

Supporting information

Novel Alkali and Alkaline Earth Metal Coordination Polymers Based on 1,4-Naphthalenedicarboxylic Acid: Synthesis, Structural Characterization and Properties

Duraisamy Senthil Raja,^{a,b} Jheng-Hong Luo,^c Chun-Ting Yeh,^b Yue-Chun Jiang,^b Kuei-Fang Hsu,^{*d} and Chia-Her Lin^{*b,c}

^aDepartment of Chemistry, National Tsing Hua University, Hsinchu 30013, Taiwan.

^bDepartment of Chemistry, Chung Yuan Christian University, Chung-Li 32023, Taiwan.

^cMaster Program in Nanotechnology, Chung Yuan Christian University, Chung-Li 32023, Taiwan.

^dDepartment of Chemistry, National Cheng Kung University, Tainan 701, Taiwan.

Corresponding Authors:

Prof. Dr. Kuei-Fang Hsu

E-mail: hsukf@mail.ncku.edu.tw

Prof. Dr. Chia-Her Lin

E-mail: chiaher@cycu.edu.tw

Tel: +886-3-2653315

Fax: +886-3-2653399

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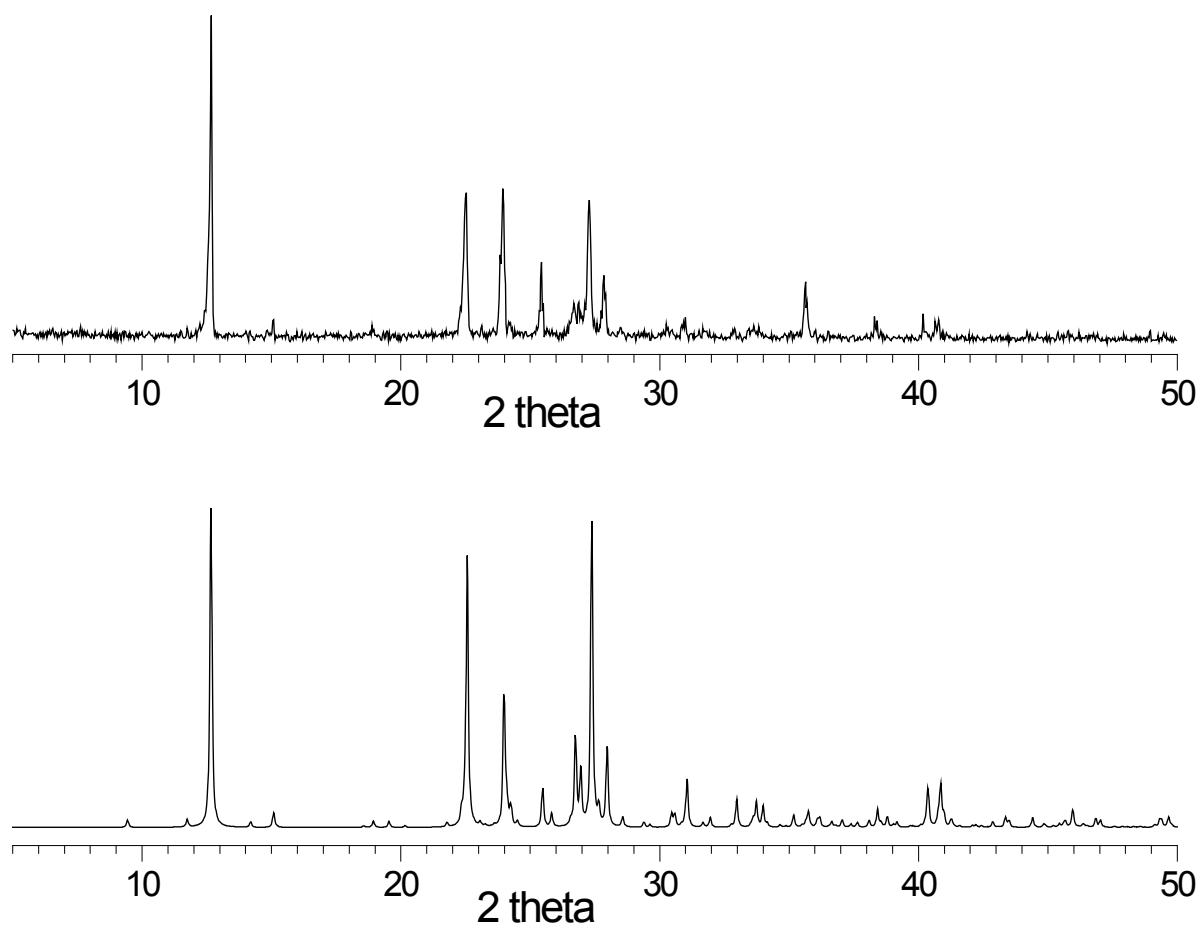


Figure S1. Powder XRD patterns of **1** (measured, top; calculated, bottom).

