Synthesis and photophysical properties of two-photon chromophores containing 1H-benzimidazole residue

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The non-centrosymmetric, trans,trans-2-{4-[2-(1H-benzimidazol-2-yl)ethenyl] -styryl}-1,3-dimethylbenzimidazole iodide and centrosymmetric, trans,trans-1,4-bis[4-(2-(1H-benzimidazol-2-yl)ethenyl)]benzene polymethine compounds based on 1H-benzimidazole residue were synthesized and characterized. Their photophysical properties in solvents of different polarity were thoroughly studied by means of absorption, emission and fluorescence quantum yield measurements. Analysis of the results clearly indicates that the compounds have strong one-photon absorption bands in the near ultraviolet region, relatively high fluorescence quantum yields and large Stokes' shifts due to the charge transfer effect. The one- and two-photon absorption properties of a selected non-centrosymmetric dye were compared to those of a centrosymmetric polymethine dye. Their two-photon absorption cross-sections in DMF were determined to be ~330 GM and ~380 GM at ca. 650 nm for the centrosymmetric and non-centrosymmetric polymethine compounds, respectively. Density functional theory calculations of one- and two-photon absorption electronic spectra of the tested compounds using CAM-B3LYP, LC-BLYP and LC-ωPBE functionals were carried out to support the experimental data.

Słowa kluczowe

Polymethine dyes, Synthesis, Absorption and emission spectra, Fluorescence lifetime, DFT calculations, Two-photon absorption

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