Supporting Information

Two novel 3D borates: porous-layer and layer-pillar framework

Dan Qin,[a] Tian-Jiao Zhang,[a] Cheng-Bing Ma,*[b] and Guo-Yu Yang*[a]

[a]*MOE Key Laboratory of Cluster Science, School of Chemistry and Chemical Engineering, Beijing Institute of Technology, Beijing 100081, China. Email: ygy@bit. edu.cn*

[b]*School of Chemistry and Materials Engineering, Fuyang Normal University, Fuyang, Anhui 236037, China. E-mail: mcb@fynu.edu.cn*

Table S1. The hydrogen bonds in **1** and **2**.

Figure S1. The PXRD patterns of compound **1** and **2**, respectively.

Figure S2. View of five types of channels A (14-MR) (a, f), B (14-MR) (b, g), C (16-MR) (c, h), D (16-MR) (d, i) and E (11-MR) (e, j) in a porous layer along different directions, respectively.

Figure S3. (a) View of the H-bonding interactions between porous layers in **1** along the *ac* plane: O7-H1...O2 (red dot line) connect 2D B-O layer and 2-connected pillar; O15-H2...O2 (black) and O15-H2...O9 (turquiose) links the adjacent porous layers. (b) The amplification of the three kinds of hydrogen bonds.

Figure S4. (a) View of the H-bonding interactions in layer-pillar structure of **2** along the [110] direction: O1-H1...O8 (red dotted line) and O1-H1...O6 (black) links 1D tubular ABO and $BO_2(OH)$ triangles; O8-H2...O13 (turquiose) connected 2D B-O layers and 1D tubular ABO. (b) Side view of the adjacent 1D tube connected by O1-H1...O8 and O1-H1...O6.

Figure S5. (a) View of the porous layer of AMH-3, showing the Si-O-Si linkers; (b) View of the porous layer of **4** in which the $[B_4O_7(OH)_2]^{4-}$ clusters as the linking pillars, showing Al-$[B_4O_7(OH)_2]$-Al linkages; (c) View of the porous layer of **5**, showing double M-O-M (M = Al/Ga) linkages as the pillars; (d) Top view of a single Si-O layer in AMH-3; (e) Top view of a single layer of **4** showing the linkages of AlO_4 units and $B_3O_6(OH)$ clusters; (f) Top view of a single layer in **5**, showing the linkages of $[AlB_4O_8(OH)]$ clusters.

Figure S6. The IR spectra of compounds **1** and **2**, respectively.

Figure S7. The TG curves of compounds **1** and **2**, respectively.

Table S1. The hydrogen bonds in**1** and **2**, respectively.

Compound	D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)	Symmetry codes
1	O7-H1...O2#9	0.69	2.26	2.919	160	#9: 1-x,-y,2-z
	O15-H2...O2#3	0.68	2.53	3.306	133	#3: 1/2-x,-1/2+y,3/2-z
	O15-H2...O9#3	0.68	2.56	3.153	148	#3: 1/2-x,-1/2+y,3/2-z
	O1-H1...O6#6	0.74	2.10	2.839	172	#6: 1/2+x,-1/2+y,z
2	O1-H1...O8#6	0.74	2.59	3.098	128	#6: 1/2+x,-1/2+y,z
	O8-H2...O13#4	0.74	2.47	3.178	161	#4: 1/2-x,1/2+y,1/2-z

