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Synthesis, DFT band structure calculations, optical and photoelectrical characterizations of the novel 5-hydroxy-4-methoxy-7-oxo-7*H*-furo [3,2-g]chromene-6-carbonitrile (**HMOFCC**)

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ABSTRACT

Reaction of 4-methoxy-5-oxo-5*H*-furo[3,2-g]chromene-6-carboxaldehyde (**1**) with hydroxylamine hydrochloride resulted in ring transformation producing the novel 5-hydroxy-4-methoxy-7-oxo-7*H*-furo [3,2-*g*]chromene-6-carbonitrile (**HMOFCC**). The structure was deduced based on its correct elemental analysis and spectral data (IR, ^{1}H NMR, ^{13}C NMR and mass spectra). The geometries of the **HMOFCC** were completely optimized by means of DFT-B3LYP/6-311++G (d,p) theoretical level. The ground state properties such as; total energy, the energy of HOMO and LUMO and Mulliken atomic charges were also determined. In addition, the two solvents; polar (methanol) and nonpolar (dioxane) were utilized to extract the electronic absorption spectra. The assignment of the detected bands was discussed by TD-DFT calculations. A cauliflower-like, as well as, needle-like leaves morphologies were observed using scanning electron microscope images. Two direct optical band gaps were extracted from the photon energy dependence of absorption coefficient at the band edges and found to be 1.16 and 2.56 eV. A characteristic emission peak of photoluminescence spectrum was observed and shifted depending on the solvent type. A remarkable rectification characteristic of **HMOFCC**/p-Si heterojunction confirms the diode-like behavior. The main important parameters like series resistance, shunt resistance and reverse saturation current show illumination dependence under influence of the illumination intensity range 20 −100 mW/cm^2. The heterojunction based **HMOFCC** showed phototransient properties under various illumination intensities which give the recommendation for the studied heterojunction in the field of optoelectronic device application.

1. Introduction

The natural occurring khellin (4, 9-dimethoxy-7-methyl-5*H*-furo [3, 2-*g*] chromen-5-one) [1], obtained from the fruits and seeds of *Ammi visnaga* L., possesses a high antiatherosclerotic and lipid-altering activity [2]. Khellin has been used for the photochemotherapeutic treatment of vitiligo and psoriasis [3]. The photodynamic characteristics of khellin in its photoreaction with DNA were previously investigated by Trabalzini et al. [4]. Generally, furochromones are known to have anti-inflammatory and analgesic [5–7], antitumor [8] and antimicrobial activities [9].

Eiden et al. [10] have investigated the structure of 6-formylvisnagin (4-methoxy-5-oxo-5*H*-furo[3,2-g]chromene-6-carboxaldehyde) as a one of the most important categories of Khellin. Another condensed studies have been achieved by Ibrahim et al. [11–14] for the chemical characteristics of γ-pyrone fused benzene as well as quinolin-2(1*H*)-ones [15,16]. As an extension of this type of studies, the present investigation aims to explore the chemical reactivity of 6-formylvisnagin towards a hydroxylamine hydrochloride and consider the optical absorption characteristics of

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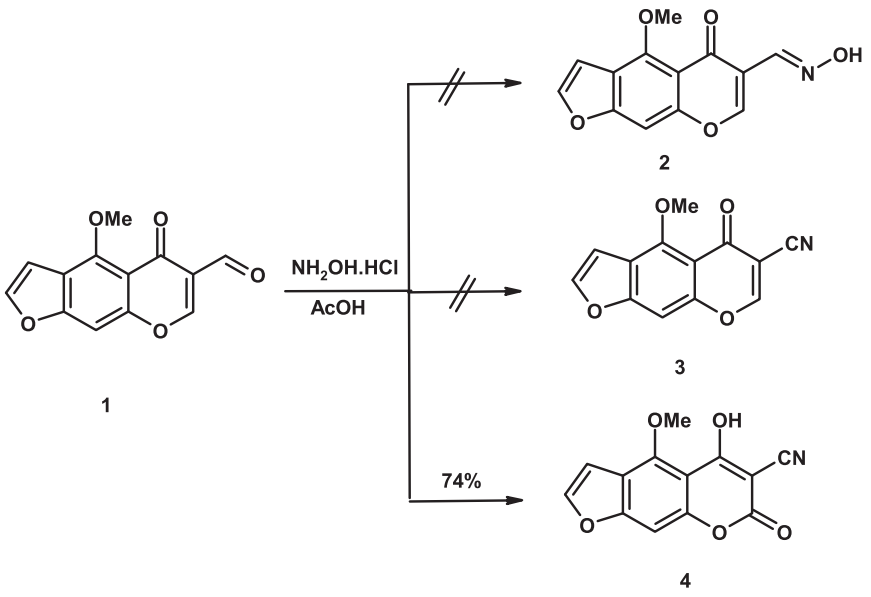

