Synthesis, characterization and optical properties of mono- and bis-chalcone

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Abstract

Mono- and bis-chalcone have been synthesized by the reaction of 3-acetyl-2,5-dimethylthiophene and N,N-di-methylbenzaldehyde/terephthalaldehyde in ethanolic NaOH in microwave oven. The structure of these compounds was established by elemental analysis, IR, 1H NMR, 13C NMR and GC–MS spectral analysis. Thin films with thickness of 100 nm of mono- and bis-chalcone were evaporated by thermal evaporation onto glass/Si wafer substrates under a vacuum of $10^{-6}$ Torr. The optical constants (absorption coefficient and optical band gap) of these films have been studied as a function of photon energy in the wavelength region 300–1100 nm. Analysis of the optical absorption data shows that the rule of non-direct transitions predominates. The optical band gaps for mono- and bis-chalcone are found to be 2.31 and 0.99 eV respectively. It has been found that the absorption coefficient changes with increasing photon energy. The peak values of the absorption coefficient are found to be at 370 nm for mono-chalcone and 460 nm for bis-chalcone thin films.

Keywords: Chalcones, Optical properties, Thin film

1. Introduction

α,β-Unsaturated ketones are commonly synthesized via the Claisen–Schmidt condensation between acetophenone and benzaldehyde. This reaction is catalyzed by acids and bases condition [1]. The members of α,β-unsaturated ketones (chalcones) and flavonoid family have attracted a great deal of interest due to their applications as antibacterial, anti-inflammatory and anticancer pharmacological agents [2–6]. Chalcones are important intermediates in the synthesis of many pharmaceuticals [7–9]. It’s also applicable in materials fields such as non-linear optical (NLO) [10], optical limiting [11], electrochemical sensing [12] and Langmuir film [13]. Various chalcone derivatives are notable materials for their second harmonic generation (SHG) [14]. Various synthetic methods have been reported so far, such as refluxing in an organic solvent [15], the solvent-free solid-phase reaction [16], ultrasonication [17] photo-sensitization [18] and microwave radiation [19]. In this paper we synthesized the mono- and bis-chalcone in microwave radiation. A lot of research has been carried out on chalcone derivatives on the bases of its application but no work has been done in thin film form. In this paper we are reporting the optical properties of chalcone as thin films. Thin films are thin material layers ranging from fractions of meters to several micrometers in thickness. Electronic semiconductor devices and optical coatings are the main applications benefiting from thin film construction. Thin film technology is based on three foundations: fabrication, characterization and applications. Some of the important applications of thin films are microelectronics, communication, optical electronics, catalysis, coating of all kinds, and energy generation and conservation strategies. It plays an important role in the high-tech industries. Progress in each area depends upon the ability to selectively and controllably deposit thin films—thickness ranging from tens of Angstroms to micrometers—with specified physical properties. This, in turn, requires control—often at the atomic level of film microstructure and microchemistry.

Keeping in view the importance of thin film technology, we have decided to prepare the films of mono- and bis-chalcones and study the optical properties of these thin films.

2. Experimental

2.1. General methods

3-Acetyl-2,5-dimethylthiophene, N,N-di-methyl benzaldehyde and terephthalaldehyde were commercially purchased (Aldrich) and used as received. HPLC-grade organic solvents (Aldrich) were used for the column chromatography. The FT-IR spectra were recorded using the KBr pellet method on a MIDAC FT-IR spectrometer within the range of 4000–400 cm$^{-1}$. The $^1$H NMR and $^{13}$C NMR spectra were obtained on a Bruker Avance 600 using CDCl$_3$ as a solvent.