

Abstract Submitted
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Disorder in NiGa₂S₄ seen with Raman and infrared spectroscopy¹ M. E. VALENTINE, Johns Hopkins University, T. HIGO, S. NAKATSUJI, University of Tokyo, D. CHAUDHURI, N. P. ARMITAGE, N. DRICHKO, Johns Hopkins University — The crystal structure of NiGa₂S₄ contains a two dimensional triangular lattice of Ni²⁺ (S = 1) ions where ferromagnetic nearest neighbor interactions and antiferromagnetic third nearest neighbor interactions lead to magnetic frustration which suppresses magnetic ordering down to at least 1.5K. We studied disorder and structural distortions in NiGa₂S₄ by Raman and IR spectroscopy on single crystals in the energy range of 10 to 600 cm⁻¹ which covers the full range of Γ -point optical modes and compared our results to DFT calculations for vibrational modes. In the Raman spectrum for temperatures below 300K, additional modes are observed between 250 and 450 cm⁻¹. These features have energies that coincide with IR vibrational modes which are Raman-forbidden based on the point group symmetry, suggesting a local loss of inversion symmetry. Also, we observe an increased line width of the phonons involving significant motion of the S atoms adjacent to Ni and responsible for superexchange interactions within the magnetic lattice. This suggests disorder of these atoms which may be the cause of the suppressed magnetic order and spin freezing observed.

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