New developments in the continuum representation of solvent effects

Morales-Lagos, D.

Gómez-Jeria, Juan S.

New developments in the continuum representation of solvent effects are presented. General expressions for the Helmholtz free energy of an arbitrary discrete charge distribution placed in spherical and spheroidal (oblate and prolate) cavities and surrounded by multiple dielectric layers are derived. The solute-solvent interaction energy is accounted for by using the multipole expansion. This dielectric partition permits the modeling of nonlinear dielectric effects (NLDE). These results are incorporated into quantum mechanical formalisms at the CNDO/2 level, giving origin to prolate spheroidal (PS) generalized Born formula (GBF), PS modified GBF, and PS self-consistent multilayered reaction field with overlap schemes. Some of these schemes incorporate nonsphericity, NLDE, or both. The Miertus and Kysel parametrization of the solute-solvent interaction is generalized. The electrostatic contributions to some selected thermodynamic properties are presented. The integrative value of this wo