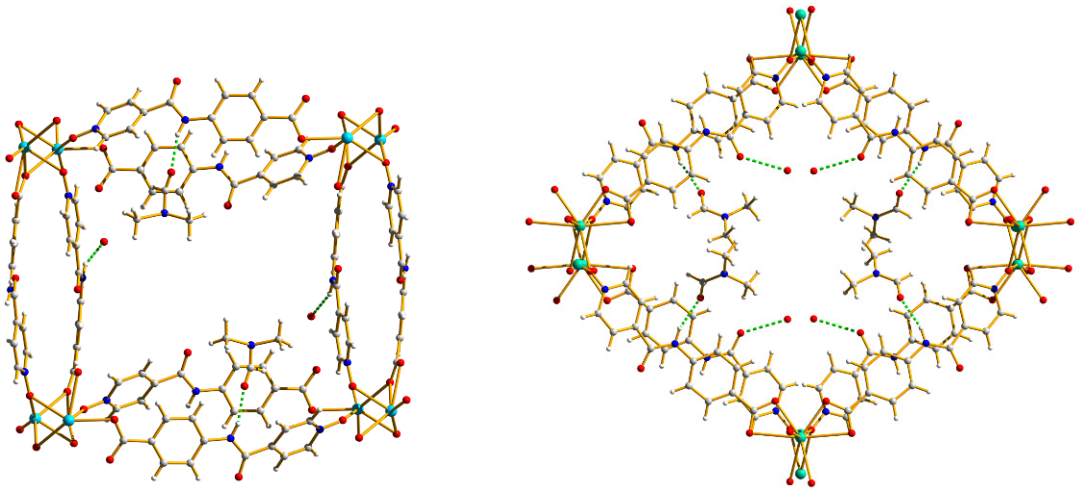

Figure S5. The hydrogen bonds (green dash lines) between the solvent molecules (DMF and water) and the amide groups in **1** (left) and **2** (right). Other solvent guest molecules that don't interact with the host are omitted for clarity.

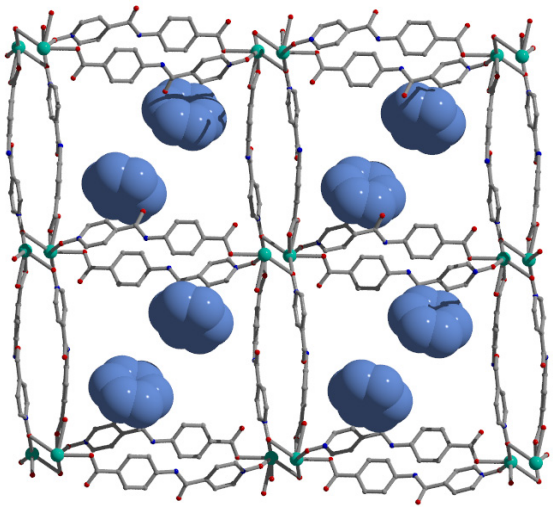

Figure S6. View of benzene guest molecules (shown in space-filling mode) hosted inside the 1D channels in **2'**. The coordination framework is shown in stick mode and H atoms are omitted for clarity.

