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The atomic arrangement and electronic interactions in vonsenite at 295, 100, and 90 K

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Abstract

Vonsenite, $Fe_2^{2+}Fe^{3+}O_2BO_3$, has been the subject of many studies in the materials science and condensed matter physics communities due to interest in the electronic and magnetic properties and ordering behavior of the phase. One such study, undertaken on synthetic material of end-member composition, reports X-ray diffraction structure refinements that indicate a phase transition from *Pbam* to *Pbnm* at or just below ~283 K, determined subsequently to arise from a Peierls-like instability. To compare the stability of the natural phase with that of synthetic material, we performed high-precision X-ray crystal-structure analyses at 295, 100, and 90 K (R_1 = 0.0119, 0.0186, and 0.0183, respectively), Mössbauer spectroscopy at 295, 220, 150, 80, and 4.2 K, and wavelength-dispersive electron microprobe analysis on a vonsenite of near-end-member composition from Jayville, New York, U.S.A. The *Pbnm* structure is observed at 100 and 90 K, suggesting similar phase stability for the natural and synthetic phases. Comparison of Mössbauer data and X-ray site occupancies between the natural and synthetic phases suggests a reinterpretation of Mössbauer site assignments. We conclude that the Peierls-like instability underlying the reported transition from *Pbam* to *Pbnm* in synthetic material also occurs in our specimen of natural near-end-member vonsenite at temperatures between 295 and 100 K.

Keywords: Vonsenite, phase transition, low-temperature structure refinements, Peierls-like instability