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Styryl dye possessing donor-π-acceptor structure : synthesis, spectroscopic and computational studies

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Abstract A novel hemicyanine dye possessing donor-π-acceptor structure that features a fixed benzimidazole ring as an electron donor and pyridinium moiety as an electron acceptor was synthesized. The structure of the hemicyanine was elucidated by means of NMR and IR spectroscopy. The dye was studied using steady-state absorption and emission spectroscopy. The analysis of experimentally recorded spectra was supported by quantum chemical calculations using density functional theory with CAM-B3LYP, LC-BLYP, LC-ωPBE and PBE0 functionals. The measurements and calculations were performed in solvents of different polarity. In particular, we found that the CAM-B3LYP and LC-ωPBE excitation energies are in very good agreement with the experimental data. Two-photon absorption of the dye was studied by Z-scan measurements.

Słowa kluczowe

Styryl dyes, Synthesis, Absorption and emission spectra, Fluorescence lifetime, Computational calculations, Two-photon absorption

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