Supporting Information

$Na_2B_{10}O_{17}\cdot H_2en$: A three-dimensional open-framework layered borate co-templated by inorganic cations and organic amines

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Table S1. X-ray crystallographic data for **1**.

Table S2. Selected bond lengths (Å) and bond valence sum (BVS) calculations for compound **1**.

Figure S1. The experimental and simulated PXRD patterns of **1**.

Figure S2. The pore size of the 9-,10- and 13-MR (the distance between two O atoms).

Figure S3. IR spectrum of **1**.

Figure S4. TG curve of compound **1** under air atmosphere (10 ºC/min).

Figure S5. UV diffuse reflectance spectrum of **1**.

Table S1. X-ray crystallographic data for **1**.

Empirical formula	$C_2H_{10}B_{10}N_2Na_2O_{17}$
M_r	488.20
crystal system	monoclinic
space group	*C2/c*
a (Å)	21.9507(10)
b (Å)	6.4172(2)
c (Å)	11.0598(5)
β (°)	103.407(4)
V (Å^3)	1515.45(11)
Z	4
D_c (g cm^{-3})	2.140
μ (mm^{-1})	0.243
F(000)	976
crystal size (mm)	0.30× 0.25 × 0.25
index ranges	3.31-25.19
GOF	1.075
collected reflcns	3220
unique reflcns (R_{int})	1369 (0.0264)
observed reflcns [$I > 2\sigma(I)$]	1180
refined parameters	150
R_1[a]/wR_2[b] [$I > 2\sigma(I)$]	0.0326/ 0.0802
R_1[a]/wR_2[b] (all data)	0.0391/ 0.0828
largest difference peak/hole	0.302/ -0.364

[a] $R_1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$, [b] $wR_2 = \{\Sigma[w(F_o^2-F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$.

Table S2. Selected bond lengths (Å) and bond valence sum (BVS) calculations for compound **1**[a].

Bond	Distance (Å)	BVS	BVS (Sum)	Bond	Distance (Å)	BVS	BVS (Sum)
B(1)-O(8)	1.356(3)	1.027	3.012	B(5)-O(3)	1.354(3)	1.033	2.990
B(1)-O(4)	1.358(3)	1.022		B(5)-O(7)	1.358(3)	1.022	
B(1)-O(9)	1.380(2)	0.963		B(5)-O(6)	1.391(3)	0.935	
B(2)-O(1)	1.432(3)	0.837	2.940	Na(1)-O(1D)	2.3154(16)	0.226	1.119
B(2)-O(2)	1.480(3)	0.735		Na(1)-O(7A)	2.5005(16)	0.148	
B(2)-O(8)	1.498(3)	0.670		Na(1)-O(5)	2.5284(16)	0.139	
B(2)-O(3)	1.499(3)	0.698		Na(1)-O(6C)	2.5352(17)	0.137	
B(3)-O(1)	1.438(3)	0.823	2.991	Na(1)-O(2D)	2.5794(16)	0.124	
B(3)-O(7A)	1.475(3)	0.745		Na(1)-O(2E)	2.8195(16)	0.072	
B(3)-O(5B)	1.481(3)	0.732		Na(1)-O(1)	2.3681(16)	0.200	
B(3)-O(4)	1.503(3)	0.691		Na(1)-O(3)	2.8156(17)	0.073	
B(4)-O(5)	1.358(3)	1.022	2.976	C(1)-N(1)	1.475(3)		
B(4)-O(2)	1.361(3)	1.014		C(1)-C(1F)	1.523(4)		
B(4)-O(6)	1.389(3)	0.940					

[a]Symmetry codes: A: *x*, -*y* + 1, *z* + 1/2; B: *x*, -*y*, *z* + 1/2; C: -*x* + 1/2, -*y* + 1/2, -*z* + 1; D: -*x* + 1/2, *y* + 1/2, -*z* + 3/2; E: *x*, *y* + 1,*z*; F: -*x*, -*y* + 1, -*z* + 1.

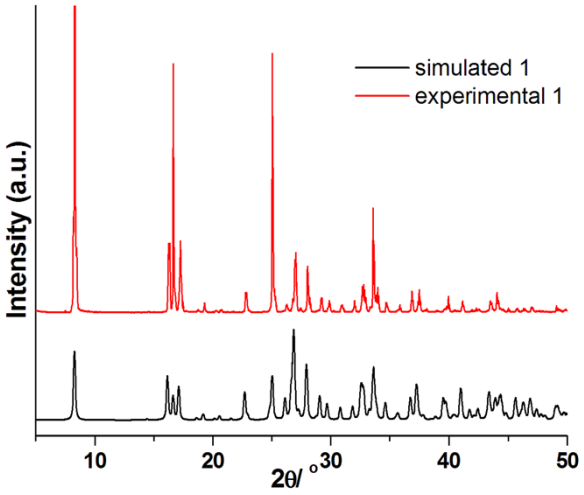

Figure S1. The experimental and simulated PXRD patterns of **1**.

