Journal of the Korean Physical Society, Vol. 35, No. 6, December 1999, pp. 492~495

Spin-Rotation Transition of Fe₇Se₇S

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(Received 30 June 1999)

Fe₇Se₇S 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 $A = 7.220 \pm 0.005$ Å and $C = 17.668 \pm 0.005$ Å. 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 ± 1 K and 256 ± 5 K, respectively. It is found that a 12.5 % substitution of S for Se in the Fe₇Se₈ crystal results in a 9 % increase in the magnetic hyperfine fields and a 1 % increase in the Néel temperature.