Electronic Supplementary Material (ESI) for Dalton Transactions.

Electronic Supporting Information

Syntheses and structures of a new 2D layered borate and a novel 3D porous-layered alunminoborate

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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) (°)
N(1) –H(1A) ···O(8)#1	0.89	1.96	2.827(3)	163.0
N(1) –H(1B) ···O(1)#1	0.89	2.45	3.170(3)	138.0
N(1) –H(1B) ···O(2)#1	0.89	2.27	3.107(3)	157.5
N(1) –H(1C) ···O(7)#2	0.89	2.17	2.958(3)	147.0
N(1) –H(1C) ···O(10)#2	0.89	2.48	3.151(3)	132.6
N(2) –H(2B) ···O(7)#4	0.89	1.94	2.811(4)	160.0
N(2) –H(2C) ···O(8)#5	0.89	2.22	2.990(3)	145.0
N(2) –H(2C) ···O(9)#5	0.89	2.41	3.165(3)	143.6
N(2) –H(2A) ···O(11)#3	0.89	2.37	3.222(3)	160.0
O(6) –H(6A) ···O(5)#4	0.82	1.95	2.766(3)	177.0
C(1) –H(1E) ···O(3)#2	0.97	2.42	3.325(3)	155.0
C(2) –H(4) ···O(9) #5	0.96	2.47	3.296(5)	143.0

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

Table S2. Hydrogen bond distances (Å) and angles (°) for the compound **2**.

D–H···A	d(D–H)	d(H···A)	d(D···A)	∠(DHA) (°)
O(1) –H(1) ···O(24)#1	0.77	2.08	2.845(6)	177.0

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

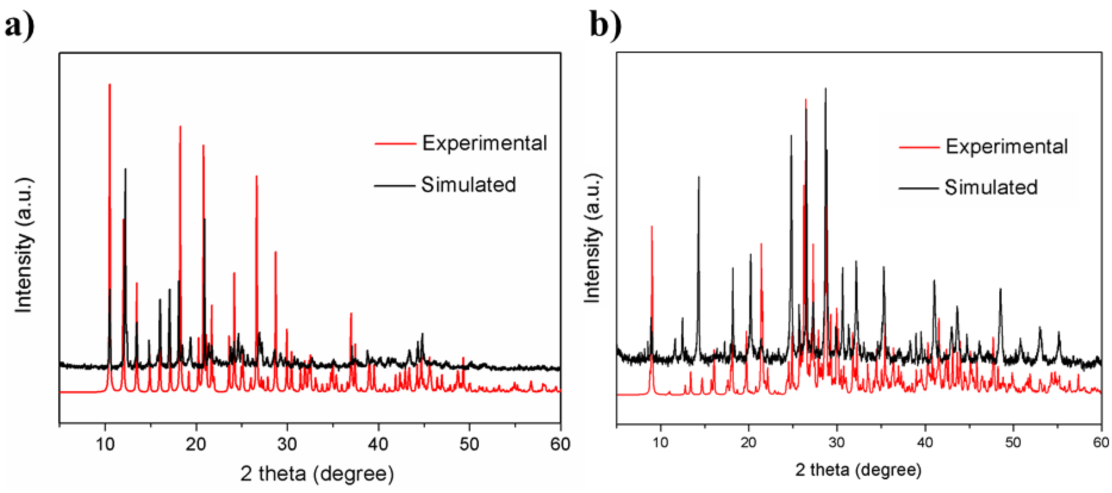

Figure S1. The PXRD patterns of **1** and **2**, respectively.

