Supporting Information

Three new aluminoborates: From 1D tube to 3D framework

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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)(°)
O(3)-H(3)···O(13)#1	0.85	1.86	2.688	166
O(12)-H(12)···O(4)#1	0.84	1.97	2.765	156
O(13)-H(13) ···O(9)#2	0.84	2.27	3.002	146

Symmetric codes: #1:1-x,1-y,-z; #2:1-x,2-y,-z.

Table S2. The BVS values of all atoms in **1**

Atoms		Bond length(Å)	BVS calculation	Atoms		Bond length(Å)	BVS calculation
B1	B(1)-O(1)	1.339(2)	3.02	O7	O(7)-B(4)	1.356(5)	2.01
	B(1)-O(5)	1.368(9)			O(7)-B(3)	1.459(5)	
	B(1)-O(2)	1.400(2)			O(7)-K#4	2.751(1)	
B2	B(2)-O(3)	1.347(1)	3.05	O8	O(8)-B(4)	1.335(8)	2.01
	B(2)-O(4)	1.368(2)			O(8)-Al#5	1.737(5)	
	B(2)-O(2)	1.378(7)			O(8)-K#4	2.762(9)	
B3	B3)-O(7)	1.459(5)	3.09	O9	O(9)-B(5)	1.394(7)	1.87
	B(3)-O(5)	1.465(4)			O(9)-B(4)	1.396(5)	
	B(3)-O(6)	1.466(7)		O10	O(10)-B(5)	1.334(4)	1.83
	B(3)-O(4)	1.474(3)			O(10)-Al	1.737(2)	
B4	B(4)-O(8)	1.335(8)	3.07	O11	O(11)-B(6)	1.332(1)	1.84
	B(4)-O(7)	1.356(5)			O(11)-Al	1.738(6)	
	B(4)-O(9)	1.396(5)		O12	O(12)-B(6)	1.366(7)	1.01
B5	B(5)-O(10)	1.334(4)	3.07	O13	O(13)-B(6)	1.385(2)	0.96
	B(5)-O(6)	1.361(1)		Al	Al-O(10)	1.737(2)	2.91
	B(5)-O(9)	1.394(7)			Al-O(8)#6	1.737(5)	
B6	B(6)-O(11)	1.332(1)	3.08		Al-O(1)#1	1.738(5)	
	B(6)-O(12)	1.366(7)			Al-O(11)	1.738(6)	
	B(6)-O(13)	1.385(2)		Cs	Cs-O(1)	3.095(3)	0.70
O1	O(1)-B(1)	1.339(2)	1.82		Cs-O(10)#7	3.127(4)	
	O(1)-Al#1	1.738(5)			Cs-O(12)#7	3.150(02)	
O2	O(2)-B(2)	1.378(7)	1.90		Cs-O(11)#1	3.26894)	
	O(2)-B(1)	1.400(2)			Cs-O(13)#8	3.320(9)	
O3	O(3)-B(2)	1.368(2)	1.31		Cs-O(8)#4	3.385(7)	
	O(3)-K	2.572(8)		K	K-O(3)	2.572(8)	1.12
O4	O(4)-B(2)	1.347(1)	1.82		K-O(5)#9	2.682(8)	
	O(4)-B(3)	1.474(3)			K-O(6)#3	2.689(2)	
O5	O(5)-B(1)	1.368(9)	2.01		K-O(7)#4	2.751(1)	
	O(5)-B(3)	1.465(4)			K-O(8)#4	2.762(9)	
	O(5)-K#2	2.682(8)					
O6	O(6)-B(5)	1.361(1)	2.02				
	O(6)-B(3)	1.466(7)					
	O(6)-K#3	2.689(2)					

Symmetric codes: #1:1-x,1-y,1-z; #2:x,1+y,z; #3:1-x,-y,1-z;; #5:1+x,y,z; #6:-1+x,y,z; #7:x,-1+y,1+z; #8:1+x,-1+y,1+z; #9:x,-1+y,z.

