A Combined Experimental and Computational Investigation on Spectroscopic and Photophysical Properties of a Coumarinyl Chalcone

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JOURNAL OF FLUORESCENCE
Volume: 26 **Issue:** 4 **Pages:** 1357-1365
DOI: 10.1007/s10895-016-1823-2
Published: JUL 2016
View Journal Impact

Abstract

Here, we synthesized a new coumarinyl chalcone derivative 3-[3-(3-Methyl-thiophen-2-yl)-acryloyl]-chromen-2-one (MTC) by simple and proficient method. A comprehensive study on the photophysics of a coumarinyl chalcone derivative having pi-conjugated potential chromophore system 3-[3-(3-Methyl-thiophen-2-yl)-acryloyl]-chromen-2-one (MTC) has been carried out spectroscopically. The electronic absorption and emission characteristic of MTC were studied in different protic and aprotic solvents using absorption and steady-state fluorescence techniques. The spectral behavior of this compound is found to be extremely sensitive to the polarity and hydrogen bonding nature of the solvent. The compound shows very strong solvent polarity dependent changes in their photophysical characteristics, namely, remarkable red shift in the emission spectra with increasing solvent polarity, change in Stokes shift, significant reduction in the fluorescence quantum yield; indicating that the fluorescence states of these compounds are of intramolecular charge transfer (ICT) character. The solvent effect on the photophysical parameters such as singlet absorption, molar absorptivity, oscillator strength, dipole moment, fluorescence spectra, and fluorescence quantum yield of the compound has been investigated in detail. The difference between the excited and ground state dipole moments (Delta mu) were estimated from solvatochromic methods using Lippert-Mataga and Reichardt's correlations. The prepared compound was also studied by density functional theory (DFT) and time-dependent density functional theory (TDDFT). The results revealed that it could be easily reproduce by computational means.

Keywords

Author Keywords: Coumarin derivative; Photophysics; ICT; Effect of solvent
KeyWords Plus: DIPOLE-MOMENTS; DENSITY; DYES

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Funding

Funding Agency	Grant Number
Research Center for Advanced Materials Science (RCAMS), King Khalid University, Abha, Saudi Arabia	

View funding text

Publisher

SPRINGER/PLENUM PUBLISHERS, 233 SPRING ST, NEW YORK, NY 10013 USA

Categories / Classification

Research Areas: Biochemistry & Molecular Biology; Chemistry

Web of Science Categories: Biochemical Research Methods; Chemistry, Analytical; Chemistry, Physical

Document Information

Document Type: Article

Language: English

Accession Number: WOS:000381197400021

PubMed ID: 27307021

ISSN: 1053-0509

eISSN: 1573-4994

Journal Information

Table of Contents: Current Contents Connect
Impact Factor: Journal Citation Reports

Other Information

IDS Number: DT0UB

Cited References in Web of Science Core Collection: 31

Times Cited in Web of Science Core Collection: 2