

Magnetic and low-temperature structural behavior of clinopyroxene-type FeGeO₃: A neutron diffraction, magnetic susceptibility, and ⁵⁷Fe Mössbauer study

**GÜNTHER J. REDHAMMER,^{1,*} ANATOLY SENYSHYN,^{2,3} GEROLD TIPPELT,¹ CLEMENS PIETZONKA,⁴
WERNER TREUTMANN,⁵ GEORG ROTH,⁶ AND GEORG AMTHAUER¹**

¹Abteilung für Mineralogie, Fachbereich Materialforschung and Physik, Universität Salzburg, Hellbrunnerstrasse 34, A-5020 Salzburg, Austria

²Forschungsneutronenquelle Heinz Maier-Leibnitz (FRM II), Lichtenbergstrasse 1, D-85747 Garching, Germany

³Fachgebiet Strukturforschung, Materialwissenschaft, Technische Universität Darmstadt, Petersenstrasse 23, D-64278 Darmstadt, Germany

⁴Fachbereich für Chemie, Philipps-University Marburg, Hans Meerweinstrasse, D-35032 Marburg/Lahn, Germany

⁵Institut für Mineralogie, Philipps-University Marburg, Hans Meerweinstrasse, D-35032 Marburg/Lahn, Germany

⁶Institut für Kristallographie, RWTH Aachen, Jägerstrasse 17/19, D-52056 Aachen, Germany

ABSTRACT

The clinopyroxene-type compound FeGeO₃ was synthesized using ceramic sintering techniques at 1273 K in evacuated silica tubes and investigated by powder neutron diffraction between 4 and 300 K, X-ray diffraction, SQUID magnetometry, and ⁵⁷Fe Mössbauer spectroscopy. The title compound shows space group *C2/c* symmetry (high pressure, HP-topology) between 4 and 900 K. No structural phase transition is present within this temperature interval, whereas lattice parameters show discontinuities around 50 and 15 K, which are due to magnetic phase transitions and the associated magneto-elastic coupling of the lattice. The magnetic susceptibility data show two maxima in their temperature dependence, one at ~47 K, the second around 12 K (depending on the external field), indicative of two magnetic transitions in the title compound. Neutron data shows that for $T < 45$ K, FeGeO₃ orders magnetically, having a simple collinear structure, with space group *C2/c*, and with the spins aligned parallel to the crystallographic *b*-axis, both on M1 and M2. The coupling within the M1/M2 band is ferromagnetic, whereas between them it is antiferromagnetic. As the bulk magnetic measurements in the paramagnetic state revealed a dominating ferromagnetic coupling, the intra-chain interactions dominate the inter-chain interaction. At 12 K, additional magnetic reflections appear, revealing a second magnetic phase transition. Spins are rotated away from the *b*-axis toward the *a-c* plane. The coupling within the M1 chain is still ferromagnetic and antiferromagnetic between the M1 chains. However, spins on M1 and M2, are no longer collinear. The moment on the M2 site is rotated further away from the *b*-axis than on M1.

Keywords: FeGeO₃, clinopyroxene, magnetic phase transition, spin structure, low-temperature neutron diffraction, SQUID magnetometry, ⁵⁷Fe Mössbauer spectroscopy