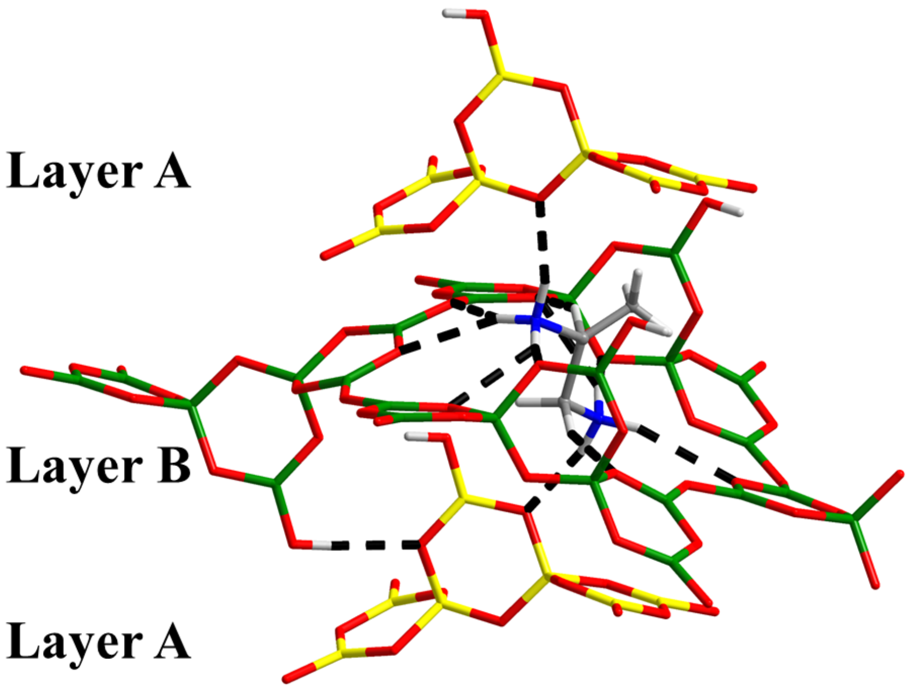

Figure S2. Hydrogen bonds between 1,2-dap molecule and inorganic framework in **1**.