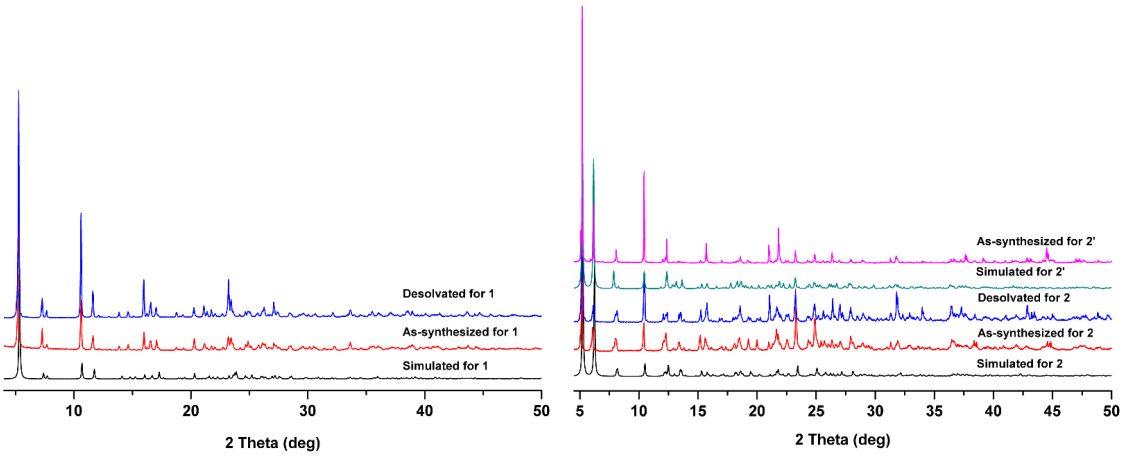

Figure S7. PXRD patterns of simulated, as-synthesized and desolvated **1** (left), **2** and **2'** (right).

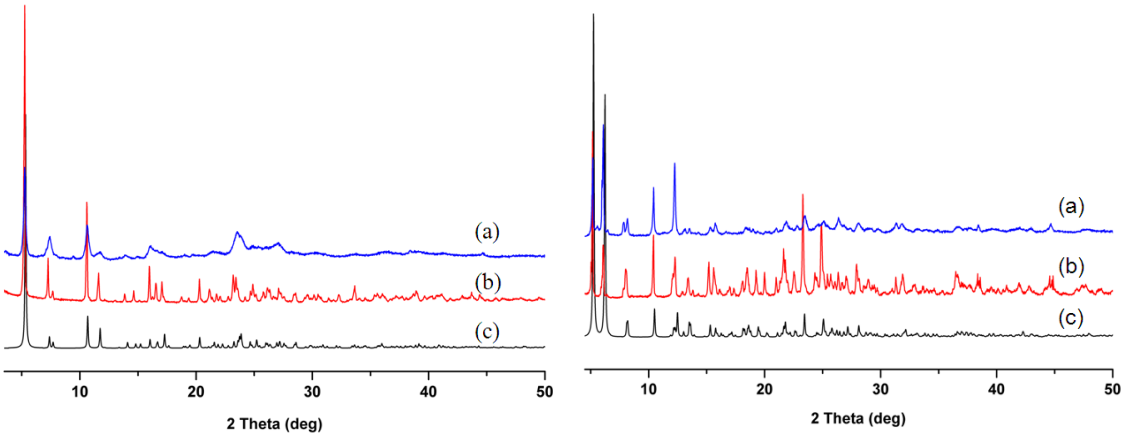

Figure S8. Powder X-ray diffraction patterns of **1** (left) and **2** (right): (a) after the catalytic reaction, (b) as-made, and (c) simulated from the X-ray crystal structure.

