



# Synthesis and characterization of efficient photosensitive and DFT studies on 2-Benzylidene-1-(5,6-diphenyl-1,2,4-triazine-3-yl)hydrazine metal complexes

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## ABSTRACT

Co(II), Cu(II) and UO<sub>2</sub>(II)-complexes of 2-Benzylidene-1-(5,6-diphenyl-1,2,4-triazin-3-yl)hydrazine (HBDHT) have been synthesized and well characterized by elemental analyses, molar conductance, electronic and FT-IR, SEM and XRD techniques. Spectral data confirmed the molecular structure of the proposed complexes. Structural parameters of the present compounds were obtained using a density function (DFT) molecular orbital calculation at the B3LYP/6-31G(d) level implemented by the Gaussian 09 program. All the synthesized compounds may attend as potential photoactive provisions as indicated from their distinctive fluorescence. Moreover, the fluorescence studies showed that the order of emission wavelengths and Stokes shifts are HBDHT-complex > Co(II)-complex > UO<sub>2</sub>(II)-complex. Investigation of the absorption coefficient close to the absorption edge implies that the type of band gap is direct allowed and has a value of 3.75 eV. The heterojunction of Cu-BDHT films/p-Si showed remarkable rectifying behavior in dark as well as demonstrated distinguished photovoltaic characteristics under illumination of 100 mW/cm<sup>2</sup>. Furthermore, the time-dependent photocurrent investigation demonstrated an acceptable response time to the influence of light. This responsivity characteristic specifies a recommendation for the prepared heterojunction for opening another point of view in photodetector applications.

## 1. Introduction

Numerous biologically important Schiff bases of 1,2,4-triazine derivatives and their complexes have been reported in literature possessing, analytical, industrial, biological, clinical, biochemical, antimicrobial, anticancer, antibacterial, antifungal and antitumor activity [1–5]. Recently, triazine compounds have a major consideration because of their interesting photophysical properties and useful applications in organic light-emitting diodes [6–9]. The eventual challenge in handling conjugated molecules for optoelectronic applications is to improve universal tactics capable of controlling excited states for efficient electron-light conversions, giving conventional fluorescence [10–12] and non-linear optical, NLO applications [13–17]. This non-linearity optical characteristic originates from the presence of extended delocalized  $\pi$ -electron distribution and used for understanding the correlation between the optical properties with the molecular structures

of organic materials [13]. Derkowska et al. [14] have presented the results on third-order nonlinear optical characteristics of various metal-substituted phthalocyanines thin films and solutions. As an extension of these investigations, Zawadzka et al. [15,16] have investigated of the influence of metallophthalocyanine on the nonlinear optical characteristics as well as the annealing processes on the stacking orientations. In addition, Iliopoulos et al. [17] have discussed the enhancement of nonlinear optical response of bis-iminopyridine-tetrathiafulvalene and its zinc metal complex. Triazine, which holds high electron affinity and good thermal stability, is suitable to demonstrate the present work. In our earlier work metal complexes of, 2-Benzylidene-1-(5,6-diphenyl-1,2,4-triazin-3-yl) hydrazine, were isolated, characterized, DFT and optoelectronic considerations were achieved [18–20]. In the management of the above-mentioned goal, we herein report the synthesis, characterization, emission spectra and optoelectronic applications of Schiff base, shown in Fig. 1, derived from the condensation of 3-hydrazino-

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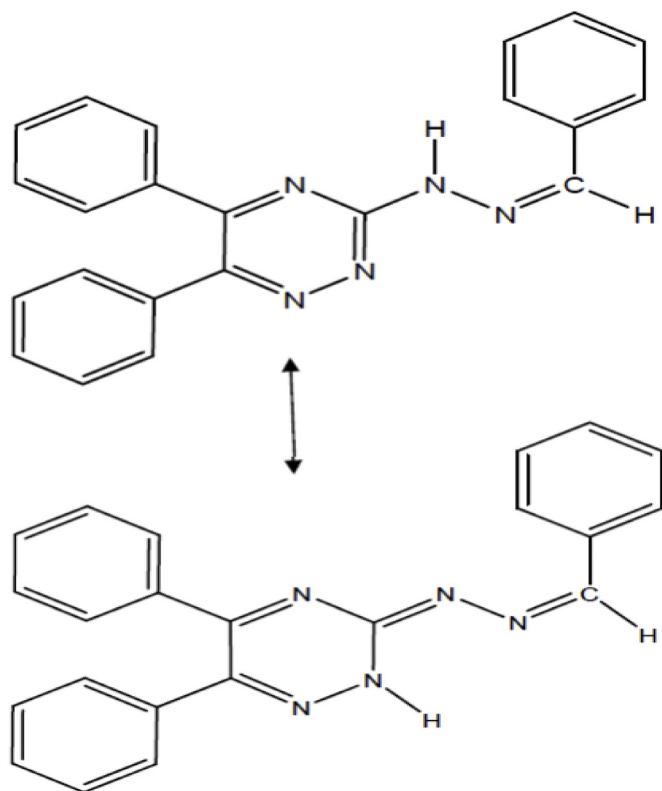


Fig. 1. Tautomerism of 2-benzylidene-1-(5,6-diphenyl-1,2,4-triazin-3-yl)hydrazine.

