The Color of An Azo Dye - A Combined Experimental and DFT Investigation of Spectral Properties of 5-(4-Sulfophenylazo) Salicylic Acid

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A study of the azo compound Mordant Yellow 10 (5-(4-sulfophenylazo)salicylic acid) was conducted, aiming to investigate factors contributing to its observed color. The compound was synthesized, and reaction mechanisms were discussed. Partly to fully deprotonated anions were investigated in solvent phase, employing an experimental approach by adjusting pH in methanolic/aqueous solutions and conducting UV-visible spectroscopy, as well as a theoretical TD-DFT study. Optimized ground-state geometries and energies were calculated using the B3LYP DFT functional with the basis sets 6-31G and 6-31G(d), later discussed based on Mulliken population analyzes. Excitation energies and absorption band intensities were obtained from TD-DFT calculations using B3LYP/6-31G+(d), with PCM to simulate methanol as dielectric medium, and were compared to experimental UV-visible absorption spectra. The absorption bands in the spectra were found to be gradually shifted toward longer wavelengths upon deprotonation of the compound, and could be correlated with a calculated decrease in the energy gap between the ground and the first excited states, as well as the HOMO-LUMO energy gap. The study provided an insight into the electronic structure of an azo dye, and why pH changes can affect the observed color of an organic dye. Comparing spectra from solutions provided some information. Improvements of the study include investigating pKa employing titration, thus more thoroughly investigating pH dependence for absorption. A valuable conclusion is the possibility of successfully employing B3LYP/6-31G(d) and TD-B3LYP/6-31G+(d) with PCM in a computational spectroscopic investigation of a newly-designed azo compound, for application as sensitizer in Grätzel photovoltaics (DSSC:s).

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