27

LATTICE ENERGY OF ALKALI HALIDE CRYSTALS

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The lattice energy of alkali halide crystals has been evaluated by Born-Mayer (1932), Huggins (1937), Cubicciotti (1959), Kachhawa *et al* (1965) and others from the knowledge of experimental compressibility values. Recently Patel *et al* (1967) modified the Varshni-Shukla (1961) potential and proposed a new potential for alkali halide molecules. In the present communication, we have calculated lattice energy of some alkali halide crystals by utilizing the above potential. According to Patel's modified Varshni-Shukla potential, the interaction energy $\phi_{ij}(r)$ between two atoms i and j separated at a distance r_{ij}, is given by

$$\phi_{ij}(r) = -\frac{e^2}{r_{ij}} + P \exp(-kr_{ij}^{3/2}) \quad .. \quad (1)$$

Here e is the electronic charge and P and k are constant. The energy of an atom in the crystal $\phi(r)$ is related to the interaction potential $\phi_{ij}(r)$ by the following expression (1956)

$$\phi(r) = \sum_j \phi_{ij}(r) \quad .. \quad (2)$$

From equation (1) and (2), we have the following relation :

$$\phi(r) = -\frac{\alpha e^2}{r} + p \exp(-kr^{3/2}) \quad .. \quad (3)$$

where α is the Madolung constant and p is a constant. The lattice energy, E_0, is given by

$$E_0 = -N\phi(r_0) \quad .. \quad (4)$$

where N is the Avagadro's number and r_0 is the closest distance between two unlike ions. The constant p of equation (3) is evaluated from the condition $\left(\frac{d\phi}{dr}\right)_{r_0} = 0$, giving

$$p = \frac{2}{3} \cdot \frac{\alpha e^2}{k r_0^{5/2}} \exp(k r_0^{3/2}) \quad .. \quad (5)$$

The second constant k is determined from Bron-Mayer's condition $\left(\frac{d^2\phi}{dr^2}\right)_r = \frac{9k_1r_0}{\beta}$, which results

$$k = \frac{5}{3r_0^{3/2}} + \frac{6k_1r_0^{5/2}}{e^2\alpha\beta} \quad .. \quad (6)$$

Here k_1 is the molecular volume (V/N) divided by r_0^3 and β is the compressibility.

Equation (4) with equations (5) and (6) gives

$$E_0 = \frac{N\alpha e^2}{r_0}\left[1 - \left(\frac{5}{2} + \frac{9k_1r_0^4}{e^2\alpha\beta}\right)^{-1}\right] \quad .. \quad (7)$$

Table 1

Crystals	r_0 (10^{-8} cm.)	β 10^{-12}/barye	α		E_0 Expt. *K.* Cal/ mole	E_0 Calc. *K.* Cal/ mole
LoCl	2.570	3.17	1.7476	2.000	201.5	201.9
NaCl	2.820	3.97	1.7476	2.000	184.7	185.5
KCl	3.147	5.50	1.7476	2.000	167.8	167.7
RbCl	3.291	6.16	1.7476	2.000	163.6	161.1
CsCl	3.571	5.55	1.7626	1.540	157.8	149.8

Calculated values of E_0 for alkali chloride crystals from equation (7) are given in table I. The data utilized in the calculations are taken from recent sources and are recorded in the table. For comparison, the experimental values of lattice energy are also listed. The calculated values of E_0 incliude the zero-point energy U_0. The agreement betweer the calculated and observed values is quite satisfactory.

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