Table S3. The BVS values of all atoms in **2**

Atoms		Bond length(Å)	BVS calculation	Atoms		Bond length(Å)	BVS calculation
B1	B(1)-O(5)	1.355(9)	3.04	O6	O(6)-B(4)	1.354(4)	1.81
	B(1)-O(4)	1.358(05)			O(6)-Al	1.721(03)	
	B(1)-O(3)	1.384(4)		O7	O(7)-B(4)	1.359(9)	2.01
B2	B(2)-O(1)	1.345(7)	2.74		O(7)-Al#5	1.740(4)	
	B(2)-O(2)	1.357(8)			O(7)-K#7	2.849(9)	
	B(2)-O(3)	1.393(9)			O(7)-Cs#5	3.210(4)	
B3	B(3)-O(2)#1	1.461(5)	3.10	O8	O(8)-B(4)	1.372(9)	1.16
	B(3)-O(2)	1.461(5)			O(8)-Cs	3.083(2)	
	B(3)-O(4)#1	1.470(08)		Al	Al-O(6)	1.721(03)	2.93
	B(3)-O(4)	1.470(08)			Al-O(5)	1.730(3)	
B4	B(4)-O(6)	1.354(4)	3.07		Al-O(7)#8	1.740(4)	
	B(4)-O(7)	1.359(9)			Al-O(1)#9	1.748(5)	
	B(4)-O(8)	1.372(9)		Cs	Cs-O(5)#8	3.051(9)	0.82
O1	O(1)-B(2)	1.345(7)	2.00		Cs-O(8)	3.083(2)	
	O(1)-Al#2	1.748(5)			Cs-O(7)#8	3.210(4)	
	O(1)-K#3	2.880(03)			Cs-O(4)#10	3.258(9)	
	O(1)-Cs#4	3.305(2)			Cs-O(1)#4	3.305(2)	
O2	O(2)-B(2)	1.357(8)	1.99		Cs-O(3)#4	3.326(8)	
	O(2)-B(3)	1.461(5)			Cs-O(3)#8	3.355(5)	
	O(2)-K	2.787(03)		K	K-O(2)	2.787(03)	0.89
O3	O(3)-B(1)	1.393(9)	2.07		K-O(2)#1	2.787(03)	
	O(3)-B(2)	1.384(4)			K-O(7)#11	2.849(9)	
	O(3)-Cs#4	3.326(8)			K-O(7)#2	2.849(9)	
	O(3)-Cs#5	3.355(5)			K-O(1)#12	2.880(3)	
O4	O(4)-B(1)	1.358(06)	1.90		K-O(1)#3	2.880(3)	
	O(4)-B(3)	1.47(04)					
	O(4)-Cs#6	3.258(9)					
O5	O(5)-B(1)	1.355(9)	1.96				
	O(5)-Al	1.730(3)					
	O(5)-Cs#5	3.051(9)					

Symmetric codes: #1:1-x,y,1/2-z; #2:-1/2+x,3/2-y,1-z; #3:1-x,2-y,1-z; #4:1-x,1-y,1-z; #5:x,1-y,1/2+z; #6:3/2-x,1/2+y,z; #7: 3/2-x,3/2+y,1/2+z; #8:x,1-y,-1/2+z; #9: 1/2+x,3/2-y,1-z; #10:3/2-x,-1/2+y,z; #11: 3/2-x,3/2-y,-1/2+z; #12:x,2-y,-1/2+z.