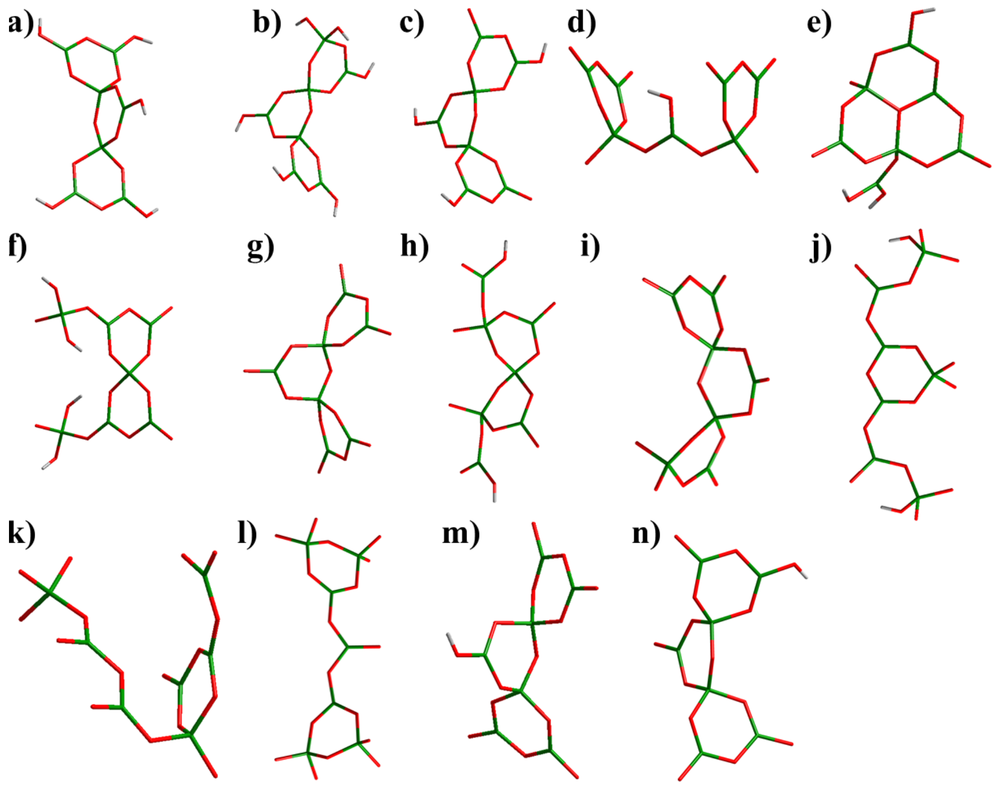

Figure S3. View of different B_7 FBBs: a) $[B_7O_9(OH)_5]^{2-}$ ([7:(5Δ+2T)]); b) $[B_7O_9(OH)_6]^{3-}$ ([7:(4Δ+3T)]); c) $[B_7O_{10}(OH)_3]^{2-}$ ([7:(5Δ+2T)]); d,e) $[B_7O_{12}(OH)_3]^{2-}$ ([7:(3:2Δ+1T) + (1: Δ) + (3:2Δ+1T)] and [7:(6:3Δ+3T) + (1: Δ)]); f) $[B_7O_{12}(OH)_4]^{7-}$([7:(1:T) + (5: 4Δ+1T) + (1:T)]); g) $[B_7O_{14}]^{7-}$ ([7:(1:T) + (5: 4Δ+1T) + (1:T)]); h) $[B_7O_{14}(OH)_2]^{9-}$ ([7: (1: Δ) + (5:2Δ+3T) + (1:Δ)]); i) $[B_7O_{15}]^{9-}$ ([7:(4Δ+3T)]); j) $[B_7O_{15}(OH)_2]^{11-}$ ([7: (2:Δ+T) + (3:2Δ+T) + (2:Δ+T)]); k) $[B_7O_{16}]^{11-}$ ([7: (3: 2Δ+T) + (3:2Δ+T) + (1: Δ)]) ; l) $[B_7O_{17}]^{13-}$ ([7: (3: Δ+2T) + (1:Δ) + (3: Δ+2T)]); m) $[B_7O_{13}(OH)]^{6-}$ ([7:(5Δ+2T)]) in **1** (This work). n) $[B_7O_{13}(OH)]^{6-}$ ([7:(5Δ+2T)]) in **2** (This work).

