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Unusual ferroelectricity induced by the Jahn-Teller effect: A case study on lacunar spinel compounds KE XU, HONGJUN XIANG, Fudan Univ — The Jahn-Teller effect refers to the symmetry-lowering geometrical distortion in a crystal (or nonlinear molecule) due to the presence of a degenerate electronic state. Usually, the Jahn-Teller distortion is not polar. Recently, GaV_4S_8 with a lacunar spinel structure was found to undergo a Jahn-Teller distortion from a cubic to ferroelectric rhombohedral structure at $T_{\text{JT}} = 38$ K. Here, we carry out a general group theory analysis to show how and when the Jahn-Teller effect gives rise to ferroelectricity. On the basis of this theory, we find that the ferroelectric Jahn-Teller distortion in GaV_4S_8 is due to the noncentrosymmetric nature of the parent phase and a strong electron-phonon interaction related to two low-energy T_2 phonon modes. Interestingly, GaV_4S_8 is not only ferroelectric, but also ferromagnetic with a magnetic easy axis along the ferroelectric direction. This suggests that GaV_4S_8 is a multiferroic material in which an external electric field may control its magnetization direction. Our study not only explains the Jahn-Teller physics in GaV_4S_8 , but also paves a way for searching and designing different ferroelectrics and multiferroics.

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