Table S3. The BVS values of all atoms in **3**

Atoms		Bond length(Å)	BVS calculation	Atoms		Bond length(Å)	BVS calculation
B1	B(1)-O(5)	1.336(3)	3.06	O6	O(6)-B(4)	1.354(4)	1.89
	B(1)-O(3)	1.361(8)			O(6)-Al	1.721(8)	
	B(1)-O(4)	1.394(1)			O(6)-Cs(1)#7	3.342(1)	
B2	B(2)-O(2)#1	1.453(4)	3.12	O7	O(7)-B(4)	1.348(5)	2.05
	B(2)-O(2)	1.453(4)			O(7)-Al#8	1.739(1)	
	B(2)-O(3)#1	1.472(7)			O(7)-Cs(1)#7	3.162(9)	
	B(2)-O(3)	1.472(7)			O(7)-Cs(2)	3.169(7)	
B3	B(3)-O(1)	1.340(7)	3.05	O8	O(8)-B(4)	1.371(9)	1.14
	B(3)-O(2)	1.363(5)			O(8)-Cs(2)#9	3.127(6)	
	B(3)-O(4)	1.391(8)		Al	Al-O(6)	1.721(8)	2.90
B4	B(4)-O(7)	1.348(5)	3.11		Al-O(7)#9	1.739(1)	
	B(4)-O(6)	1.371(9)			Al-O(5)	1.743(04)	
	B(4)-O(8)	1.354(4)			Al-O(1)#10	1.750(1)	
O1	O(1)-B(3)	1.340(7)	2.04	Cs1	Cs(1)-O(2)	3.056(4)	1.09
	O(1)-Al#2	1.750(1)			Cs(1)-O(2)#1	3.056(4)	
	O(1)-Cs(1)#3	3.115(9)			Cs(1)-O(1)#11	3.115(9)	
	O(1)-Cs(2)#4	3.279(6)			Cs(1)-O(1)#3	3.115(9)	
O2	O(2)- B(3)	1.361(8)	2.02		Cs(1)-O(7)#2	3.162(9)	
	O(2)- B(2)	1.472(7)			Cs(1)-O(7)#12	3.162(9)	
	O(2)-Cs(1)	3.056(4)			Cs(1)-O(6)#12	3.342(1)	
	O(2)-Cs(2)#5	3.473(6)			Cs(1)-O(6)#5	3.342(1)	
O3	O(3)-B(1)	1.361(8)	1.87	Cs2	Cs(2)-O(5)	3.077(3)	0.80
	O(3)-B(2)	1.472(7)			Cs(2)-O(8)#8	3.127(6)	
	O(3)-Cs(2)#6	3.313(03)			Cs(2)-O(7)	3.169(7)	
O4	O(4)-B(3)	1.391(8)	1.99		Cs(2)-O(4)#4	3.230(4)	
	O(4)-B(1)	1.394(1)			Cs(2)-O(1)#4	3.279(6)	
	O(4)-Cs(2)#4	3.230(4)			Cs(2)-O(3)#7	3.313(04)	
O5	O(5)-B(1)	1.336(3)	1.98		Cs(2)-O(2)#10	3.473(6)	
	O(5)-Al	1.743(04)					
	O(5)-Cs(2)	3.077(3)					

Symmetric codes: #1:1-x,y,1/2-z; #2:1/2+x,3/2-y,1-z; #3:1-x,2-y,1-z; #4:1-x,y,3/2-z; #5:1/2+x,3/2-y,1-z; #6:1/2-x,3/2+y,-1/2+z; #7:1/2-x,3/2-y,1/2+z; #8:x,1-y,1/2+z; #9:x,1-y,-1/2+z; #10:-1/2+x,3/2-y,1-z; #11:x,2-y,-1/2+z; #12:1/2-x,3/2-y,-1/2+z.

