Electronic Supporting Information

Syntheses, Structures and Optical Properties of Two B_3O_7 Cluster-based Borates

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Table S1. Hydrogen bond distances (Å) and angles (°) for the compound **1**.

D–H···A	d(D–H)	d(H…A)	d(D…A)	∠(DHA) (°)
O(11)–H(2)…O(2)#1	0.82	2.47	3.130(2)	138.0
O(11)–H(2)…O(3)#1	0.82	2.46	3.071(5)	132.5
N(1)–H(1A)…O(7)#2	0.89	1.89	2.780(8)	176.0
N(1)–H(1B)···O(10)#3	0.89	1.98	2.862(7)	173.0
N(1)–H(1C)···O(1)#3	0.89	1.96	2.836(3)	170.0
N(2)–H(2A)···O(7)#4	0.89	1.89	2.746(7)	160.0
N(2)–H(2A)···O(8)#4	0.89	2.59	2.884(9)	100.6
N(2)–H(2B)···O(2)#4	0.89	2.08	2.927(6)	158.0
N(2)–H(2B)···O(8)#4	0.89	2.52	2.884(9)	105.8
N(2)–H(2B)···O(3)#5	0.89	2.31	2.877(8)	121.6
N(2)–H(2C)···O(6)#6	0.89	2.56	3.028(6)	113.0
N(2)–H(2C)···O(8) #6	0.89	2.45	3.258(3)	151.5
C(1)–H(1D)···O(9)#7	0.97	2.51	3.407(3)	154.0
C(3)–H(3B)···O(6)#6	0.96	2.55	3.367(2)	143.0

Symmetric codes: #1: 2-x,1/2+y,1/2-z; #2: -1+x,1/2-y,-1/2+z; #3: 1-x,-1/2+y,1/2-z; #4: -1+x,y,z; #5: x,1/2-y,1/2+z; #6: -1+x,1/2-y,1/2+z; #7: 2-x,-1/2+y,1/2-z.

Table S2. Hydrogen bond distances (Å) and angles (°) for the compound **1**.

D–H…A	d(D–H)	d(H…A)	d(D…A)	∠(DHA) (°)
O(6)–H(1)…O(2)#1	0.82	2.43	3.135(9)	145.0

Symmetric codes: #1: x,-1+y,z.

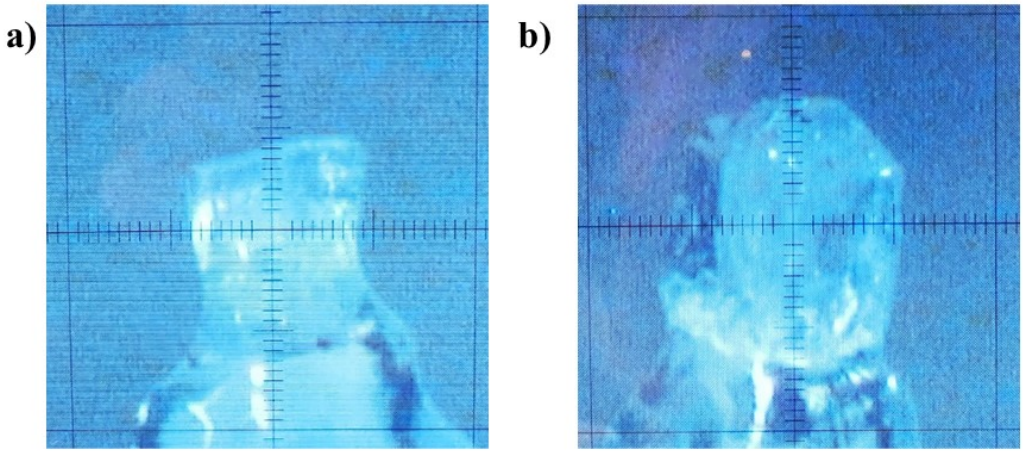

Figure S1. a) Crystals of **1**. b) Crystals of **2**. Each grid represent 0.01mm.

