

Electronic Supplementary Information for:

**MCuB<sub>7</sub>O<sub>12</sub>·nH<sub>2</sub>O (M=Na, K ): A new copper borate with  
14-ring channel**

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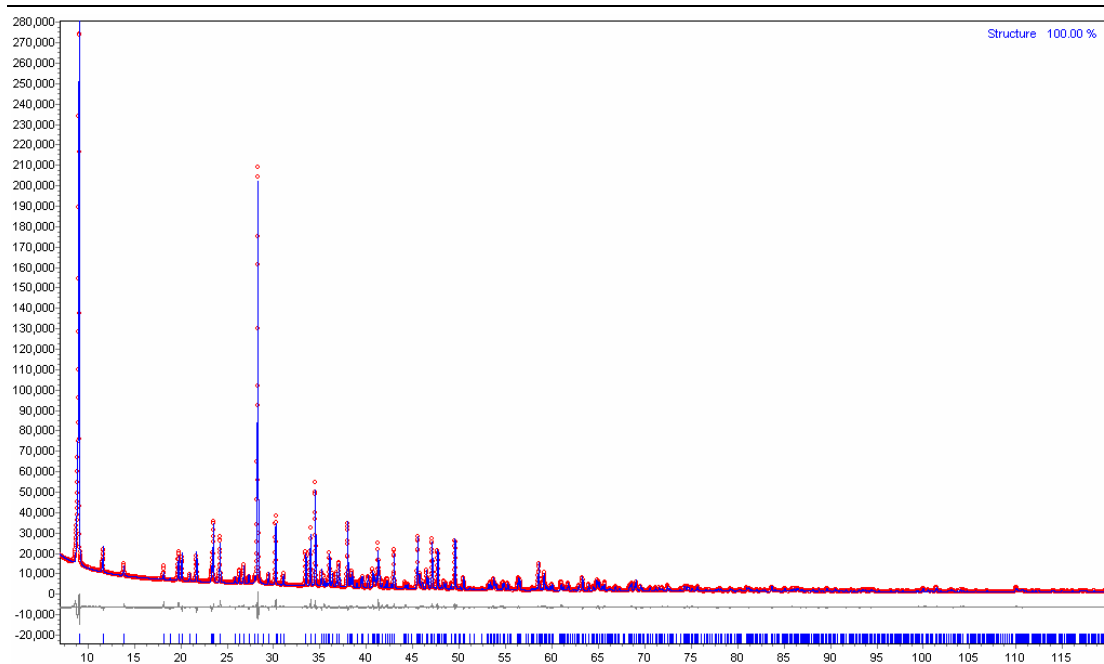


Figure S1. Rietveld plot of the powder X-ray diffraction pattern of  $\text{NaCuB}_7\text{O}_{12} \cdot n\text{H}_2\text{O}$ . The symbol  $\bullet$  represents observed pattern and the solid line is the calculated pattern; the marks below the diffraction patterns are the reflection positions and, the difference curve is also shown below the diffraction curves.

Table S1. Refined atomic parameters of  $\text{NaCuB}_7\text{O}_{12} \cdot n\text{H}_2\text{O}^*$

site	x	y	z	$U_{\text{eq}}$
Na	0.2094(3)	0.4090(8)	0	0.0783(2)
Cu	0	0	0.40044(7)	0.0093(4)
B1	0.1218(7)	0.438(2)	0.5	0.0088(2)
B2	0.1846(5)	0.561(1)	0.1913(4)	0.0088(2)
B3	0.0622(6)	0.207(1)	0.2181(4)	0.0088(2)
B4	0.1740(5)	0.411(1)	0.3467(4)	0.0088(2)
O1	0	0	0.1851(3)	0.0051(1)
O2	0.0697(4)	0.1811(9)	0.5	0.0051(1)
O3	0.1114(3)	0.3773(7)	0.1613(2)	0.0051(1)
O4	0.1402(2)	0.5730(6)	0.4228(2)	0.0051(1)
O5	0.2553(3)	0.2111(7)	0.3696(2)	0.0051(1)
O6	0.0794(3)	0.2304(7)	0.3103(2)	0.0051(1)
O7	0.2025(3)	0.6145(6)	0.2789(2)	0.0051(1)
O8	0.9018(5)	0.047(2)	0	0.1591(2)

\* Pnmm (No. 58),  $a = 12.73720(8) \text{ \AA}$ ,  $b = 4.69546(3) \text{ \AA}$ ,  $c = 15.17928(9) \text{ \AA}$ ,  $V = 907.83(2) \text{ \AA}^3$ ,  $R_p$   
 $= 0.038$ ,  $R_{wp} = 0.053$

