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Nonlinear Optical Property Of 6'-Amino-5-Fluoro -2-Oxo-3'-Propyl-2'*H*-Spiro[Indoline-3,4'-Pyrano [2,3-*C*]Pyrazole]-5'-Carbonitrile- A Theoretical Approach

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Abstract

We present a DFT based study of the non-liniear optical property of 6'-Amino-5-fluoro-2-oxo-3'-propyl-2'H-spiro[indoline-3,4'-pyrano[2,3-c] pyrazole]-5'-carbonitrile. The geometry optimization first static hyperpolarizability, dipole moment and polarizability of the compound are performed using B3LYP/6-311+G(d,p) level of theory. The calculated hyperpolarizability, dipole moment and polarizability of the title compound is compared with urea at the same level of theory. The study reveals that the title compound possesses large value than urea hence in general may have potential application in the development of nonlinear optical material.

Keywords: DFT; Hyperpolarizability; Dipole Moment; Polarizability

Abbreviations: DFT: Density Functional Theory; PES: Potential Energy Surface; NLO: Nonlinear Optics

Introduction

The Nonlinear Optics (NLO) of materials was started after the Kerr's observations of quadratic electric field induced changes in the refraction index, known as the Kerr effect [1] in 1875. This was followed by the observation of the Pockel's effect. The organic compounds with large optical nonlinearities have become the focus of current research in view of their potential applications in various photonic technologies, including all optical switching and data processing. Organic molecules that exhibit extended pi conjugation, in particular, show enhanced second order NLO properties. The equilibrium geometry and NLO property of 6'-Amino-5-fluoro-2-oxo-3'-propyl-2'H-spiro[indoline-3,4'-pyrano[2,3-c]pyrazole]-5'-carbonitrile have been calculated by using Density Functional Theory (DFT).

Computational Details

In the present study all the DFT calculations were performed with the help of Gaussian 09 program [2] using a hybrid functional B3LYP and employing 6-311+G (d,p) as a basis set. The geometry of the title compound was fully optimized without any constraint in Potential Energy Surface (PES). The optimized structure of the molecule has been visualized by the use of the Gauss View 5.0 molecular visualization program [3].

Result and Discussion

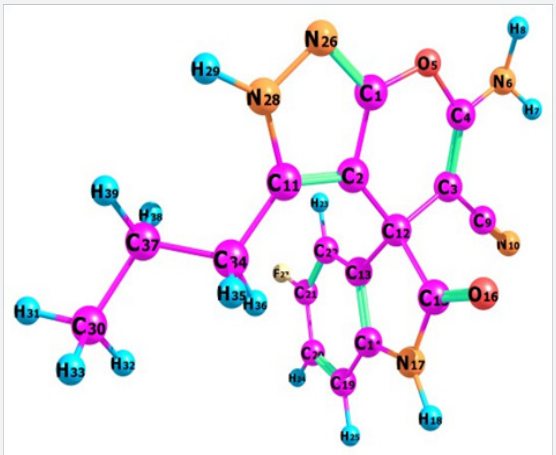

Figure 1: (a) Optimized geometry of title compound with labeled atom.

The optimized geometry of the 6'-Amino-5-fluoro-2-oxo-3'-propyl-2'*H*-spiro[indoline-3,4'-pyrano[2,3-c]pyrazole]-5'-carbonitrile is shown in Figure 1 with proper atomic labeling. The compounds that shows asymmetric polarization induced by electron donor and acceptor groups in pi electron conjugated molecules are candidates for electro optic and NLO applications [4] (Figure 1).

