Continuum, Discrete and Explicit Solvation Models for Describing the Low-Lying Absorption Spectrum of the Pterin Acid in Aqueous Environment.

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The absorption spectrum of the acid form of pterin in water was investigated theoretically. Different procedures using continuum, discrete and explicit models were used to include the solvation effect on the absorption spectrum, characterized by two bands. The discrete and explicit models used Monte Carlo simulation to generate the liquid structure and time dependent density functional theory (B3LYP/6-31G+(d)) to obtain the excitation energies. The discrete model failed to give the correct qualitative effect on the second absorption band. The continuum model, in turn, has given a correct qualitative picture and a semi-quantitative description. The explicit use of 29 solvent molecules, forming a hydration shell of 6 Å, embedded in the electrostatic field of the remaining solvent molecules (below), gives absorption transitions in excellent agreement with the S0-S1 and S0-S2 absorption bands that characterize the experimental spectrum of pterin in water environment.