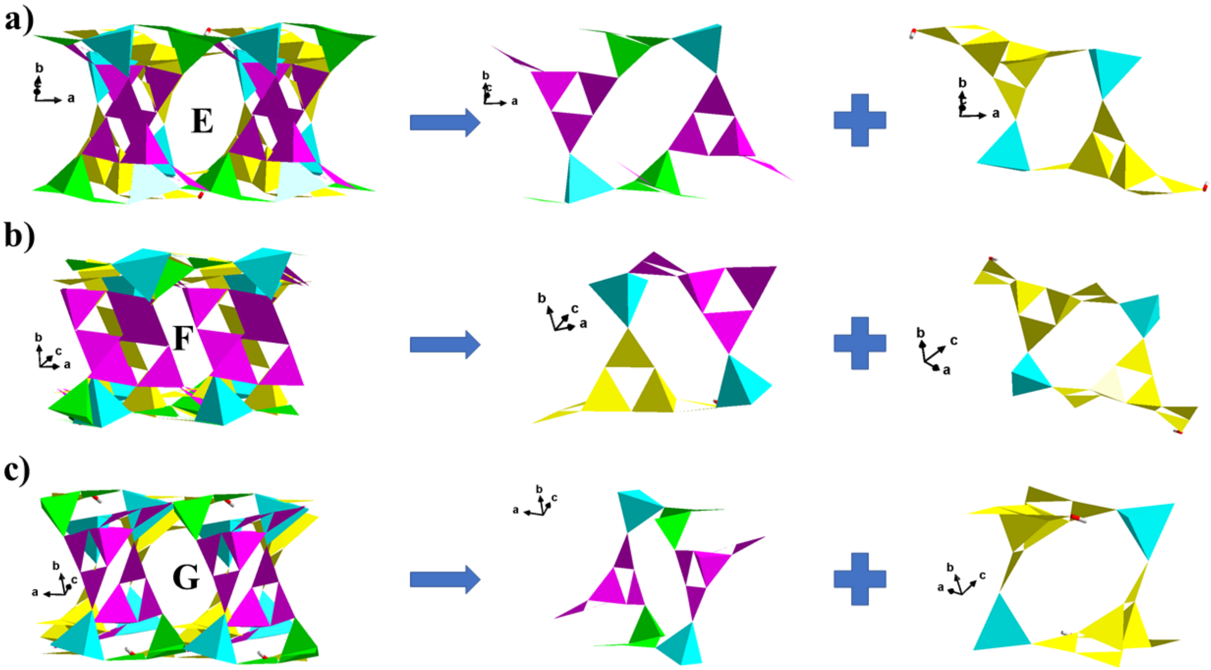

Figure S4. View of compositions of channel E (a), F (b) and G (c).

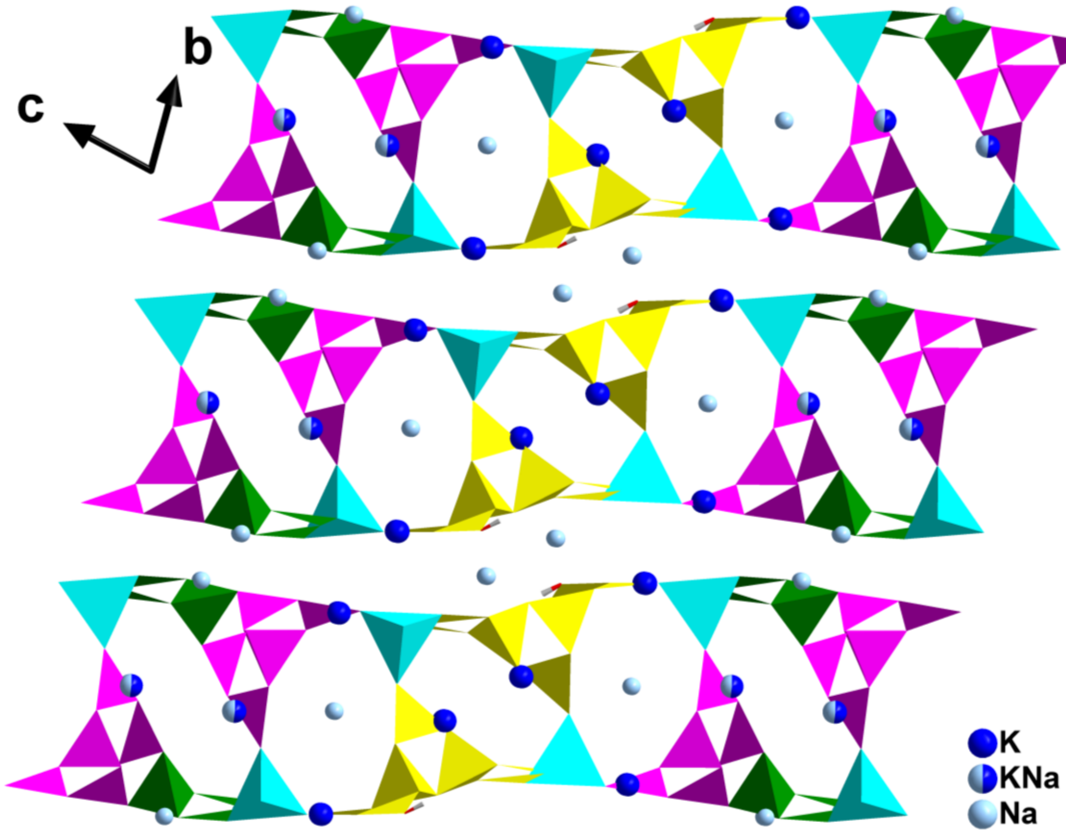

Figure S5. The metal ions positions in the inorganic framework in **2**.

