NOVEL WAY OF CALCULATING THERMOCHEMICAL RADII OF NON-SPHERICAL IONS

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The radii of non-spherical ions such as OH^-, NO_3^- and SO_4^{2-} cannot be determined by the convensional physical methods such as X-ray and neutron defraction analysis. They are generally obtained either by using experimental data such as molar volumes and conductivities or by the use of molecular models. However, the values obtained vary significantly depending on the nature of the data employed in the calculation.

Yatismirskii[1] has shown that it is possible to determine the apparent values of the ionic radii of these indirectly from the lattice energy of compounds containing them using a Born-Haber cycle.

Since, the above mentioned technique requires data which are very often difficult to determine, the Extended Lattice[2] model has been employed to evaluate the radii. This procedure requires only the density and the geometry of the substance. Interionic distance of the crystal (γ) is given by the equation.

$$\gamma = k \left(\frac{M}{nd} \right)^{1/3}$$

Where k is a constant and M,n and D are the relative molar mass, the number of ions and the density, respectively. Some of the results obtained are given below.

ION	Calculated radius	Observed radius[2]
OH^-	1.47	1.4
CLO_3^-	2.30	2.36
CrO_4^{2-}	2.44	2.40
SO_4^{2-}	2.26	2.3

References:

Yatismirsi K.B. (1948 Invest. Alcad. Nauk SSR
Wijayananyake R.H. and Griffith T.R. (1981) Ionic Liquids, New York:Plenum Press. P.79