Ab-initio calculations of the elastic, piezoelectric and dielectric tensors of Diisopropylammonium bromide molecular ferroelectric Crystal

AHMAD ALSAAD, Department of Physics, Jordan Univ. of science and Technology, Irbid 22110, Jordan, NABIL AL-AQTASH, RENAT SABIRIANOV, Department of Physics, University of Nebraska at Omaha, 6001 Dodge Street Omaha, NE 68182 — The elastic, piezoelectric and dielectric properties of Diisopropylammonium bromide molecular ferroelectric crystal are investigated by first-principles methods. The Born effective charge tensor is reported to reveal the relation between Br-N bond hybridization and the ferroelectric structural distortion. As the crystal symmetry is reduced, the Born effective charges of Br and N atoms show a relatively large anisotropic trend demonstrated by the off diagonal nonzero components. The spontaneous polarization is found to be 22.7 $\mu$C/cm$^2$, which is very close to the reported experimental value. The dielectric tensor is found by applying an external electric field of 0.02 eV/Å. The values of the principle components of the electronic contribution to the dielectric tensor are found to be about 50% of the corresponding values of orthorhombic KNbO$_3$ ferroelectric crystal recently reported. The components of the piezoelectric tensor are calculated. The $e_{15} = 0.22$ C/m$^2$ component is smaller than $e_{35} = -0.203$ because they correspond to applying uniaxial strain in the direction perpendicular to the Br-N bond. Therefore, a large change in polarization is expected upon strain in Br-N bonds because ferroelectric behavior in $P2_1(\alpha)$ phase is determined primarily by the strongly hybridized bond between the Br and N atoms. We calculated the elastic tensor and explain its relation with the crystal symmetry. We found the ionic relaxation contributions to the total elastic tensor to be larger than the lattice contributions.

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