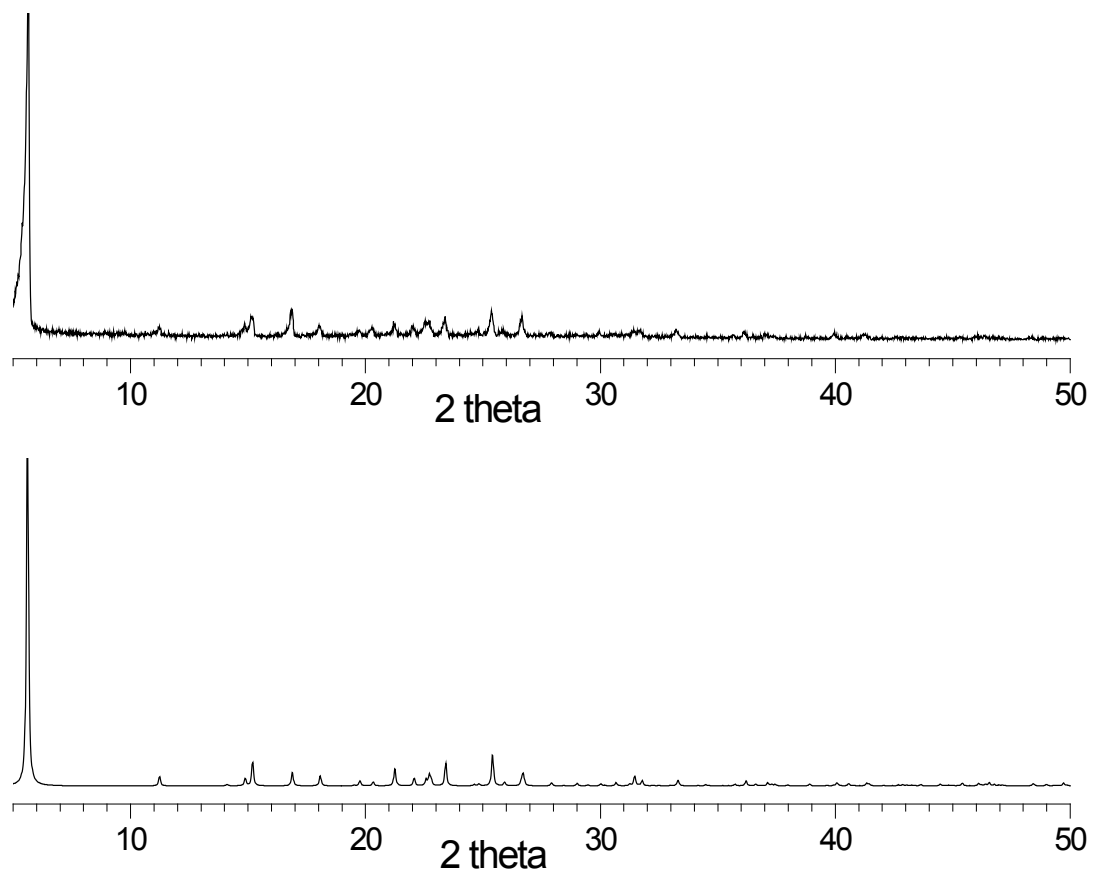


Figure S2. Powder XRD patterns of **2** (measured, top; calculated, bottom).

