On the SCF theory of continuum solvent effects representation: Introduction of local dielectric effects

Contreras, Renato

Aizman, Arie

The introduction of local dielectric effects within the SCF theory of continuum solvent effects representation is examined at a semiempirical level. The formalism is developed in the frame of the reaction field theory within the effective charge approximation. The solvation free energies of Li+, Na+, F?, and Cl? ions in water were calculated in order to illustrate the reliability of the proposed model. The extension to molecules and molecular ions was performed including a desolvation corrective term related to the specific neighborhood of each atomic center. The results show a qualitative agreement with experimental data. A comment on the solvatonlike models for incorporating the solvent effect into the Hamiltonian is also given.