Supporting Information

Open-framework aluminoborates co-templated by two types of primary amines

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Table S1 Hydrogen bond lengths (Å) and bond angles (°) for compounds **1**-**4**.

Fig.S1 a) View of the asymmetric units of **1**-**4**, respectively.

Fig. S2 View of the elliptical 8-ring (a) and 14-ring (b) openings situated on bc plane in **1**.

Fig. S3 View of the 11-ring openings in **1** located on ac (a)and ab (b) planes, respectively.

Figure S4 View of the elliptical 14-ring (a) and 8-ring (b) openings situated on ab plane in **4**.

Fig. S5 View of the crystallographically independent templates and water molecules situated in channels in **1** (a), **2** (b), **3** (c) and **4** (d).

Fig. S6. IR spectra of **1**-**4**.

Fig. S7. Optical diffuse reflectance spectra for **1**-**4**.

Fig. S8. TG curves of **1**-**4**.

Table S1 Hydrogen bond lengths (Å) and bond angles (°) for compounds **1-4**.

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
1				
N1-H1D···O3#3	0.89	1.95	2.807(2)	161.0
N1-H1E···O6	0.89	1.90	2.785(2)	170.9
N1-H1F···O2#6	0.89	1.93	2.813(2)	170.3
N1-H1F···O4#6	0.89	2.51	3.126(2)	126.5
N2-H2D···O7	0.90	1.91	2.801(2)	172.9
N2-H2C···O9#7	0.90	2.07	2.890(2)	150.4
N2-H2C···O8#7	0.90	2.38	3.177(2)	147.5
2				
N1-H1C···O3	0.89	1.97	2.824(3)	160.5
N1-H1D···O6#3	0.89	1.90	2.786(3)	177.5
N1-H1E···O2#2	0.89	1.99	2.880(3)	173.3
N1-H1E···O4#2	0.89	2.48	3.072(3)	124.0
N2-H2D···O9#3	0.90	2.06	2.872(3)	150.3
N2-H2D···O8#3	0.90	2.36	3.145(3)	146.4
N2-H2E···O7#1	0.90	1.94	2.833(3)	169.5
3				
N1-H1C···O9#7	0.89	2.03	2.904(3)	168.3
N1-H1C···O8#7	0.89	2.58	3.113(3)	119.2
N1-H1D···O7#8	0.89	1.94	2.816(3)	167.5
N1-H1E···O5	0.89	1.95	2.825(3)	169.3
N2-H2D···O2#1	0.90	2.09	2.874(3)	144.4
N2-H2D···O4#1	0.90	2.26	3.063(4)	148.1
N2-H2E···O3	0.90	1.88	2.772(3)	170.4
OW-H1W···O10#7	0.85	2.32	3.166(2)	179.8
4				
N1-H1C···O7	0.89	1.99	2.846(5)	159.8
N1-H1C···O10	0.89	2.46	3.033(5)	122.5
N1-H1D···O3#1	0.89	1.99	2.866(4)	166.7
N1-H1E···O6#5	0.89	1.99	2.865(6)	167.7
N2-H2D···O1	0.89	2.03	2.888(5)	161.9
N2-H2D···O2	0.89	2.52	3.002(5)	114.7
N2-H2E···O2W	0.89	1.88	2.770(8)	174.9
N2-H2F···O10#6	0.89	2.13	2.996(5)	163.9
O1W-H1W···O2W#4	0.85	1.89	2.743(7)	179.0
O1W-H2W···O4#5	0.85	2.11	2.956(6)	179.4
O2W-H3W···O5#7	0.85	2.06	2.822(5)	148.4

[a] Symmetry codes for **1**: #3 -x+1, -y+1, -z+1; #6 -x+3/2, y+1/2, z; #7 -x+1, y-1/2, -z+1/2. for **2**: #1 x, -y+1/2, z+1/2; #2 x-1/2, -y+1/2, -z+1; #3 -x+1, -y, -z+1. for **3**: #1 -x, y+1/2, -z+3/2; #7 -x-1/2, y-1/2, z; #8 -x, -y, -z+2. for **4**: #1-x, -y+1, z-1/2; #4 x+1/2, -y+1/2, z; #5 x, y, z-1; #6 -x+1/2, y-1/2, z+1/2; #7 -x+1/2, y-1/2, z-1/2.

