



## PAPER

## Synthesis, DFT calculations and optical nonlinear properties of two derived Schiff base compounds from ethyl-4-amino benzoate

RECEIVED  
27 October 2021REVISED  
26 November 2021ACCEPTED FOR PUBLICATION  
3 December 2021PUBLISHED  
31 January 2022Hasanain A Abdullmaged<sup>1</sup>, H A Sultan<sup>2</sup>, Rafid H Al-Asadi<sup>1</sup>, Qusay M A Hassan<sup>2</sup> , Asaad A Ali<sup>1</sup> and C A Emshary<sup>2</sup><sup>1</sup> Department of Chemistry, College of Education for Pure Sciences, University of Basrah, Basrah 61001, Iraq<sup>2</sup> Department of Physics, College of Education for Pure Sciences, University of Basrah, Basrah 61001, IraqE-mail: [qusayali64@yahoo.co.in](mailto:qusayali64@yahoo.co.in)**Keywords:** Schiff base, DFT, Z-scan, NRI, OLg, optical materialsSupplementary material for this article is available [online](#)**Abstract**

Two Schiff base compounds viz., Ethyl (E)-4-((3-ethoxy-2-hydroxybenzylidene)amino)benzoate (EHB) and Ethyl (E)-4-(((2-hydroxynaphthalen-1-yl)methylene)amino)benzoate (ENB) are synthesized by condensation of ethyl-4-amino benzoate with 2-hydroxy-3-ethoxy benzaldehyde and 2-hydroxy-1-naphthaldehyde. The two compounds are studied and identified by FT-IR, UV-visible, Mass, <sup>1</sup>H-NMR, and <sup>13</sup>C-NMR spectroscopies. The nonlinear refractive index (NRI) of the two compounds are determined, for ENB compound via the diffraction ring patterns (DRPs) and the Z-scan and via Z-scan for the EHB compound, using continuous wave (CW) low power laser beam, and founds of the order of  $10^{-7} \text{ cm}^2 \text{ W}^{-1}$  due to the first technique and  $10^{-8} \text{ cm}^2 \text{ W}^{-1}$  due to the second technique. The optical limiting (OL) property of both compounds is studied too with OLg thresholds of 16.5 mW and 11 mW for the compounds EHB and ENB respectively, which makes these two compounds as candidates to be used as an optical limiter (OLr). The DRPs are numerically simulated based on the theory of Fresnel-Kirchhoff with reasonable agreement compared to the experimental findings.

**1. Introduction**

The passage of a continuous wave (CW) laser beam through a medium of the intensity-dependent index of refraction together with the coefficient of absorption leads to the number of amazing phenomena viz., self-focusing (SF) and defocusing (SDF), spatial ring formations, self-phase modulation (SPM), etc [1–11]. Based on the SPM and generally on the spatial self-phase modulation (SSPM) two types of interferences occur viz., destructive and constructive within the laser beam leads to a set of circular diffraction ring patterns (DRPs) depending on the laser beam power. SSPM has been extensively studied in different materials that suffer thermal-dependent changes in their index of refractions [12–22], liquid crystals [23], atomic vapors [24], photorefractive crystals [25], Kerr media [26], and nanosheet dispersion [27]. The number of rings per pattern generally depends on the nonlinear phase shift of the laser beam suffered during the passage through the nonlinear media. The phase shift amount depends on the beam input power, thickness of the sample, etc. The index of refraction change of the medium and the nonlinear refractive index (NRI) can be determined based on the number of rings at the maximum input power. The Z-scan [28], is another technique used to determine the medium NRI and its sign and real part and imaginary part of the nonlinear susceptibility.

Because of the widespread use of lasers in various areas of daily life, especially the low-power CW laser beam, the human eye needs a device that protects it against CW laser beams because it will be damaged when exposed even for short times to sub-Watt CW laser beam. This device is called the optical limiter (OLr). An OLr is a photonic device that has an ideal characteristic of optical limiting (OL). It shows three types of transmission viz., high linear at low power input, nonlinear at medium input power, and constant at high input power. Therefore, we find that work continues until today by researchers around the globe to study the thermal-optical effects in