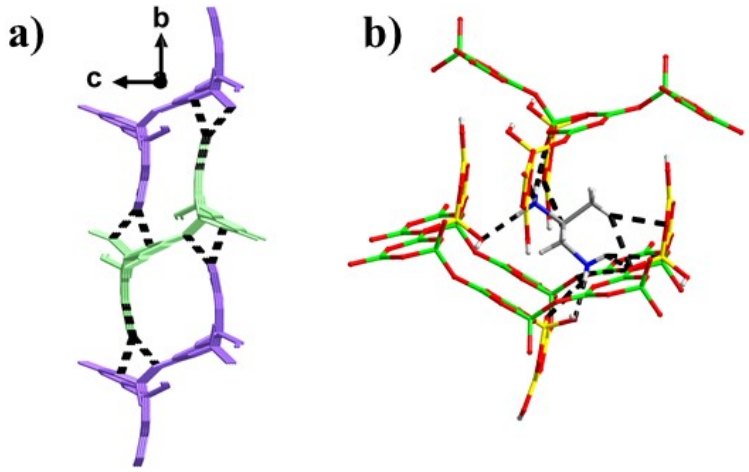

Figure S2. a) Interlayered H-bonds in **1**. b) H-bonds between 1,2-dap molecules and oxoboron layers in **1**.

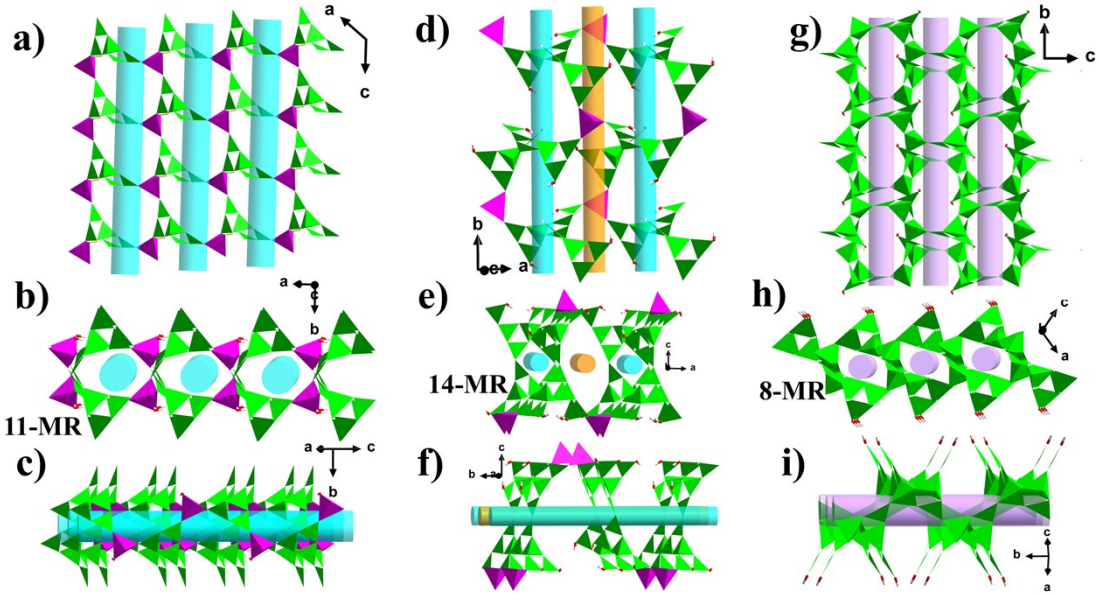

Figure S3. a-c) 2D fluctuant layer with 11-MR unclosed channels in $[Zn(dien)_2][\{Al(OH)\}\{B_5O_9F\}]$. d-f) 2D fluctuant layer with a pair of 14-MR helical channels in $[M(dap)_3]_2\{Al[B_5O7(OH)_3][B_5O_8(OH)_2][B_6O_9(OH)_2]\}$. g-i)2D fluctuant layer with 8-MR unclosed channels in $LiCs[B_5O_8(OH)]\cdot H_2O$.

