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PLACE: KOLHAPUR

Research Student
Shri. **UDAY .S. RAIKAR**

DATE:

A Study on Combination of Varshni's Potential Functions for Diatomic Molecules

U. S. RAIKAR and M. K. SOUDAGAR

*Department of Physics, Shivaji University,
Kolhapur - 416 004, India.*

In this paper we have proposed a super position potential function as below:

$$U(r) = D_0 \left\{ 1 - \exp \left[-n \left(\frac{r^2 - r_0^2}{2 r_0^2} \right) \right] \right\}^2 + D_0 \left[1 - \left(\frac{r_0}{r} \right)^n \right]^2 - 2 D_0$$

where the constant $n = \left(\frac{\Delta}{2} \right)^{\frac{1}{2}}$, Δ being the sutherland parameter. Employing Varshni's method the following expressions for α_0 and $w_0 x_0$ have been obtained

$$\alpha_0 = \left[\left(\frac{\Delta}{2} \right)^{\frac{1}{2}} - 1 \right] \frac{6 B_0^2}{w_0}$$

$$w_0 x_0 = \left[4 \Delta - 3 \left(\frac{\Delta}{2} \right)^{\frac{1}{2}} - 7 \right] \frac{w}{r_0^2 \mu_A}$$

These are applied to a large number of diatomic molecules. The estimated value of α_0 are in good agreement with the respective experimental values. However, the calculated $w_0 x_0$ values are found to be considerably low. The potential energy curves for a few typical molecules are also calculated.

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