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Computational Modeling of Solvent Effects on Electronic Spectra of Carbonyl Chromophores

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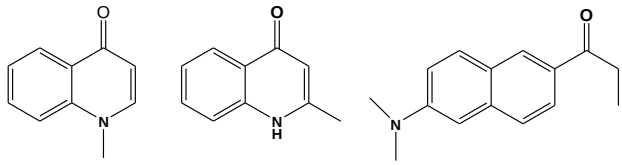
Interpretations of observed solvent effects on light absorption and emission by dye molecules have traditionally been associated during recent decades with time dependent density functional theory.[1] More sophisticated theoretical approaches have been applied to small molecular examples only. Here we compare some ways of accounting for the solvent effect using model specific solvent-solute interactions in continuum in the ground S_0 and the fluorescent first excited state singlet (S_1), considering specifically registered and predicted electronic spectra of hydrogen-bonded complexes. Comparisons of TD DFT predictions with more recent DLPNO-STEOM-CCSD[2] computational results are presented.



Keywords: electronic spectra, general and specific solvent effect, TD-DFT and STEOM-CCSD computing

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