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

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— 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 μC/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/AA. 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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