

DENSITY FUNCTIONAL THEORY STUDY OF THE ELECTRONIC AND NONLINEAR OPTICAL PROPERTIES OF 3-((E)-((4-(((E)-3-NITROBENZYLIDENE)AMINO)PHENYL)IMINO)METHYL)PHENOL

Suberu J. O*, Prof. N. O Obi-Egbedi*, Dr. N. D Ojo*, and Dr. Nnenna W.O
 *Department of Chemistry, Faculty of Science, University of Ibadan, Nigeria
 Email: joshuasuberu8@gmail.com

1 Introduction

- Despite progress in clean energy access, 645 million people will still lack electricity and 1.8 billion will rely on polluting fuels for cooking by 2030 [1]
- Efficient light-harvesting materials, such as Schiff bases, can help address this energy gap sustainably.
- To explore this potential, 3-((E)-((4-(((E)-3-nitrobenzylidene)amino)phenyl)imino)methyl)phenol (NBA) was investigated.

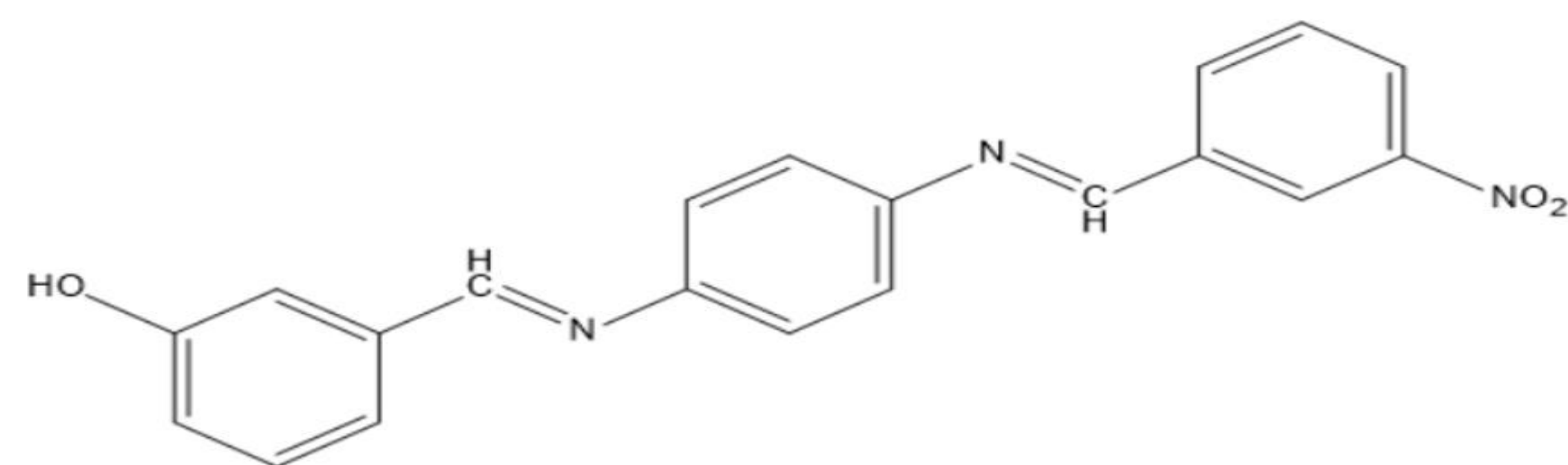


Fig. 1: Structure of NBA

- Schiff bases with promising electronic, optical, and nonlinear optical properties.