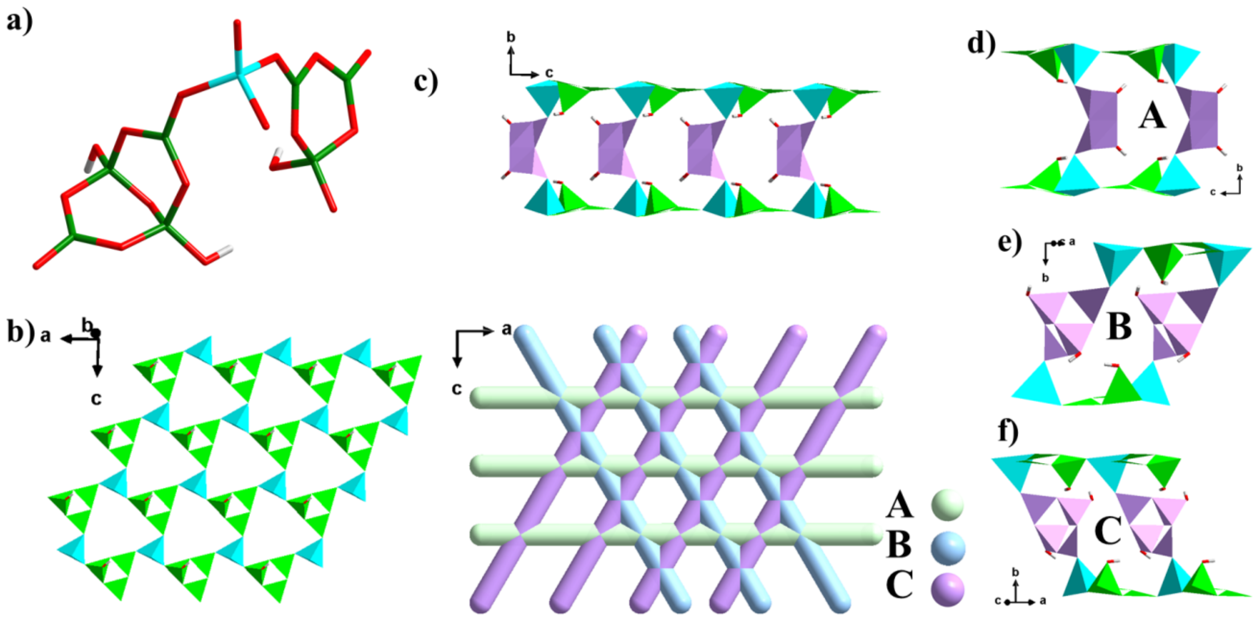

Figure S6. View of a) *FBB*; b) 2D ABO monolayer; c) 3D ABO porous layer; d) The intercommunicated channel system; e,f ,g) Three types of 14-MR channels in **3**.