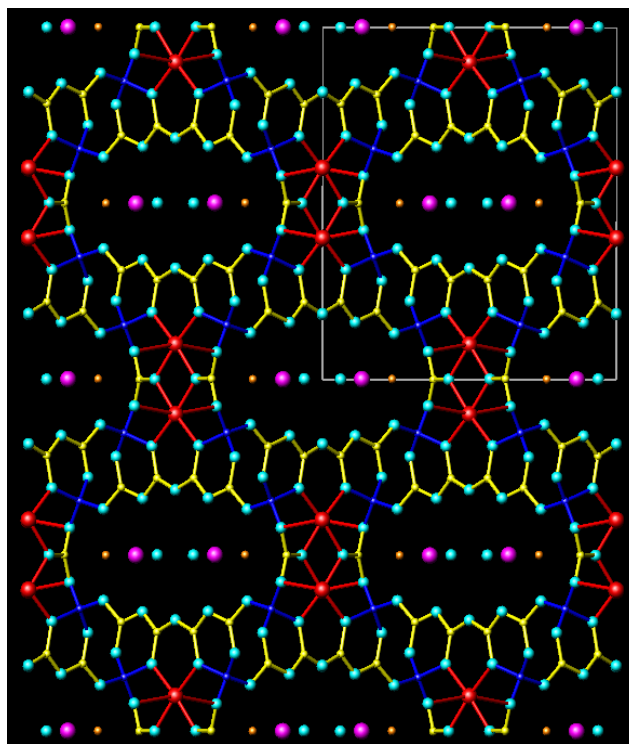


Figure S2. A view along the b axis of the structure of  $\text{Li}_{0.45}\text{Na}_{0.55}\text{CuB}_7\text{O}_{12} \cdot n\text{H}_2\text{O}$ .

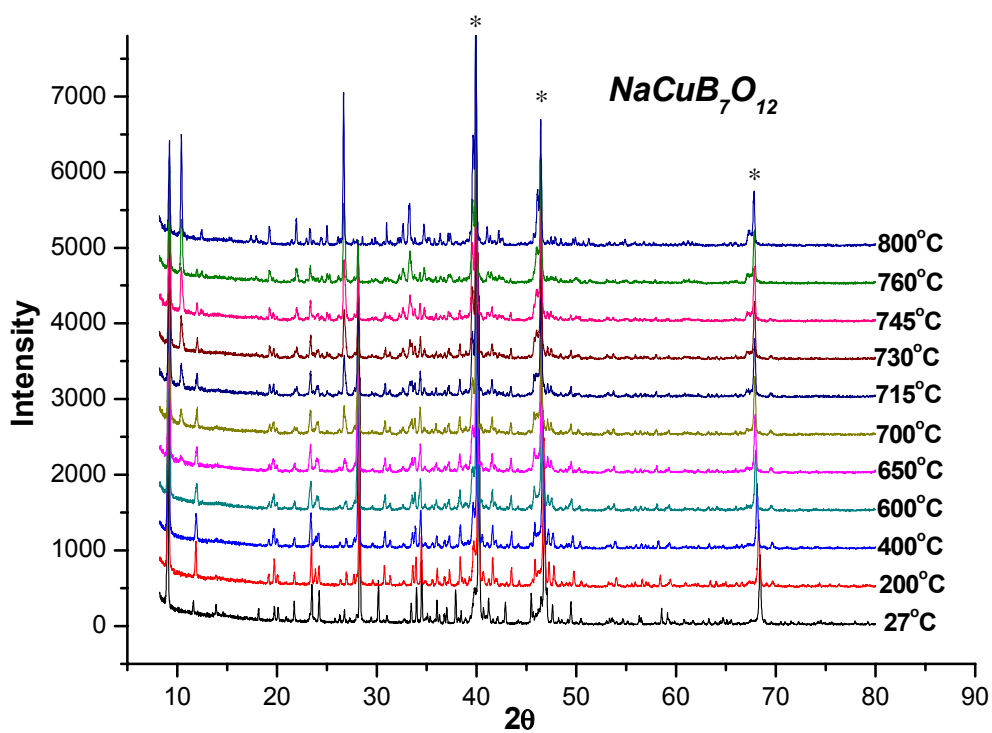


Figure S4. In situ powder X-ray diffraction of  $\text{NaCuB}_7\text{O}_{12} \cdot n\text{H}_2\text{O}$ . The peaks marked with \* correlated to the Pt substrate on which our sample was placed.

