Electronic Supplementary Material (ESI) for CrystEngComm

Supporting Information:

From Discrete Borate Cluster to Three-Dimensional Open Framework

Lian-Zhi Wu, Lin Cheng, Jin-Ni Shen and Guo-Yu Yang*

State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian 350002, China. Fax:+86-591/8371-0051; E-mail: ygy@fjirsm.ac.cn.

Table S1. Hydrogen bonds for **1** [Å and °].

D-H···A	d(D-H)	d(H···A)	d(D···A)	∠(DHA)
O(1)-H(1A)···O(7)#2	0.82	1.91	2.730(4)	177.3
O(8)-H(8A)···O(3)#3	0.82	1.96	2.736(4)	157.8
O(12)-H(12A)···O(2)#4	0.82	1.94	2.736(3)	164.0
N(2)-H(2C)···O(6)#2	0.89	2.01	2.888(4)	170.6
N(2)-H(2D)···O(5)#5	0.89	2.12	2.977(4)	162.4
N(2)-H(2D)···O(13)#5	0.89	2.62	3.072(4)	112.6
N(2)-H(2E)···O(13)#2	0.89	2.15	2.938(4)	147.0
N(3)-H(3C)···O(8)#6	0.89	1.94	2.768(4)	154.2
N(3)-H(3C)···O(3)#7	0.89	2.53	3.096(4)	122.1
N(3)-H(3D)···O(2)#5	0.89	2.67	3.297(4)	128.4
N(3)-H(3E)···O(5)#5	0.89	2.04	2.798(4)	142.3
N(3)-H(3E)···O(4)#5	0.89	2.31	3.074(4)	143.8

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

Table S2. Hydrogen bonds for **2** [Å and °].

D-H···A	d(D-H)	d(H···A)	d(D···A)	∠(DHA)
N(1)-H(1A)···O(3W)	0.90	1.89	2.723(5)	153.1
N(1)-H(1B)···O(12)	0.90	2.04	2.930(4)	169.9
N(1)-H(1C)···O(8)#5	0.90	2.00	2.857(4)	158.3
N(1)-H(1C)···O(10)#5	0.90	2.31	3.030(4)	137.0
N(2)-H(2A)···O(2W)#11	0.89	2.01	2.834(5)	153.3
N(2)-H(2B)···O(20)#11	0.89	1.89	2.773(4)	170.4
N(2)-H(2C)···O(6)#9	0.89	2.12	2.904(4)	146.6
N(3)-H(3A)···O(3W)#9	0.90	2.45	3.211(6)	142.5
N(4)-H(4A)···O(1W)#1	0.89	2.03	2.784(5)	141.2
N(4)-H(4B)···O(1)#1	0.89	2.06	2.813(4)	141.5
N(4)-H(4B)···O(2)#1	0.89	2.51	3.127(4)	126.8
N(4)-H(4C)···O(18)#6	0.89	2.10	2.965(4)	162.3
N(4)-H(4C)···O(5)#6	0.89	2.60	3.312(4)	138.1
N(5)-H(5A)···O(4W)	0.90	1.87	2.762(5)	170.8
N(5)-H(5B)···O(5)#7	0.90	1.95	2.838(4)	168.3
N(5)-H(5C)···O(11)	0.90	1.89	2.785(4)	174.3
N(5)-H(5C)···O(14)	0.90	2.65	3.249(4)	124.6
N(6)-H(6A)···O(1W)	0.90	2.11	2.868(4)	141.0
O(3W)-H(3WA)···O(4)	0.85	2.56	3.343(6)	154.0
O(3W)-H(3WA)···O(6)	0.85	2.58	3.201(6)	130.7
O(3W)-H(3WB)···O(2W)#4	0.85	2.61	3.359(6)	148.3

Symmetry transformations used to generate equivalent atoms: #1 -x+3,y-1/2,-z+2; #2 -x+3,y+1/2,-z+3; #3 -x+2,y+1/2,-z+2; #4 x,y+1,z; #5 -x+2,y+1/2,-z+3; #6 x,y-1,z; #7 -x+2,y-1/2,-z+2; #8 -x+3,y+1/2,-z+2; #9 -x+2,y-1/2,-z+3; #10 -x+3,y-1/2,-z+3; #11 x-1,y,z

