Hydrogen bond. Environmental effects on proton potential curves. An SCRF MO CNDO/2 calculation of a water dimer

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A solvent and/or environmental effect has been introduced into the MO CNDO/2 calculation of a model hydrogen bonded system. Proton potential curves, potential energy, dipole moments, the polarizability component parallel to the reaction field, and the second order perturbation effects associated to the dispersion forces, have been studied as a function of a solute-solvent coupling parameter. This parameter may be related, through the self-consistent reaction field theory of solvent effects, to both the macroscopic dielectric properties of the solvent and to the local order (if any) around the solute. Numerical results corresponding to a water dimer are discussed. © 1976.