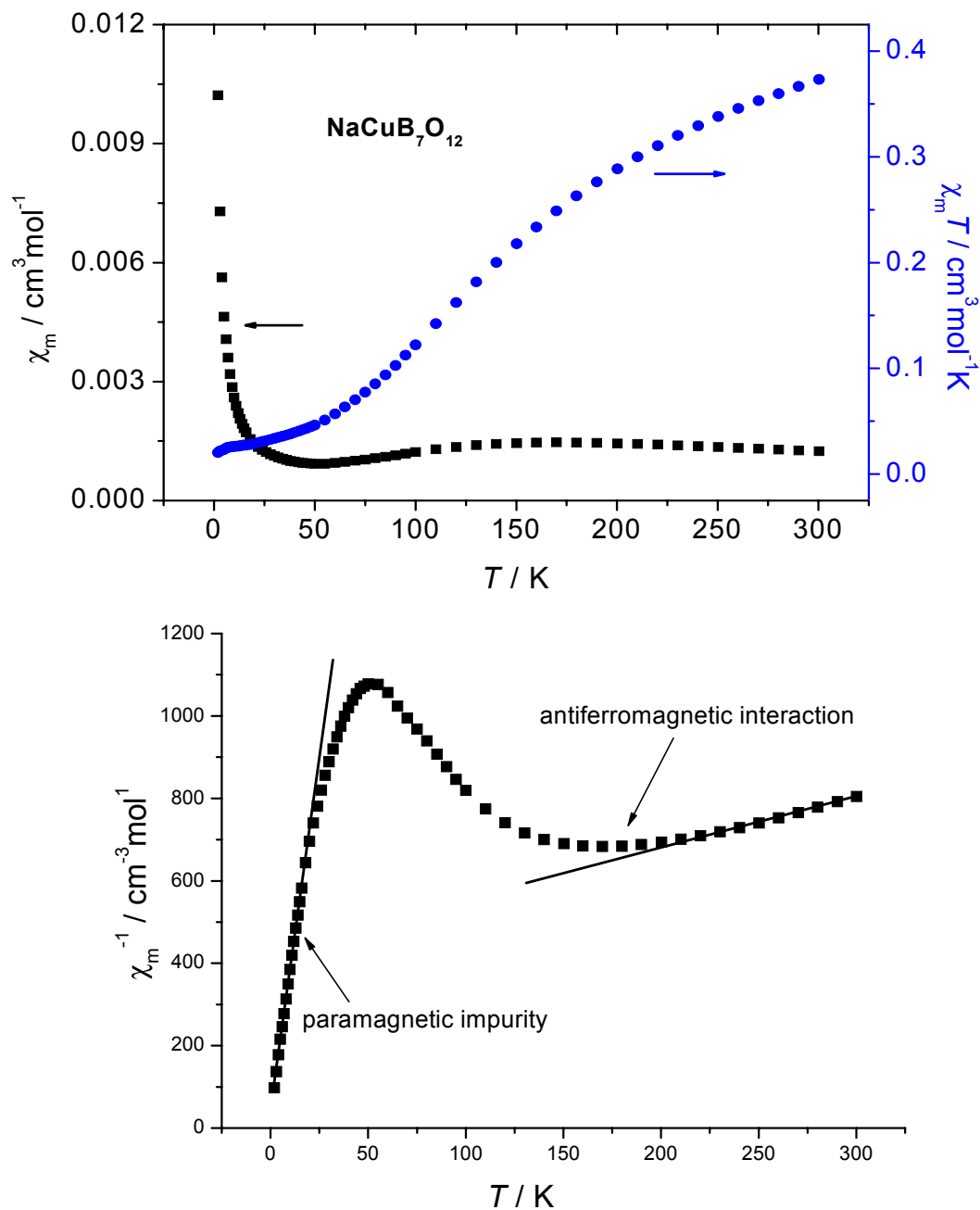


Figure S4. The temperature dependence of the magnetic susceptibility of  $\text{NaCuB}_7\text{O}_{12} \cdot n\text{H}_2\text{O}$  in an applied field of 5000 Oe. Because the existence of paramagnetic impurity, the data above 250K fit the Curie-Weiss law with the  $\theta = -323\text{K}$ .