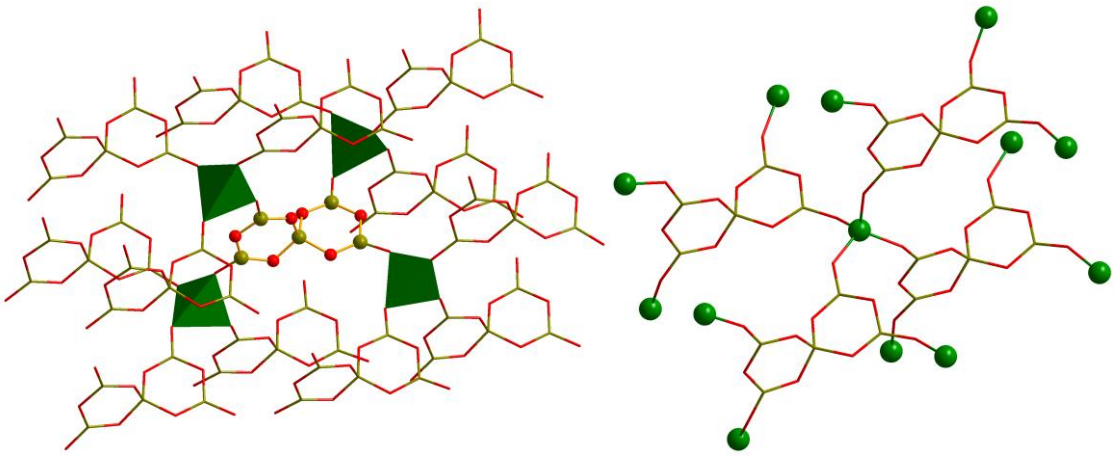

Figure S1. Views of the linkage of B_5O_{10} cluster units and AlO_4 groups in **2**. Each B_5O_{10}/AlO_4 units is bridged by four AlO_4/B_5O_{10} groups to 12 other B_5O_{10}/AlO_4 units.

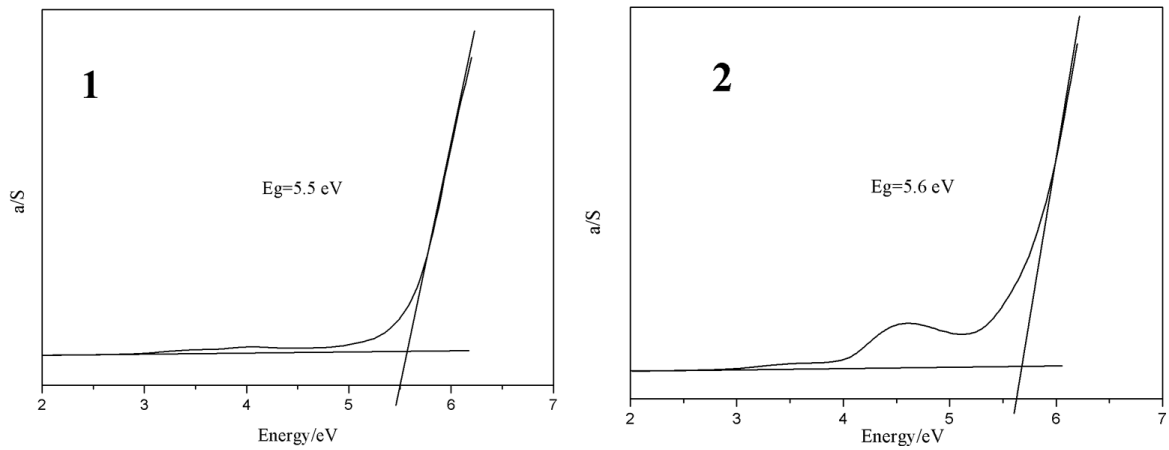

Figure S2. Optical diffuse reflectance spectra for **1** (a) and **2** (b), respectively.

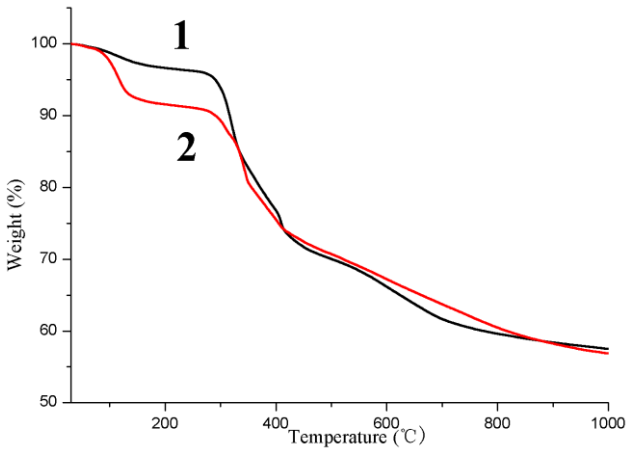

Figure S3. TG curve of **1** and **2**, respectively.