Fig. 1. Reaction of 6-formylvisnagin with hydroxylamine hydrochloride.

the synthesized product and its applications. El Harmoudi et al. [17] have reported the characterization of chitin and chitosan by infrared spectroscopy, nuclear magnetic resonance and theoretical calculation of UV–Vis spectra. They proposed theoretical approach depending on geometry optimization and relating quantum chemical calculations based on semi-empirical PM3 method within a framework of the confined Hartree–Fock approach. In addition, Arslan et al. [18] have calculated the vibrational frequencies and geometric parameters of the 5-chloro-10-oxa-3-thia-tricyclo [5.2.1.0^{1,5}]dec-8-ene-3,3-dioxide (COTDO) compound in the ground state to recognize the essentials from the exploratory vibrational frequencies and geometric parameters by utilizing the Hartree-Fock and density functional using Becke's three-parameter hybrid method with the Lee, Yang, and Parr correlation functional methods (B3LYP) with the standard 6-31G(d,p) and 6-311G(d,p) basis sets. Moreover, El Kouari et al. [19] have presented the theoretical calculations of UV spectra and second-order frequency-dependent molecular hyperpolarizability to propose NLO analysis of Anthocyanin's derivatives on a molecular scale. They explored that the quantum chemical calculations results can furnish the rule for finding of acquiescence of the calculated and experimental electronic properties in these types of molecules.

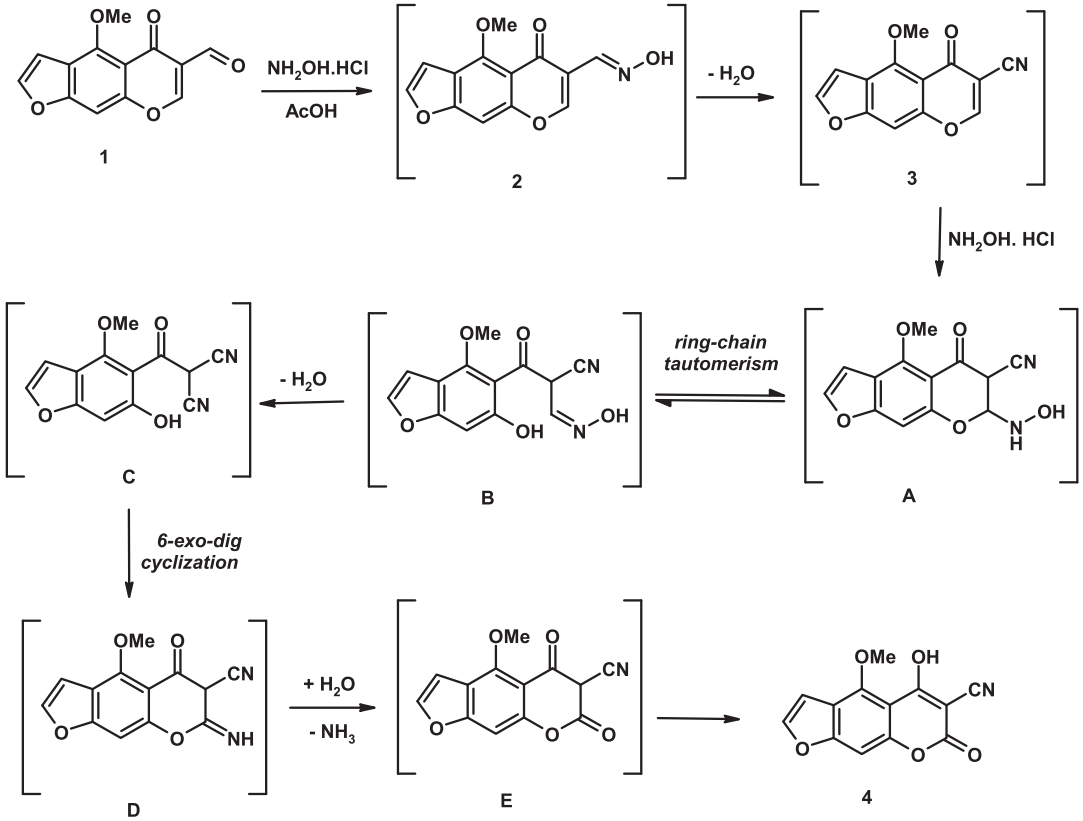

Fig. 2. The proposed mechanism for the formation of **HMOFCC**.