Binding Energy and Dissociation Energy of Alkali Halide and Alkali Hydride Molecules

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The interection potential model (IPM) by Rittner is- $U(r) = - z_1 z_2 \frac{e^2}{r} + \Psi_R(r)$ .....(1)

Considering the effect of the polarizability of the molecules, covalent effect and effect of Van der Walls dispersive force in the IPM is now be expressed as--

$$U(r) = -\frac{e^2}{r} - \frac{e^2(\alpha_1 + \alpha_2)}{2r^4} - \frac{c}{r^6} + \Psi_R(r) \text{.....(2)}$$

General form of repulsive interactions is $\Psi_R(r) = (S_i/r^m)\exp(-r^n / \rho_i)$ Where S_i, ρ_i, m, n are potential parameter. S_i is the repulsive strength parameter and ρ_i is the repulsive softness parameter.

Theoretical evaluation of molecular spectroscopic constants like binding energy and dissociation energy are calculated for 20 alkali halides and 5 alkali hydrides using the equation - 2

ABSTRACT

Theoretical evaluation of molecular spectroscopic constants is of considerable importance for the understanding of the nature of chemical bonding in the molecules. Binding energy and dissociation energy are calculated for 20 alkali halides and 5 alkali hydrides using the modified Rittner model or T-Rittner model. Polarizability of the molecules and effect of Van der Walls dispersive force are considered in this interaction potential

model (IPM). Four form of repulsive interactions suggested by Born-Mayer (BM), Hellmann (Hm), Varshni Shukla (VS) and Ali-Hasan (AH) are used here. The aim of the present work is to show the relative merit of the IPM in predicting the spectroscopic constants of diatomic molecules (alkali halides and alkali hydrides) like binding energy and dissociation energy.

KEY WORDS : Binding Energy and dissociation energy of Alkali halide and alkali hydride molecules.