



STATIC AND THERMO-ELASTIC PROPERTIES OF ALKALI CYANIDE CRYSTALS

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ABSTRACT

In the present paper authors have made an attempt to analyse the thermo-elastic properties of alkali cyanide crystals by estimating the values of their cohesive energy, Bulk-modulus and their pressure derivatives, Debye-temperature and Gruneisen parameter. A modified form of the three-body force shell model has been employed to calculate these values. The model used in the present study consists of long-range Coulomb and three-body interactions, short-range overlap repulsion of HZ-type, and van der Waals interactions. The van der Waals interaction coefficients are determined using the Kirkwood-Muller theory. Results obtained are compared with the available experimental data. A good agreement is found.
