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MÖSSBAUER STUDIES FOR FeV_2Se_4

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Here we present magnetic susceptibility, XRD and Mössbauer spectroscopy studies of FeV_2Se_4. The inverse susceptibility of FeV_2Se_4 changes its slope at 74 K, which is due to a phase transition in the system. The effective Bohr magneton value is obtained to be 0.138 μ_B. Crystallographic structure, cation distribution, anion positions are determined by the Rietveld refinement of the Fullprof program. The crystal symmetry is found to be a monoclinic space group of *I2/m* [Fe (2a); Cr (4i); S (4i(u,0,w)] with its lattice constants, a_0=6.152Å, b_0=3.458Å, c_0=11.726 Å, and β=91.30 °, respectively. The cation distribution from the x-ray diffraction refinements result show that V^{3+} exists on the A and B sites as $[Fe_{0.95}^{2+}V_{0.05}^{3+}]_A[Fe_{0.05}^{2+}V_{1.95}^{3+}]_BSe_4$.

The Mössbauer spectra severely distorted the asymmetric 8-line shape below 85 K, denoting a large orbital contribution. It agrees with the result of the temperature dependent susceptibility measurements. While, it shows a quadrupole doublet above 85 K, of which value decreases with increase of the temperature. It is noticeable that, in the temperature region 85 K $\leq$ T $\leq$ 300 K, the ratio of the intensity of the two lines $R_q=A_1/A_2$ increases rapidly from 1 to 1.30, where A_1, A_2 correspond to the Mössbauer absorption area of the quadrupole splitting for the lower and higher energies, respectively. It is attributed to Goldanskii-Karyagin effect. We interpret it, that it is closely related to the anisotropic atomic vibration for an iron atom in FeV_2Se_4. Also, it accords with the result of the XRD refinement, slightly distorted local environment of the Se ions along the c-axis.

Table I: Results of refinement parameters of X-ray diffraction on FeV_2Se_4 [I2/m: A site (2a); B site (4i); S (4i (*u*,0,w))].

Lattice constants	
a_0 (Å)	6.152
b_0 (Å)	3.458
c_0 (Å)	11.726
β (°)	91.30
$[Fe_{0.95}^{2+}V_{0.05}^{3+}]_A[Fe_{0.05}^{2+}V_{1.95}^{3+}]_BSe_4$	

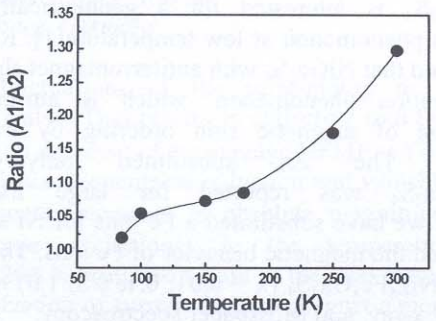

Figure 1. Temperature dependence on the ratio of intensity of the two line $R_q=A_1/A_2$, where A_1, A_2 correspond to Mössbauer absorption area.