

Poster Presentation

MM.P02

Symmetry Relations Between Space Groups in Layered Germanate Structures: Modeling Crystal Structures

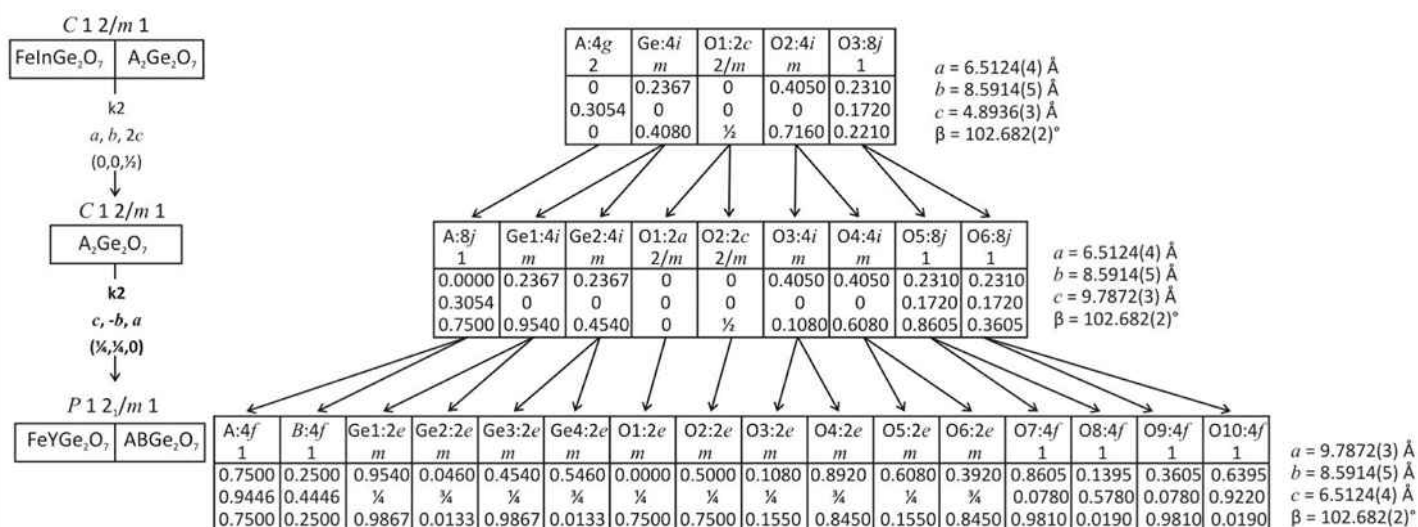
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Structural models for the new layered germanates ScInGe₂O₇ and ScFeGe₂O₇ were analyzed within the framework of symmetry relations between space groups. These compounds were supposed to be hettotypes of the thortveitite mineral, (Sc,Y)2Si₂O₇, which was considered as the aristotype. Thortveitite crystallizes in the monoclinic system, and the symmetry is described by the space group type C2/m. Other monoclinic hettotypes for the thortveitite are FeInGe₂O₇ (PDF 01-070-8447, ICSD - 94487), space group C2/m (No. 12); TbInGe₂O₇ (PDF 01-072-6515, ICSD - 96360), space group C2/c (No. 15); and FeYGe₂O₇ (PDF 01-072-6099, ICSD - 95935), space group P21/m (No. 11). All these space groups are related by symmetry. By the use of these relations, we proposed starting models for the crystal structures of ScInGe₂O₇ and ScFeGe₂O₇. For ScInGe₂O₇ this was found to be isostructural to FeInGe₂O₇ reported by our laboratory [1]. The structural data for this compound were obtained by conventional Rietveld refinement of the powder diffraction data of X-rays, using the GSAS program and EXPGUI [2, 3] interface. For ScFeGe₂O₇ the symmetry related structural model was found in the triclinic system by symmetry reduction from the space group C2/m (unique axis b) to the triclinic space group P1 (figure 1). Rietveld refinement was performed reaching to the following results: lattice parameters a = 5.3434 (8), b = 5.3145 (8), c = 4.8732 (7) Å, α = 99 468 (2), β = 97 257 (2), γ = 104 609 (2)°, V = 130.03 (5) Å³, Z = 1; WRp = 0.047, Rp = 0.04 and reduced χ² of 2.176 for 64 variables. This study was sponsored by CONACYT project CB-2011/167624.

[1] L. Bucio, J.L. Ruvalcaba-Sil, I. Rosales, J. García-Robledo y E. Orozco. *The Crystal Structure of FeInGe₂O₇*. *Zeit. Krist.* 216 (2001) 438-441., [2] A.C. Larson and R.B. Von Dreele. *General Structure Analysis System (GSAS)*. Los Alamos National Laboratory Report LAUR 86-748 (2000)., [3] B. H. Toby. *EXPGUI, a graphical user interface for GSAS*. *J. Appl. Cryst.* 34 (2001) 210-213.

Figure 1



Keywords: Symmetry relations, layered structures, models for Rietveld refinement