Non-linear optical property

The NLO property provides useful information for optical modulation, optical switching and optical logic for the developing new technologies in area of communication. Previously, It has been reported that molecules having conjugated pi electrons are found to possess large values of polarizability [5-8]. The intra-molecular charge transfer from electron rich system to electron poor system through a conjugated path can induce a large aberration in both the molecular dipole as well as molecular polarizability. The abnormally high value of hyperpolarizability β, which is a critical parameter of non linear activity of molecular systems, can be presumably linked to intramolecular charge transfer, as a consequence of electron cloud movement through pi conjugated system. The first-order hyperpolarizability (β_0) and related properties (μ_0 and $|\alpha_0|$) of 6'-Amino-5-fluoro-2-oxo-3'-propyl-2'*H*-spiro[indoline-3,4'-pyrano[2,3-c]pyrazole]-5'-carbonitrile have been calculated at the B3LYP/6-311+G (d, p) level of theory. First hyperpolarizability is a third rank tensor of order three that can be described by a 3×3×3 matrix. The 27 components of the order 3 matrix can be reduced to 10 components using the Kleinman Symmetry [9] and it can be presented in the lower tetrahedral format. The components of β0 are defined as the coefficient in the Taylor series expansion of the energy in the external electric field.

The total dipole moment (μ_0), anisotropy of the polarizability($|\alpha_0|$), the mean polarizability (Δα) and the total first hyperpolarizability (β_0) using x, y and z components are

$\mu 0 = (\mu_x^2 + \mu_y^2 + \mu_z^2)1/2$ defined as [47],

$$|\alpha_0| = 1/3(\alpha_{xx} + \alpha_{yy} + \alpha_{zz})$$

$$\beta 0 = (\beta_x^2 + \beta_x^2 + \beta_x^2)1/2$$

Where,

$$\Delta\alpha = 1/21/2\left[(\alpha_{xx} - \alpha_{yy})2 + (\alpha_{yy} - \alpha_{zz})2 + (\alpha_{zz} - \alpha_{xx})2\right]1/2$$

The calculated first-order hyperpolarizability (β_0), dipole moment (μ_0) and mean polarizability ($|\alpha_0|$) for the

Molecule is listed in Table 1. It can be seen that the calculated β0 and μ0 values of title compound are more than the value of urea and are also listed in Table 1. Hence it can be said that the molecule exhibits promising nonlinear optical property (Table 1).

Table 1: The calculated hyperpolarizability βtot (× 10-30 esu), polarizability (× 10-24 esu), dipole moment (μ in Debye) of 6'-Amino-5-fluoro-2-oxo-3'-propyl-2'H-spiro[indoline-3,4'-pyrano[2,3-c]pyrazole]-5'-carbonitrile and Urea at B3LYP/6-311+G (d, p) level.

First order molecular hyperpolarizability	Urea	Carbonitrile
β_{xxx}	0.0035	84.0340
β_{xxy}	37.74	271.5962
β_{xyy}	-0.0047	-8.6442
β_{yyy}	-63.7591	47.8002
β_{xxz}	-3.9319	25.8471
β_{xyz}	-0.0013	61.4904
β_{yyz}	-2.9356	27.6061
β_{xzz}	0.0034	19.1140
β_{yzz}	-33.0484	82.9696
β_{zzz}	12.7984	47.8746
β_0	0.51286	3.6405
Dipole moment		
μ_x	0.0004	-4.4850
	-4.3607	2.3181
μ_z	1.2339	0.3830
μ_0	4.5319	5.0632
Polarizability μy		
α_{xx}	36.7020	232.4715
α_{xy}	-0.0004	5.2350
α_{yy}	38.5858	269.0669
α_{yz}	0.00008	6.0684
αzx	0.2407	-5.7932

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α_{zz}	24.1111	192.4789
$\|\alpha_0\|$	4.9102	34.280
Δ_α	2.02006	9.8329

Conclusion

We have performed theoretical study on molecular structure and NLO properties of 6'-Amino-5-fluoro-2-oxo-3'-propyl-2'H-spiro[indoline-3,4'-pyrano[2,3-c]pyrazole]-5'-carbonitrile with the help of density functional theory. Significantly high non linearity is observed in first order molecular hyperpolarizability and polarizability. So this molecule may have potential application in the development of NLO materials.

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