



Quantum Chemical Calculations of (2-Amino, 3-Amino, 4-Amino and 4-Hydrazino) Benzene Sulfonamides Compounds by DFT

DR. ANIL BATTA

PROFESSOR & HEAD,
DEPARTMENT OF MEDICAL BIOCHEMISTRY
GOVT. MEDICAL COLLEGE, AMRITSAR

This study represents an integral approach towards understanding the electronic properties of (2-amino, 3-amino, 4-amino and 4-hydrazino) benzene sulfonamides compounds 1-4 by DFT/B3LYP method using 6-31G (d,p) to predict their applications. The geometrical parameters of these compounds are obtained by the same method. The predicted MEP figure revealed the negative regions of the molecules, which was subjected to the electrophilic attack of these compounds. The calculated HOMO and LUMO energies confirm that charge transfer occurs within the molecules. The structure-chemical reactivity relations of the compounds were determined through global reactivity descriptors by conceptual DFT methods. Mulliken population analysis was also carried out. NBO analysis was made and it indicated the intra molecular charge transfer between the bonding and anti-bonding orbitals. The linear polarizability ($\hat{\alpha}$) and the first order hyper polarizability ($\hat{\alpha}^2_{tot}$) values of the title compounds have been computed and results illustrated that the compounds 1-4 might not have the NLO behavior.



Biography – Prof. Dr. Anil Batta is presently professor & Head with senior consultant in Govt. Medical College, Amritsar. He did his M.B.B.S. and M.D. in Medical Biochemistry from Govt. