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Synthesis and investigation of nonlinear optical properties of Para Red: Z-scan technique and quantum mechanical calculations

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In this study, we present a systematic study of linear and nonlinear optical properties of Para Red with the aim of Z-scan technique and quantum mechanical calculations. The Z-scan experiments were performed using a 532 nm Nd: YAG (SHG) CW laser beam. Para Red exhibited a strong nonlinear refractive index, nonlinear absorption coefficient and third-order nonlinear susceptibility 3.487×10^{-6} cm^2/W, 2.341×10^{-1} cm/W and 2.157×10^{-4} esu, respectively. Also, quantum chemical analysis was used for the calculation of the dipole moment μ, dipole polarizability α, anisotropy of polarizability Δα and molecular hyperpolarizabilities (β, γ). The results revealed that Para Red has large first and second hyperpolarizabilities. However, from the obtained results, it was found that Para Red can be a promising material for applications in the development of non-linear optical materials.

Keywords: *azo dye; nonlinear optics; nonlinear refractive index; Z-scan technique; polarizability; hyperpolarizability*

1. Introduction

Organic materials with extensive conjugated π system are expected to have relatively strong nonlinear optical properties because of delocalized electrons at π-π* orbitals [1]. This expectation explains extensive search for better nonlinear optical (NLO) materials among organic crystals. Nonlinear optical materials can be used in a wide variety of optoelectronic and photonic devices [2–5]. Over the years, organic molecules with nonlinear optical properties have gained great interest because of their very high nonlinear response, chemical stability, ease of molecular design, lower density and fast response time to optical excitation [6–10].

In recent years, various types of organic compounds have been studied to obtain materials with large third-order nonlinearity. NLO organic molecules possess a strong donor-acceptor intermolecular interaction due to the presence of easily polarizable delocalized π-electrons in the system [11–16].

A large number of organic materials have been found to exhibit NLO properties [17–21]. Further research on organic materials with excellent nonlinear optical properties and vigorous application has been carried out. Among organic compounds, azo dyes have also attracted attention due to their potential applications in many aspects, such as polarized photo-induced anisotropy and nonlinear optical effects [22, 23]. The π-conjugated organic azo dyes having good photothermal stability and easy preparation virtue were also found to have high optical nonlinearity, good optical power limiting properties and high damage resistance.

The molecular structure of azo dyes has the general structure Ar–N=N–Ar'. Azo dyes can be incorporated in cis and trans isomerization reaction upon light illumination. This transmission is reversible, which changes the absorption coefficient.

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Transitions of n $\rightarrow$ π^* and $\pi \rightarrow \pi^*$ type occur in these molecules which require low energy, and take place at longer wavelengths. In general, the greater the length of a conjugated system in a molecule, the nearer the λ_{max} comes to the visible region and the observed color is changing accordingly [24, 25].

Besides, in aromatic systems, a strong electron-donating group and a strong electron withdrawing group, para to one another on the aromatic ring is another factor which increases the intensity and wavelength of the absorption. Such absorptions arise from a charge transfer process, where electrons are moved from one part of the system to another due to the energy provided by the visible light.

The electronically excited state produced upon absorption of light has dipolar character that is stabilized relatively to the ground state, thus the ground state absorbs light of lower energy than could be expected for an analogous molecule without the electron donating/withdrawing groups.

Moreover, azo dyes can be readily prepared with a wide range of donor and acceptor groups in order to change their absorption band according to demands and lead to higher optical activity [26–28].

In this study, we have investigated nonlinear optical properties of Para Red. In first section, the nonlinear optical properties of Para Red (PR) have been measured by Z-scan technique according to the procedure reported by Sheik-Bahae et al. [29]. This is a simple and effective tool for determining the nonlinear refractive index n_2, nonlinear absorption coefficient β and the third-order nonlinear electric susceptibility $\chi^{(3)}$. This method can provide the magnitude of nonlinear absorption and the sign and magnitude of nonlinear refraction simultaneously. Therefore it has been widely used in material characterization [30, 31].

In the second section, the electric dipole moment μ, dipole polarizability α, first and second hyperpolarizability β, γ and the anisotropy of the polarizability $\Delta\alpha$ are calculated using quantum mechanical methods.

2. Experimental

2.1. Material and methods

The linear absorption spectra of the sample were recorded with a double-beam Shimadzu 1700 spectrophotometer. To perform the Z-scan experiments, a Q-switched NdVYVO4 laser from the EKSPLA Company (model NL640) was used. The light source was coupled to a second harmonic generation unit (SHG) which generates 532 nm laser pulses with 10 ns pulse duration and 200 Hz repetition rate. The beam waist radius at the focal point was 80 μm.

All quantum chemical calculations were carried out with the Gaussian program 09 [32], as basic program and Gaussian Viewer as graphical medium. The calculations of DFT were carried out by using the three B3LYP functional. The usual 6-31G basis set was employed in the DFT calculations.

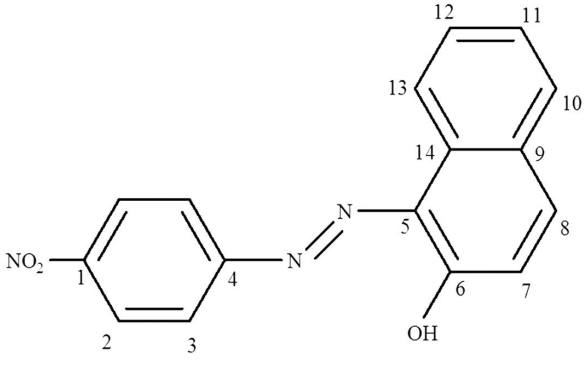

Fig. 1. Molecular structure of Para Red.

2.2. Synthesis of 1-[(E)-[(4-nitrophenyl) diazenyl]-2-naphthol PR

Para Red was synthesized by the method reported in the literature [33]. To a stirred solution of 4-nitroaniline (1 g, 7 mmol), in 1 M sulfuric acid (10 mL) at 0 °C, sodium nitrite solution in water (1 M, 10 mL) was added slowly so that no gas formation or coloring occurred. Then, a solution of 1 g (7 mmol) of 2-naphthol in 10 mL of 2.5 M sodium hydroxide was added into the flask in an ice bath, at vigorous stirring for 30 min. The mixture was

acidified with 1 M sulfuric acid. The formed precipitate was filtered and washed with water. The crude product was purified by recrystallization. The red product was characterized by FT-IR, UV, and HNMR spectroscopy. Yield: 75 %; purity >98 %; mp: 245 °C to 246 °C. Molecular structure of Para Red is presented in Fig. 1.

IR (KBr, cm^{-1}): 3423 (m, OH), 1593 (s, C=C), 1501 (s, asym NO_2), 1338 (s, sym NO_2), 860 (s, C–H), 836 (s, C–H).

^{1}H NMR: δ_H(ppm) (300 MHz, CDCl3): 4.69 (1H, s, OH) 6.70 (1H, d, J = 9 Hz, Ar-H7) 7.34 to 7.50 (1H, m, Ar-H11) 7.50 to 7.61 (2H, m, Ar-H10,12) 7.64 to 7.78 (3H, m, Ar-H3,8) 8.33 (2H, d, J = 9 Hz, Ar-H2) 8.42 (1H, d, J = 8 Hz, Ar-H13), 16.13 (1H, NH).

Accurate mass: $C_{16}H_{12}N_3O_3$ requires 292.0719, found 292.0727.

3. Results and discussion

The Z-scan measurement is a common technique which utilizes a tightly focused laser beam onto a nonlinear sample medium. The sample under investigation is moved along the laser beam direction (z direction) in and out of the laser focal point and the power transmitted through the sample is measured. An open aperture Z-scan is produced when all of the transmitted energy is collected. However, when an aperture is placed after the sample, a closed aperture Z-scan is produced [29, 34].

The measurements of the nonlinear absorption coefficient β and the nonlinear refractive index n_2 for Para Red in the acetonitrile solution has been carried out using open and closed apertures, respectively.

3.1. UV-Vis absorption spectrum

The UV-Vis absorption spectrum of Para Red is presented in Fig. 2. As can be seen, the spectrum shows absorption peaks at 285 nm (n → π), 324 nm (π → π*) and 482 nm (π → π*) and it is almost transparent in the near infrared region.

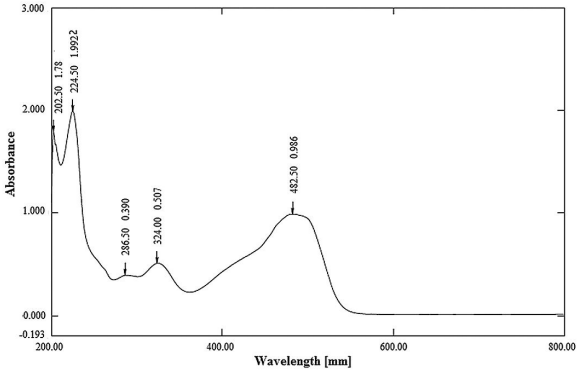

Fig. 2. UV-Vis absorption spectra of Para Red in acetonitrile.

3.2. Nonlinear absorption coefficient

Essentially, in the open-aperture Z-scan (S = 1), the laser pulse energy can remain constant, but the beam intensity at the sample varies as the sample position is changed in the z-direction due to the changing beam diameter at the sample. For measuring the nonlinear absorption coefficient, the open-aperture Z-scan has been used. In other word, there is no aperture in front of the detector and the whole signal is measured. Then a normalized transmittance graph has been plotted as a function of sample position [34]. The normalized transmittance of open aperture Z-scan at the wavelength of 532 nm of Para Red is presented in Fig. 3.

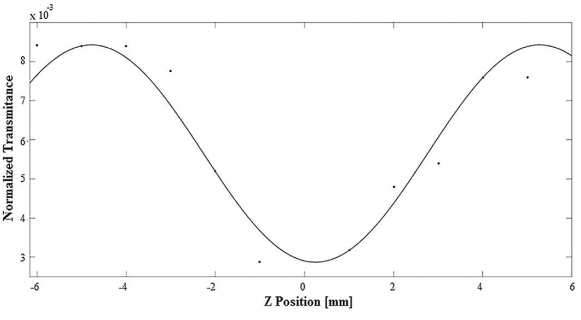

Fig. 3. Open aperture Z-Scan data for Para Red solution.

As it is seen in Fig. 3, the open aperture curve indicates a valley shape which is a signature of a positive nonlinear absorption (NLA) coefficient which is in agreement with the two-photon absorption process.

The nonlinear absorption cross-section of the Para Red can be easily calculated from the data of transmittance curve in open-aperture Z-scan, using the following equations [35, 36]:

$$T(z, s=1) = \sum_{m=0}^{\infty} \frac{\left[\frac{\beta I_o L_{eff}}{1+\left(\frac{Z}{Z_0}\right)^2}\right]^m}{(m+1)^{\frac{3}{2}}} \quad (1)$$

where

$$Z_0 = \frac{K\omega_0^2}{2} \quad (2)$$

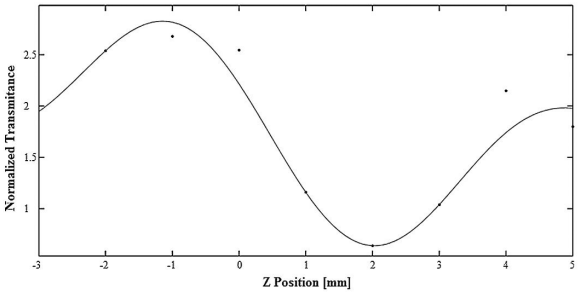

Fig. 4. Closed aperture Z-Scan data for Para Red solution.

In the above equations, T is the total transmittance, β is NLA coefficient, I_0 is the peak on-axis irradiation at the focus, Z is the sample position at the minimum transmittance, Z_0 is diffraction length, and L_{eff} is the effective thickness of the sample; it can be expressed by equation 3:

$$L_{eff} = \frac{[1-\exp(-\alpha L)]}{\alpha} \quad (3)$$

where

$$\alpha = -\frac{1}{L}\ln\left(\frac{P}{P_0}\right) \quad (4)$$

The nonlinear absorption coefficient of Para Red is shown in Table 1. From the presented results, it is evident that the nonlinear absorption coefficient β is positive, and two-photon absorption occurred in this case.

3.3. Nonlinear refractive index

For measuring the nonlinear index of refraction n_2, the Z-scan setup has been used in its closed-aperture form. In this experiment, the aperture is placed in front of detector. Therefore, only the central region of the cone of light is reached to the detector. The amount of energy transmitted through the aperture depends on the sample position and sign of nonlinear refractive index n_2. In Fig. 4, the normalized transmittance of closed aperture Z-scan is plotted as a function of distance from the focus point (Z = 0). As can be seen, the curve exhibits a peak followed by a valley, indicating a negative nonlinearity.

$\Delta T_{p\text{-}v}$ is the distance between the peak and valley transmittance which is obtained from Fig. 4. However, $\Delta T_{p\text{-}v}$ is related to the nonlinear refractive index n_2 by the following equation [35, 36]:

$$\Delta T_{p\text{-}v} = 0.406(1-S)^{0.25}\left(\frac{2\pi}{\lambda}\right) n_2 I_0 L_{eff} \quad (5)$$

where n_2 is the nonlinear refractive index and I_0 is the intensity in the focused sample as follows:

$$I_0 = \frac{2p}{\pi\omega^2} \quad (6)$$

and S is the linear transition which is given by:

$$S = 1 - exp\left(\frac{-2r_a^2}{\omega_a^2}\right) \quad (7)$$

where r_a is the radius of aperture and ω_a is the radius of the beam at the aperture.

Additionally, we can estimate the induced refractive index change Δn using equation 8:

$$\Delta n = n_2 I \quad (8)$$

The nonlinear refractive index n_2 and the induced refractive index change Δn have been calculated from equation 5 to equation 8 and presented in Table 1. These results indicate that the nonlinearity in this case is of thermal origin.

Thermal processes can lead to large nonlinear optical effects. When a high intensity laser beam

propagates through an optical material, some fraction of the incident laser power is absorbed. Consequently, the temperature of the illuminated portion of the material increases, and induced refractive index changes, which leads to self-focusing or defocusing of the laser beam [37].

3.4. Third order susceptibility $\chi^{(3)}$

Experimentally obtained value of nonlinear refractive index n_2 and nonlinear absorption coefficient β are related to the real and imaginary parts of the third-order susceptibility $\chi^{(3)}$ as follows [38]:

$$Re\chi^{(3)}(esu) = \left(\frac{10^{-4}\varepsilon_0 c^2 n_0^2}{\pi}\right) n_2, \quad \text{in} \left[\frac{\text{cm}^2}{\text{W}}\right] \tag{9}$$

$$Im\chi^{(3)}(esu) = \left(\frac{10^{-2}\varepsilon_0 c^2 n_0^2\,\lambda}{4\pi^2}\right)\beta, \quad \text{in} \left[\frac{\text{cm}}{\text{W}}\right] \tag{10}$$

where n_2 is the nonlinear refractive index, n_0 is the linear refractive index, c is the speed of light in vacuum and ϵ_0 is the vacuum permittivity.

However, the absolute value of the third-order nonlinear optical susceptibility can be obtained by:

$$\left|\chi^{(3)}\right| = \left\{\left[Re(\chi^{(3)})\right]^2 + \left[Im(\chi^{(3)})\right]^2\right\}^{1/2} \tag{11}$$

The values of the third order nonlinear susceptibility and the related properties obtained for Para Red are listed in Table 1.

From the obtained results, it is found that Para Red possess a large third-order nonlinear susceptibility with a magnitude of the order of 10^{-4} esu (Table 1).

3.5. Quantum mechanical calculations

The theoretical analysis performed by computer simulation is an invaluable and inexpensive tool for clarifying the electronical, mechanical and optical properties of different molecules. In this section, we used the quantum mechanical calculations for predicting the molecular NLO properties of Para Red.

We have reported the calculations of the electric dipole moment μ, dipole polarizability α, first and second hyperpolarizability β, γ and the anisotropy of the polarizability Δα of Para Red.