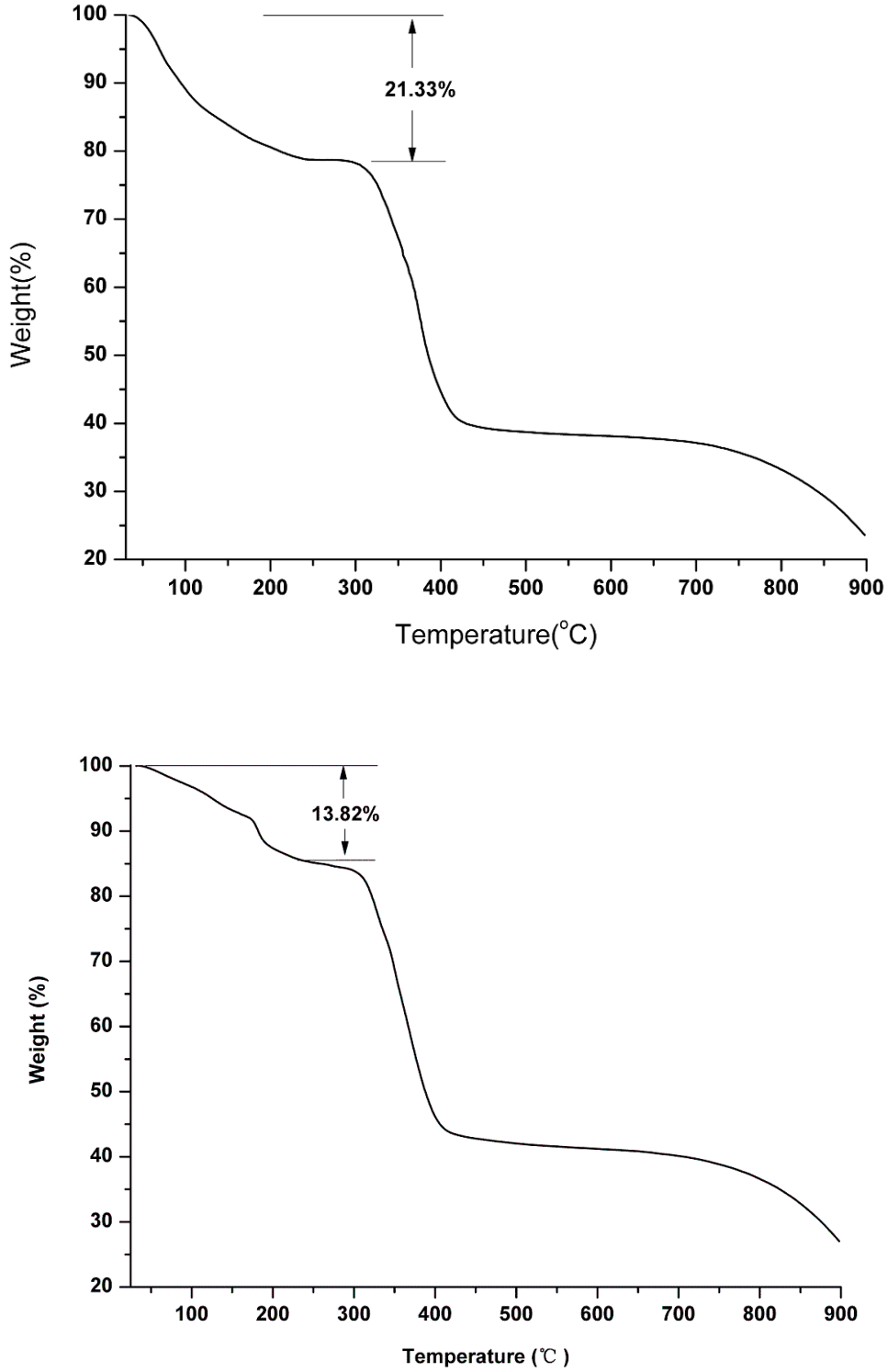

Figure S9. The TGA curves of **1** (top) and **2** (bottom).

Table S1. Selected bond lengths (Å) and bond Angles (°) for 1, 2 and 2'.

1		**2**		**2'**	
Pb(1)-O(2)#1	2.438(5)	Pb(1)-O(5)#1	2.402(6)	Pb(1)-O(6)#1	2.423(3)
Pb(1)-O(2)	2.438(5)	Pb(1)-O(2)	2.468(7)	Pb(1)-O(1)	2.508(3)
Pb(1)-O(4)#2	2.470(5)	Pb(1)-O(1)	2.562(6)	Pb(1)-O(2)	2.556(3)
Pb(1)-O(4)#3	2.470(5)	Pb(1)-O(8)	2.616(7)	Pb(1)-O(8)	2.647 (3)
O(2)#1-Pb(1)-O(2)	71.7(2)	O(5)#1-Pb(1)-O(2)	85.0(2)	O(6)#1-Pb(1)-O(1)	85.20(11)
O(2)#1-Pb(1)-O(4)#2	83.68(17)	O(5)#1-Pb(1)-O(1)	77.7(2)	O(6)#1-Pb(1)-O(2)	78.26(11)
O(2)-Pb(1)-O(4)#2	82.77(17)	O(2)-Pb(1)-O(1)	51.5(2)	O(1)-Pb(1)-O(2)	51.54(9)
O(2)#1-Pb(1)-O(4)#3	82.77(17)	O(5)#1-Pb(1)-O(8)	79.2(2)	O(6)#1-Pb(1)-O(8)	80.39(10)
O(2)-Pb(1)-O(4)#3	83.68(17)	O(2)-Pb(1)-O(8)	127.9(2)	O(1)-Pb(1)-O(8)	128.63(10)
O(4)#2-Pb(1)-O(4)#3	163.3(2)	O(1)-Pb(1)-O(8)	76.6(2)	O(2)-Pb(1)-O(8)	77.23(9)

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