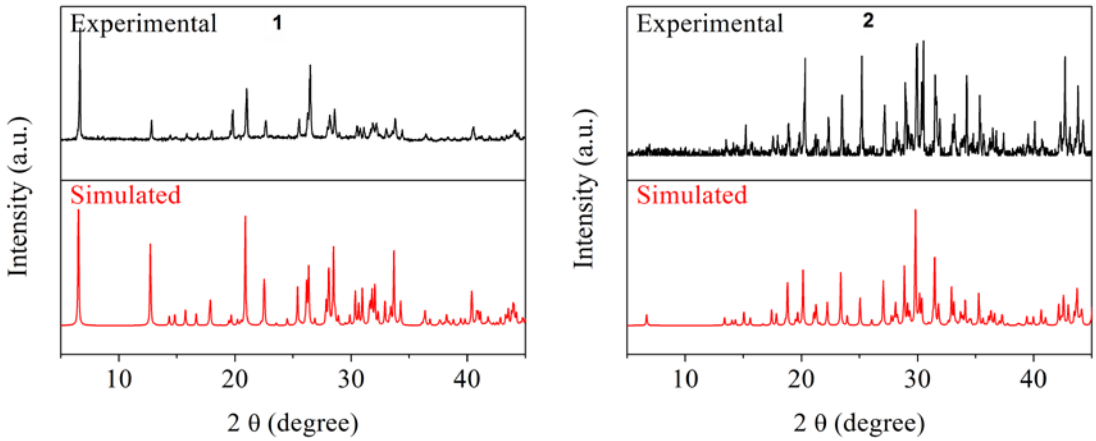

Figure S1. The PXRD patterns of compounds **1** and **2**, respectively.

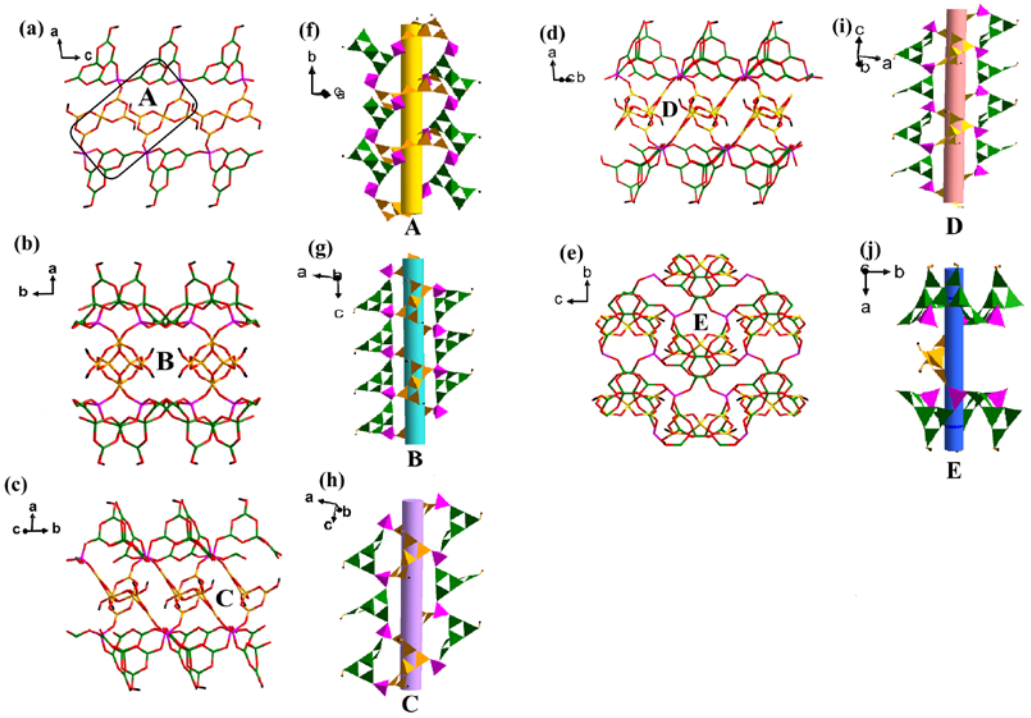

Figure S2. View of five types of channels A (14-MR) (a, f), B (14-MR) (b, g), C (16-MR) (c, h), D (16-MR) (d, i) and E (11-MR) (e, j) in a porous layer along different directions, respectively.