Photodetectors



Frequency Doublers



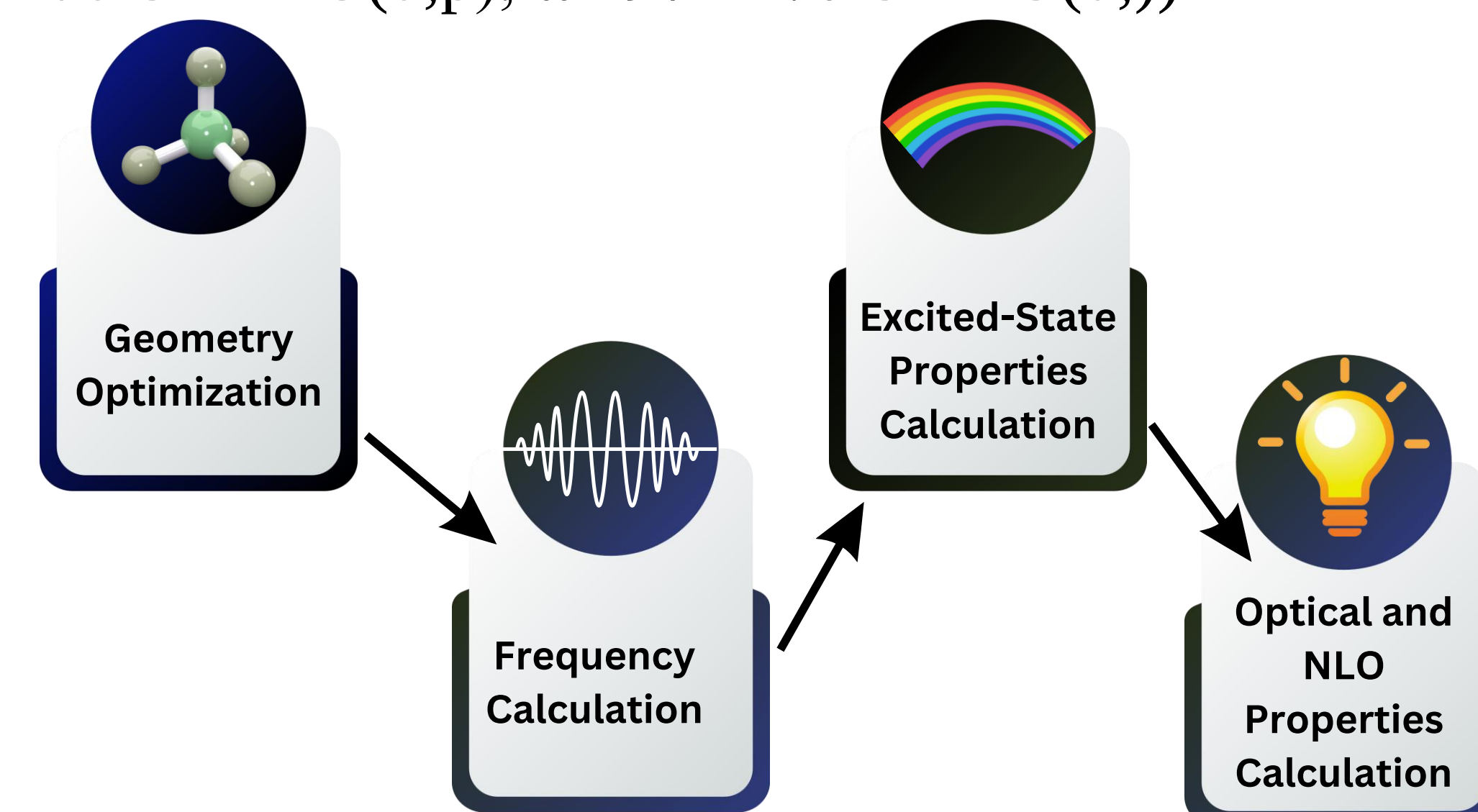
Optical Switches

2 Objectives

- To optimize the geometry of the compound.
- To perform frequency calculation.
- To compute the excited-state properties.
- To compute the optical and nonlinear optical properties.

3 Methodology

- GaussView 6.0.16 → structure building
- Gaussian 09 → quantum calculations
- DFT (B3LYP/6-311++G(d,p), ωB97XD/6-311+G(d,))



