Abstract Submitted
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Effect of Bromine Deficiency on the Lattice Dynamics and Dielectric Properties of Alpha-Phase Diisopropyl Ammonium Bromide Molecular Crystals .[1] AHMAD ALSAAD, Jordan Univ., of Science and technology, CHRIS MARIN, University of Nebraska-Lincoln, NABIL ALAQTASH, The Hashemite University, HSIEN-WEN CHAO, TSUN-HSU CHANG, National Tsing Hua University, CHIN LI CHEUNG, University of Nebraska-Lincoln, RENAT SABIRIANOV, University of Nebraska at — Diisopropyl ammonium bromide (DIPAB) molecular ferroelectric crystals exhibiting a large electric polarization (˜23μC/cm^2), a large dielectric constant and a low tangent loss of 0.00068-0.0008 in the α-phase. Although XRD shows overall excellent crystallinity, the analysis of vibrational spectra of α-DIPAB obtained by FT-IR and Raman spectrometry suggests the presence of disorder in synthesized crystals as indicated by the presence of broad features in Raman spectra. Using vdW + DF2 calculations, we identified majority of vibrational modes present in experimental spectra, specifically analyzing the ones due to Br-disorder. We find that the Br deficiency strongly affects the electric properties of α-DIPAB. Particularly, the experimentally measured dielectric constant is large (˜20), while DFT-based calculations of the ideal DIPAB give much smaller values (˜2-3). However, the Br-deficiency leads to a drastic increase of the calculated dielectric constant (˜15-20). Finally, using vdW+DF2 method we show that the van der Waals forces have only a slight effect on the structural parameters.

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