Construction of Hydrothermally Stable Beryllium Phosphite Open-Frameworks with High Proton Conductivity

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1. TGA and DSC

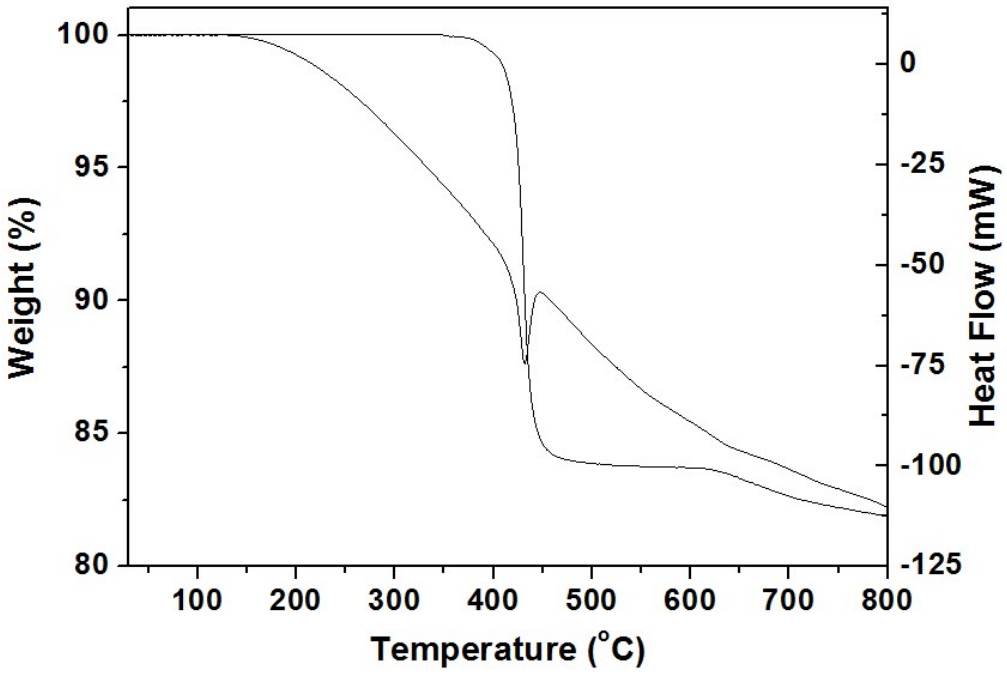

Fig. S1. The TGA and DSC curves of compound **1**.

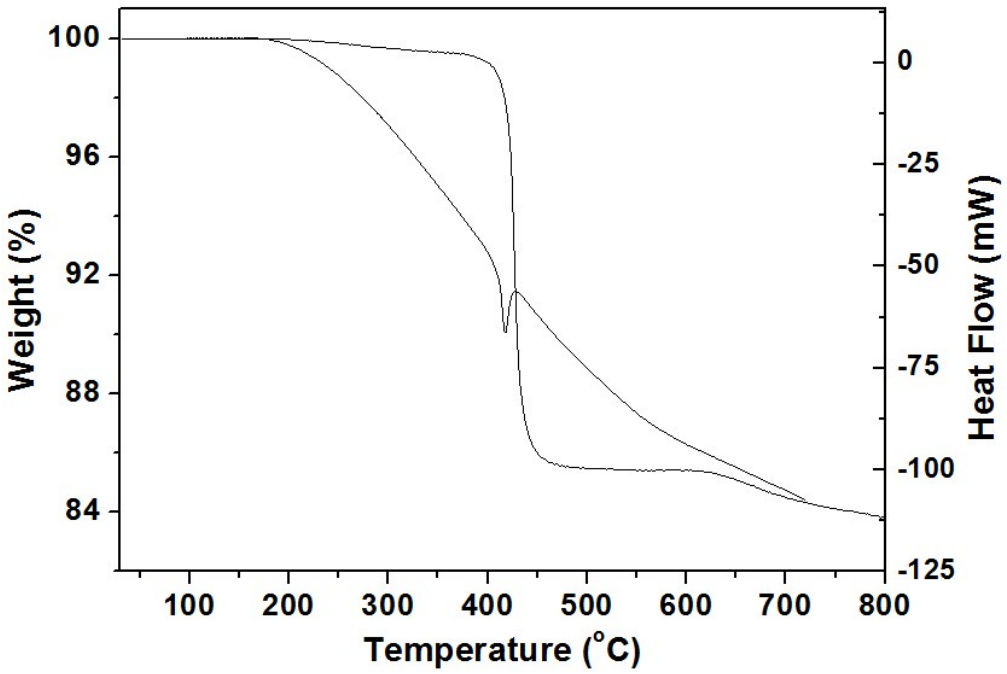

Fig. S2. The TGA and DSC curves of compound **2**.