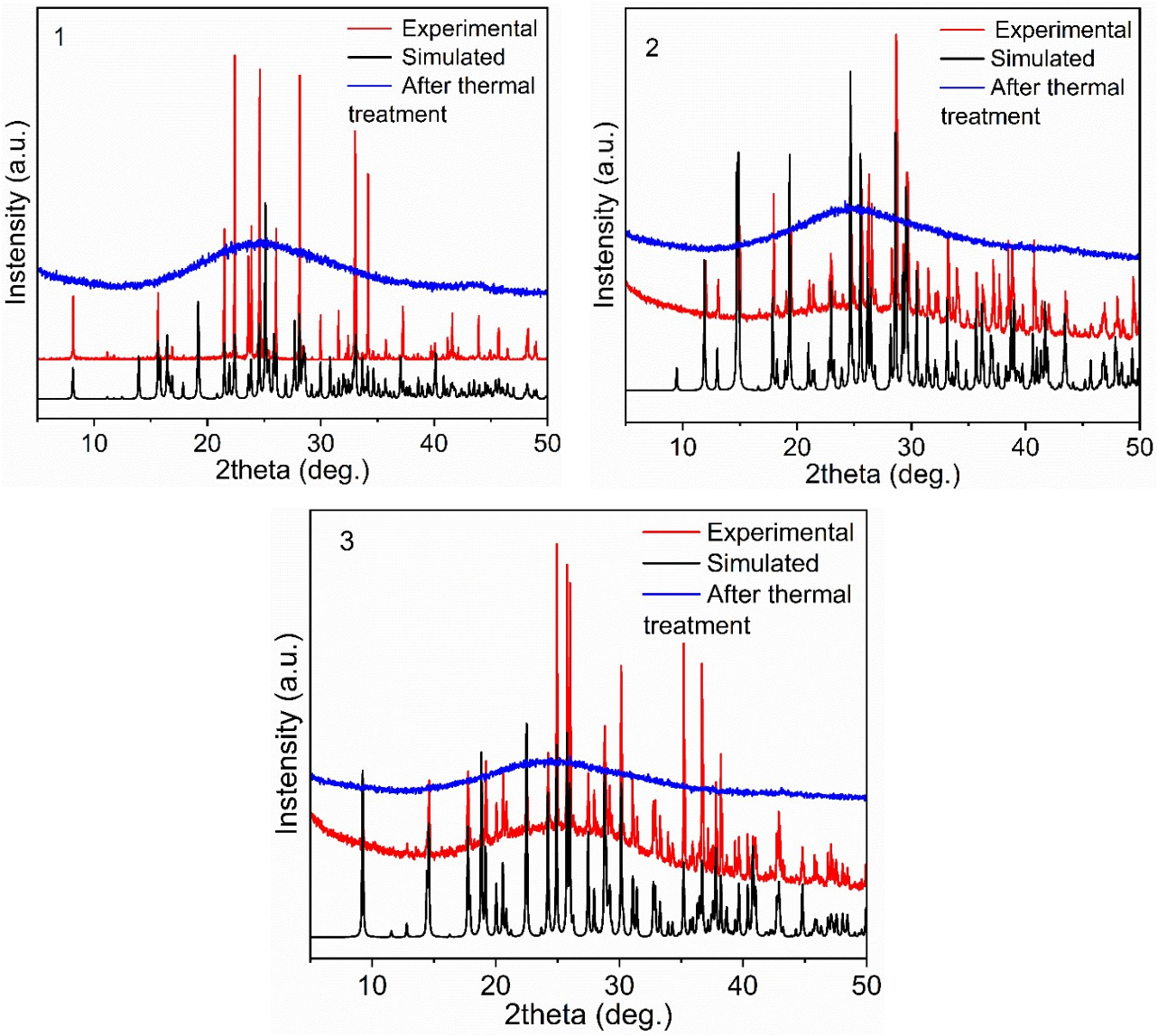

Figure S1. The PXRD patterns before and after thermal treatments of compounds **1-3**, respectively.

