

Spin-Rotation Transition of $\text{Fe}_7\text{Se}_7\text{S}$

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(Received 30 June 1999)

$\text{Fe}_7\text{Se}_7\text{S}$ has been studied by Mössbauer spectroscopy, X-ray diffraction, and magnetic-moment measurement. The crystal is found to have the "3c" hexagonal superstructure of the NiAs structure with lattice constants $A = 7.220 \pm 0.005 \text{ \AA}$ and $C = 17.668 \pm 0.005 \text{ \AA}$. The quadrupole shifts change substantially over the temperature range from 120 to 130 K, suggesting that a spin-rotation transition takes place. The iron ions at all three sites are found to be in highly covalent ferrous states. The Néel temperature and the Debye temperature are found to be $450 \pm 1 \text{ K}$ and $256 \pm 5 \text{ K}$, respectively. It is found that a 12.5 % substitution of S for Se in the Fe_7Se_8 crystal results in a 9 % increase in the magnetic hyperfine fields and a 1 % increase in the Néel temperature.