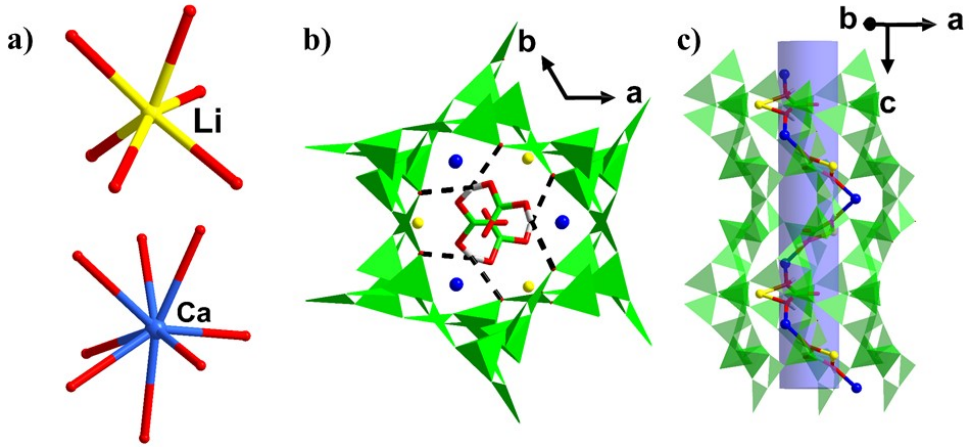

Figure S4. a) LiO_6 and CaO_8 coordination geometries in **2**. b) H-bonds between $BO(OH)_2$ groups and oxoboron framework in **2**. c) 1D-3D interpenetrating structure of **2**.

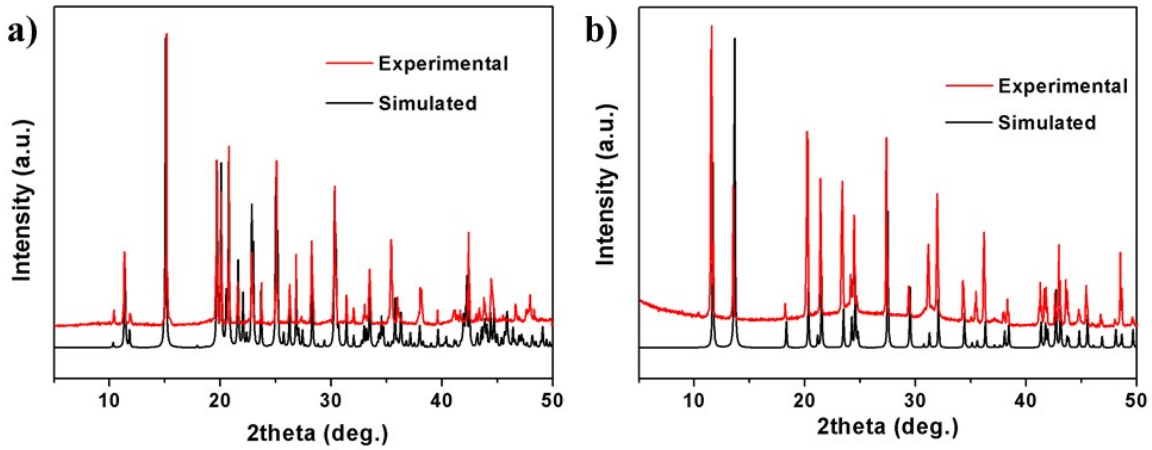

Figure S5. PXRD of **1** (a) and **2** (b).

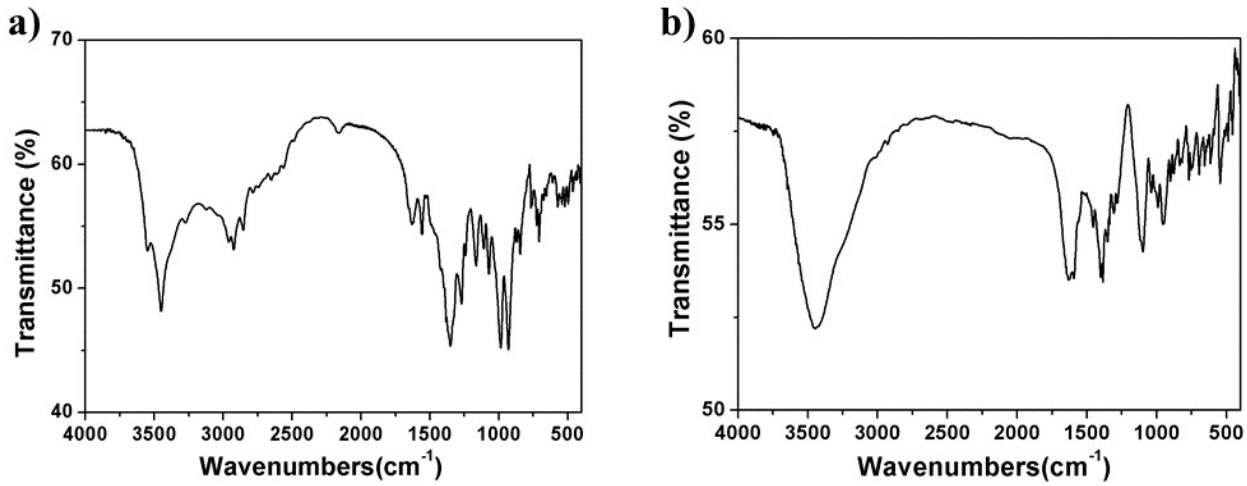

Figure S6. IR spectra of **1** (a) and **2** (b).

