On the SCF theory of continuum solvent effects representation II. Quantum chemical calculation of thermodynamic properties of some acid?base equilibria in solution

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Further developments in the local reaction field (LRF) model of solvent effects are presented. The improved formalism, including dielectric saturation effects, permits a better description of the solvent polarization vector. As a result, the calculation of entropies of solvation is significantly improved with respect to the standard reaction field models, allowing a complete thermodynamic picture of ion solvation to be obtained. The calculated thermodynamic functions of solvation are combined with gas?phase proton affinities to yield theoretical estimates of solution equilibrium properties in some acid?base processes. Some preliminary results concerning the basicity of primary alkylamines in water are used to illustrate the reliability of the present approach.