Ion solvation from isoelectronic processes at the nucleus

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A Kohn-Sham (KS) like formalism for the calculation of solvation energies of singly charged ions is presented. The approximate theory is based on a simple model that represents embedding an atomic ion into a polarizable liquid, through successive isoelectronic processes at its nucleus. In this way, the controversial procedure of selecting appropriate ionic radii, as involved in the computation of solvation energies via the Born formula, is avoided and replaced by energy changes involving a varying nuclear charge. The effective KS potential is derived within the framework of a linear response model. It is written in terms of the electrostatic potential at the nucleus of an auxiliary transition state pseudo-atom, and the electron density induced by the electrostatic external perturbation. As an illustration, the formalism was implemented within the Hartree?Fock?Slater Xa approximation. This is discussed in detail.