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New coumarin-based disperse disazo dyes: synthesis, spectroscopic properties and theoretical calculations

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Abstract

5-amino-4-aryldiazo-3-methyl-1H-pyrazoles (**3a-l**) have been diazotised and coupled with 4-hydroxycoumarin to give rise to the coumarin-based disperse disazo dyes (**3a-l**). The newly synthesized twelve coumarin-based disperse disazo dyes have been characterized by using the elemental analysis and the spectral methods. The solvatochromic behavior of these dyes in various solvents is evaluated. Substituent, acid and base effects on the visible absorption spectra of the dyes substituted with electron-withdrawing and electron-donating groups at their *o*-, *m*-, *p*-position are also reported in detail. Molecular geometries and spectroscopic properties of the compounds considered in this work are also analyzed by using ab initio calculation methods based on the density functional theory (DFT) in the ground state. The theoretical results obtained from DFT are compatible with the experimental results.

Keywords: Coumarin, Pyrazole, Disperse dyes, Disazo dyes, Solvatochromism, DFT

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