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Octahedral distortion induced Phonon Vibration and Electrical conduction in

 A_2NdSbO_6 (A = Ba, Sr, Ca)

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Keywords: Ceramics; double perovskite; phonons; grain boundaries; small polaron.

Abstract:

A meticulous comparison of crystal structures and vibrational degrees of freedom in the light

of A-site substitution for polycrystalline double perovskite oxides A₂NdSbO₆ (A= Ba, Sr, Ca)

has been carried out for accurate identification of crystal symmetry and distortions in these

materials. Raman spectra, correlated with group theoretical calculations, characterizes the

normal modes of vibrations associated with the oxygen octahedra and establishes a

rhombohedral structure for Ba₂NdSbO₆ and monoclinic structure for Sr₂NdSbO₆ and

Ca₂NdSbO₆ supporting the X-ray diffraction results. The symmetric stretching mode

occurring at the highest frequency is identified as the breathing vibration of the SbO₆

octahedra. The frequency and temperature responses of electrical properties studied by

impedance spectroscopy show the dominant effect of grain boundaries on the conduction

process. The conductivity spectroscopic plots reveal a semiconducting nature. A correlation

has been drawn between the vibrational and electrical measurements showing the interplay

between the phonon and electronic properties.

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