Temperature-Driven Phonon Anomalies in Quasi-2D $AgCrP_2S_6$ Probed by Raman Spectroscopy

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Abstract

$AgCrP_2S_6$ serves as a rich platform for exploring quasiparticle dynamics and a series of temperature-driven phase transitions involving polar, lattice, and spin degrees of freedom [1]. Using detailed temperature- and polarization-dependent Raman scattering on single crystals, supported by first-principles phonon calculations, we uncover multiple transitions associated with short- and long-range spin ordering within the 1D Cr-chain sublattice at ~90 K and ~20 K [2]. These transitions are marked by clear anomalies in phonon self-energy parameters and intensities. Contrary to expectations for heavy Ag ions, we find evidence for a quasi-antipolar ordering near ~200 K, followed by antipolar ordering around ~140 K (Fig.1). These features are reflected in strong phonon renormalization that persists across all temperatures. Moreover, a large number of additional phonon modes emerge between ~200-140 K as the antipolar order develops. The nearly doubled number of modes below ~200 K indicates a lowering of lattice symmetry from the high-temperature C_2h phase to a low-temperature C_2 or C_s structure [3].

References

[1] C. Payen, P. Molinié, P. Colombet, and G. Fillion, *J. Magn. Magn. Mater.*, vol. 84, (1990) pp. 95–101.
[2] C. B. Auti, A. G. Chakkar, S. Semwal, S. Selter, Y. Shemerliuk, B. Büchner, S. Aswartham, K. Pal, P. Kumar, *Journal of Materials Chemistry C* (2026).
[3] R. Loudon, The Raman effect in crystals, Adv. Phys. **13**, 423 (1964).

Figures

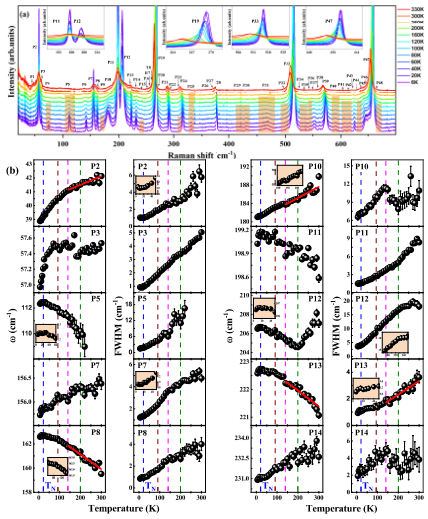

Figure 1: (a) Temperature evolution of the Raman spectrum. (b) Temperature evolution of the mode frequency and FWHM of phonon modes, brown, pink, and green dash line indicates anomalies ~90K, 140K, and 200K. Blue dash line indicates antiferromagnetic transition ~20K.