E/Z Isomerization of Brilliant Yellow: A Theoretical Study of Its Photoactive Forms

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Brilliant Yellow (BY) is an azo dye exhibiting photoinduced E/Z isomerization, which governs its optical properties and potential applications in photonic and bioanalytical systems. In this work, a comprehensive theoretical investigation of multiple conformational and configurational isomers of BY was performed in order to elucidate their structural and spectroscopic characteristics. Geometry optimizations were performed by applying density functional theory (DFT), followed by time-dependent DFT (TD-DFT) to simulate the electronic absorption spectra in solution. Several exchange–correlation functionals in combination with basis sets were employed to evaluate their potential applicability in predicting the excitation energies and spectral features. The nature of the electronic transitions was analyzed based on molecular orbital contributions, showing that the main absorption bands originate predominantly from π→π* transitions localized on the azo chromophore. The calculated UV/Vis spectra reveal distinct differences among the isomers, with significant shifts in absorption maxima and oscillator strengths depending on the E/Z configuration. The theoretically obtained results are further compared to experimental data to provide evidence of the most suitable combination of a method/ basis set. Falling in line with other studies provided in scientific literature, the presented results demonstrate that photoinduced interconversion between photoactive forms can indeed lead to measurable spectral changes, thus providing insight into the structure–property relationship in azo dyes and supporting their application in photoresponsive systems [1-2].

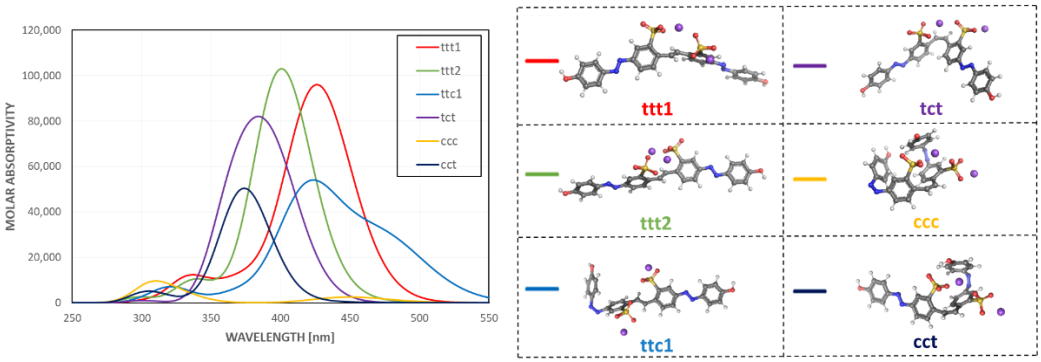

Figure 1. Optimized geometries and simulated UV–Vis absorption spectra of the six possible conformational isomers of the BY-2Na dye

Funding:

This research was financed by the Bulgarian National Science Fund, grant number KP-06-M98/01 of 01.12.2025 (project “Azo Dyes in Polymer Matrices as Media for Optical recording”).

References:

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