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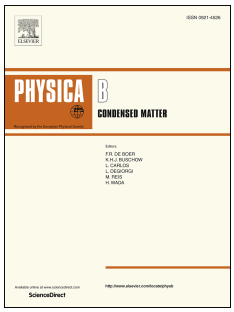

Relationships between lattice energies of inorganic ionic solids

Savaş Kaya

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Relationships between Lattice Energies of Inorganic Ionic Solids

Savaş KAYA*

Cumhuriyet University, Faculty of Science, Department of Chemistry, 58140, Sivas/TURKEY

Corresponding author e-mail address: **savaskaya@cumhuriyet.edu.tr**

Fax: 0346 219 10 10

Abstract: Lattice energy, which is a measure of the stabilities of inorganic ionic solids, is the energy required to decompose a solid into its constituent independent gaseous ions. In the present work, the relationships between lattice energies of many diatomic and triatomic inorganic ionic solids are revealed and a simple rule that can be used for the prediction of the lattice energies of inorganic ionic solids is introduced. According to this rule, the lattice energy of an AB molecule can be predicted with the help of the lattice energies of AX, BY and XY molecules in agreement with the experimental data. This rule is valid for not only diatomic molecules but also triatomic molecules. The lattice energy equations proposed in this rule provides compatible results with previously published lattice energy equations by Jenkins, Kaya, Born-Lande, Born-Mayer, Kapustinskii and Reddy. For a large set of tested molecules, calculated percent standard deviation values considering experimental data and the results of the equations proposed in this work are in general between %1 to 2%.

Keywords: Lattice energy, inorganic solids, a simplified rule

1.1. Introduction

Lattice energy is very useful concept in terms of the thermodynamic analysis of existence and stability of simple and complex inorganic ionic systems. Actually, it is not possible to determine the lattice energy as direct experimental because an inorganic ionic solid can be decomposed into gaseous atoms, not gaseous ions. Indirect experimental determination of the lattice energy is made via Born-Fajans-Haber thermochemical cycle. This thermochemical cycle is applied to inorganic ionic systems based on Hess's law. Hess's law states that formation enthalpy of inorganic ionic solids can be calculated taking into consideration the enthalpy changes of the accompanying individual steps.

Born-Lande [1], Born-Mayer [2] and Kapustinskii [3] equations are the ones proposed to predict the lattice energies (U) of inorganic ionic solids in the light of electrostatic approach. The disadvantage of Born-Lande and Born-Mayer equations included the use of Madelung constant is that these equations can be applied only to crystals of which lattice type is certain. Kapustinskii equation that can be also used for the simple ionic crystals of which lattice type is uncertain is given below.

$$U(kJ/mol) = \frac{Bz^{+}z^{-}n}{r^{+}+r^{-}}\left[1-\frac{0.345}{r^{+}+r^{-}}\right] \quad (1)$$

In this equation, z+, z− are cation, anion charges in electron unit. *Q* is softness parameter. In the Kapustinskii equation, *Q* = 0.345 Å is for the alkali metal NaCI-type structures, and *B*=