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$In_{1.06}Ho_{0.94}Ge_2O_7$: a thortveitite-type compound

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A new indium holmium digermanate, $In_{1.06}Ho_{0.94}Ge_2O_7$, with a thortveitite-type structure, has been prepared as a polycrystalline powder material by high-temperature solid-state reaction. This new compound crystallizes in the monoclinic system (space group $C2/c$, No. 15). The structure was characterized by Rietveld refinement of powder laboratory X-ray diffraction data. The In^{3+} and Ho^{3+} cations occupy the same octahedral site, forming a hexagonal arrangement on the *ab* plane. In their turn, the hexagonal arrangements of $(In/Ho)O_6$ octahedral layers are held together by sheets of isolated diortho groups comprised of double tetrahedra sharing a common vertex. In this compound, the Ge_2O_7 diortho groups lose the ideal D_{3d} point symmetry and also the C_{2h} point symmetry present in the thortveitite diortho groups. The Ge—O—Ge angle bridging the diortho groups is 160.2 (3)°, compared with 180.0° for Si—O—Si in thortveitite ($Sc_2Si_2O_7$). The characteristic mirror plane in the thortveitite space group ($C2/m$, No. 12) is not present in this new thortveitite-type compound and the diortho groups lose the C_{2h} point symmetry, reducing to C_2.

Comment

Previous work on a series of isomorphous germanates $MRGe_2O_7$ (where M is In, Mn, Fe, Y, Sc, Ga or Al, and R is a rare earth) has included compounds such as $FeInGe_2O_7$ (Bucio *et al.*, 2001) and $InYGe_2O_7$ (Juarez-Arellano, Bucio *et al.*, 2002), described by the space group $C2/m$ (No. 12) and adopting the thortveitite structure, $FeRGe_2O_7$ (where R is La, Pr, Nd or Gd; Bucio *et al.*, 1996) and $NdAlGe_2O_7$ (Jarchow *et al.*, 1985), taking space group $P2_1/c$ (No. 14), and $FeRGe_2O_7$ (R is Y or Tb–Yb; Cascales *et al.*, 1998), $GdMnGe_2O_7$ and $EuMnGe_2O_7$ (Taviot-Gueho *et al.*, 1999; Juarez-Arellano *et al.*, 2001), with space group $A222$ (No. 21). Interesting optical, electrical and magnetic properties have been reported in these kinds of compounds.

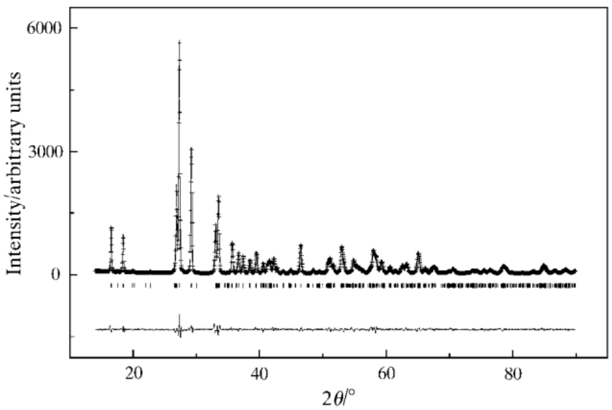

Figure 1
The observed (crosses), calculated (solid line) and difference (at the bottom) X-ray powder diffraction profile for $In_{1.06}Ho_{0.94}Ge_2O_7$ at room temperature. Vertical marks correspond to the position of the allowed Bragg reflections.

In recent years, compounds with rare earth cations (especially Gd^{3+}, Tb^{3+}, Eu^{3+} and Ho^{3+}) have been developed and employed as scintillators for radiation detectors used in medical diagnostics, industrial inspection, dosimetry, nuclear medicine and high-energy physics. In each application, the scintillator is the primary radiation sensor that emits light or scintillates when it is struck by high-energy photons (Greskovich & Duclos, 1997). Polycrystalline ceramic scintillators are a relatively new class of materials developed for quantitative detection accuracy. Ceramic scintillators have been attracting increasing attention because their complex compositions, which cannot be grown by single-crystal methods, can be synthesized by relatively inexpensive ceramic processes.

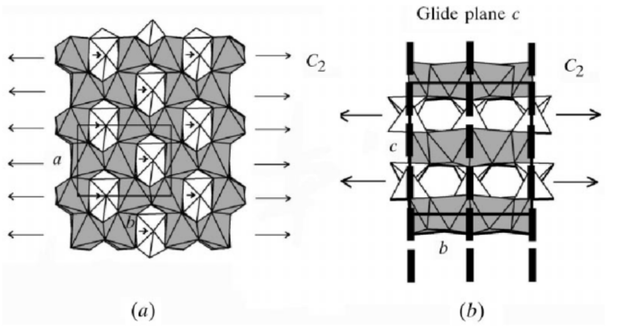

Figure 2
A projection of $In_{1.06}Ho_{0.94}Ge_2O_7$ on the *ab* plane, showing the honeycomb-like arrangement of $(In/Ho)O_6$ octahedra (in dark grey). (*a*) The Ge_2O_7 diortho groups (light grey) link at three points to the hexagonal rings of octahedra. The displacement of bridging O atoms to the right-hand side (black arrows) is clearly seen, changing the C_{2h} symmetry of the Ge_2O_7 diortho groups to C_2. (*b*) $(In/Ho)O_6$ octahedral layers (dark grey) are held together alternately along the *c* axis by sheets of isolated Ge_2O_7 diortho groups (in light grey).

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