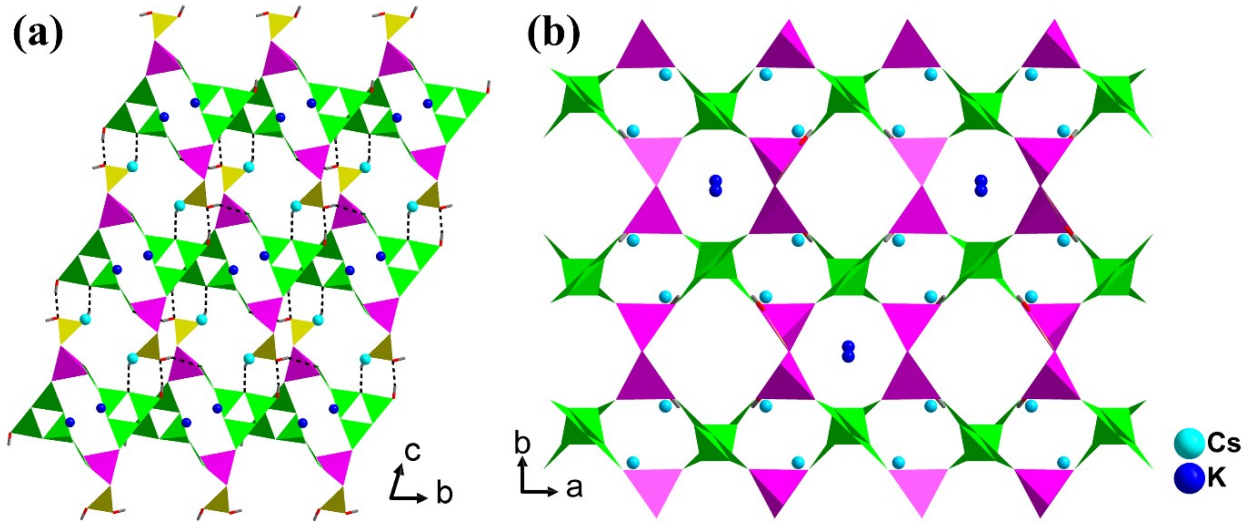

Figure S2. Metal positions in the framework for **1** (a) and **2** (b).

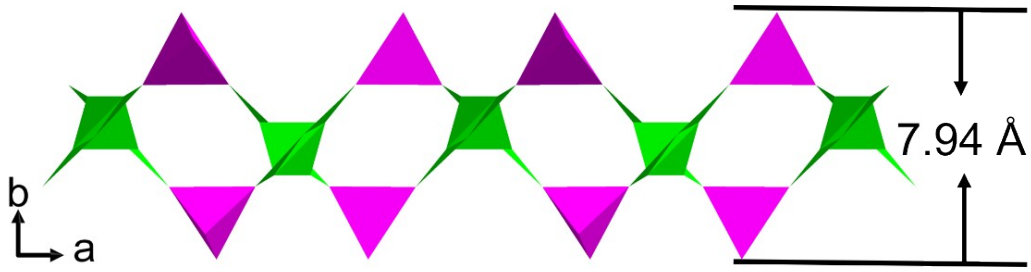

Figure S3. Side view of 2D ABO layer with a thickness of 7.94 Å.