2. Structural illustration and selected bond lengths and angles

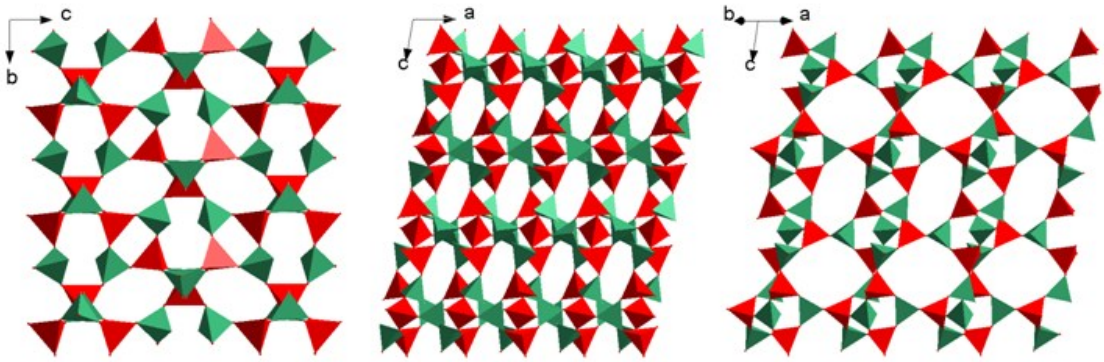

Fig. S3. Polyhedral view of compound **1** along different directions.

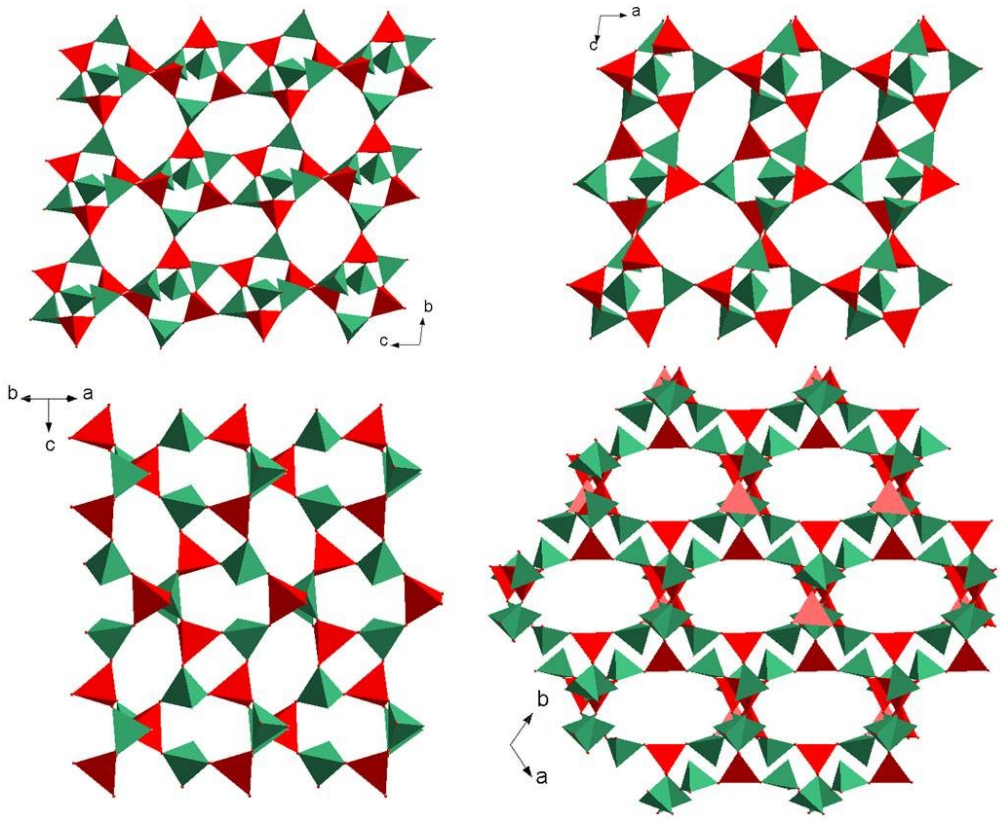

Fig. S4 Polyhedral view of compound **2** along different directions.

