THEORETICAL DETERMINATION OF NLO, CHEMICAL REACTIVITY AND TD PARAMETERS OF (1S*, 4R*,7S*)-(E)-7-(2,5-DIMETHOXYPHE NYL)-3,3-DIMETHOXY-5-(2NITROVINYL)BICYCLO[2.2.2]OCT-5-EN-2- ONE USING DFT METHOD

Abstract

FMO (Frontier molecular orbital) method was used to understand the stability of the (1S*,4R*,7S*)-(E)-7-(2,5 Dimethoxyphenyl)-3,3-dimethoxy-5-(2nitrovinyl)bicycle [2.2.2] oct-5-en-2-one (DNB) molecule. Non-linear optical properties like dipole moment and hyperpolarizability were calculated, and common thermodynamic parameters also estimated for DNB.

Keywords: NLO, Parameters, Chemical reactivity

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I. INTRODUCTION

(1S*,4R*,7S*)-(E)-7-(2,5-Dimethoxyphenyl)-3,3-dimethoxy-5-(2nitrovinyl)bicycle [2.2.2] oct-5-en-2-one (DNB) molecule was synthesized by Sharma et al[1]. It belongs to hypervalent iodine chemistry, and acts as good reagents in synthesis of organic molecules [2]. To generate the masked o-benzoquinones and benzoquinone monoamines, hypervalent molecules plays a vital role [3]. Diels-Alder reaction of o-benzoquinones and benzoquinone monoamines is identified as key step of producing biologically dynamic molecules [4] and many natural products [5-6]. However, the calculations of Non-linear optical properties, chemical reactivity and thermodynamic parameters are yet to appear in literature. We computed such quantum chemical calculations recently [7-15] and now extended the investigations to the selected molecule DNB, in this article.

II. COMPUTATIONAL INFORMATION

Computational quantum chemical estimations carried out by using DFT, incorporated in 09 Gaussian window package [16,17] with 6-311++G(d,p) basis set. NLO properties of the DNB calculated by DFT method of finite field [18]. The Chemical reactivity of the selected molecule also determined using the methods [19-23]. By assuming a rigid-rotor harmonic approximation [24], we estimated the thermodynamic parameters for the chosen molecule.

III. RESULTS AND DISCUSSIONS

1. **Molecular Geometry:** DNB molecule is optimized with above said method. The geometry parameters were excellent agreement with the experimental values [1]. By the calculation the DNB molecule has been belongs to C_1 symmetry and its optimized molecular structure as shown in figure.

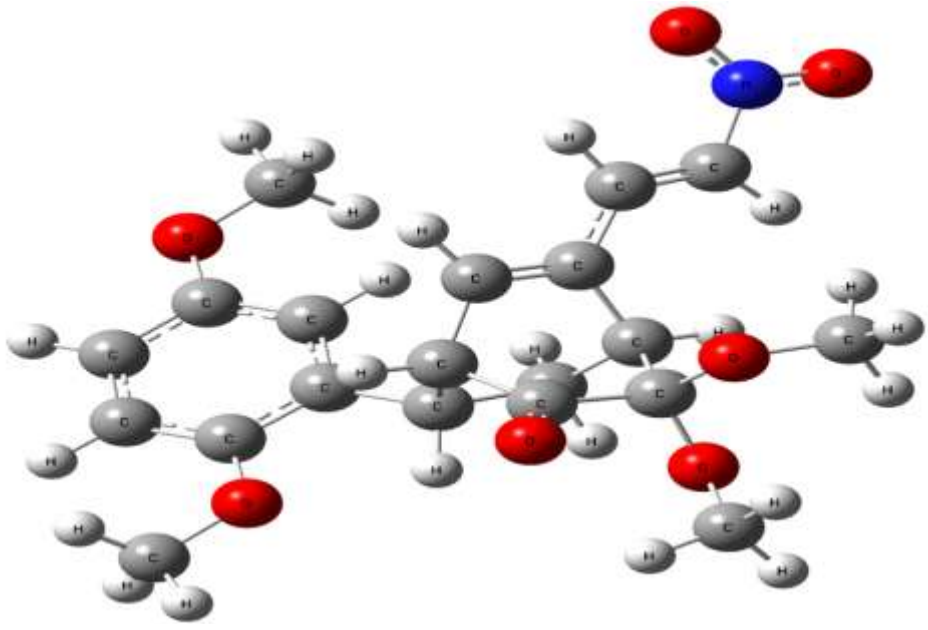

Figure 1: Optimized structure of DNB

2. **NLO Properties:** When Electromagnetic radiation interacts with NLO material, then change occurse in phase, amplitude, frequency, or gives the new propagation field characteristics [25]. If this change is significant then the NLO material used in signal processing, optical inter-connections telecommunications and optical memory [26-29]. Using DFT techniques, expansively investigate organic NLO materials [30-34].

The NLO behavior of selected compound is judged by comparing the related quantities of Urea. For Urea, hyper polarizability (β_t) and dipole moment(μ_t) are 372.8 × 10^{-33} $cm^{5/}$esu and 1.3732 Debye, respectively. For DNB, these values are β_t = 8272.174 × 10^{-33} $cm^{5/}$esu and μ_t = 2.415 Debye. The estimated values are very high compared with that of Urea; hence DNB is a sturdy contender for the enlargement of novel NLO materials. β_t components are very helpful to identify the delocalization of charge in the DNB.

3. **Chemical Reactivity:** The parameters of FMO were calculated for the molecule DNB. From the calculations we observed that the energy gap, linking the LUMO and HOMO orbital energies is 2.340 eV. It is comparatively small, worth to characterize a conjugated molecule. The chemical potential (μ) is negative for DNB, and is stable [35, 36].

4. **Thermodynamic Parameters:** Thermodynamic parameters such as entropy, C_v, C_p were determined (183.955, 101.541 and 103.526) in cal mol^{-1} K^{-1}. ZPV energy and TT energy (256.040 and 273.100 kcal mol^{-1}), SCF energy -1357.486 Hartree were calculated for chosen molecule. Further, the rotational constants were A, B and C also calculated as (0.201, 0.138 and 0.088 GHz) for the selected molecule.

IV. CONCLUSION

The Following Inferences are Drawn from the Calculations

- DNB molecule has the non-planar structure acquiring point group of C_1 symmetry. Theoretically calculated geometric parameters of DNB are excellent agreement with the values of experimental.
- DNB is a good candidate for NLO materials.

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