

STRUSCTURAL, ELASTIK AND THERMODYNAMIC PROPERTIES
OF HEXAGONAL BiTeBr CRYSTAL

Mehmet Nurullah Secuk¹, Rana Eda Bicer², Harun Akkus³,
Bahattin Erdinc⁴, Murat Aycibin⁵, Emel Kilit Dogan⁶, Sinem
Erden Gulebaglan⁷

^{1,2,3,4,5,6} *Yuzuncu Yil University, Department of Physics, Faculty of
Science, Van, Turkey*

⁷*Department of Electric Program, Vocational School of Van, Yuzuncu Yil
University, Van, Turkey*

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Abstract

The geometric structural optimization, elastic properties and thermodynamic functions of total energy (E) Helmholtz free energy (F), constant volume heat capacity (Cv) and entropy (S) have been investigated by linearized augmented plane wave method using the density functional theory under the generalized gradient and local density approximations for hexagonal BiTeBr crystal in this study. Ground state properties of topographic ferroelectric BiTeBr structure were studied. Calculated lattice parameters, ground state properties and experimental results are consistent with literature. We could not find any experimental data to compare our calculated results for thermodynamic and elastic properties.

Keywords: Structural properties, thermodynamic properties, elastic properties

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¹nurullahsechuk@gmail.com

²redabicer@gmail.com

³physicsthakkus@gmail.com

⁴bahattinerdinc@yyu.edu.tr

⁵aycibin@gmail.com

⁶ekilit@yahoo.com

⁷sinemerden@gmail.com