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*P*4/*n* and *P*4*nc* long-range ordering in low-temperature vesuvianites

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ABSTRACT

Low-temperature vesuvianites crystallize in the two space groups *P*4/*n* or *P*4*nc* due to different arrangements of Ca-dodecahedra and $M^{2+,3+}$ square pyramids that form strings along the fourfold axes. Long-range ordered vesuvianites of acentric *P*4*nc* symmetry may have the same diffraction symmetry as centrosymmetric disordered *P*4/*nnc* vesuvianites. In contrast, *P*4/*n* long-range ordered vesuvianites exhibit glide plane violating reflections and can easily be identified. We report the first successful X-ray single-crystal structure refinement of a *P*4*nc* vesuvianite, $a = 15.487(2)$, $c = 11.764(2)$ Å from the N'chwaning II mine of the Kalahari manganese fields (RSA). This untwinned crystal has Cu^{2+} and Mn^{2+}, Mn^{3+} forming the square pyramid and exhibits an acentric ordering pattern with 85% string A and 15% string B. This is compared to a reinvestigation of the structure of a *P*4/*n* vesuvianite from Asbestos Quebec (Canada), $a = 15.531(2)$, $c = 11.817(2)$ Å. The crystal is composed of a merohedral (110) twin with a close to 1:1 twin ratio and has mainly Fe^{3+} in square pyramidal coordination. In this centric structure, string A is 84% and string B is 16% occupied. Criteria to determine the symmetry of low-temperature vesuvianites, studied by diffraction experiments, are discussed.