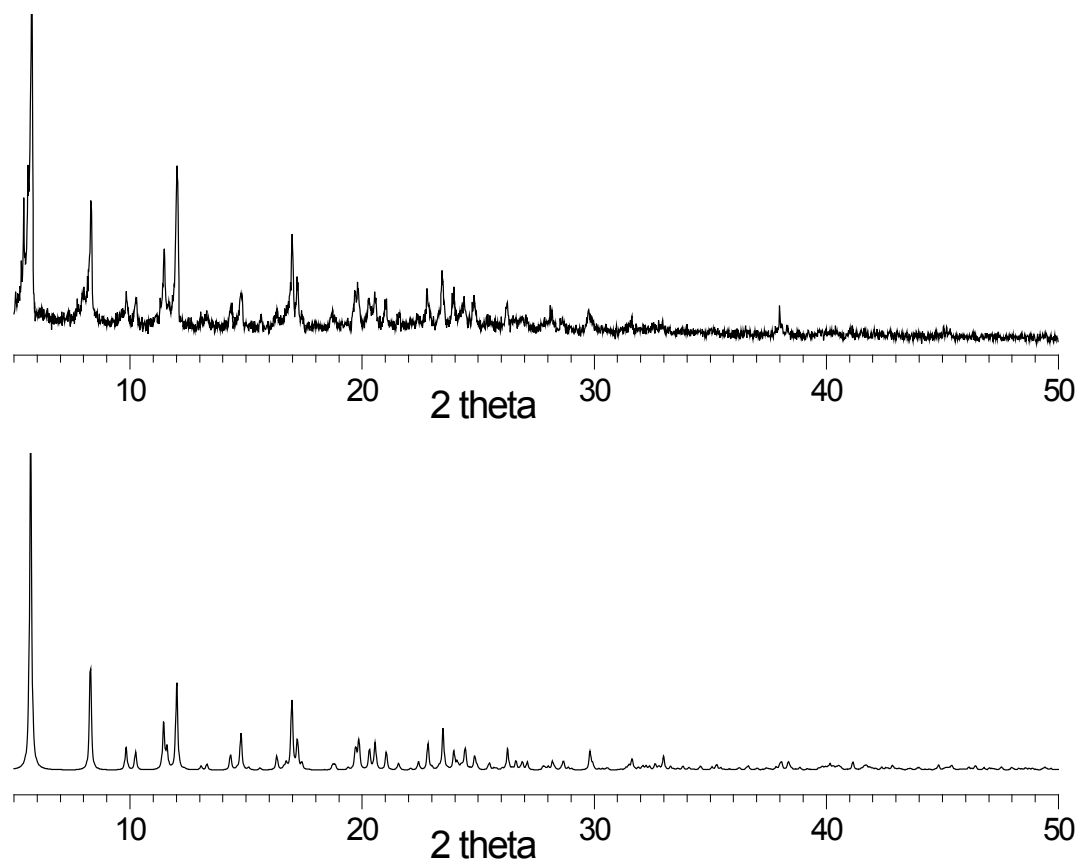


Figure S3. Powder XRD patterns of **3** (measured, top; calculated, bottom)

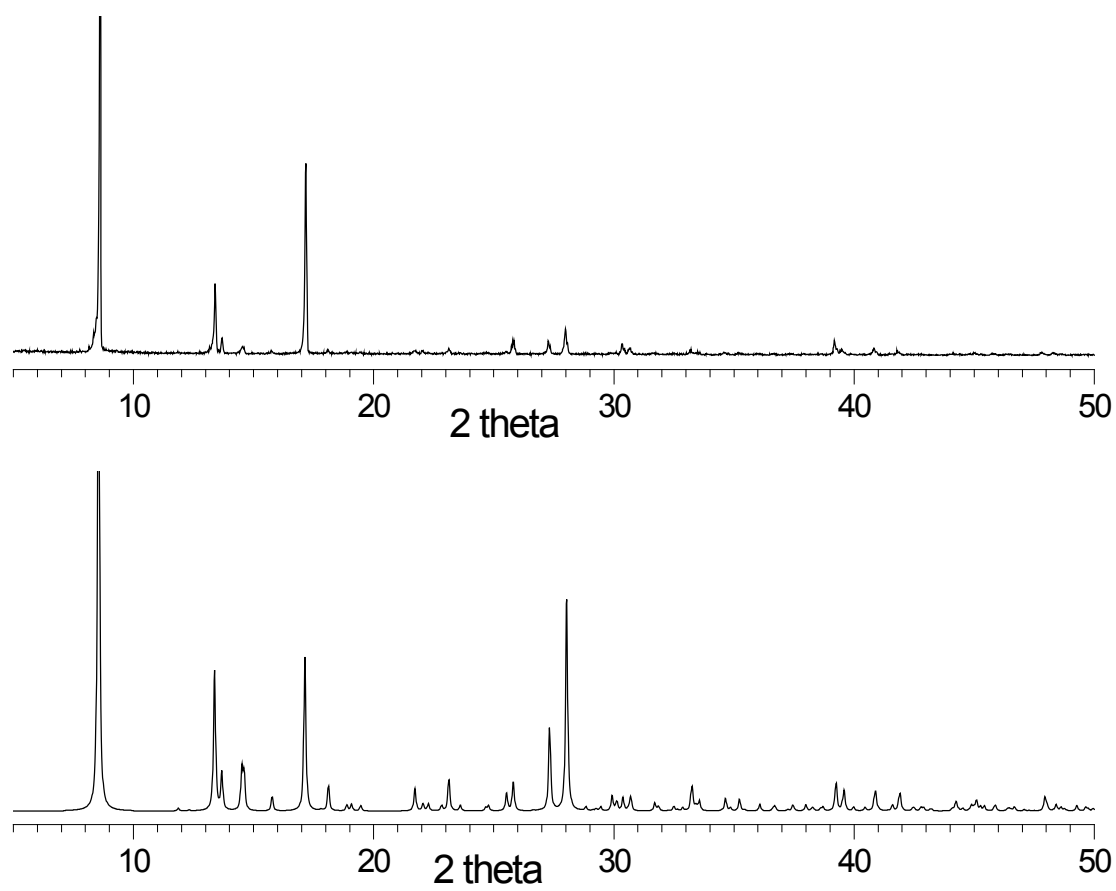


Figure S4. Powder XRD patterns of **4** (measured, top; calculated, bottom)