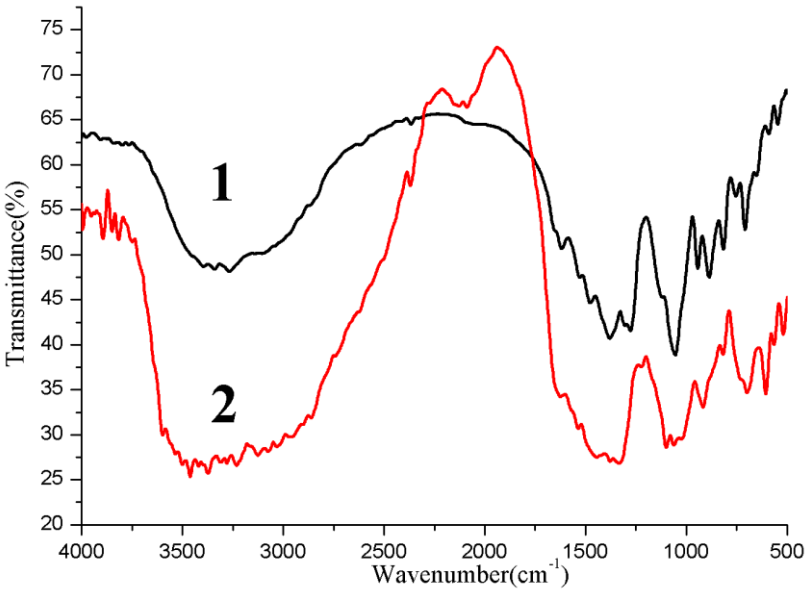

Figure S4. IR spectra of **1** and **2**.

Infrared spectroscopy was used to verify the nature of the borate groups and the presence of amine in the structure. For **1**, the strong bands at ~1377, 1276 cm^{-1} in the spectra are consistent with the existence of trigonally coordinated boron, while the bands at 1057, 945 and 886 cm^{-1} are characteristic of tetrahedral boron.[1, 2] The broad bands in the range of 3401–3059 cm^{-1} correspond to the stretching bands of the N-H, C-H, and O-H. The bending bands of N-H and C-H are presented at about 1617-1478 cm^{-1}. For **2**, the bands at ~1329, ~1377 cm^{-1} in the spectra are consistent with the existence of trigonally coordinated boron, while the bands at 1100-1014 cm^{-1} are characteristic of tetrahedral boron.[1,2] The broad bands at 3460–2851 cm^{-1} correspond to the stretching bands of the N-H and C-H. The bending bands of N-H and C-H are presented at about 1634-1441 cm^{-1}. In addition, the bands at 912-700 cm^{-1} are characteristic of the stretching vibrations of tetrahedral AlO_4 groups.[3]

1. C. E. Weir, *Journal of Research of the National Bureau of Standards Section a-Physics and Chemistry*, 1966, **A70**, 153.
2. C. E. Weir and R. Schroeder, *Journal of Research of the National Bureau of Standards Section a-Physics and Chemistry*, 1964, **A68**, 465.
3. S. Cavalu and V. Simon, *Journal of Optoelectronics and Advanced Materials*, 2007, **9**, 3297.

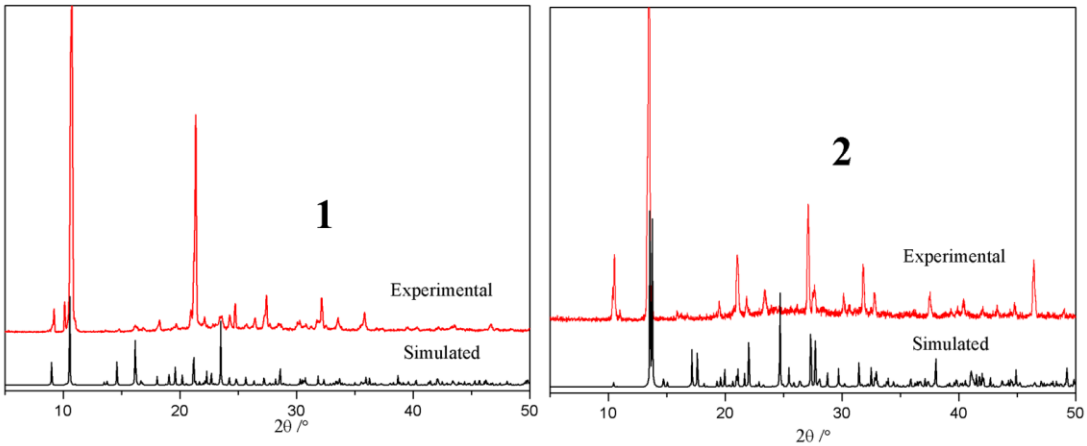

Figure S5. Simulated and experimental powder XRD patterns of **1** and **2**, respectively.

The powder X-ray diffraction patterns for **1** and **2** are in good agreement with the patterns based on each single- crystal X-ray solution in position, indicating the phase purity of the as-synthesized samples of the two compounds.