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Crystallographic and magnetic properties of FeGa$_2$S$_4$

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The synthesis of the FeGa$_2$S$_4$ was accomplished by the direct reaction of the high-purity elements Fe, Ga, S, in an evacuated 10$^{-6}$ torr quartz tube. The crystal structure of FeGa$_2$S$_4$ has a trigonal (space group P3(-)m1), with the lattice constants $a = 3.669$ Å, $c = 12.096$ Å, respectively. The cation and anion parameters are determined to be Fe(0,0,1/2), Ga(1/3,2/3,0.208), S$_1$ (1/3,2/3,0.863), S$_2$(1/3,2/3,0.390) by the Rietveld refinement. The sample is semiconductor and the magnetic behavior shows an antiferromagnetic character.

The Mössbauer spectra were obtained at various temperatures from 4.5 to 600 K. The Mössbauer spectra show severely distorted 8-line shape, which denotes a large electric quadrupole contribution at low temperature. Magnetic hyperfine field and electric quadrupole interactions at 4.5 K have been fitted, yielding the following results: $H_{hf} = 113.9$ kOe, $\Delta E_0 = 1/2e^2qQ(1+1/3\eta^2)^{1/2} = 1.28$ mm/s, $\theta = 45^\circ$, $\varphi = 0^\circ$, $\eta = 0.5$, and $R = 1.60$, where $\theta$ and $\varphi$ are the polar and azimuthal angles, respectively. $\eta$ is the asymmetric parameter and $R$ is the ratio of electric quadrupole interaction to magnetic dipole interaction. In the temperature region 295 K $\leq T \leq$ 600 K, the ratio of intensity of two line $R_q = A_1/A_2$ increases rapidly from 1.0 to 2.7, where $A_1$, $A_2$ correspond to Mössbauer absorption area of the quadrupole splitting for lower and higher energies, respectively. We conclude that it occurs from Goldanskii-Karyagin effect for an iron atom in FeGa$_2$S$_4$. 

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