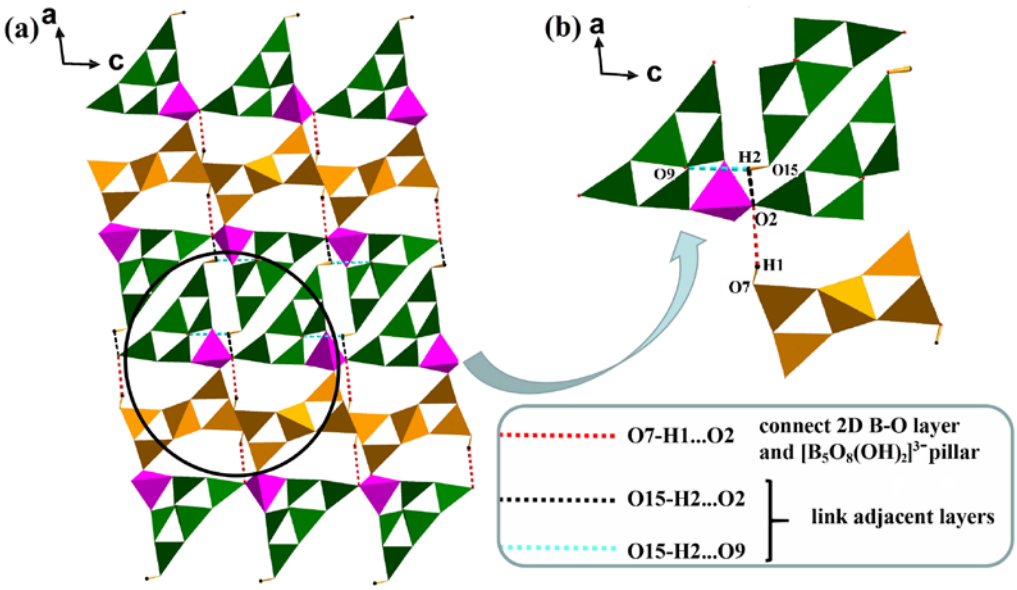

Figure S3. (a) View of the H-bonding interactions between porous layers in **1** along the *ac* plane: O7-H1...O2 (red dot line) connect the 2D B-O layer and the 2-connected pillar; O15-H2...O2 (black) and O15-H2...O9 (turquiose) links the adjacent porous layers. (b) The amplification of the three kinds of hydrogen bonds.

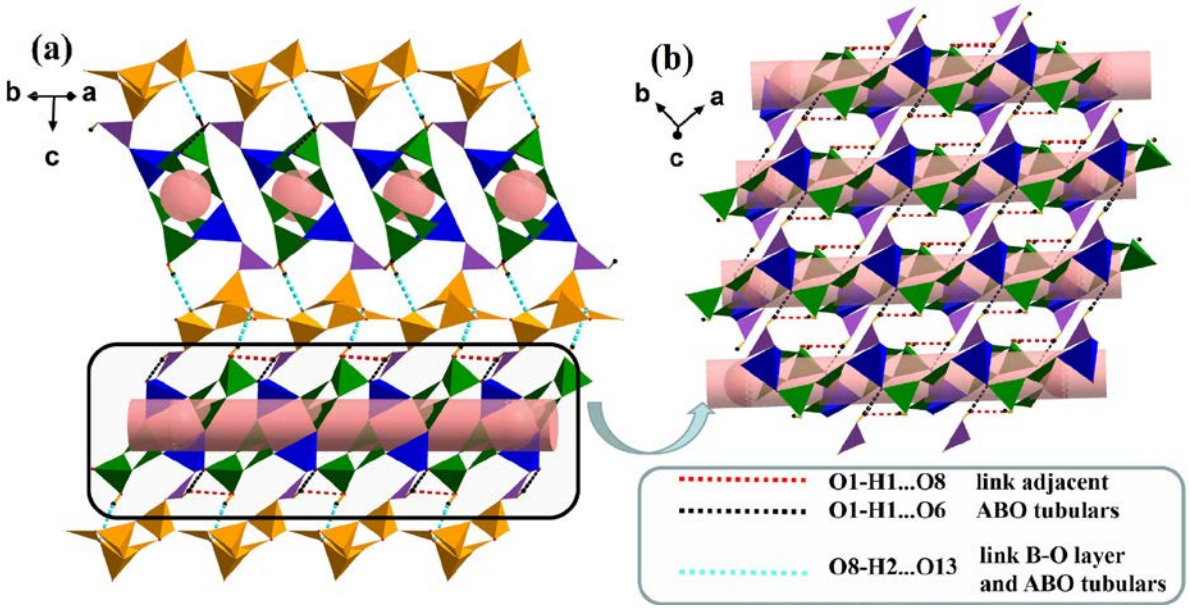

Figure S4. (a) View of the H-bonding interactions in layer-pillar structure of **2** along the [110] direction: O1-H1...O8 (red dot line) and O1-H1...O6 (black) links the 1D tubular ABO and the $BO_2(OH)$ triangles; O8-H2...O13 (turquiose) connected the 2D B-O layers and the 1D tubular ABO. (b) Side view of the adjacent 1D tubular connected by O1-H1...O8 and O1-H1...O6.

