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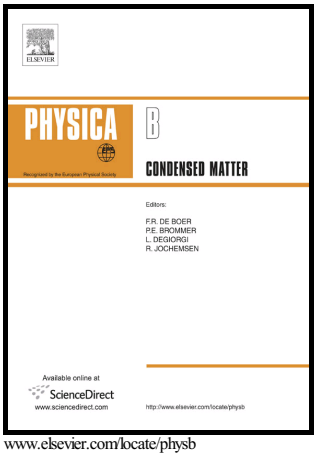

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A Novel Lattice Energy Calculation Technique for Simple Inorganic Crystals

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Abstract

In this pure theoretical study, a hitherto unexplored equation based on Shannon radii of the ions forming that crystal and chemical hardness of any crystal to calculate the lattice energies of simple inorganic ionic crystals has been presented. To prove the credibility of this equation, the results of the equation have been compared with experimental outcome obtained from Born-Fajans-Haber- cycle which is fundamentally enthalpy-based thermochemical cycle and prevalent theoretical approaches proposed for the calculation of lattice energies of ionic compounds. The results obtained and the comparisons made have demonstrated that the new equation is more useful compared to other theoretical approaches and allows to exceptionally accurate calculation of lattice energies of inorganic ionic crystals without doing any complex calculations.

Keywords: Lattice energy, Chemical Hardness, Shannon radii of ions, A new equation based on molecular hardness and Shannon radii of ions.

1. Introduction

The absolute hardness is an important quantity in terms of describing the reactivity and stabilities of chemical species [1,2]. Chemical principles such as Hard and Soft acid-base (HSAB) [3-6] principle and Maximum Hardness Principle (MHP) [7-9] based on chemical hardness concept are very useful in order to provide theoretical justification to many experimental results obtained. According to Maximum Hardness Principle, a chemical system tends to arrange itself so as to achieve maximum hardness and chemical hardness can be considered as a measurement of stability. In other words, soft molecules are in general more reactive than hard molecules. In recent times, we have a few sorts of new equations to