Ion solvation energies from density functional theory

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Electrostatic solvation energies of singly charged monoatomic ions may be predicted from the knowledge of an electrostatic potential buildup from a physically meaningful ionic radius. Since the asymptotic behavior of the electrostatic potential for cations and anions do not follow the same pattern, different methodologies are needed. The reaction field potential required for the calculation of Born's solvation energies of singly charged cations may be obtained from the simple Thomas?Fermi?Dirac theory, based on the condition that the electrostatic potential of the ground?state atomic ions do exactly equal the negative of their chemical potentials. For singly charged anions, electrostatic solvation energies may be directly obtained from Sen?Politzer electrostatic potentials. Numerical results are presented for two representative series of ions and compared with experimental data.