Crystallographic, vibrational modes and optical properties data of α-DIPAB crystal

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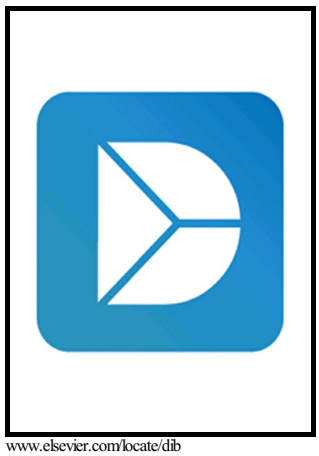

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Data Brief article

Title: ***Crystallographic, vibrational modes and optical properties data of α-DIPAB crystal***

Authors: Ahmad Alsaad,[1,a)] Chris M. Marin,[2] Nabil Alaqtash,[3] Hsien-Wen Chao,[4] Tsun-Hsu Chang,[4] Chin Li Cheung,[2,a)] A. Ahmad,[1] I.A. Qattan,[6] and Renat F. Sabirianov[5,a)]

Affiliations: [1]*Department of Physical Sciences, Jordan University of Science and Technology, P.O. Box 3030, Irbid 22110, Jordan*
[2]*Department of Chemistry, University of Nebraska-Lincoln, Lincoln, NE 68588, United States*
[3]*Department of Physics, The Hashemite University, P.O. Box 330127, Zarqa 13133, Jordan*
[4]*Department of Physics, National Tsing Hua University, Hsinchu 300, Taiwan*
[5]*Department of Physics, University of Nebraska at Omaha, Omaha, NE 68182, United States*
[6]*Department of Applied Mathematics and Sciences, Khalifa University of Science, Technology and Research, P.O. Box 127788, Abu Dhabi, UAE.*
Contact emails: alsaad11@just.edu.jo; rsabirianov@unomaha.edu; ccheung2@unl.edu

Abstract

The Crystallographic data of the α-DIPAB sample was measured using powder X-ray diffraction (PXRD). The crystal structure was also optimized using density functional based method. The calculations were performed both including van der Waals (vdW) interactions and excluding them to quantify the effects of vdW interaction on the crystal formation. The vibrational modes of DIPAB crystal corresponding to the Bromine deficient samples are calculated and presented. These show the origin of drastic change in dielectric response in Br deficient samples as compared to the ideal stoichiometric DIPAB crystal [Effect of bromine deficiency on the lattice dynamics and dielectric properties of alpha-phase diisopropylammonium bromide molecular crystals. [Ref. 4]]. Optical properties of an idealα-DIPAB were calculated using GGA and HSE06 hybrid functional methods implemented in VASP package. We mainly calculated the real and imaginary parts of the frequency-dependent linear dielectric function, as well as the related quantities such as the absorption, reflectivity, energy-loss function, and refractive index of α-DIPAB in the energy window of (0-12) eV.

Keywords

Powder X-Ray Diffraction; Density Functional Theory; van der Waals interactions; Vibrational modes; Bromine deficient samples; GGA approximation; HSE06 hybrid functionals

Specifications Table

Subject area	Physics, Chemistry
More specific subject area	Molecular Ferroelectric Crystals
Type of data	Table, (x-ray diffraction), graph, figure
How data was acquired	The crystallographic data of the α-DIPAB sample was measured using powder X-ray diffraction (PXRD).The crystal structure was also optimized using density functional based method. The calculations were performed both including van der Waals (vdW) interactions and excluding them to quantify the effects of vdW interaction on the crystal formation. The vibrational modes of DIPAB