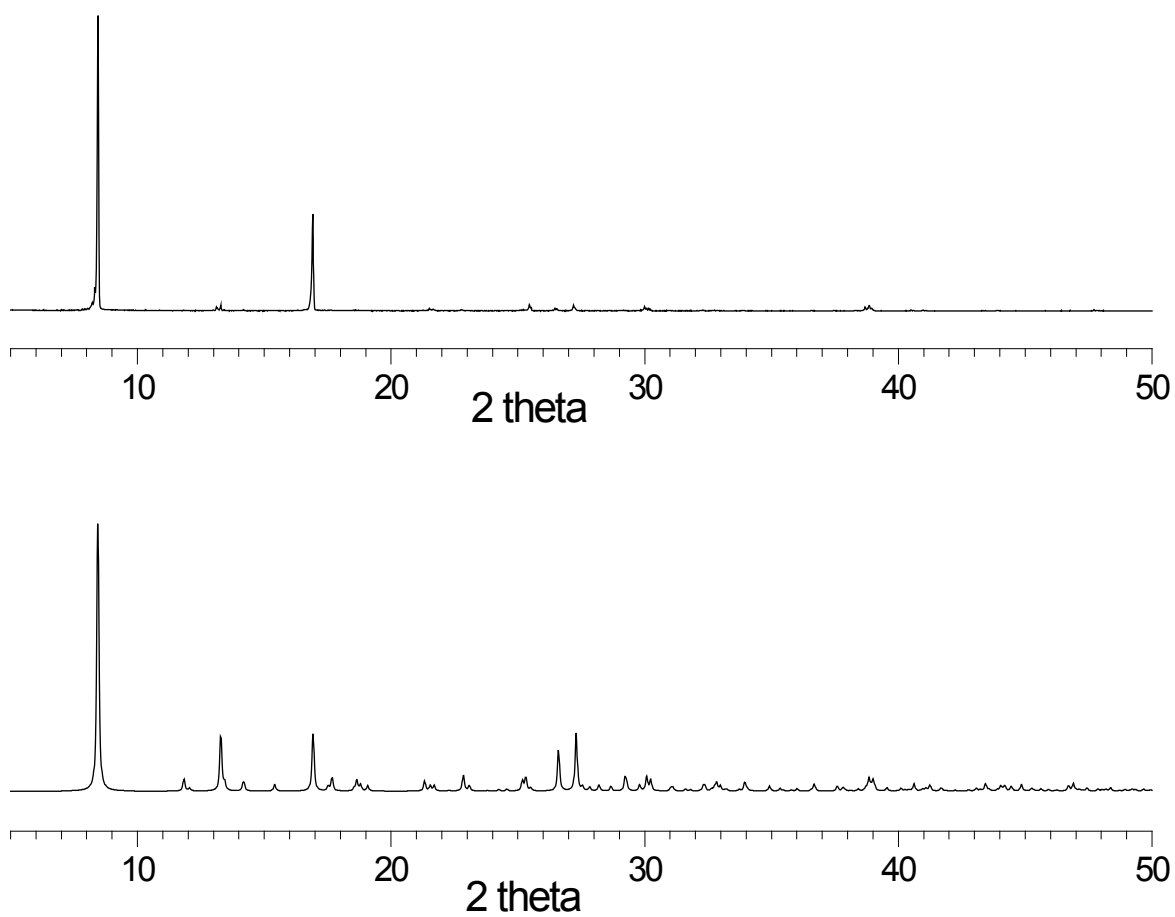


Figure S5. Powder XRD patterns of **5** (measured, top; calculated, bottom)

