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on 11 & 12 May 2023 and presented a paper (Oral) entitled *Structural analysis and hydrogen bonding interactions on 2,2-Benzene-2,4-dicybis(imino aceto nitrile)(BDIN) and water mixture by density Functional Theory.*

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Structural Analysis and hydrogen bonding interactions on 2,2-Benzene-2, 4-diylbis(imino aceto nitrile) (BDIN) and Water mixture by Density Functionl Theory

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Abstract

The geometrical parameters, different inter and intra molecular interactions of 2,2-Benzene-2, 4-diylbis(imino aceto nitrile) (BDIN) and its water complex (BDIN.H₂O) has been performed using density functional theory (DFT) method with 6-311++G(D,P) basis set. Natural bonding orbital (NBO) analysis and optimized molecular structure show the clear evidence for electronic interaction of within the molecules. HOMO- LUMO energy gap local softness and electrophilicity indices selected atomic site of the BDIN and its water complex were determined. The first and second order hyperpolarizability confirm the NLO property of the Molecules.

Keywords:DFT;NBO;HOMO-LUMO;NLO.

1. Introduction

Non-linear optical (NLO) materials have recently engaged a lot of concentration due to their potential use in the fields like laser technology, optical communication, optical data storage and optical signal processing. In this respect organic nonlinear optical materials are found to have high nonlinear coefficient equated to those of inorganic materials. In the present work the structural analysis of NLO compound 2,2-Benzene-2, 4-diylbis(imino aceto nitrile) (BDIN) and its water complex (BDIN.H₂O) have been performed. The review of literature explore that there is no detailed theoretical spectroscopic study on BDIN have been performed. This encourages performing the structural analysis of BDIN and BDIN.H₂O complex compounds. In the present investigation, the structural and spectral analysis of the NLO compounds BDIN and BDIN.H₂O complex have been selected for comparative study, and their calculations were performed with the help of density functional theory (DFT) approach. BDIN and BDIN.H₂O complex has been selected to compare the structure activity, relationship and NLO activity by computational methods.

2. Computational methods

Gaussian'09 software package as used for theoretical calculation. The quantum chemical calculations were performed by applying DFT method with Becke3-Lee-YangParr (B3LYP) supplemented with the standard 6-311G(d,p) basis set[1]. The optimized geometry corresponding to the minimum on the potential energy surface has been secure by solving self-

consistent field equation iteratively. The natural bonding orbital (NBO) calculations were performed using NBO 3.1 [2] program and were implemented in the Gaussian software. HOMO- LUMO energy gap local softness and electrophilicity indices selected atomic site of the BDIN and its water complex was prepared by using the gaussian 2.2 program. The hyperconjugative interaction energy was deduced from the second order perturbation approach [3]. The polarizability first and second order hyperpolarizability were calculated using Gaussian 09 software package at B3LYP/6-311 G(d,p) basis set level.

3. Result and Discussion

Optimized geometre of the compound BDIN and BDIN.H₂O complex with atom numbering scheme adopted in the computation are shown in fig.1 and 2

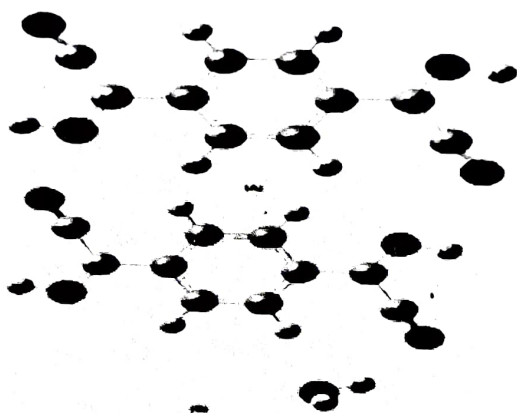


Fig 3.1. Optimized structure of (A). BDIN and BDIN.H₂O complex

In BDIN and BDIN.H₂O, both inter and intera molecular hydrogen bonds can be described as H-donor X-H and H-acceptor(y). In BDIN.H₂O, both inter and intera molecular hydrogen bonds can be described as H-donor X-H and H-acceptor(y). In BDIN.H₂O complex C4-H9 bond length is increased when compared with BDIN. This is due to C4-H9...O21 hydrogen bonding interaction. The corresponding stabilization energy is 60 kJmol⁻¹. In BDIN and BDIN.H₂O complex the ring C-C-C bond angle is 120°. This indicates Ring is perfectly aromatic nature. The C2-C2-C3-C16, C2-C1-C6-C111 Dihedral angle is 0° and 180°. This shows title molecule is perfectly planar nature. The calculated value of electrophilicity index 3.84, which shows more NLO active nature of BDIN WATER complex while comparing with

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BDIN (2.35). The electric-field induced second-order hyperpolarizability, $\gamma(-2)$ for BDIN and BDIN.H₂O is found to be 10.684×10^{-33} and 14.813×10^{-33} e.s.u. The calculated value of polarizability, first and second order hyperpolarizability shows more NLO active nature of BDIN.H₂O while comparing with BDIN.

4. Conclusion

The theoretically predicted optimized geometry of BDIN and BDIN-H₂O complex by DFT method suggests the possibility of strong C-H...O hydrogen bonding networks. The lowering of HOMO and LUMO energy gap of BDIN.H₂O complex while comparing with BDIN indicates the charge transfer interaction within the molecule by which it leads to an NLO activity. NBO analysis confirms the possibility of strong C-H...O hydrogen bonding networks. While comparing the HOMO and LUMO energy gap the lowering of BDIN.H₂O with BDIN leads to an NLO activity. The DFT, NBO analysis, HOMO-LUMO energy gap, first order hyperpolarizability, and electrophilicity index shows the BDIN.H₂O complex is the more NLO active compared with BDIN.

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CORSIKA based muon ratio at DEASA detectors for a proton primary in Quark Gluon String Jet Model.

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Abstract

Cosmic ray particles with energy $\geq 10^{14}$ eV can be measured by the extensive air shower phenomenon. An extensive air shower is generated when a highly energetic cosmic ray enters atmosphere resulting in soft, hard and nucleonic components which can be measured by array of detectors on the ground. These phenomena have been studied by many groups including Stockholm