Supporting Information

Short-Range Structure of the Brownmillerite-Type Oxide Ba₂In₂O₅ and its Hydrated Proton-Conducting Form BaInO₃H

Johan Bielecki,^{1,2,*} Stewart F. Parker,³ Dharshani Ekanayake,¹ Seikh Mohammad Habibur Rahman,⁴ Lars Börjesson,¹ and Maths Karlsson^{1,†}

¹Department of Applied Physics, Chalmers University of Technology, SE-41296 Göteborg, Sweden ²Department of Cell and Molecular Biology, Uppsala University, Box 596, SE-75124 Uppsala, Sweden ³ISIS Facility, STFC Rutherford Appleton Laboratory, Chilton, Didcot, Oxon OX11 0QX UK ⁴Department of Chemical and Biological Engineering, Chalmers University of Technology, SE-41296 Göteborg, Sweden *johanb@xray.bmc.uu.se, †maths.karlsson@chalmers.se



Fig. S1. (a) TGA curve for the BaInO₃H sample under a flow of N₂(g), as measured with an F1 Iris spectrometer from Netzsch, with a heating rate of 10 °C/min. The mass loss when heating from 30 to 900 °C corresponds to a hydration degree of approximately 110%. The fact that the mass loss corresponds to a hydration level slightly higher than 100% may be related to the presence of a small amount of adsorbed surface water. (b) Room temperature X-ray powder diffraction patterns for the Ba₂In₂O₅ and BaInO₃H samples, measured with a Bruker AXS D8 ADVANCE VARIO powder diffractometer (CuK $\alpha_1 = 1.5406$ Å). The diffraction data of Ba₂In₂O₅ indicates an orthorhombic crystal structure and that of BaInO₃H a tetragonal structure, in agreement with the literature.^{1,2} No peaks related to impurities were detected. Tick marks indicate the position of the Bragg peaks predicted by structural models based on *Ibm2* symmetry for Ba₂In₂O₅ and on *P4/mmm* symmetry for BaInO₃H.

¹ W. Fisher, G. Reck, T. Schober, *Solid State Ion.* **116** (1999) 211–215.

² S. A. Speakman, J. W. Richardson, B. J. Mitchell, S. T. Misture, Solid State Ion. 149 (2002) 247–259.