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Combined single-crystal X-ray and neutron powder diffraction structure analysis exemplified through full structure determinations of framework and layer beryllate minerals

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Abstract

Structural analysis, using neutron powder diffraction (NPD) data on small quantities (<300 mg) and in combination with single-crystal X-ray diffraction (SXD) data, has been employed to determine accurately the position of hydrogen and other light atoms in three rare beryllate minerals, namely bavenite, leifite/IMA 2007-017, and nabesite. For bavenite, leifite/IMA 2007-017, and nabesite, significant differences in the distribution of H, as compared to the literature using SXD analysis alone, have been found. The benefits of NPD data, even with small quantities of H-containing materials, and, more generally, in applying a combined SXD-NPD method to structure analysis of minerals are discussed, with reference to the quality of the crystallographic information obtained.

Keywords: Hydrogen, beryllium, minerals, powder neutron diffraction