

A NOTE ON THE LATTICE ENERGY CALCULATIONS OF PbSe AND PbTe

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The lattice energies of PbSe and PbTe have been calculated, and found to be respectively 686.8 kcal/mole and 671.0 kcal/mole, neglecting the contributions due to multipole interactions and zero point energy.

Semiconductors of $A^{IV} B^{VI}$ type, generally denoted as polar semiconductors, are known to have an ionic crystal structure^{1, 2, 3}. Because of their application as infrared detectors and thermoelements, they have been intensively investigated by many workers. As the crystal structure is determined by the dominant binding force, the main part of the binding energy in these crystals is due to Coulomb attraction between the ions. However, according to Tsidil¹ Kovskii⁴ the above classification is not well founded, especially with regard to PbTe and PbSe.

The type of binding is deduced from the lattice energy, dimensions and polarizabilities of ions and from differences in the electronegativities of components. Although some calculations of lattice energy of PbSe have been reported by Sherman⁵, the corresponding value for PbTe is not available.

According to Born⁶ the energy per unit cell is given by the equation :

$$\phi = - \frac{\alpha^2 e^2 \mu A}{R} + \frac{B}{R^n} \quad (1)$$

where e is the electronic charge,

α is the largest common factor in the valencies of the ions,

μ is the number of stoichiometric molecules in the unit cell,

A is the constant depending only on the structure of the crystal (Madelung Constant), and n is the repulsive exponent.

At the equilibrium separation $\frac{\partial \phi}{\partial R} = 0$, we get

$$\frac{\alpha^2 e^2 \mu A}{R_0^2} - \frac{n B}{R_0^{n+1}} = 0$$

where R_0 is the distance between adjacent ions.

Using this relation to eliminate B from (1) we obtain

$$\phi_0 = - \frac{\alpha^2 e^2 \mu A}{R_0} \left(1 - \frac{1}{n} \right) \quad (2)$$

Now, the lattice energy per mole is given by

$$U_o = - \frac{N \phi_o}{\mu} \quad (3)$$

where N is the Avogadro's number.

Substituting the value of ϕ_o in (3) we get

$$U_o = \frac{\alpha^2 e^2 A N}{R_o} \left(1 - \frac{1}{n} \right) \quad (4)$$

As both PbSe and PbTe have the same structure as sodium chloride, the value of Madelung constant A is taken to be 1.747558. Using the value of R_o for PbSe and PbTe from available X-ray crystallographic data⁷ and the values of n from the same consideration as that used by Sherman and others (i.e. $n=11.0$ for PbSe and $n=12.0$ for PbTe) we have calculated the values of lattice energy for PbSe and PbTe.

Substituting the values of R_o , α , A , N , e and n in equation (4) we obtain :

$$U_o = 686.8 \text{ kcal/mole for PbSe.}$$

$$U_o = 671.0 \text{ kcal/mole for PbTe.}$$

In these calculations we have not taken into consideration the contributions due to Van-der Waals attraction between the ions, i.e. multipole interactions and the contribution of the zero point energy. However, according to Mott and Gurney⁸ these factors do not contribute more than 1 to 2 per cent to the total lattice energy.

A C K N O W L E D G E M E N T

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R E F E R E N C E S

1. SCANLON, W. W., "Solid State Physics" (Academic Press, New York) 1959.
2. BURSTEIN, E. & EGLI, P., "Advances in Electronics & Electron Physics" (Academic Press, New York) 1955.
3. BUSCH, G., *Z. Angew. Maths. Phys.*, 1 (1950), 3; 2 (1950), 81.
4. TSIDL'KOVSKII, I. M., "Thermomagnetic Effects in Semiconductors" (Infosearch Ltd., London) 1962.
5. SHERMAN, J., *Chem. Rev.*, 11 (1932), 153.
6. BORN M., "Handbuch der Physics" (Verlag Von Julius Springer, Berlin) 1933.
7. "Handbook of Physics & Chemistry", (Chemical Rubber Publishing Co., USA) 1962.
8. MOTT, N. F. & GURNEY, R. W., "Electronic Processes in Ionic Crystals" (Clarendon Press, Oxford) 1948.