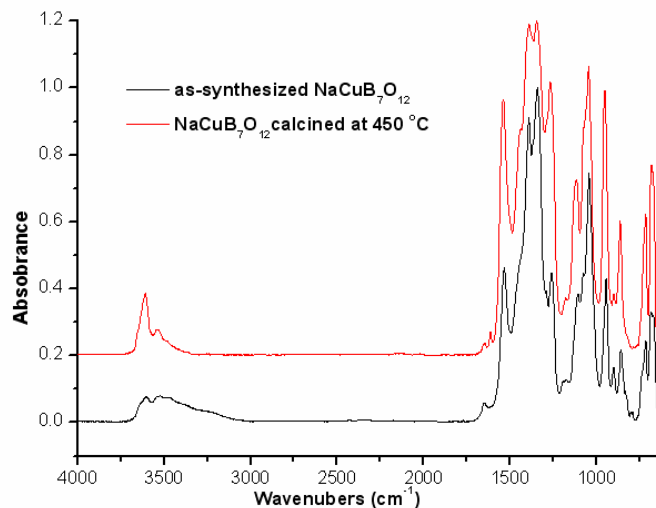


Figure S5. The IR spectra of the as-synthesized NaCuB<sub>7</sub>O<sub>12</sub>·nH<sub>2</sub>O ( in black ) and the NaCuB<sub>7</sub>O<sub>12</sub>·nH<sub>2</sub>O ( calcined at 450 °C, in red ). It shows that the framework remains intact after heating and an obvious dehydrate-rehydrate behavior of water. The heated powder can rehydrate just the time we test its IR spectrum. The peaks between 1000 cm<sup>-1</sup> to 1200 cm<sup>-1</sup> correspond to the BO<sub>4</sub> group of the structure and that between 1200 cm<sup>-1</sup> to 1400 cm<sup>-1</sup> correspond to the BO<sub>3</sub> group. The existence of water can be distinguished by the peaks about 3600 cm<sup>-1</sup>.

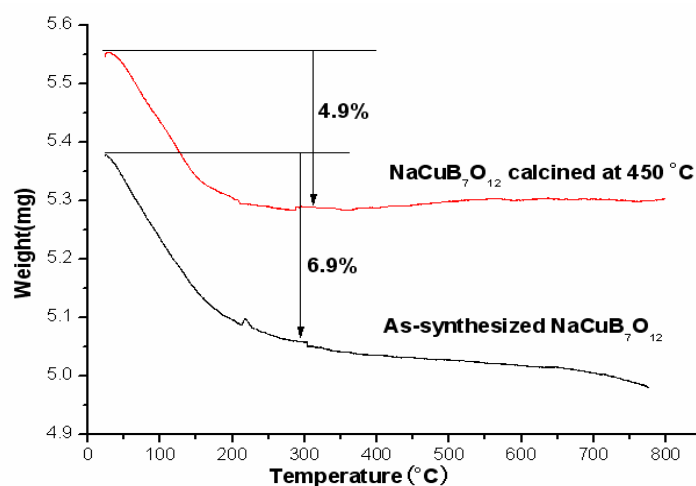


Figure S6. The TGA analysis of the as-synthesized  $\text{NaCuB}_7\text{O}_{12} \cdot n\text{H}_2\text{O}$  ( in black) and the  $\text{NaCuB}_7\text{O}_{12} \cdot n\text{H}_2\text{O}$  which are calcined at  $450^\circ\text{C}$  and then exposed itself to air for several hours ( in red ), gives another evidence that it has a dehydrate-rehydrate behavior of water.

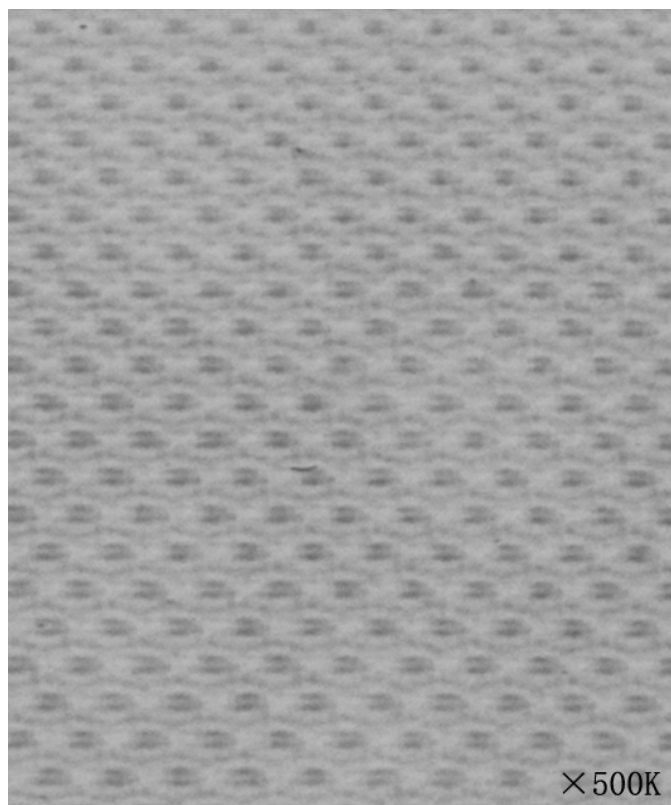


Figure S7. The HRTEM image of  $\text{NaCuB}_7\text{O}_{12} \cdot n\text{H}_2\text{O}$  in the 010 zone carried on an H-9000 transmission electron microscope.