Polarizability is the ability to form instantaneous dipoles. It is a property of matter. The isotropic (or average) linear polarizability α expresses the capacity of the charge density of a system to be changed under the influence of an external field. Magnitude of the average polarizability α_{av} and anisotropy of polarizability Δα, were calculated from the polarizability components as follows [39]:

$$\alpha_{ve} = \frac{1}{3}(\alpha_{xx} + \alpha_{yy} + \alpha\alpha_{zz}) \tag{12}$$

$$\Delta\alpha = \frac{1}{2}\left[(\alpha_{xx} - \alpha_{yy})^2 + (\alpha_{xx} - \alpha_{zz})^2 + (\alpha_{yy} - \alpha_{zz})^2\right]^{1/2} \tag{13}$$

The total first hyperpolarizability β that is often studied using second-harmonic generation (SHG) in solution, can be calculated using following equation [40, 41]:

$$\beta_{tot} = \left[(\beta_{xxx} + \beta_{xyy} + \beta_{xzz})^2 + (\beta_{yyy} + \beta_{yzz} + \beta_{yxx})^2 + (\beta_{zzz} + \beta_{zxx} + \beta_{zyy})^2\right]^{1/2} \tag{14}$$

The third-order optical nonlinearity γ of molecules is often studied using third-harmonic generation (THG) in solution. In an isotropic liquid, one has to consider only the rotational average of γ_{ijkl}, for which one gets [42–44]:

$$\gamma \equiv \gamma_{zzzz} = \frac{1}{5}\left[\gamma_{xxxx} + \gamma_{yyyy} + \gamma_{zzzz} + 2\left(\gamma_{xxyy} + \gamma_{xxzz} + \gamma_{yyzz}\right)\right] \tag{15}$$

The components of the electric dipole moment μ, dipole polarizability α, first and second hyperpolarizability β, γ and the anisotropy of the polarizability Δα of Para Red are shown in Table 2.

The magnitude of the molecular hyperpolarizability β and total dipole moment, are two key factors in NLO system. As can be seen from Table 2,

Table 1. Calculated third order nonlinear optical parameters of Para Red.

$n_2 \times 10^{-6}$ [cm^2/W]	$\beta \times 10^{-1}$ [cm/W]	Re $\chi^{(3)} \times 10^{-4}$ [esu]	Im $\chi^{(3)} \times 10^{-4}$ [esu]	$\chi^{(3)} \times 10^{-4}$ [esu]
3.487	2.341	–1.6088	1.438	2.157

Table 2. The electric dipole moment μ, dipole polarizability α, first and second hyperpolarizability β, γ and the anisotropy of the polarizability $\Delta\alpha$ of Para Red.

μ [debye]	α [a.u]	$\Delta\alpha$ [a.u]	β [a.u]	$\langle\gamma\rangle$ [a.u]
5.3970	131.2442	255.5163	188.1372	3512.5055

Para Red has large hyperpolarizabilities and total dipole moment, so it may have potential applications in the development of NLO materials. Therefore it is an attractive target for future studies of nonlinear optical properties.

This investigation proves that the nonlinear optical properties of Para Red can be successfully predicted by B3LYP method with the used basis sets.

4. Conclusions

In this research, nonlinear optical properties of Para Red have been studied successfully by Z-scan technique and quantum chemical calculations. The measured nonlinear refractive index, first hyperpolarizability β and third order nonlinear susceptibility were 3.487×10^{-6} cm^2/W, 2.341×10^{-1} cm/W and 2.157×10^{-4} esu, respectively. Also, this investigation proved that the nonlinear optical properties of Para Red can be successfully predicted by DFT methods with B3LYP basis sets. The calculated value of first hyperpolarizability β was 1.625×10^{-30} esu.

The obtained results, which are optimal for possible application in different optoelectronic devices, showed that Para Red might have the good NLO properties. These attractive properties of Para Red could be exploited in developing it as a NLO material, for future photonic and optoelectronic applications.

Information obtained for electric dipole moment μ, dipole polarizability α, first and second hyperpolarizability β, γ and the anisotropy of the polarizability $\Delta\alpha$ are a valuable part of planning chemical experiments, as well as a support for the explanation of obtained experimental results. In addition, the computation analysis of this compound is in excellent agreement with all the experimental findings. We hope that the combination of theoretical and experimental data will provide relevant information on the nonlinear optical properties of materials.

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