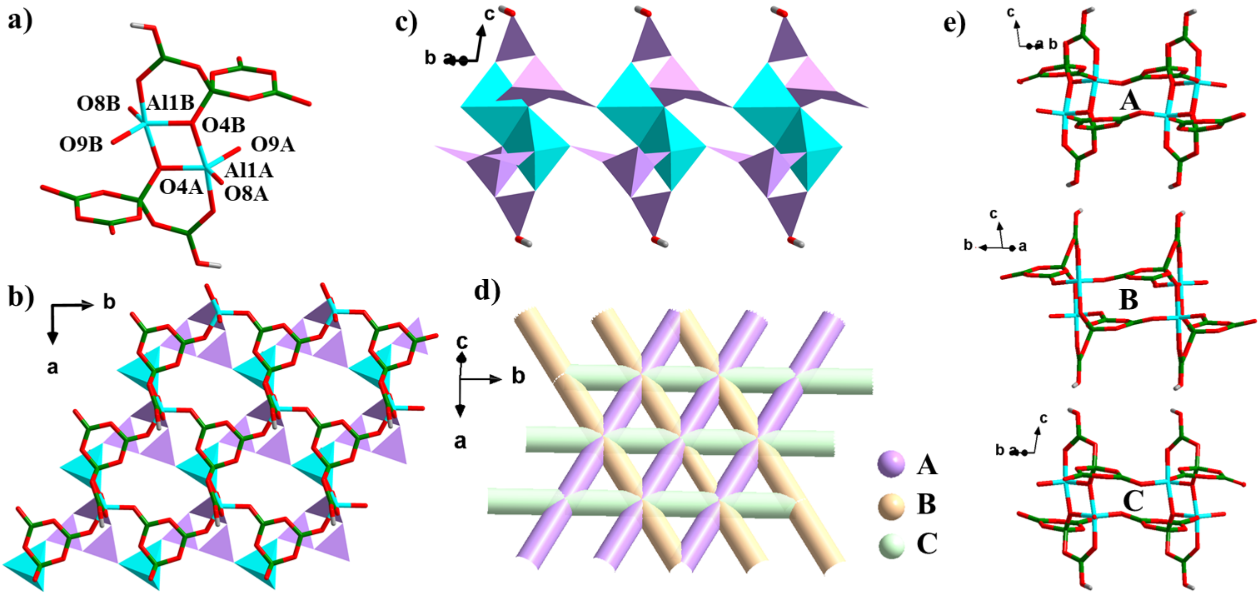

Figure S7. a) The $[Al_2B_8O_{20}(OH)_2]^{12-}$ dimeric clusters in **4**; b) Top view of 3D porous layer showing interlaced 9-MR windows in **4**; (c) Side view of 3D porous layer; d)The intercommunicated channel system of **4** (A, B and C); e) The three types of 6-MR windows along the [010], [110] and [1-10] directions, respectively.

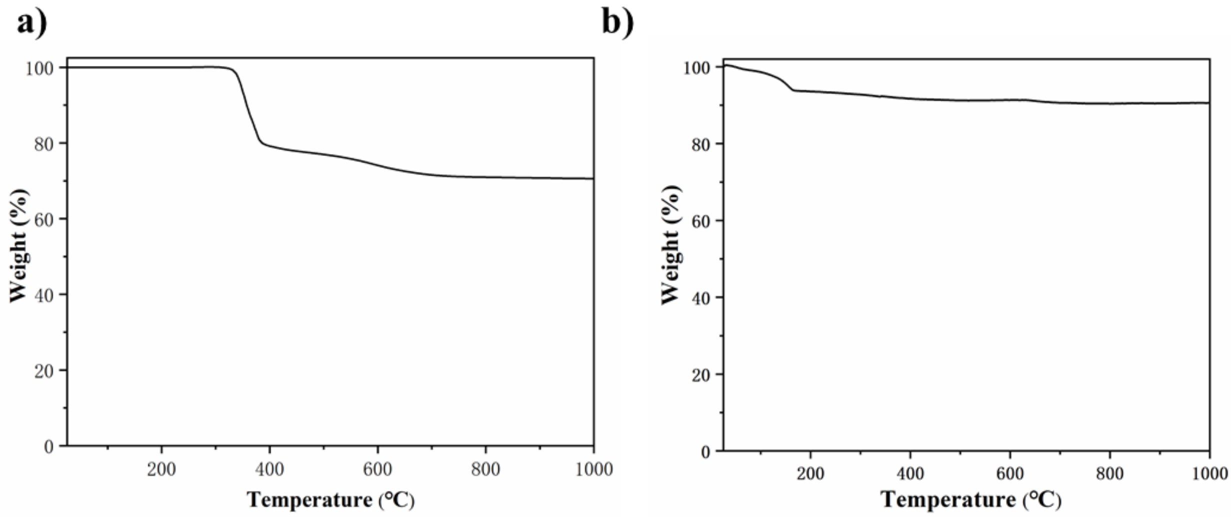

Figure S8. The TG curves of **1** and **2**, respectively.