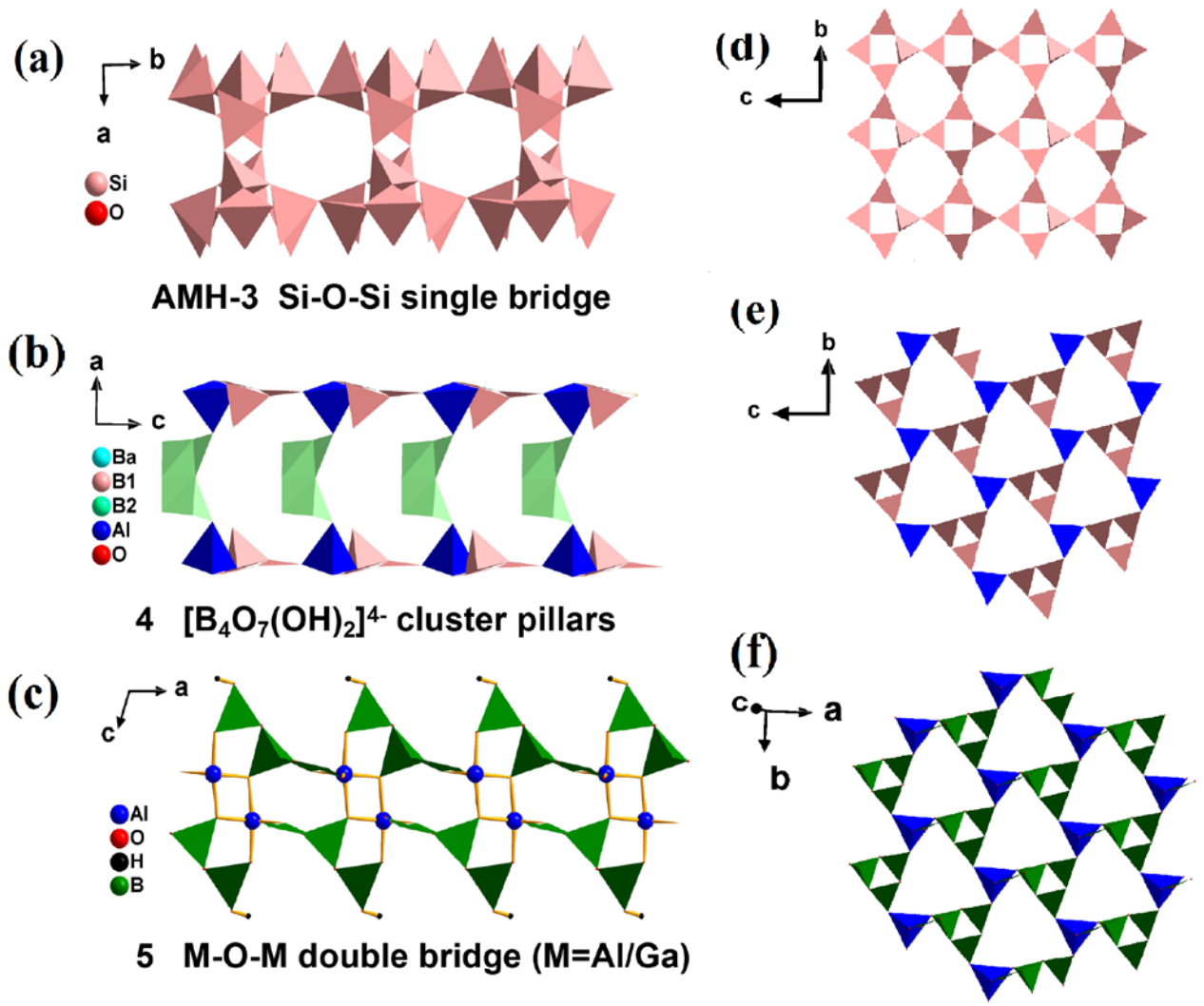

Figure S5. (a) View of the porous layer of AMH-3, showing the Si-O-Si linkers; (b) View of the porous layer of **4** in which the $[B_4O_7(OH)_2]^{4-}$ clusters as the linking pillars, showing Al-$[B_4O_7(OH)_2]$-Al linkages; (c) View of the porous layer of **5**, showing double M-O-M (M = Al/Ga) linkages as the pillars; (d) Top view of a single Si-O layer in AMH-3; (e) Top view of a single layer of **4** showing the linkages of AlO_4 units and $B_3O_6(OH)$ clusters; (f) Top view of a single layer in **5**, showing the linkages of $[AlB_4O_8(OH)]$ clusters.