5,6-diphenyl-1,2,4-triazine with benzaldehyde and its Cu(II), Co(II) and UO<sub>2</sub>(II) metal complexes. Furthermore, computational studies were achieved on the basis of DFT at the B3LYP/6-31G (d) level embedded with the *Gaussian 09* program. Moreover, molecular, thermal, photoluminescence, optical and morphological properties were investigated. In addition, the electrical characteristics in dark and under lightening conditions are considered to comprehend the prime parameters of the heterojunction to investigate the photosensitivity properties for photodiodes applications.

## 2. Experimental

### 2.1. The preparation process

3-Hydrazino-5,6-diphenyl-1,2,4-triazine (DHT), was synthesized as described elsewhere [18]. A mixture of DHT (5.26 g, 20 mmol) and C<sub>6</sub>H<sub>5</sub>CHO (4.20 g, 20 mmol) was refluxed for 30 min in 50 mL of C<sub>2</sub>H<sub>5</sub>OH and left overnight at room temperature. The solid compound, obtained by adding cold water, was then recrystallized using aqueous ethanol (1: 3). Yield 5.15 g (72%) of the comparing Schiff base 2-Benzylidene-1-(5,6-diphenyl-1,2,4-triazin-3-yl) hydrazine (HBDHT), shown in Fig. 1, is obtained and the analytical and physical data are recorded in Table 1.

### 2.2. Preparation of the solid complexes

The solid complexes of Cu(II), Co(II) and UO<sub>2</sub>(II) were prepared by adding a respective metal ion dissolved in 20 mL of ethanol to the ligand HBDHT in 25 mL ethanol with continuous stirring for 30 min. The resultant solution was filtered off and let stand overnight. The resulting crude crystals are brown for Cu (II) and Co (II) complexes and yellow for UO<sub>2</sub> (II) complex. The obtained complexes were recrystallized from 1,2-dichloroethane (DCE).

### 2.3. Materials and methods

Chemicals and solvents employed were of analytical grade. The molecular structure investigations by FT-IR spectra using a Shimadzu FT-IR-8101 spectrometer in the region 4000–400 cm<sup>-1</sup>. A Perkin-Elmer 550S spectrophotometer was used to measure the electronic absorption. Magnetic moments were acquired utilizing an MSB-AUTO magnetic susceptibility balance by the Gouy method [21–23].

Thin films of Cu-BDHT complex were fabricated by employing POLOS spin coater. The topography of the films was explored utilizing type JEOL-JSM-636A OLA, scanning electron microscopy (SEM). The photoluminescence properties were determined by using RF-5301. The optical absorption characteristics of the films were recorded by JASCO 670 spectrophotometer. Single crystalline p-type Si (100) wafers were cleaned and etched to remove the oxygen layer by using the CP4 solution (HF: HNO<sub>3</sub>: CH<sub>3</sub>COOH with ratio 1:6:1). The electrical measurements were accomplished by utilizing Keithley type 2635 A. A halogen tungsten lamp was used for the illumination condition and the intensity of the light source was measured by using TM-206 solar power meter instrument.

## 3. Results and discussion

The structure of the ligand is shown in Fig. 1(a) and the proposed structures for the complexes are illustrated in Fig. 6. The acquired buildings are high stability in air, and sparingly soluble in water and other basic solvents yet are effortlessly solvent in polar coordinating (i.e. DMF and DMSO). The physical attributes of systematic information and molar conductance information of metal complexes are given in Table 1 and are in good agreement with the proposed form.

### 3.1. Molar conductance measurements

The molar conductance estimations of the present complexes were measured at room temperature for their methanolic solutions (10<sup>-3</sup> M) and the outcomes are recorded in Table 1. The values are 13, 62 and 55 Ω<sup>-1</sup> cm<sup>-1</sup> mol<sup>-1</sup> for Co(II)-, Cu(II)- and UO<sub>2</sub>(II)-complex, respectively, suggesting the non-electrolytic nature of Co(II)-complex. However, the molar conductance values of Cu(II)- and UO<sub>2</sub>(II)-complexes, reveal to either 1:1 electrolyte or partially ionization in methanol solution and/or replacement of solvent to the nitrate anion [24,25].

### 3.2. Molecular structural characterizations

The important molecular structural characterization obtained from infrared spectral data of the Schiff base and its metal complexes are listed in Table 2. The IR spectra of the Schiff base exhibited a strong band around 3454 cm<sup>-1</sup> which can be attributed to NH stretching vibration of HBDHT that disappeared in the resultant complexes. The results of the ligand and its complexes confirm the coordination modes of the ligand during complex formation. Thus, the red shift in the azomethine band, 1612 cm<sup>-1</sup> in free ligand, to the range (1590–1605 cm<sup>-1</sup>) in the IR spectra of the metal complexes, indicates that the azomethine nitrogen atom is coordinated to the metal ion. Likewise, a strong band at 1515 cm<sup>-1</sup> observed in the spectrum of free ligand, which might assigned to ν(C...C) + ν(C...N) group of triazine ring was shifted to a higher frequency of 1522–1575 cm<sup>-1</sup> in the complexes. This finding was further confirmed by observation of a new absorption band in the range (450–474 cm<sup>-1</sup>) due to the ν(M–N) [24].

### 3.3. Surface morphology characterization

The images of SEM of the spin-coated Cu(II)-complex films for different magnifications (5,000x and 20,000 x), as a representative example, are represented in Fig. 2(a–c). It is clear that the prepared films

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