

CRYSTAL AND MAGNETIC SPIN STRUCTURE OF GERMANIUM- HEDENBERGITE, $\text{CaFeGe}_2\text{O}_6$

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Structure-property relations in pyroxenes have been studied for many decades. The interest was then mainly triggered by the important role of pyroxenes as rock forming minerals in the lower crust and upper mantle, especially with respect of phase transitions at non ambient conditions. In the last years it was established that the transition metal bearing pyroxenes also have a rich magneto-chemistry (e.g. REDHAMMER et al. 2011, 2012). As part of our ongoing studies on magnetic properties of minerals / pyroxenes we here present results of the magnetic and nuclear structure of $\text{CaFeGe}_2\text{O}_6$, the germanium-analogue to the mineral Hedenbergite.

The title compound has been synthesized at 1273 K in evacuated SiO_2 -glass - tubes. Powder neutron diffraction data collected between 4 K and 300 K were used to evaluate the magnetic spin as well as the nuclear crystal structure and its T - evolution. $\text{CaFeGe}_2\text{O}_6$ is monoclinic, $C2/c$, $a = 10.1778(5)$ Å, $b = 9.0545(4)$ Å, $c = 5.4319(3)$ Å, $\beta = 104.263(3)^\circ$, $Z = 4$ at room temperature. No change of symmetry was observed down to 4 K. Below 43 K, additional magnetic Bragg reflections appear, which can be indexed on the basis of a commensurate magnetic propagation vector k [1,0,0]. The successful description of the magnetic spin structure reveals a ferromagnetic spin coupling within the Fe^{2+}O_6 M1 chains, while the coupling between the chains is antiferromagnetic. Spins are oriented collinearly within the a - c plane and form an angle of $\sim 60^\circ$ with the crystallographic a -axis. The magnetic moment at 4 K amounts to about 4.4 μB . The observed magnetic structure is similar to that of other Ca-clinopyroxenes. The present data is put into context with the structural and magnetic properties of other pyroxenes – among them magnetoelectric and multiferroic pyroxene-type compounds.

REDHAMMER, G.J., SENYSHYN, A., MEVEN, M., ROTH, G., PRINZ, S., PACHLER, A., TIPPELT, G., PIETZONKA, C., TREUTMANN, W., HOELZEL, M., PEDERSEN, B., AMTHAUER, G. (2011): Phys. Chem. Minerals, 38, 139-157.

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