The electronic states and vibronic absorption spectrum of berberine in aqueous solution

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Abstract

The time-dependent density functional theory (TD-DFT) was used to calculate the vibronic absorption spectrum of berberine (BER) in an aqueous solution. The best agreement with the experimental spectrum gives the O3LYP functional. Functionals with long-range correction showed poor agreement with experiment. The molecular orbitals of BER involved in the electronic transition during light absorption in the visible spectral region have been obtained. The dipole moments and atomic charges of the ground and excited states of the BER molecule have been calculated. Maps of BER electron density and electrostatic potential have been drawn. A significant photoinduced electron transfer from the outer di-oxygen five-membered heterocycle to the center of the BER chromophore has been found. According to our calculations, vibronic coupling and Boltzmann distribution play a significant role in the absorption spectrum of BER.

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