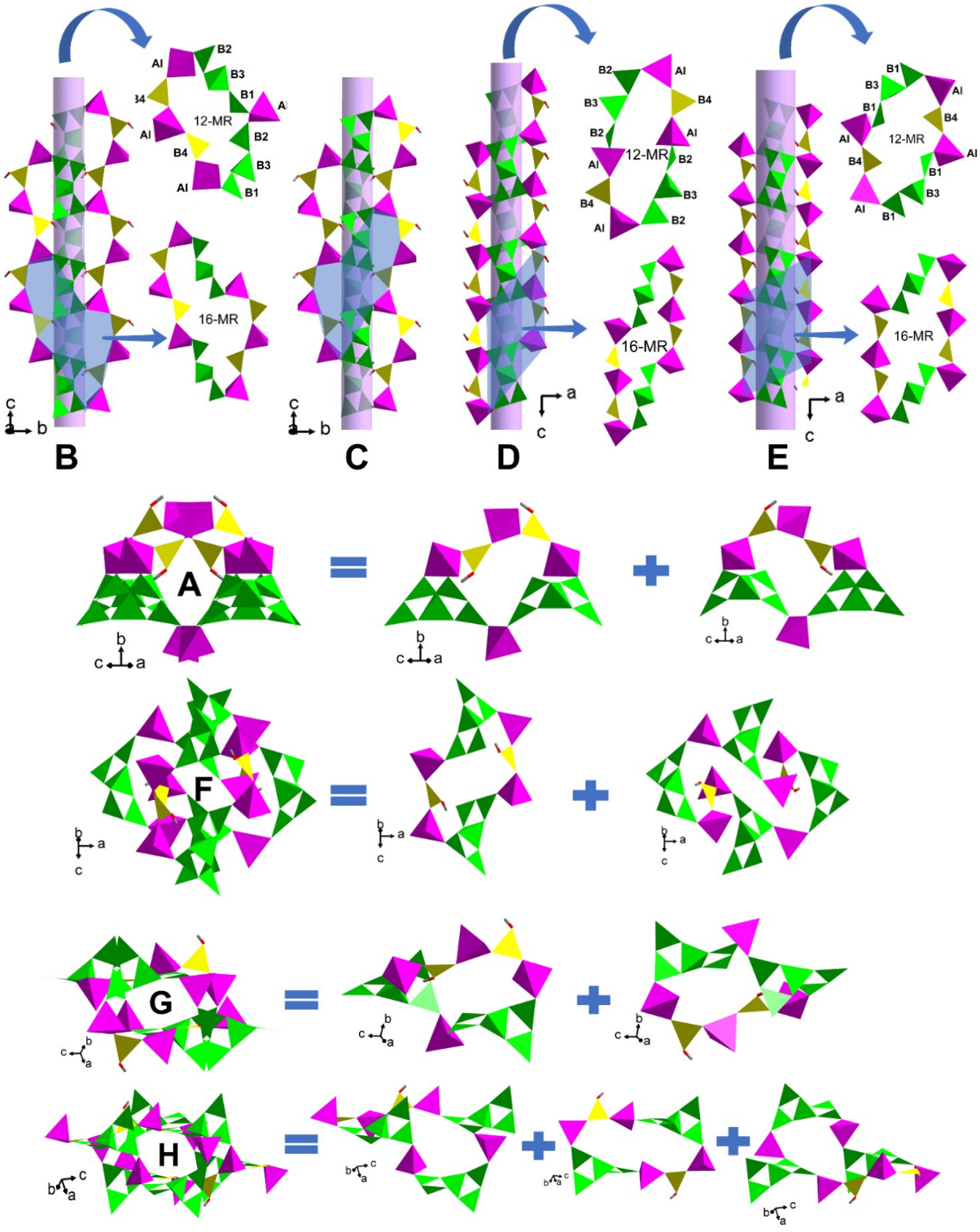

Figure S4. The eight types of channels in **2**.

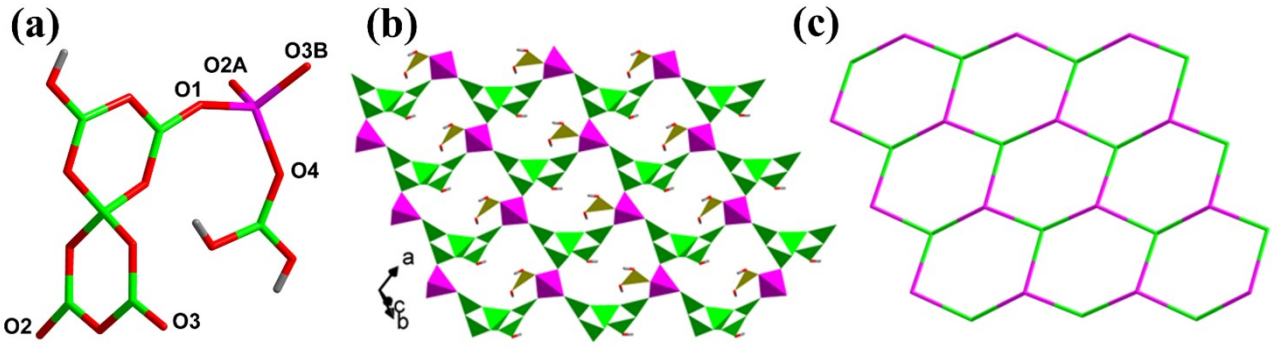

Figure S5. (a) The asymmetric unit in **4**; (b) View of 2D layer; (c) The topology network in **4**.

