

PREFACE

This dissertation deals with the investigations carried out by the author during 1988-91 on the topic entitled "Spectroscopic studies on Diatomic molecules". The dissertation has been written in two chapters.

Chapter I deals with the experimental potential energy curves for different electronic states of SiN, SiCl, AsN, SbO, BiF, AsO⁺, and RbH molecules by the method of RKR and Jarman. The dissociation energies of the diatomic molecules have been computed by fitting an empirical potential function to the experimental potential energy curves for the electronic ground states of the molecules. The five parameter Hulbert-Hirschfelder function has been used. The estimated dissociation energies are 4.43 ± 0.10 , 4.46 ± 0.09 , 4.43 ± 0.09 , 4.33 ± 0.09 , 2.61 ± 0.05 , 7.12 ± 0.14 , and 1.64 ± 0.04 eV for SiN, SiCl, AsN, SbO, BiF, AsO⁺ and RbH respectively. The estimated dissociation energies are in excellent agreement with the literature values. Birge-Sponer extrapolation and Hildenbrand and Murad methods are also employed for the estimation of dissociation energies of the above molecules.

From these studies it is concluded that the above methods yield different values in giving dissociation

energies for the molecules in ionic in nature. It is in conformity with the view of Gaydon that for the molecules with the strong ionic bonding the linear extrapolation gives much too low or high values and is of little use. It is also observed that it works well for the case of Covalent molecules (AsN).

Sharma and Hussain proposed relation has been used for the evaluation bond lengths for various diatomic Hydride molecules. The estimated bond lengths are in excellent agreement with the values reported in literature. New empirical relations have been derived for the calculation of bond orders and vibrational - rotational constants of about twenty five hetero nuclear diatomic hydride molecules. For the purpose of comparison, Reddy et al and Pekeris relations are also employed and results are presented in the same table. The estimated values are in excellent agreement with the literature values. The estimated bond orders for OH, HF, AlH, GaH, RbH, CsH and SiH, SrH and BaH have same q values 1.3 and 1.45 respectively. It has no meaning in having the same bond orders for different molecules.

The ambiguity arising from the above equation is also discussed. The present study supports the view of Politzer that $q/(0.05re)^2$ is the correct definition for bond order. The chief merit of the proposed equation for α_e is that knowledge of ' $w_e x_e$ ' and B_e is enough to evaluate α_e where as in Pekeris's relation an addition of w_e is also needed. The

estimated values of α_e are in good agreement with the experimental values.