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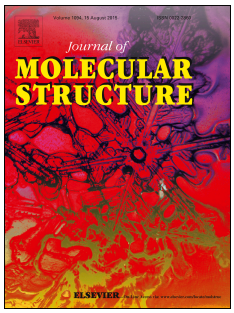

Green synthesis, structure and fluorescence spectra of new azacyanine dyes

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ACCEPTED MANUSCRIPT

Green synthesis, structure and fluorescence spectra of new azacyanine dyes.

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Abstract*:*
A series of symmetric and unsymmetric monomethine azacyanine dyes (monomethine azacyanine and merocyanine sulfobetaines) were synthesized with moderate to high yields via a novel method using microwave irradiation. The compounds are derived from a condensation reaction between 2-thiomethylbenzotiazolium salts and 2-imino-3-methylbenzothiazolines proceeded under microwave irradiation. The synthetic approach involves the use of green solvent and absence of basic reagent. TD-DFT calculations were performed to simulate absorption and fluorescent spectra of synthesized dyes. Absorption maxima, λ_{max}, of the studied dyes were found in the range 364-394 nm. Molar absorbtivities were evaluated in between 40300-59200 mol^{-1} dm^3 cm^{-1}. Fluorescence maxima, λ_{fl}, were registered around 418-448 nm upon excitation at 350 nm. A slight displacements of theoretically estimated absorption maxima according to experimental ones is observed. The differences are most probably due to the fact that the DFT calculations were carried out without taking into account the solvent effect. In addition, the merocyanine sulfobetaines also fluorescence in blue optical range (420-480 nm) at excitation in red range (630-650 nm).

Keywords: azacyanine dyes; green chemistry; UV-vis; fluorescence; quantum chemical calculations;

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