

Electrostatic contributions to thermodynamic properties of aqueous ions from electrostatic potentials defined in the context of density functional theory

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Density functional theory provides physically meaningful ionic radii to build up electrostatic potentials for singly charged negative and positive monoatomic ions. On the basis of these electrostatic potentials, electrostatic contributions to extensive properties such as free energy, entropy, ionic volume, and ionic compressibility for a representative series of singly charged monoatomic cations and anions are calculated and compared with experimental data. © 1993.