TD-DFT/DFT study of Toluidine blue O in aqueous solution: vibronic transitions and electronic properties

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Abstract

The vibronic absorption spectrum of Toluidine blue O (TBO) dye in an aqueous solution was calculated using the time-dependent density functional theory (TD-DFT). The calculations were performed using all hybrid functionals supported by Gaussian16 software and 6-31++G(d,p) basis set with IEFPCM and SMD solvent models. The IEFPCM gave underestimated values of λmax in comparison with the experiment, what is a manifestation of the TD-DFT "cyanine failure". However, the SMD made it possible to obtain good agreement between calculated and experimental spectra. The best fit was achieved using the X3LYP functional. The dipole moments and atomic charges of the ground and excited states of the TBO molecule were calculated. Photoexcitation leads to an increase in the dipole moment of the dye molecule. An insignificant photoinduced electron transfer was found in the central ring of the chromophore of the TBO molecule. Vibronic transitions play a significant role in the absorption spectrum of the dye.

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