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Geochemical applications of the simple salt approximation to the lattice energies of complex materials

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ABSTRACT

The lattice energies for a variety of compounds that can be classified as double salts are calculated by summing the lattice energies of the constituent simple salts. A comparison with the lattice energies obtained from the Born-Haber or other thermodynamic cycles shows that the simple salt approximation reproduces these values generally to within 1.2%, even for compounds that have considerable covalent character. Application of this method to the calculation of the lattice energies of silicates, using the sum of the lattice energies of the constituent oxides are, on average, within 0.2% of the value calculated from the experimental enthalpies of formation. The implications of the simple salt approximation for the thermodynamics of geochemically important processes are discussed.