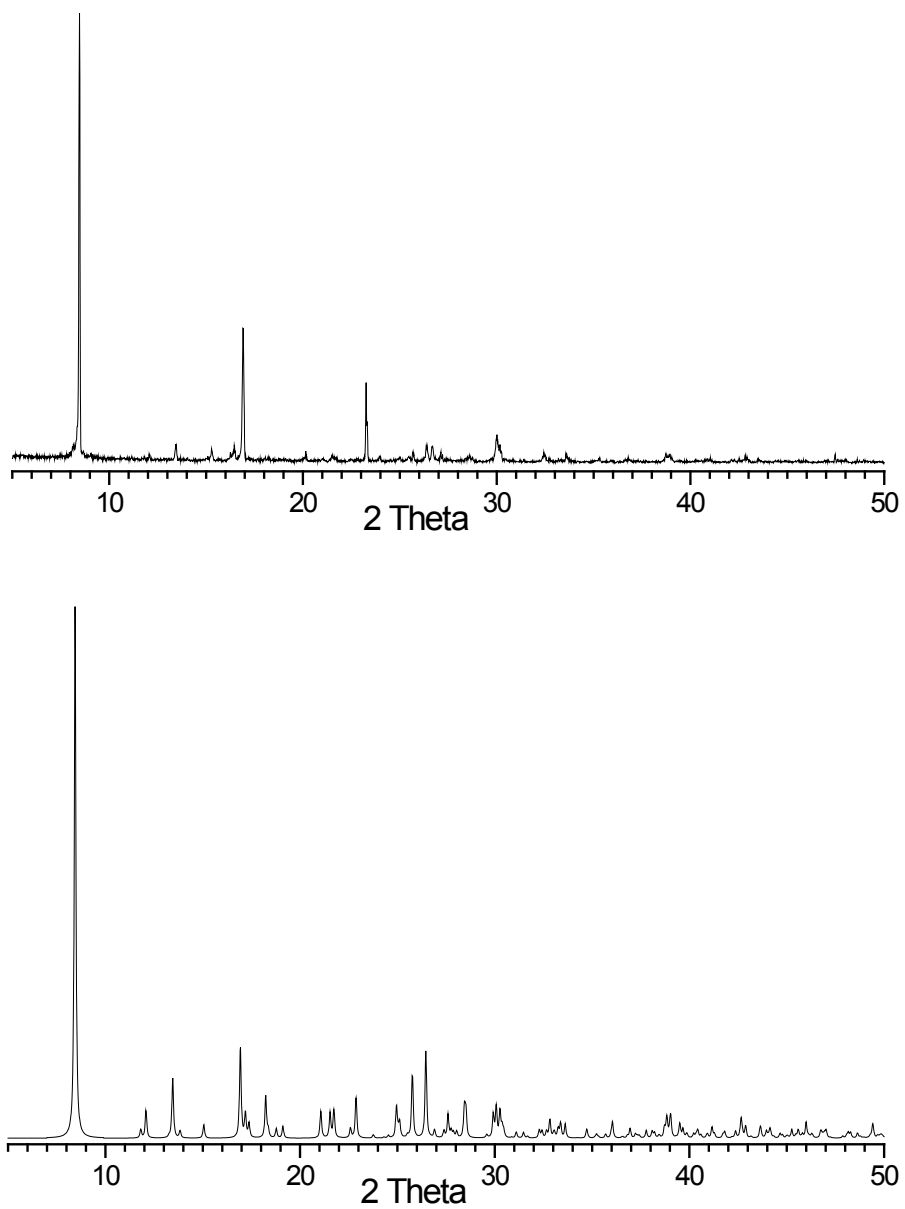


Figure S6. Powder XRD patterns of **6** (measured, top; calculated, bottom).

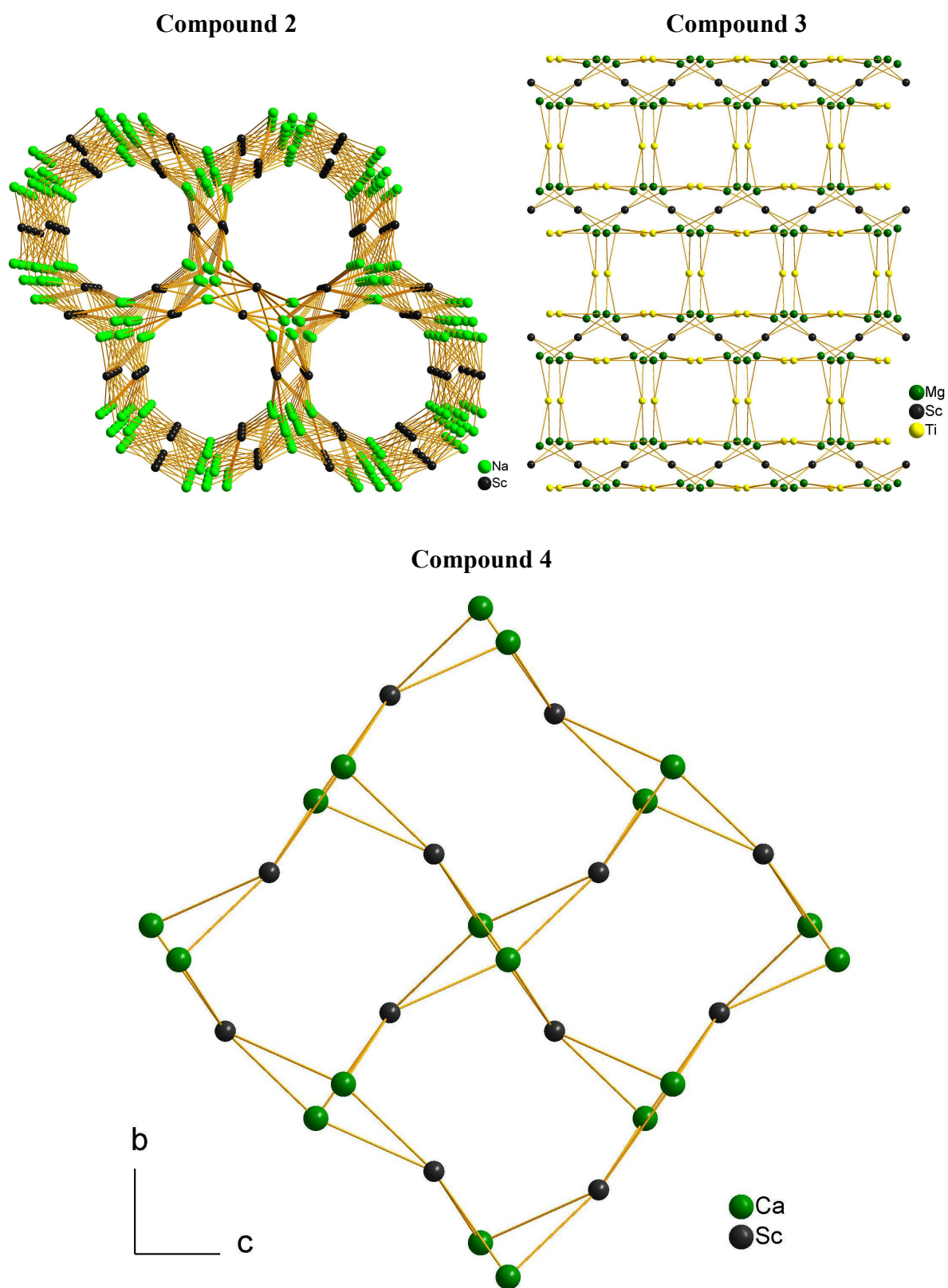


Figure S7. The topological representation of compound 2-4.

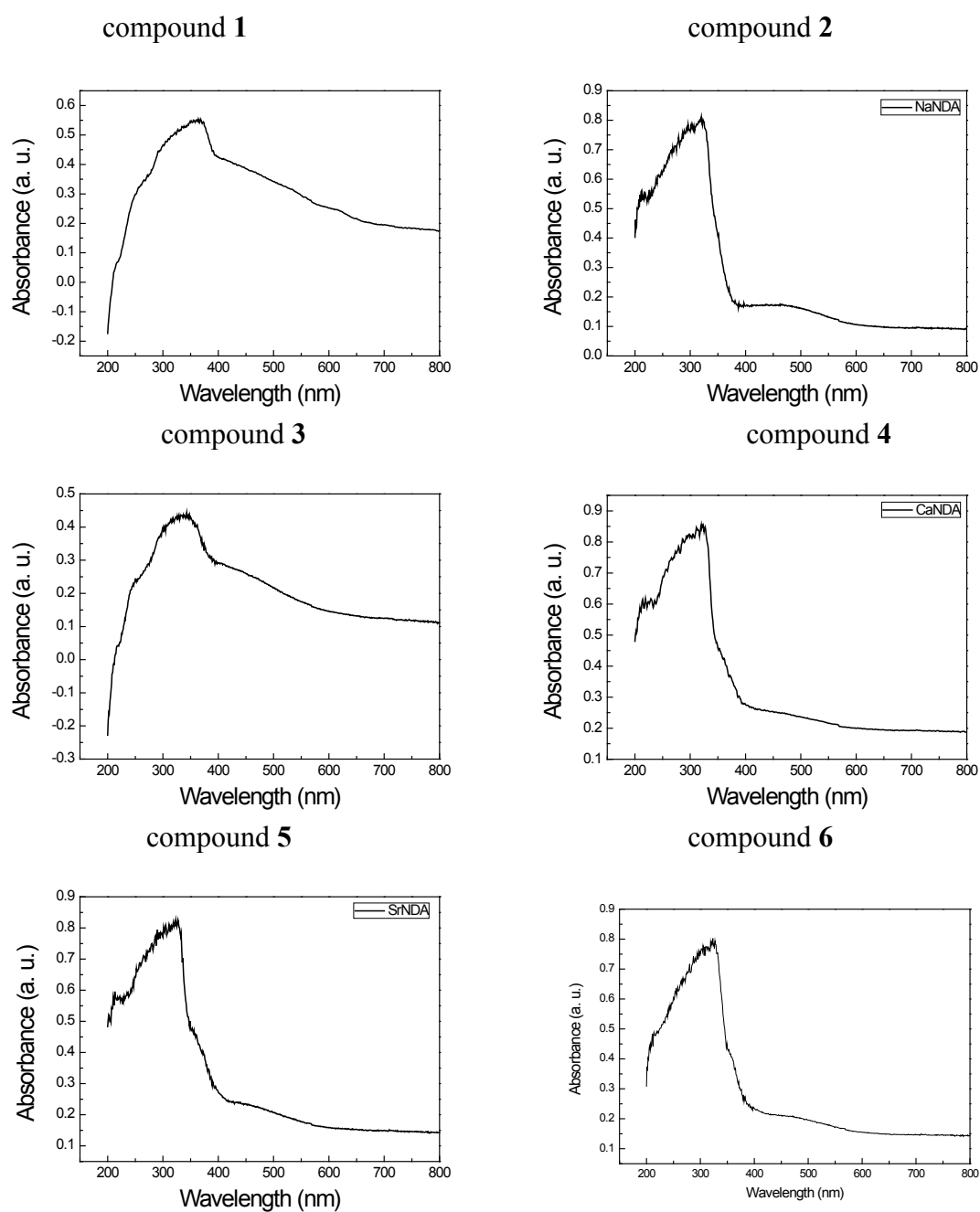


Figure S8. UV-vis absorption spectra for 1-6.

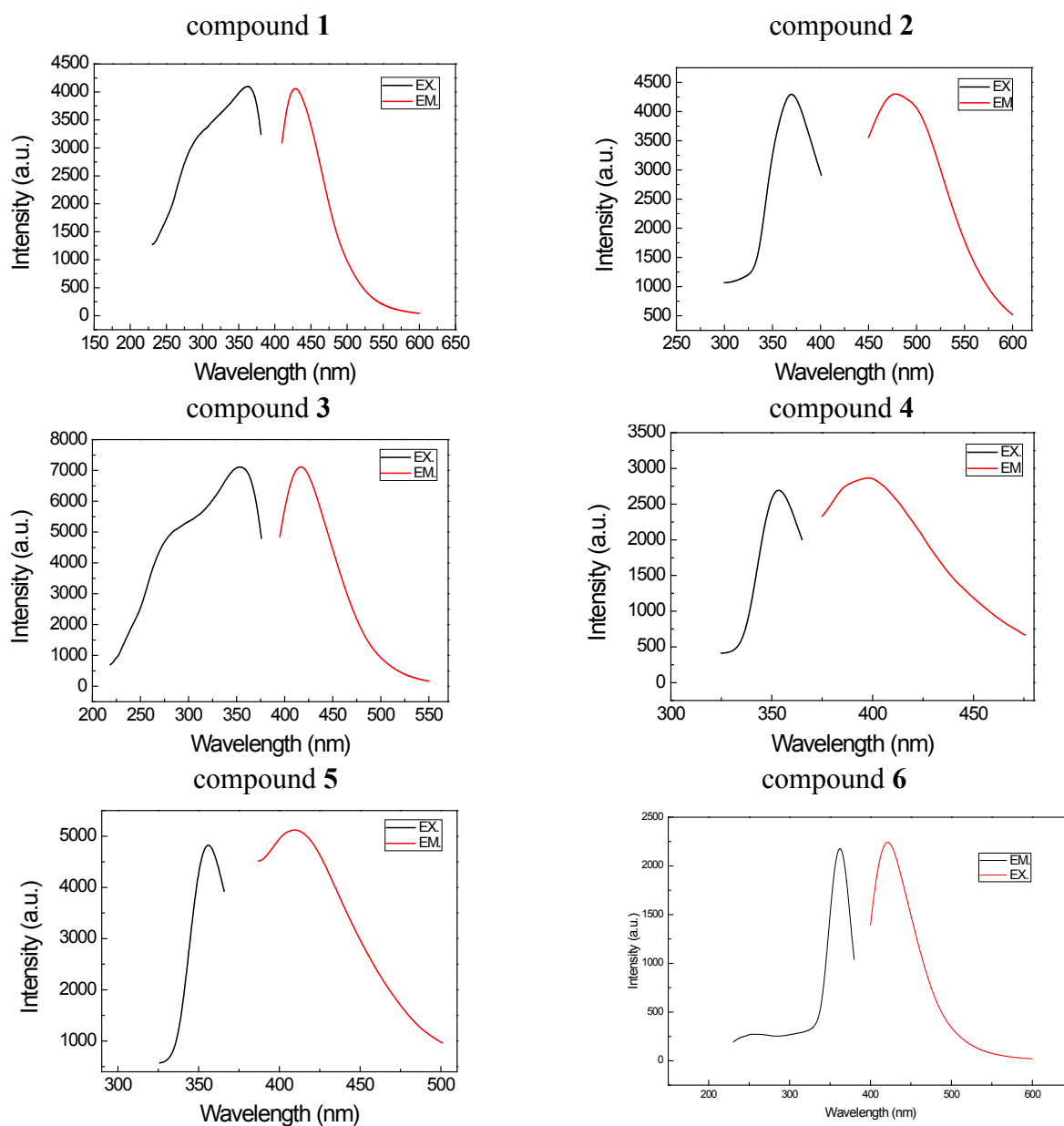


Figure S9. Photoluminescence emission spectra for 1-6.

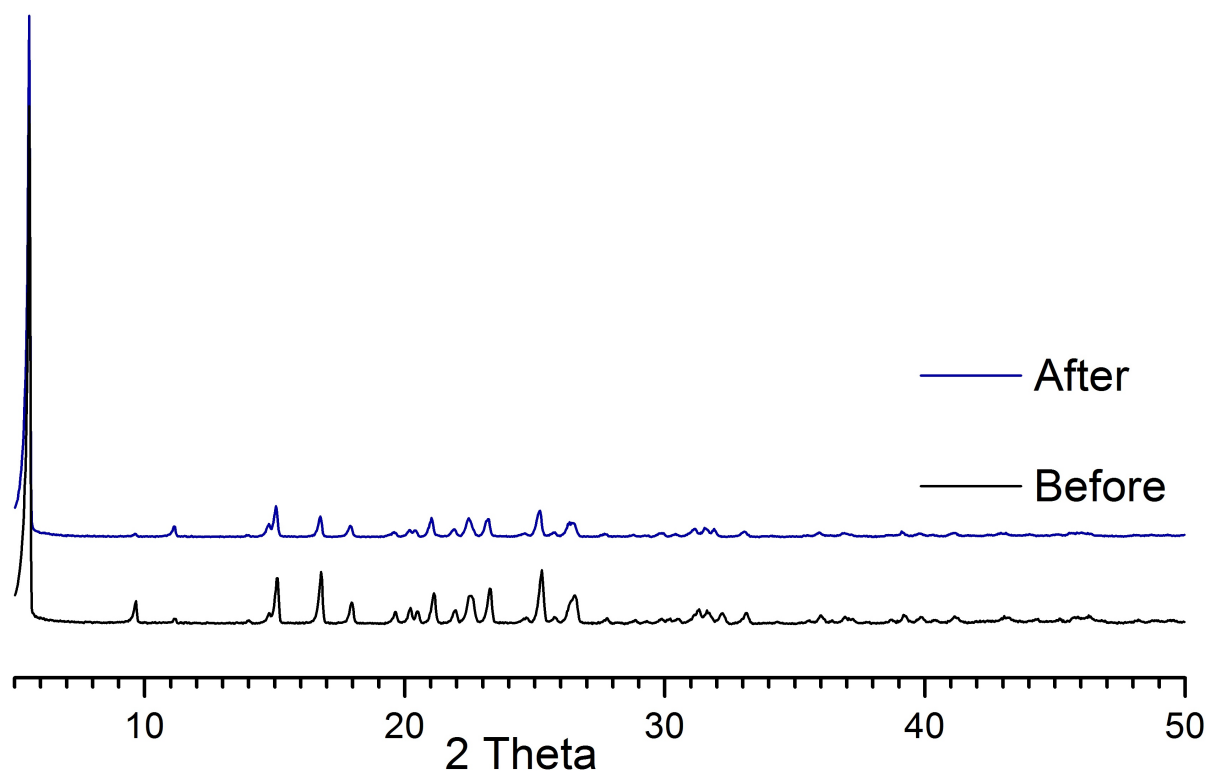


Figure S10. PXRD patterns of **2** before and after gas sorption studies.

Table S1. Selected bond lengths (Å) for **1-6**.

1			
Li(1)-O(2W)	1.895(3)	Li(1)-O(4)#1	1.934(3)
Li(1)-O(1W)	1.903(3)	Li(1)-O(1)	2.018(2)
2			
Na(1)-O(4)#1	2.262(2)	Na(2)-O(3)#3	2.302(2)
Na(1)-O(2)#2	2.285(2)	Na(2)-O(1)#6	2.341(2)
Na(1)-O(4)#3	2.445(2)	Na(2)-O(1S)	2.346(3)
Na(1)-O(2)	2.508(2)	Na(2)-O(2)#4	2.378(2)
Na(1)-O(1)	2.547(2)	Na(2)-O(4)#1	2.388(2)
Na(1)-O(3)#3	2.635(2)		
3			
Mg(1)-O(4)	2.014(2)	Mg(2)-O(7)	1.951(2)
Mg(1)-O(3)	2.026(2)	Mg(2)-O(8)	2.012(2)
Mg(1)-O(2)	2.052(2)	Mg(2)-O(5)	2.051(2)
Mg(1)-O(1S)	2.073(2)	Mg(2)-O(2W)	2.125(2)
Mg(1)-O(1)	2.1029(19)	Mg(2)-O(6)	2.129(2)
Mg(1)-O(1W)	2.144(2)	Mg(2)-O(1)	2.2592(19)
4			
Ca(1)-O(1S)	2.2808(14)	Ca(1)-O(2)#4	2.4603(12)
Ca(1)-O(3)#1	2.3167(13)	Ca(1)-O(1)	2.4939(11)
Ca(1)-O(4)#2	2.3305(13)	Ca(1)-O(2)	2.5394(11)
Ca(1)-O(1)#3	2.4471(13)		
5			
Sr(1)-O(1S)	2.435(3)	Sr(1)-O(4) #4	2.5781(19)
Sr(1)-O(3)#1	2.463(2)	Sr(1)-O(1)	2.644(2)
Sr(1)-O(2)#2	2.474(3)	Sr(1)-O(4)	2.677(2)
Sr(1)-O(1)#3	2.559(2)		
6			
Ba(1)-O(1S)	2.634(3)	Ba(1)-O(1)#4	2.754(3)
Ba(1)-O(3)#1	2.642(3)	Ba(1)-O(1)	2.812(2)
Ba(1)-O(4)#2	2.665(3)	Ba(1)-O(2)	2.825(2)
Ba(1)-O(2)#3	2.690(3)		

Symmetry transformations used to generate equivalent atoms: for complex **1**, #1 $-x+1, y+1/2, -z+3/2$; for complex **2**, #1 $y, -x+y+1, z+1/6$, #2 $-y+1, x-y, z-1/3$, #3 $x-y, x-1, z-1/6$, #4 $-x+y+1, -x+1, z+1/3$, #6 $-y+1, x-y, z+2/3$, #7 $y+1, -x+y+1, z+1/6$, #8 $x-y+1, x, z-1/6$; for complex **4**, #1 $-x+1/2, -y+1, z+1/2$, #2 $-x, y-1/2, -z+1/2$, #3 $x-1/2, -y+1/2, -z+1$, #4 $x+1/2, -y+1/2, -z+1$; for complex **5**, #1 $-x-1/2, -y-1, z+1/2$, #2 $-x, y-1/2, -z-3/2$, #3 $x+1/2, -y-3/2, -z-1$, #4 $x-1/2, -y-3/2, -z-1$; for complex **6**, #1 $-x+1/2, -y+1, z+1/2$, #2 $-x, y+1/2, -z+1/2$, #3 $x+1/2, -y+3/2, -z+1$, #4 $x-1/2, -y+3/2, -z+1$.