



Contents lists available at ScienceDirect

Optik

journal homepage: www.elsevier.com/locate/ijleo

Synthesis, theoretical properties using DFT method, and nonlinear optical properties of 4-methyl umbelliferone derivative

Ayat Adil ^a, Qusay M.A. Hassan ^{b,*}, Tahseen A. Alsalm ^a, H.A. Sultan ^b, Rafid H. Al-Asadi ^a, C.A. Emshary ^b

^a Department of Chemistry, College of Education for Pure Sciences, University of Basrah, Basrah 61001, Iraq

^b Department of Physics, College of Education for Pure Sciences, University of Basrah, Basrah 61001, Iraq

ARTICLE INFO

Keywords:

Coumarin derivative
DPS
Z-scan
All-optical switching

ABSTRACT

4-methyl umbelliferone compound is synthesized from resorcinol with ethyl acetoacetate under ultrasound irradiation as an assistant of reaction. The coumarin derivative, COM-ester compound, is synthesized from the 4-methyl umbelliferone with chloroethyl acetate also using ultrasound irradiation. The COM-ester compound is characterized via spectroscopic, FTIR and ¹H NMR methods. The geometrical optimization and thermodynamic characterization of the COM-ester compound are theoretically investigated via DFT. To determine the HOMO, LUMO, Mullikan atom charges and electronic spectrum of the investigated COM-ester compound, the hybrid functional B3LYP and CAM- B3LYP procedures are applied. Nonlinear optical (NLO) properties of the COM-ester compound are studied via the diffraction patterns (DPS) and Z-scan techniques where its nonlinear refractive index (NLRI), n_2 , is obtained using cw, low power laser beam. As high as $4.658 \times 10^{-11} \text{ m}^2/\text{W}$ of n_2 is obtained. The all-optical switching (AOS) of the COM-ester compound is tested using two 473 and 532 nm cw, visible laser beams, both static AOS and dynamic AOS.

1. Introduction

Coumarins are a class of benzopyrones that are widely dispersed in nature and may be found in different parts of various plant species [1,2]. Some plants or spices are used as nutraceuticals, have large amounts of natural coumarin components [3–6]. The explore for new materials that might be used in variety of uses viz., optical phase conjunction [7], data storage [8], optical switching [9], optical-bistability [10], optical limiting [11], etc., is an ongoing matter for the last four decades. Variety of materials have been tested for such applications viz., fluoride glasses [12], polymers [13], photo-refractive materials, Buckminsterfullerenes have been investigated. We have studied during the last 4 years so many available materials [14], so many materials whose properties have been improved by the addition of other materials [15,16], and so many new synthesized materials [17–19]. Such materials that can be used in the previous mentioned applications must have large nonlinear refractive indexes (NLRI), n_2 , and respond fast to the incident low power laser beams with low nonlinear absorption coefficients (NLACs) [20].

When high intensity laser beams are incident on a homogenous medium, a diffraction pattern of beam divergence is observed at a distance, and its phase is modulated by its own light intensity. Such effect is known in nonlinear optics as spatial self-phase modulation

* Corresponding author.

E-mail address: qusayali64@yahoo.co.in (Q.M.A. Hassan).

<https://doi.org/10.1016/j.ijleo.2023.171320>

Received 4 July 2023; Received in revised form 16 August 2023; Accepted 16 August 2023

Available online 19 August 2023

0030-4026/© 2023 Elsevier GmbH. All rights reserved.