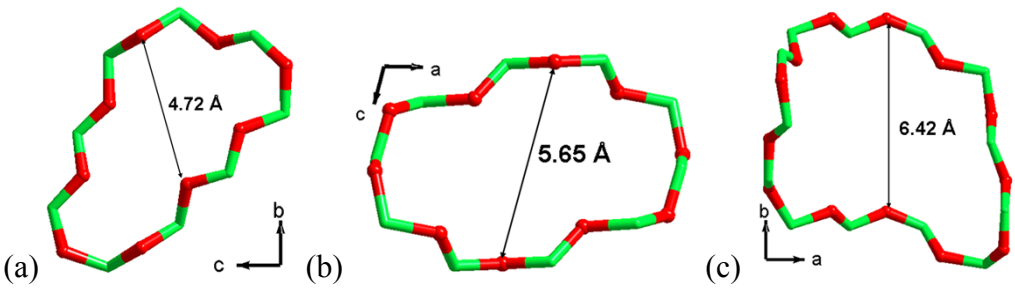

Figure S2. The pore size of the 9-,10- and 13-MR (the distance between two O atoms).

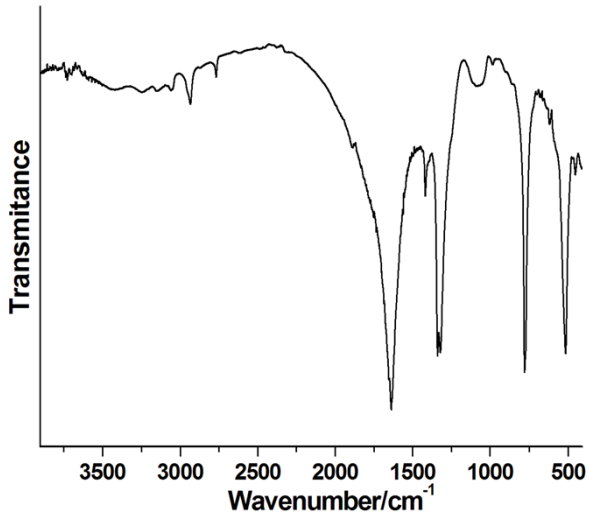

Figure S3. IR spectra of **1**.

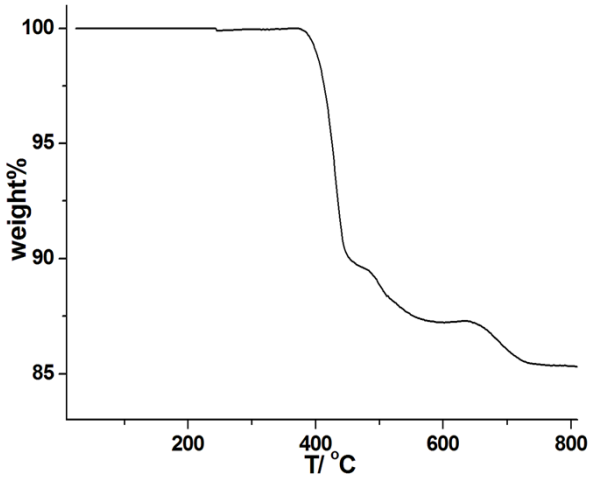

Figure S4. TG curve of compound **1** under air atmosphere (10 ºC/min).

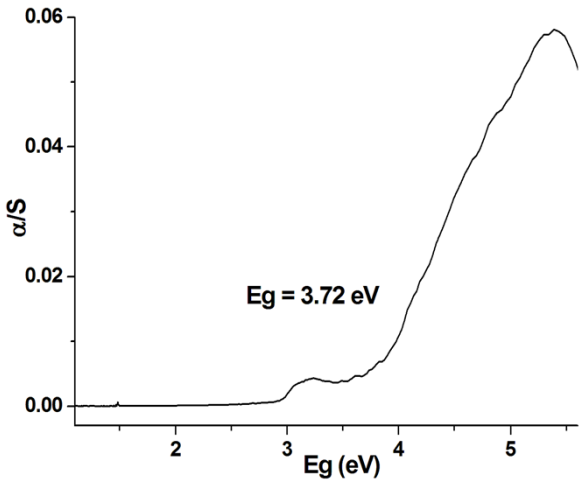

Figure S5. UV diffuse reflectance spectra of **1**.