4 Results

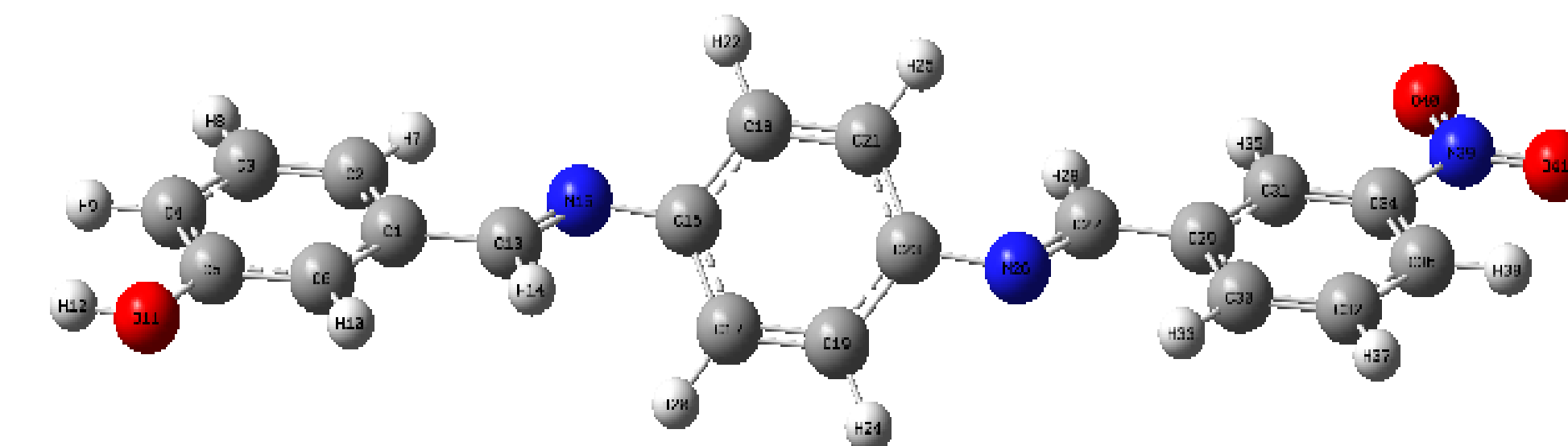


Fig. 2: Optimised Structure of NBA

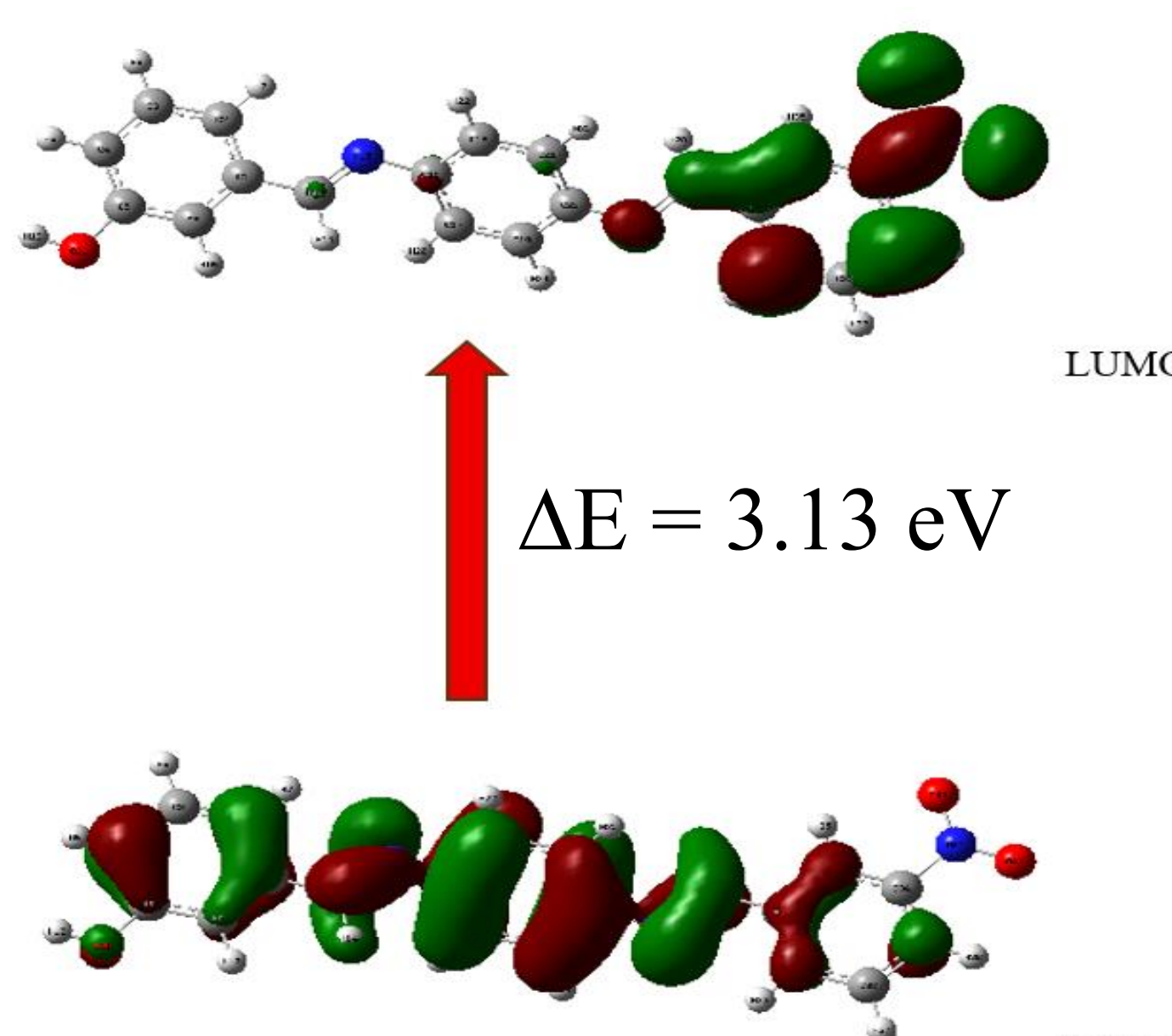


Fig. 3 HOMO–LUMO gap of NBA

Solvent	E _{ex} (eV)	λ (nm)	f	LHE (%)
Vacuum	3.77	329	0.78	84
n-Hexane	3.74	331	0.98	89
CCl ₄	3.74	331	0.97	89
THF	3.77	329	0.98	90
Ethanol	3.79	327	0.98	90
Methanol	3.79	327	0.97	89
Acetonitrile	3.79	327	0.98	90