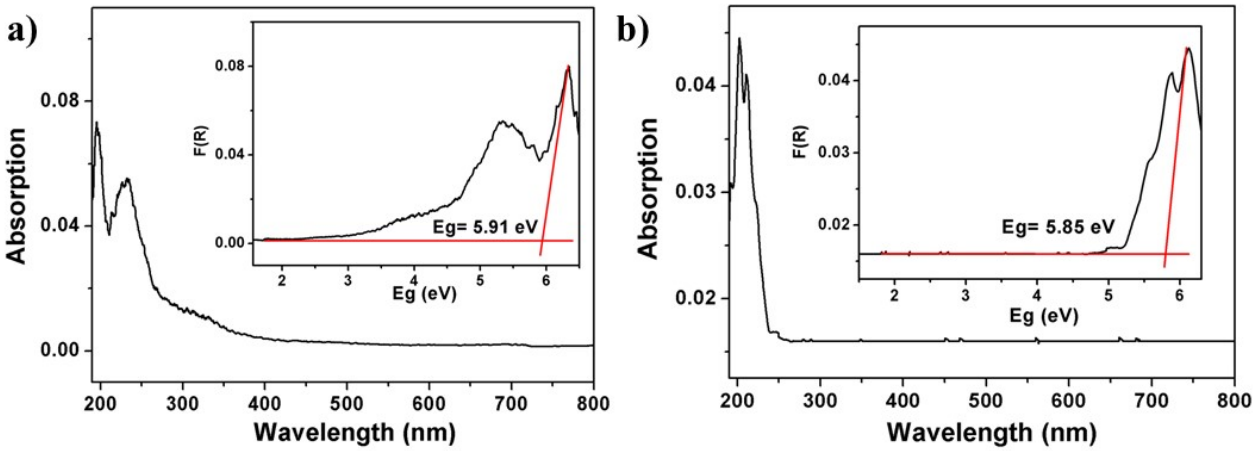

Figure S7. UV-Vis spectra of **1** (a) and **2** (b).

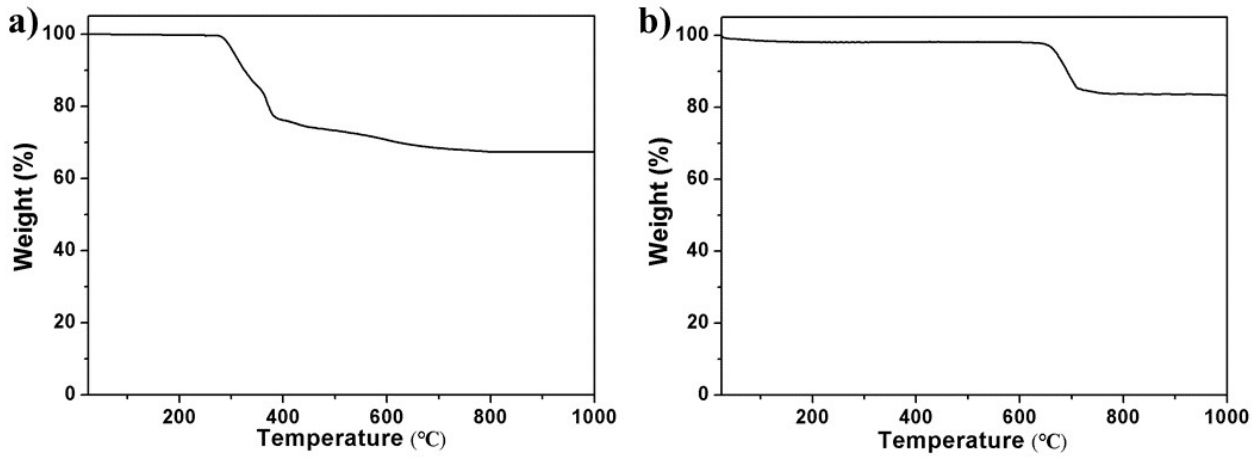

Figure S8. TG curves of **1** (a) and **2** (b).