EXPERIMENTAL AND THEORETICAL STUDIES ON THE ELECTRONIC ABSORPTION SPECTRA OF QUINOLINE CARBOXYALDEHYDES

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We have investigated electronic spectra of some quinoline carboxaldehydes dissolved in water by UV-vis measurements in the range of 190-1100 nm and by theoretical calculations with density functional theory (DFT). The geometrical structures of the quinoline carboxaldehydes have been obtained at the B3LYP/6-311++G(d,p) level, while the electronic absorption spectra have been simulated in water by using time-dependent DFT at the same level. Theoretical and experimental spectra agree to each other very well.

Keywords: Electronic spectra, Quinoline carboxaldehydes, DFT