Table 1: Excitation energies, wavelength, Oscillator strength and LHE

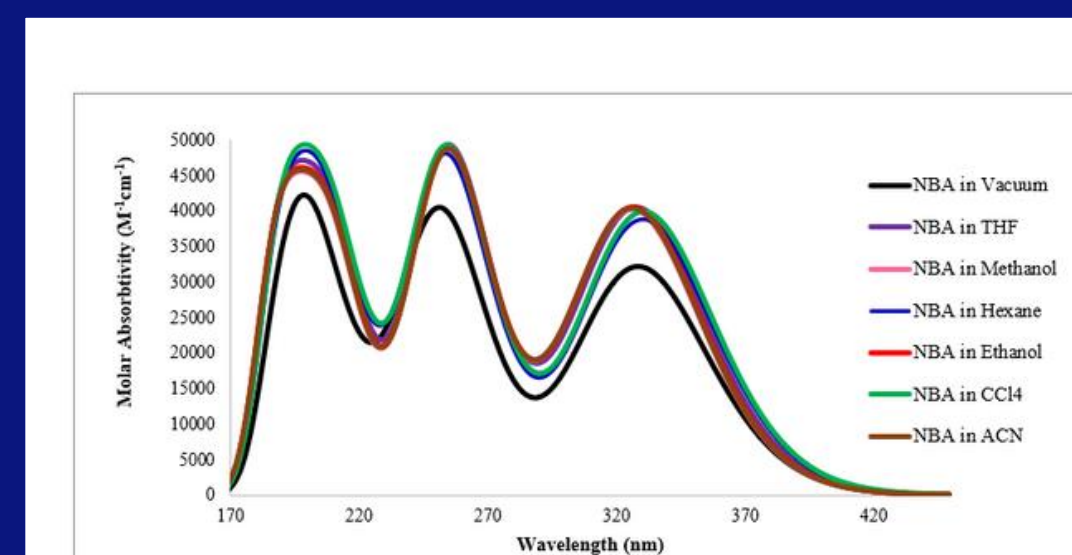


Fig. 4: UV–Vis spectrum of NBA

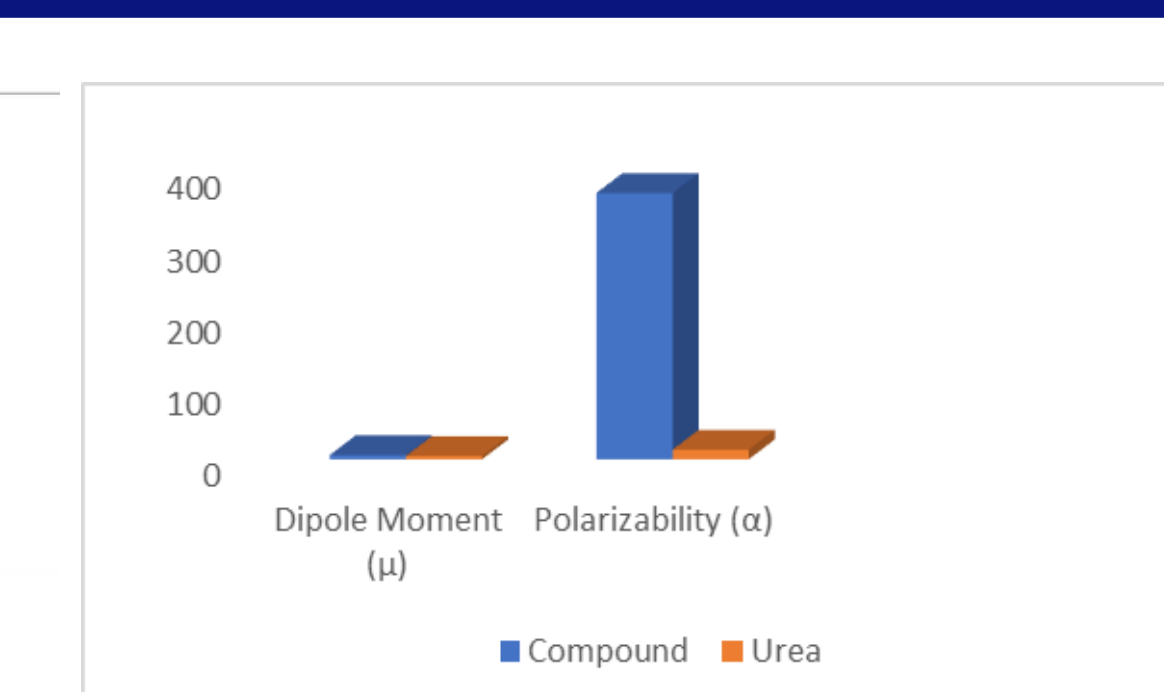


Fig. 5: Dipole moment & polarizability (μ, α)

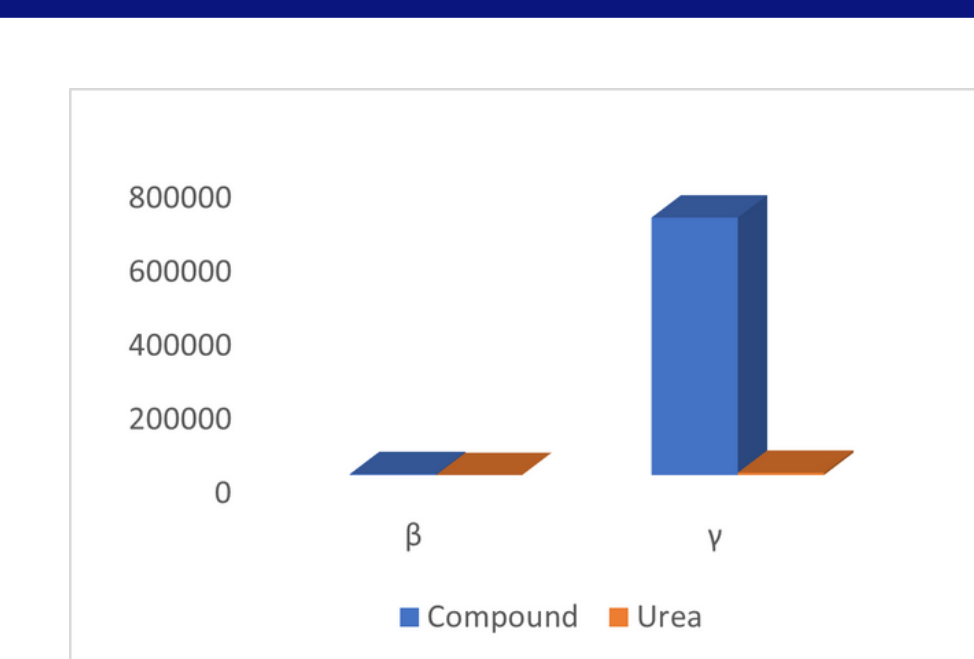


Fig. 6: First- and second-order hyperpolarizabilities (β, γ)

5 Conclusion

- NBA has a small HOMO–LUMO gap, showing semiconductor behavior, efficient charge transfer, and strong electronic activity.
- Efficient charge transfer makes it suitable for photonics and energy applications, e.g., green laser pointers, optical switches, solar cells, and photodetectors.
- High polarizability and hyperpolarizability enhance nonlinear optical performance.
- High oscillator strength and 90% LHE indicate excellent light absorption and energy conversion.
- SDG 7: NBA is promising for affordable and clean energy devices.
- SDG 12: Computational design reduces experimental waste, supporting sustainable materials development.

6 Acknowledgement

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- Dr. N. D. Ojo
- Dr. Nnenna W. O.
- Department of Chemistry, University of Ibadan, Nigeria

7 References

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- [2] Obi-Egbedi, N. O., & Ojo, N. D. 2021. Synthesis, light harvesting efficiency, photophysical and nonlinear optical properties of 3-(5-(4-hydroxybenzylideneamino) naphthalen-1-yl)iminomethyl) phenol. Springer, 47(12), 5249–5266. <https://doi.org/10.1007/S11164-021-04579-4>
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