

W0096

Novel Mineral Structure of $\text{LiNaSiB}_3\text{O}_7(\text{OH})$ from Lab Powder Diffraction Data and *Ab-Initio* Quantum Optimization. P.S. Whitfield¹, Y. Le Page¹, J.D. Grice², C.J. Stanley³, G.C. Jones³, M.S. Rumsey³, C. Blake⁴, A.C. Roberts⁵, J.A.R. Stirling⁵ & G.J.C. Carpenter⁶, IICPET, National Research Council, 1200 Montreal Rd, Ottawa, Canada, ²Canadian Museum of Nature, PO Box 3443, Stn D, Ottawa, Canada, ³Dept. of Mineralogy, Natural History Museum, London, UK, ⁴Rio Tinto, Unit 34, Hither Green Industrial Estate, Clevedon, Somerset, UK, ⁵Geological Survey of Canada, 601 Booth St, Ottawa, Canada, ⁶Materials Technologies Laboratories, Natural Resources Canada, 568 Booth St, Ottawa, Canada.

Agglomerates of crystals smaller than $5\mu\text{m}$ of a new mineral (IMA 2006-36) with the title composition were discovered in a drill core from the Jadar Basin in Serbia. The crystals are too small for standard laboratory single crystal X-ray diffractometry, so structure solution from laboratory X-ray powder diffraction data was attempted.

The structure was solved by simulated annealing in TOPAS (Bruker-AXS) from capillary X-ray data indexed by singular value decomposition algorithm. A mixture of z-matrices and soft bond-length constraints were used in the structure solution step, but removed for final refinement except the O-H bond length. Obtaining neutron diffraction data of this material is problematic due to high boron content, so VASP *ab-initio* optimization in the *Materials Toolkit* framework was used to validate the structure and to better localize the H atom.

The unit cell is monoclinic ($P2_1/c$) with $a = 6.7620(1)\text{\AA}$, $b = 13.8016(3)\text{\AA}$, $c = 7.6878(2)\text{\AA}$, and $\beta = 124.0894(9)^\circ$. The structure contains a layer of corner-sharing, tetrahedrally coordinated Li, Si and B, decorated with triangular BO_3 groups. The H forms a weak intra-layer hydrogen bond, whilst the Na is situated between the layers in a distorted octahedral site. The structure appears to be unique and has no known direct structural analogues.