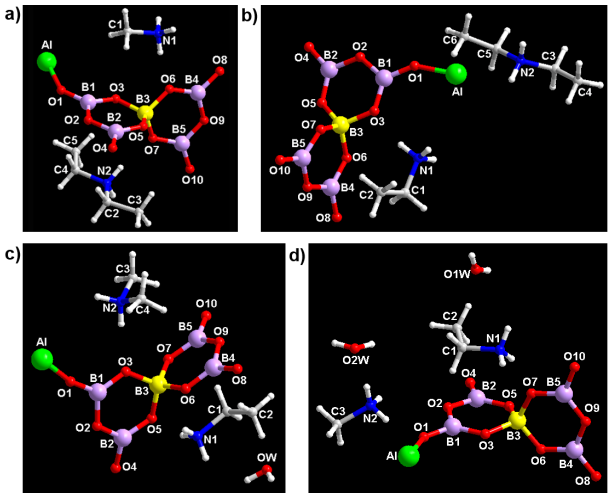

Fig. S1. View of the asymmetric units of **1** (a), **2** (b), **3** (c) and **4** (d), respectively.

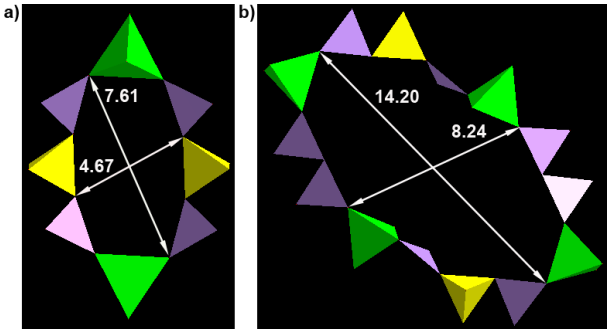

Fig. S2. View of the elliptical 8-ring (a) and 14-ring (b) openings situated on the *bc* plane in **1**.

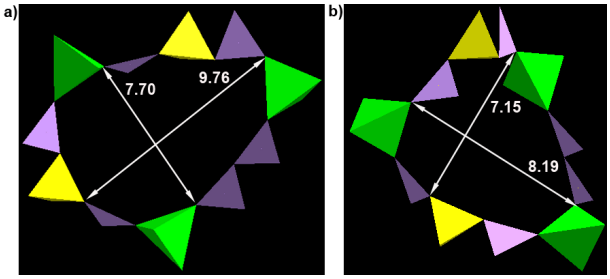

Fig. S3. View of the 11-ring openings in **1** located on the *ac* (a) and *ab* (b) planes, respectively.

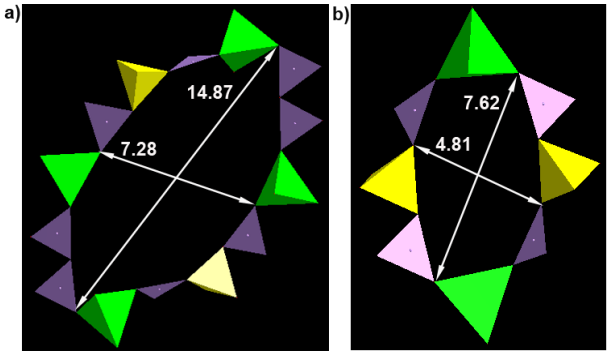

Fig. S4. View of the elliptical 14-ring (a) and 8-ring (b) openings situated on the *ab* plane in **4**.

