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DFT calculation and nonlinear optical properties of (E)-(2)-((8-hydroxyquinolin-5yl)diazenyl)-5-sulfamoylpheneyl)mercury (II) chloride

Dhia A. Hassan [a], H.A. Sultan [b], Rafid H. Al-Asadi [a], Qusay M.A. Hassan [b,*], C.A. Emshary [b], Tarek Fahad [a]

[a] Department of Chemistry, College of Education for Pure Sciences, University of Basrah, Basrah, 61004, Iraq
[b] Department of Physics, College of Education for Pure Sciences, University of Basrah, Basrah, 61004, Iraq

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ABSTRACT

The molecular structure of mercurated azo compound (A1), (E)-(2-((8-hydroxyquinolin-5-yl)diazenyl)-5-sulfamoylphenyl)mercury(II) chloride, is investigated theoretically by the DFT with the GGA approximation, PEB level and DNP as basis set. The nonlinear optical (NLO) properties of the synthesized azo compound are investigated using a continuous wave (cw), low power, with TEM_{00} mode laser beam using the methods diffraction ring patterns (DRPs) and Z-scan. The nonlinear refraction index (NRI) is calculated based on both methods where as high as 5.28×10^{-7} cm^2/W of the NRI is determined via the DRPs. The optical limiting (OLg) property of the A1 compound is examined with limiting threshold of 10 mW is determined. The experimentally determined DRPs are simulated via Fresnel-Kirchhoff integral with good accord of experimental and theoretical results.

1. Introduction

The exploration of new different materials showing high optical nonlinear response in short times to laser lights is the object of continuous intense research during the last forty years. The interaction of coherent laser light with nonlinear medium leads to many effects in the spatial dimensions viz., self-phase modulation (SPM), self-focusing (SF) and defocusing (SDF) etc. SPM effect is the result of intensity dependent complex refractive index, CRI, which was noticed to occur in so many materials viz., liquid crystals [1], atomic vapors [2], nanostructured materials [3], polymers [4], dyes [5–11], etc. The formation of diffraction ring patterns (DRPs) is one of the results that occur due to SPM. These DPRs can be adopted in the calculation of changes in the medium refraction index (Δn) and nonlinear refraction index (NRI), n_2, via the total rings number of in the PDRs. The deformation of the laser beam wavefront, leads to the Z-scan [12] which is very useful in the determination of the NRI, n_2, the nonlinear absorption coefficient, NAC, etc.

Nonlinear optical (NLO) materials are essential of many applications such as optical computing [13], all-optical switching [14, 15], optical limiting [16–30], optical communication [31], phase conjugation [32], modulation [33], and data storage [34–37].

The azo compounds are considered as one of the largest group of organic compounds and the biggest industrial compounds in dyeing market. It represents more than 60% of the total pigments in the world [38,39]. Azo dyes have many important applications such as printing, pharmaceutical, textile, cosmetics, food, paper manufacturing, etc. [40]. Azo dyes have –N=N–group which is attached to at least one aromatic ring or both are aromatic or heteroaromatic systems, it absorb light in the visible region because of their structures. The colors of azo compounds can be determined by azo group that associate with chromogens, auxochromes, and other chromophores exhibit high intensity of color and brightness [41,42].

Mercurated azo compounds were used in synthesis of organtellurium. It is prepared by mercuration of azobenzen then transmetallation with $TeCl_4$ [43,44]. These compounds have received substantial attention because of their biological activity [45,46]. There are few reports on mercurated azo compounds. The stability, anti-bacterial and antifungal activities of these compounds were studied, together with their molecular structure and energies were

* Corresponding author.
E-mail address: qusayali64@yahoo.co.in (Q.M.A. Hassan).

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