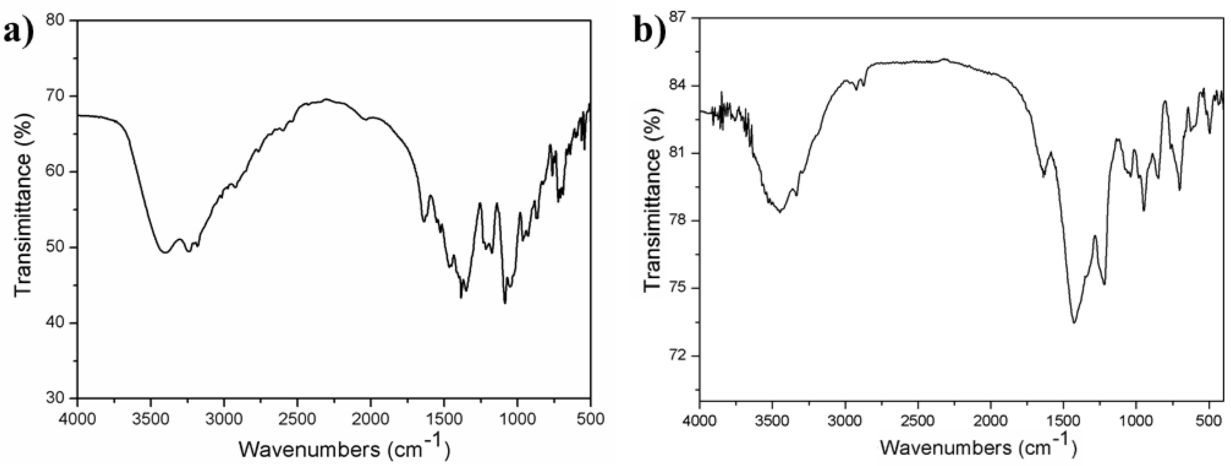

Figure S9. IR spectra of **1** and **2**, respectively.

As shown in Fig. S9, for **1**, the bands around 3400 cm^{-1} are the characteristic peaks of the asymmetric stretching vibrations of O-H, N-H and C-H bonds. The bands appear at 1662-1607 cm^{-1} belong to the bending vibrations of O-H, N-H and C-H bonds. The absorption peaks from 1483-1336 cm^{-1} are attributed to the asymmetrical stretching vibrations of BO_3 triangles, while the peaks ranging from 1148-985 cm^{-1} are the asymmetrical stretching peaks of BO_4 tetrahedrons. For **2**, the absorption peaks occurring from 3452-3172 cm^{-1} are the asymmetric stretching vibrations of O-H bonds. The peak at 1637 cm^{-1} and 1465 are the characteristic peaks of C-O bonds, which confirm the existence of CO_3^{2-}.[1-2] The peaks appear in the range of 1465-1210 cm^{-1} and 1058-942 $cm^{-1}$are the asymmetric stretching vibrations of BO_3 and BO_4, respectively. The bands in the region of 740-900 cm^{-1} are the Al-O stretching vibrations of tetrahedral AlO_4 groups.

[1] Z. H. Cheng, A. Yasukawa, K. Kandori and T. Ishikawa. *Langmuir.*, 1998, **14**, 6681-6686.

[2] J. A. Toledo-Antonio, S. Capula, M. Antonia Corte´s-Ja´come, C. Angeles-Cha´vez, E. Lo´pez-Salinas, G. Ferrat, J. Navarrete and J. Escobar. *J. Phys. Chem. C*. 2007, **111**, 10799-10805.