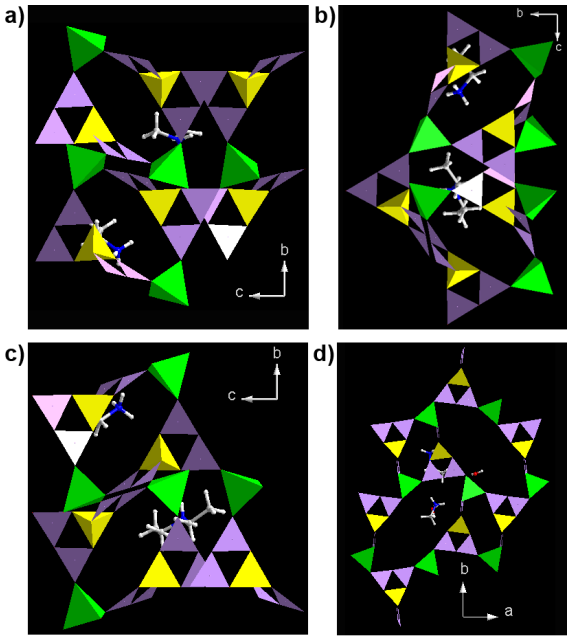

Fig. S5. View of the crystallographically independent templates and water molecules situated in channels in **1** (a), **2** (b), **3** (c) and **4** (d).

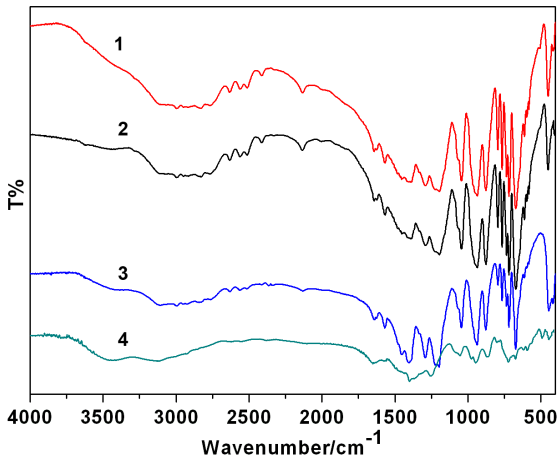

Fig. S6. IR spectra of **1**-**4**.

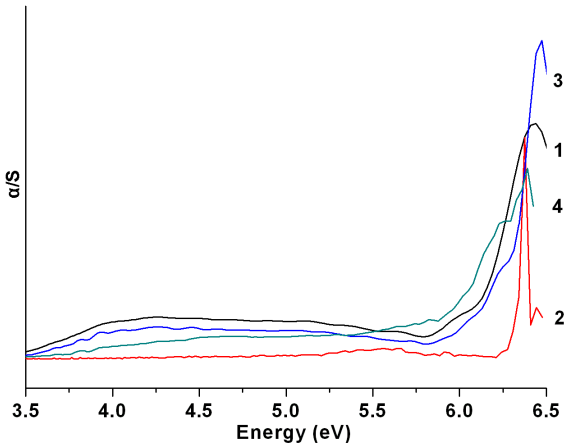

Fig. S7. Optical diffuse reflectance spectra for **1**-**4**.

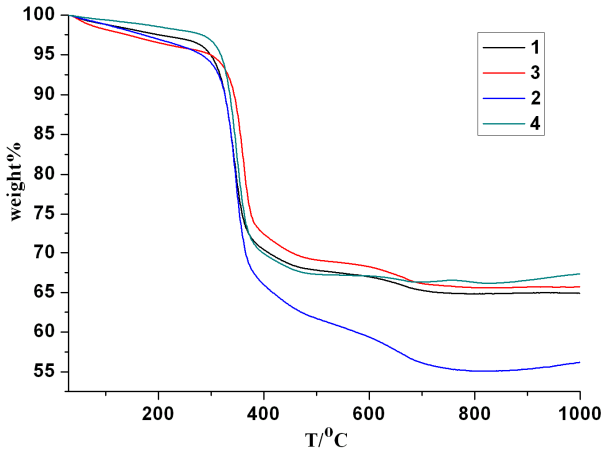

Fig. S8. TG curves of **1**-**4**.

Thermal Stability Analyses: The thermal stabilities of **1**-**4** were examined on powder samples by TG analysis in dry air atmosphere from 30 to 1000°C. These compounds show similar thermal behavior. For **1**-**3**, the TG curve shows a weight loss of 29.68% for **1**, 33.87% for **2** and 29.03% for **3** from 30 to 400°C, corresponding to the release of free water molecules and the decomposition of organic amines (calcd 30.53%、33.22% and 29.51%). The TG curves of **4** shows one-step of weight loss in the range of 30-630 °C. The total weight loss (found 32.93%) is assigned to the loss of free water molecules, organic amines (calcd 32.09 %).