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Repulsion potential parameters and effective ion charges in binary crystals with cubic crystal lattice

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Using an ionic model of chemical bonding from equilibrium internuclear distances in binary crystals and in their corresponding diatomic molecules, the parameters of the potential of the "non-Coulomb" (Born) repulsion of ions are determined. Using these parameters and the compressibility of crystals, the effective charges of ions and the corresponding ionic chemical bond are found. The dependence of the ionic bond on the structural parameters of the crystal, as well as on the electronegativity difference and on the valence of the initial atoms is obtained.

Keywords: electronegativity, ionic compounds, crystal lattice type and coordination number, internuclear distances in crystals and molecules, Born repulsion potential, effective ion charge.

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