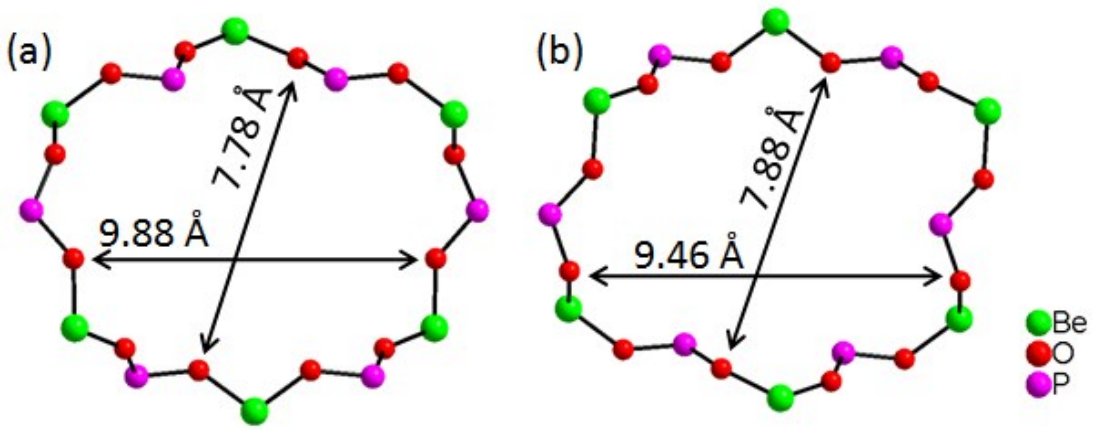

Fig. S5. The 12-members ring window contained in compound **1** (a) and **2** (b).

Table S1 The selected bond lengths [Å] and angles [°] of compound **1**.

Be1-O2[1]	1.625(4)	Be2[3]-O1	1.623(3)
Be1-O3	1.627(3)	P1-O1	1.520(2)
Be1-O4	1.617(4)	P1-O2	1.505(2)
Be1-O5[2]	1.625(4)	P1-O3	1.507(2)
Be2-O1[3]	1.632(3)	P1-O4	1.506(2)
Be2-O1[4]	1.632(3)	P2-O5	1.509(2)
Be2-O6	1.623(3)	P2-O6	1.512(2)
Be2-O6[5]	1.623(3)	Be1[2]-O5	1.625(4)
O2[1]-Be1-O3	109.8(2)	P1-O1-Be2[3]	141.6(2)
O2[1]-Be1-O5[2]	104.4(2)	P1-O2-Be1[1]	138.0(2)
O2[1]-Be1-O4	110.8(2)	P1-O3-Be1	137.2(2)
O3-Be1-O4	109.6(2)	P2-O4-Be1	140.7(2)
O4-Be1-O5[2]	116.7(2)	P2-O5-Be1[2]	144.4(2)
O3-Be1-O5[2]	105.3(2)	P2-O6-Be2	135.5(2)
O1[3]-Be2-O1[4]	110.7(3)	O2-P1-O1	110.8(2)
O6-Be2-O1[3]	107.8(2)	O2-P1-O3	114.1(2)
O6[5]-Be2-O1[4]	107.8(2)	O3-P1-O1	109.4(2)
O6[5]-Be2-O1[3]	111.3(2)	O4-P2-O5	113.68(2)
O6-Be2-O1[4]	111.3(2)	O4-P2-O6	110.8(2)
O6[5]-Be2-O6	107.8(3)	O5-P2-O6	110.9(2)

[1]1-X,1-Y,1-Z; [2]1-X,+Y,3/2-Z; [3]3/2-X,1/2-Y,1-Z; [4]1/2+X,1/2-Y,1/2+Z; [5]2-X,+Y,3/2-Z

Table S2. The selected bond lengths [Å] and angles [°] of compound **2**.

Be1-O2[1]	1.619(5)	Be2[2]-O1	1.630(5)
Be1-O3	1.628(5)	P1-O1	1.521(3)
Be1-O4	1.595(5)	P1-O2	1.509(3)
Be1-O7	1.633(5)	P1-O3	1.502(3)
Be2-O1[2]	1.630(5)	P3-O4	1.511(3)
Be2-O5	1.627(5)	P3-O5	1.511(3)
Be2-O8[3]	1.619(5)	P3-O6	1.505(5)
Be2-O12[4]	1.624(5)	Be1[1]-O2	1.619(5)
Be3-O6	1.610(5)	P2-O7	1.512(3)
Be3-O9	1.605(5)	Be2[6]-O8	1.619(5)
Be3-O10	1.634(5)	P2-O8	1.509(3)
Be3-O11[5]	1.632(5)	P4-O11	1.513(3)
O2[1]-Be1-O3	109.6(3)	P1-O1-Be2[2]	141.1(2)
O2[1]-Be1-O7	104.0(3)	P1-O2-Be1[1]	137.6(3)
O3-Be1-O7	104.5(3)	P1-O3-Be1	140.2(2)
O4-Be1-O2[1]	111.5(3)	P3-O4-Be1	142.5(2)
O4-Be1-O3	110.2(3)	P3-O5-Be2	136.5(2)
O3-Be1-O7	116.6(3)	P3-O6-Be3	145.2(2)
O5-Be2-O1[2]	107.6(3)	O2-P1-O1	110.9(2)
O8[3]-Be2-O1[2]	111.0(3)	O3-P1-O1	109.3(2)
O8[3]-Be2-O12[4]	107.7(3)	O3-P1-O2	114.5(2)
O12[4]-Be2-O1[2]	110.7(3)	O7-P2-O9	113.53(2)
O6-Be3-O10	105.5(3)	O8-P2-O7	110.9(2)
O6-Be3-O11[5]	105.1(3)	O5-P3-O4	110.7(2)
O9-Be3-O6	116.6(3)	O10-P4-O12	110.0(2)
O9-Be3-O10	108.7(3)	O11-P4-O12	113.3(2)

