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Characterizations of structural and optical properties of 2-(pyranoquinolin-4-yl) malononitrile

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ABSTRACT

Thin films of 2-(pyranoquinolin-4-yl) malononitrile, PQM, are deposited by thermal evaporation technique. X-ray diffraction pattern of the powder and thin films with different thicknesses are investigated. Crystallite size, strain and dislocation are determined. Optical properties of PQM thin films are studied in wavelength range of 200–2500 nm using spectrophotometric measurements of transmittance and reflectance. The optical constants are calculated. Direct and indirect optical energy gaps of PQM thin films are estimated. Dispersion parameters as oscillator energy and dispersion energy are determined using single-oscillator model. The real and imaginary parts of dielectric constant show maxima at 1.24, 1.49, 2.75, 3.54 eV.

1. Introduction

Molecular materials with nonlinear optical properties are currently attracting considerable attention because of their potential applications in the optoelectronic devices of telecommunications, information storage and optical switching [1]. Organic semiconductors are of steadily growing interest as active components in electronics and optoelectronics [2,3]. Quinolines are heterocyclic aromatic organic compounds and they are π-conjugated semiconductor materials. The physical properties of a functional organic material arise from delocalised π electrons, adsorbed species, defect sites and the presence of functional groups [4]. Conjugated polyquinolines has an excellent electron- accepting and transport properties. Thus, they are promised to act as electronic and optoelectronic materials [5]. Quinolines and their substituted derivatives are of major interest for their application in optoelectronic, organic electronics [6], light emitting diodes, solar cell [7–9] and ion sensor devices [10]. Organic thin films enable to fabricate low cost electronic [11]. The optical properties of organic films are significant since they are directly linked to their atomic structure, electronic band structure and electrical properties that helps in designing materials for specific applications such as optoelectronic devices [12,13].

In the present work, the characteristic structural and optical properties of 2-(pyranoquinolin-4-yl) malononitrile, PQM, are investigated.

2. Experimental technique

The powder of 2-(pyranoquinolin-4-yl) malononitrile, PQM, was synthesized as proposed by Hassanin [14]. The chemical structure of PQM was shown in Fig. 1. All reagents were purchased from Sigma & Aldrich company and used without further purification. A mixture of 4-chloro-6-ethyl-3-nitro-pyrano [3,2-*c*] quinoline-2,5-dione (3.20 g, 10 mmol) and malononitrile

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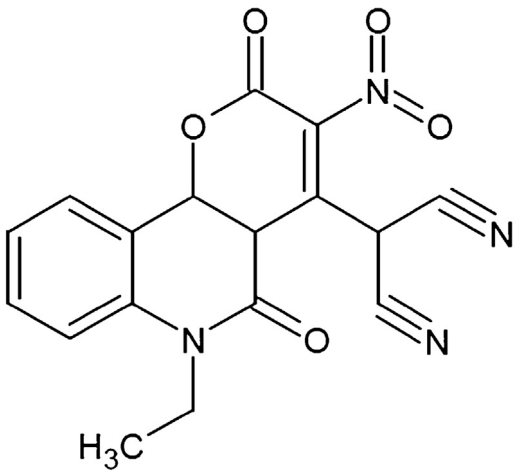

Fig. 1. The chemical structure of PQM.

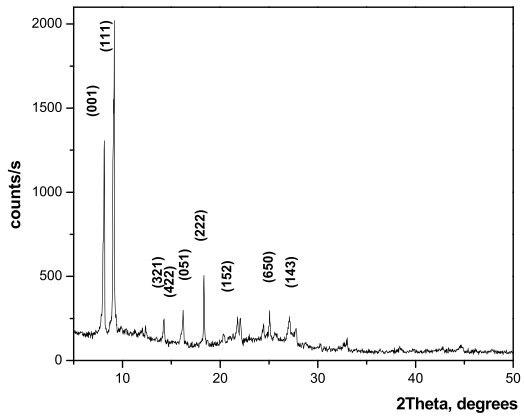

Fig. 2. XRD pattern for the powder of PQM.

(0.70 g, 10 mmol), in absolute ethanol (50 mL) containing few drops of triethylamine, was stirred for 2 h. The solid was deposited after cooling. Then it was filtered and crystallized from methanol to give 2-(pyranoquinolin-4-yl) malononitrile (PQM) as yellow crystals.

Thin films of PQM were prepared by thermal evaporation technique using a high vacuum coating unit (Edward's, E306A, UK). PQM films were deposited onto optical flat and well-cleaned glass substrates in a vacuum of 4×10^{-4} Pa. The deposition rate and film thickness were controlled using a quartz crystal thickness monitor (Edwards, FTM4). X-ray diffraction measurements for the powder and thin films of PQM were carried out by the X'Pert diffractometer which operated at 25 kV and 30 mA. Optical measurements for thin films of PQM were performed using a double-beam spectrophotometer (JASCO model V-570-UV/vis/NIR). Transmittance, T, and reflectance, R, of the thin film samples are carried out at room temperature and at normal incidence of light in the wavelength range 200–2500 nm. The absolute values of T and R were used to calculate optical constants, the refractive index (n), the absorption index ((*k*)), and absorption coefficient (α) according to the relations in Refs. [15,16].

3. Results and discussion

XRD pattern recorded for the powder of -(pyranoquinolin-4-yl) malononitrile (PQM) is shown in Fig. 2. The powder of PQM shows polycrystalline nature. Using Crysfire and Checkcell programs [17,18], the crystal structure of PQM and lattice constants are determined. The crystal structure of PQM is an orthorhombic with a = 25.748 Å, b = 31.477 Å, c = 10.997 Å. Miller indices (hkl) are listed in Table 1. The crystallite size (D) and the strain ($\in$), for the powder PQM were calculated from Lorentzian function and Gaussian function [19] as follow:

$$\left(d_{hkl}\beta_{hkl}\cos\theta\right)^2 = \frac{0\cdot 95}{D}\left(d_{hkl}^2\beta_{hkl}\cos\theta\right) + \left(\frac{\in}{2}\right)^2 \quad (1)$$