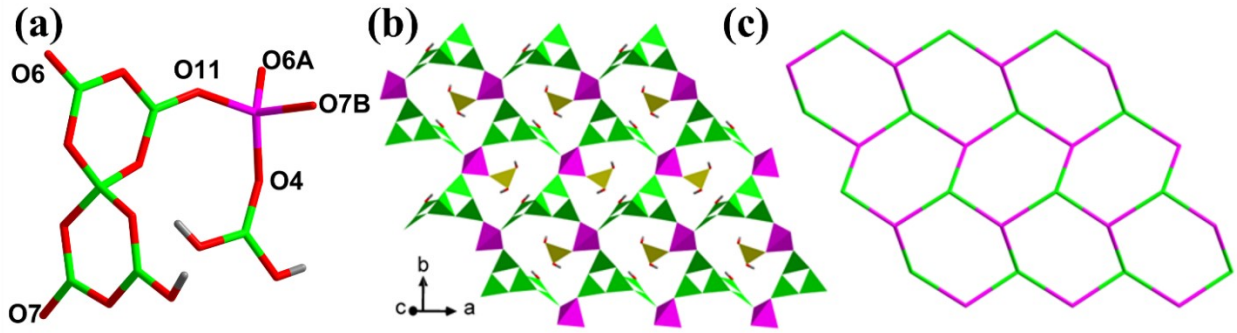

Figure S6 (a) The asymmetric unit in **5**; (b) View of 2D layer; (c) The topology network in **5**.

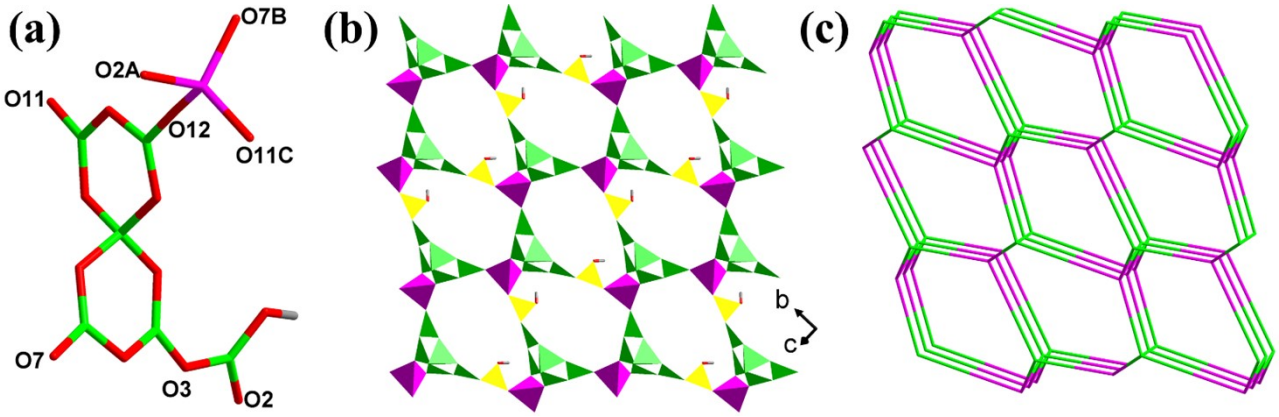

Figure S7 (a) The asymmetric unit in **6**; (b) View of 3D framework; (c) The topology network in **6**.

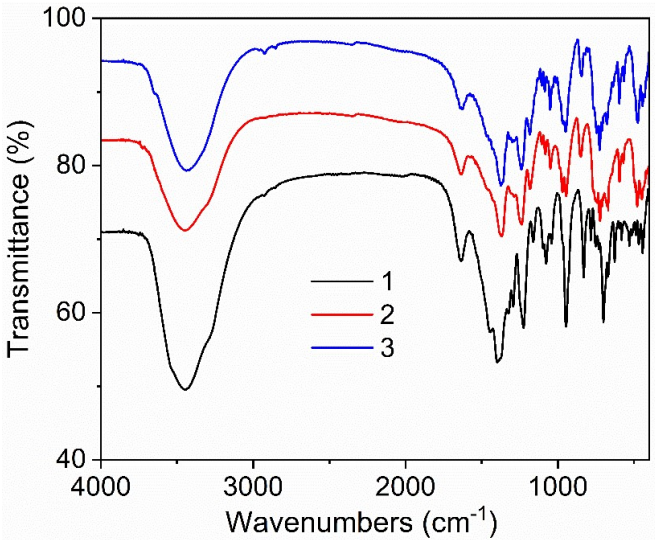

Figure S8. The IR spectra of compounds **1-3**, respectively.

