Supporting Information

High-Temperature, High-Pressure Hydrothermal Synthesis, Crystal Structure, Thermal Stability, and Solid State NMR Spectroscopy of an Aluminum Borate, Ba[AlB4O8(OH)]

Chun-Chi Peng,^a Hsin-Kuan Liu,^a and Kwang-Hwa Lii*^{a,b}

^aDepartment of Chemistry, National Central University, Zhongli, Taiwan 320, R.O.C.

^bInstitute of Chemistry, Academia Sinica, Taipei, Taiwan 115, R.O.C.

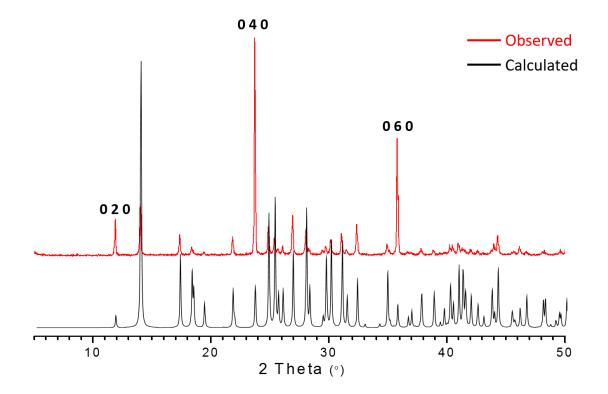


Figure S1. The observed and simulated X-ray powder patterns of $Ba[AlB_4O_8(OH)]$. The differences between the observed and calculated intensities are due to the effect of preferred orientation. Several 0*k*0 reflections are indicated.

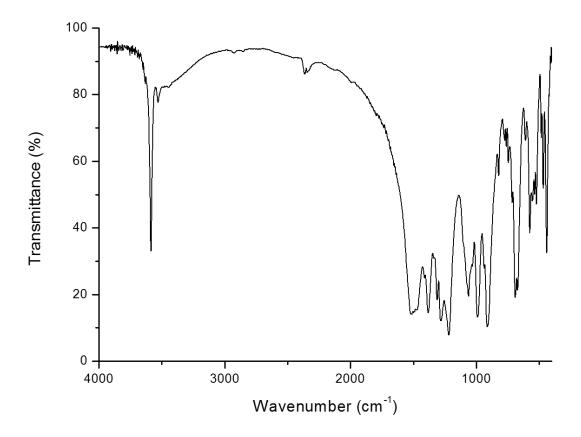


Figure S2. The infrared spectrum of Ba[AlB₄O₈(OH)] (KBr pellet method). The peak at 3580 cm⁻¹ is due to the O-H stretching vibration. The bands from 1508 to 1218 cm⁻¹ correspond to antisymmetric stretching vibrations of the BO₃ groups. The bands from 1062 to 950 cm⁻¹ correspond to antisymmetric stretching vibrations of BO₄ and AlO₄ groups. The bands from 800 to 500 cm⁻¹ are bending vibrations.

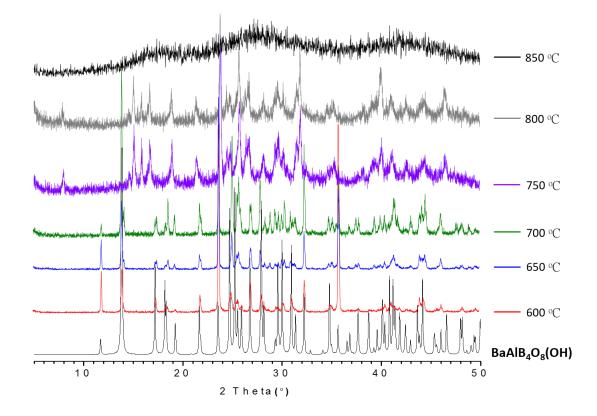


Figure S3. X-ray powder patterns of a sample of $Ba[AlB_4O_8(OH)]$ which were taken after being heated in a Pt crucible in air at 600, 650, 700, 750, 800, and 850 °C for 2 h and cooled to room temperature.

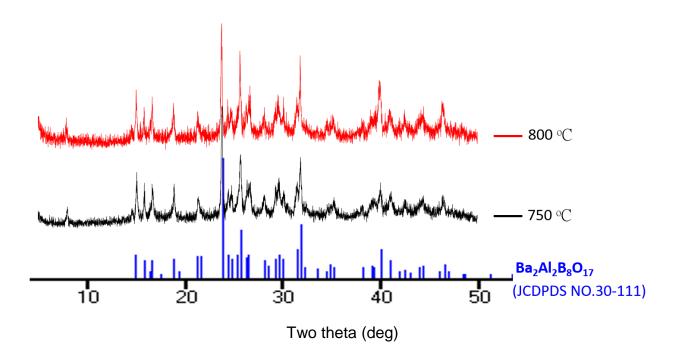


Figure S4. X-ray powder patterns of a sample of Ba[AlB₄O₈(OH)] which were heated at 750 and 800 $^{\circ}$ C are compared with that of Ba₂Al₂B₈O₁₇.