LIST OF PUBLICATIONS

1. Raikar U.S., Patil V.M. and Soudagar M.K.,"Binding Energy calculations for Heavy Metal Halides" Ind. J.Pure and Appl. Phys.(In Press).

2. Raikar U.S., Patil V.M. and Soudagar M.K., "Binding Energy Calculations for Alkali Halides and Hydrides and Heavy Metal Halide Molecules" National Seminar on Chemical Physics, Pondicherry, Feb. 9-11, 1990, Paper No.TCP-07.

3. Patil V.M. and Soudagar M.K.," A New Generalized Combination Potential for Diatomic Molecules" (Communicated to Ind. J. Pure and Appl. Phys.)

4. Patil V.M. and Soudagar M.K. "RKRV Curves and Dissociation Energies for AgH, Br_2, CrO Molecules" (Communicated to Ind. J. Pure and Appl. Phys.).

5. Patil V.M. and Soudagar M.K., "Generalized Exponential And Logarithmic Potentials for Alkali Halides And Hydrides And Havy Metal Halide Molecules" 8^{th} National Workshop on Atomic and Moleculear Physics, Hydrabad, to be held during Dec.6-12, 1990.(Communicated).

BINDING ENERGY CALCULATIONS FOR ALKALI HALIDES AND HYDRIDES AND HEAVY METAL HALIDE MOLECULES†

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Expressions for binding energy have been obtained by considering two newly suggested ionic potential energy functions :

Potential I :

$$U(r) = -\frac{e^2}{r} + B'' \exp\left(K'' r^{5/2}\right)$$

$$D_i = \frac{e^2}{r_e}\left(\frac{2 k_e r_e^3 + 5 e^2}{2 k_e r_e^3 + 7 e^2}\right) \qquad \text{I}$$

Potential II :

$$U(r) = -\frac{e^2}{r} + S \log\left(8 + \frac{t}{r^2}\right)$$

$$D_i = \frac{e^2}{r_e}\left[1 + \left(\frac{2 e^2}{2 k_e r_e^3 + e^2}\right) \log\left(\frac{4 e^2}{k_e r_e^3 + e^2}\right)\right]$$

where B'', K'', S and t are potential parameters, while other symbols have their usual meanings.

Using these expresssions the binding energies of 27 alkali halides, 13 alkali hydrides and 14 heavy metal halide molecules have been calculated. The average percentage errors in D_i are found to be $\pm$ 3.71 ($\pm$ 0.06), $\pm$ 5.88 ($\pm$ 6.38) and $\pm$ 0.59 ($\pm$ 4.89) on Potential I [Potential II] respectively for alkali halides and hydrides and heavy metal halides. For comparison, average % errors are calculated on some well known potentials in the literature. It is seen that our Potential I is superier to the Gaussian and modified Gaussian potential functions, while Potential II is found to be equally good in estimating binding energies as other logarithmic potentials do.

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