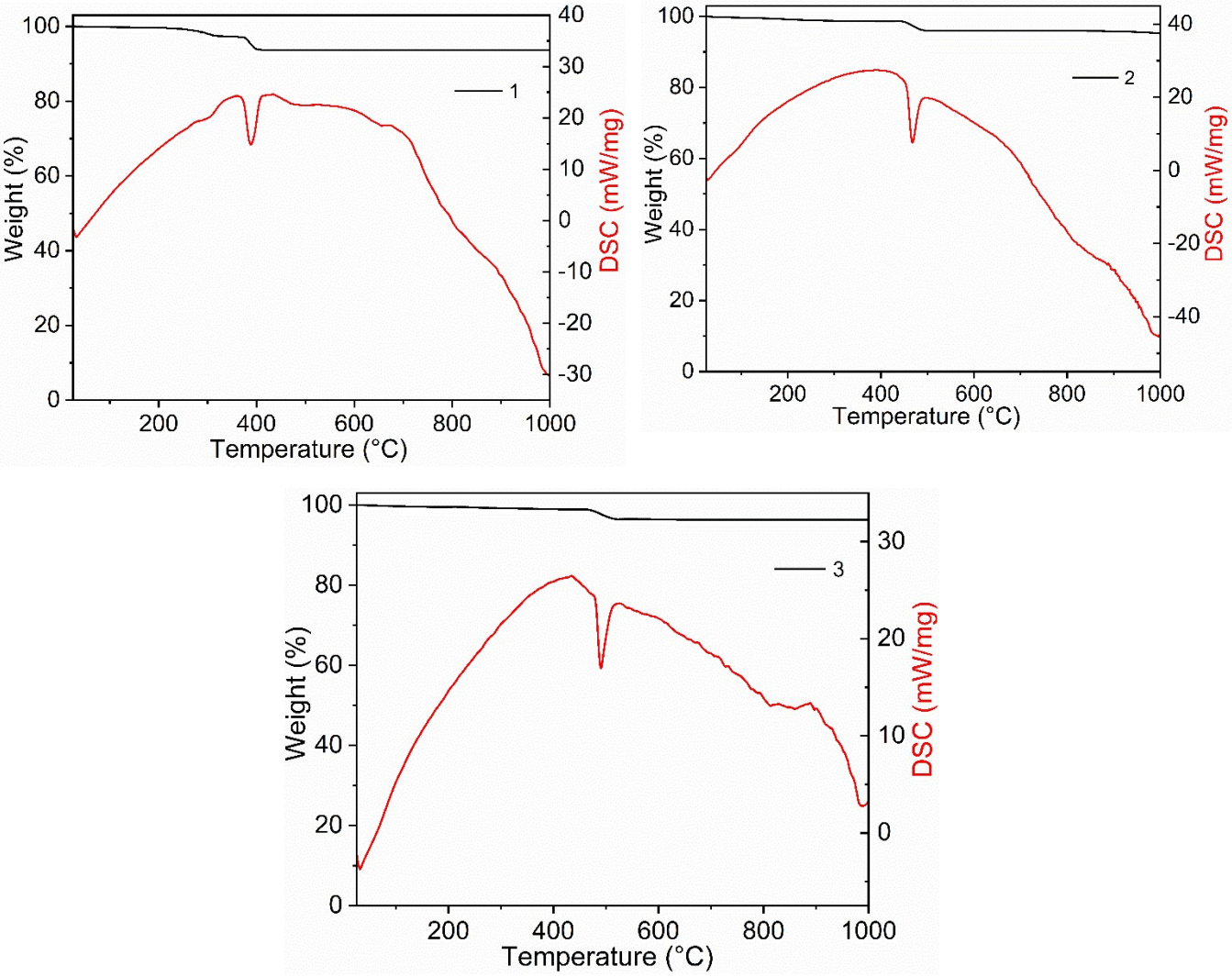

Figure S9. The TG-DSC curves of compounds **1-3**, respectively.