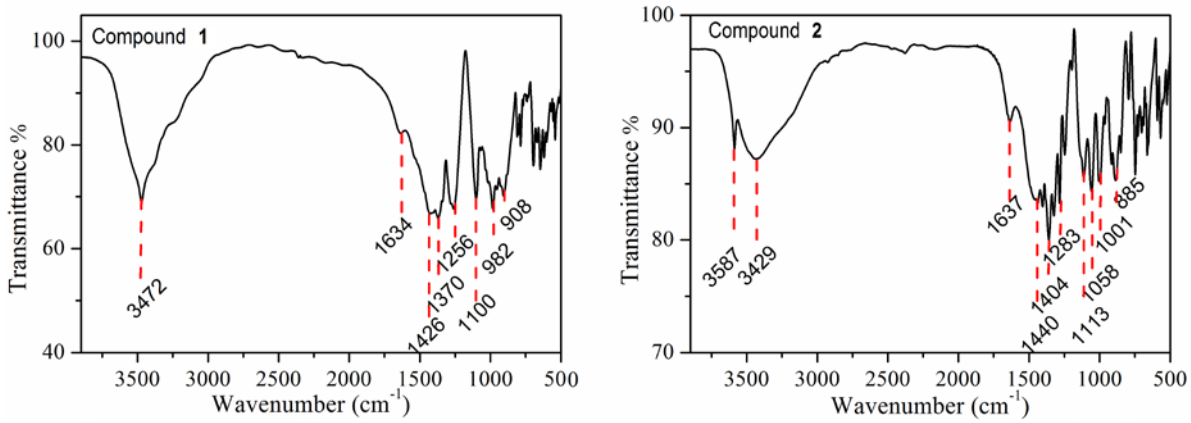

Figure S6. The IR spectra of compounds **1** and **2**, respectively.

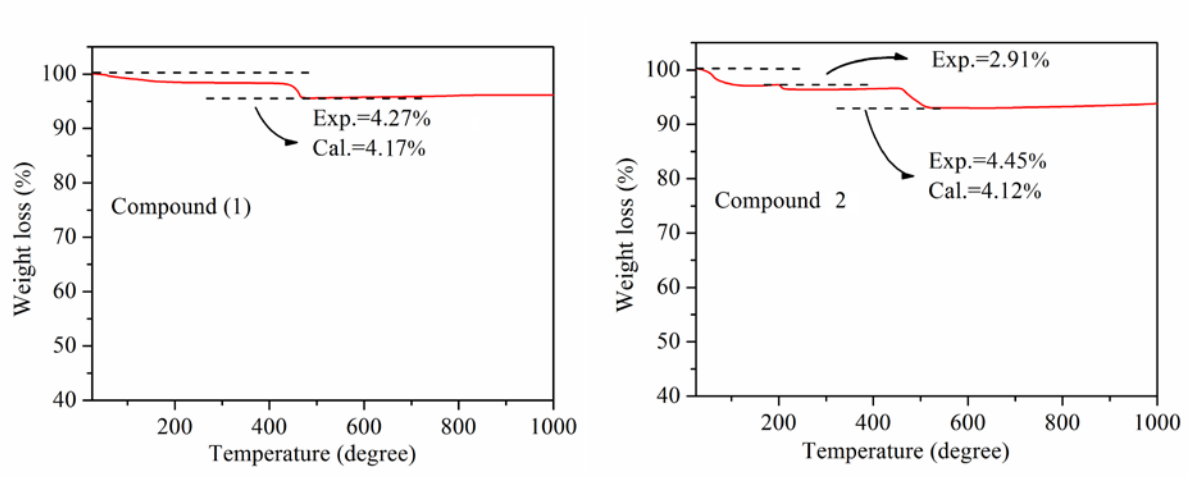

Figure S7. The TG curves of compounds **1** and **2**, respectively.