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Understanding Local Structure and Magnetically-Driven Phase Transitions in LiMO_2 ($M=\text{V}, \text{Co}$) J. CAO, J.T. HARALDSEN, K. GIESFELDT, J.L. MUSFELDT, University of Tennessee, W. TIAN, D. MANDRUS, T. BARNES, University of Tennessee and Oak Ridge National Laboratory — We report the variable temperature optical properties of high-quality, nearly stoichiometric LiVO_2 through the magnetic phase transition to probe the role of the lattice in this process. In contrast to the symmetry-consistent spectra of LiCoO_2 , LiVO_2 shows extra vibrational structure in both low and high temperature phases. These extra peaks can not be accounted for within a traditional symmetry analysis, suggesting that the local structure and bulk structure are different. Leading phase transition mechanisms focus on trimer formation at low temperature phase as well as orbital ordering processes. Considering the Jahn-Teller local distortions in LiVO_2 , a different picture of the magnetically-driven transition seems to emerge.

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