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Ferroelectric to paraelectric transition in YCrO_3 revisited RAJEEV GUPTA, Department of Physics and Materials Science Programme, IIT Kanpur, Kanpur 208016, India, ASHISH MALL, Materials Science Programme, IIT Kanpur, Kanpur 208016, India, ASHISH GARG, Department of Materials Science and Engineering, IIT Kanpur, Kanpur 208016, India — X-ray diffraction (XRD) and Raman spectroscopy measurements are used to explore the origin of ferroelectricity in the orthorhombic ferroelectric oxide, YCrO_3 . Temperature dependent XRD studies carried out up to 900K and subsequent Reitveld refinement of the data shows that there is no evidence of any structural phase transition in YCrO_3 across the ferroelectric to paraelectric phase transition at $T_c = 470\text{K}$. Temperature dependent unpolarized Raman spectroscopy measurements, from 300 K to 600 K, were carried out to investigate structural changes near T_c locally within the material. All Raman modes below 600 cm^{-1} were assigned to phonon modes of Pnma structure and for further analysis of the Raman data, the line shape parameters were obtained by fitting a Lorentzian function to each peak. Surprisingly, despite absence of observation of any structural change in XRD measurements, YCrO_3 shows a strong anomalous temperature variation near T_c in the peak positions and line widths for selected modes as a function of temperature. It is believed that YCrO_3 is an improper ferroelectric and ferroelectricity arises due to local rotations of CrO_6 octahedra leading to non-centrosymmetry. Our results seem to suggest that YCrO_3 undergoes an iso-structural transition across T_c .

Rajeev Gupta
Department of Physics and Materials Science Programme, IIT Kanpur, Kanpur 208016, India

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