[1]1-X,1-Y,1-Z; [2]-X,1-Y,1-Z; [3]-1+X,-1+Y,+Z; [4]-X,1-Y,-Z; [5]1-X,1-Y,-Z; [6]1+X,1+Y,+Z

3. Nyquist plots of compounds **1** and **2** at different conditions.

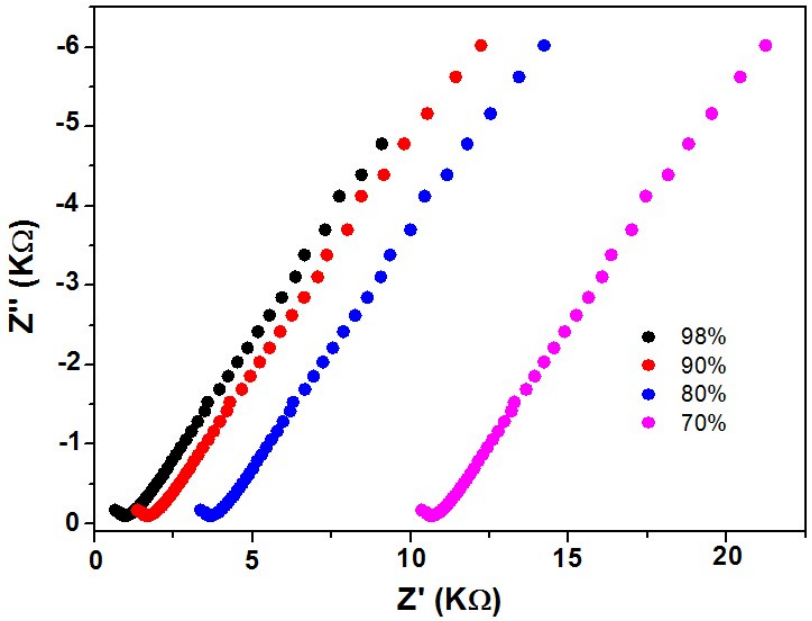

Fig. S6. Nyquist plots of compound **1** at 90 °C under different relative humidity from 70% to 98%.

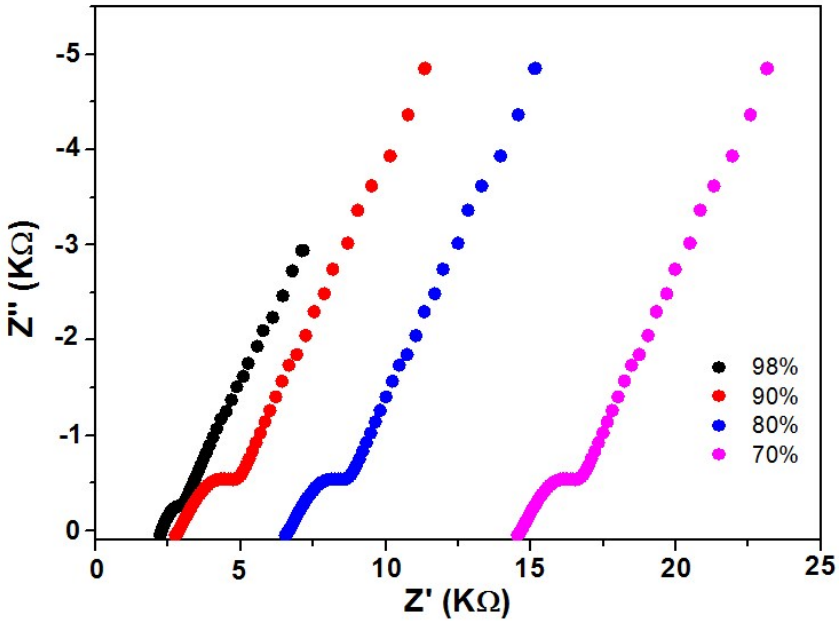

Fig. S7 Nyquist plots of compound **2** at 90 °C under different relative humidity from 70% to 98%.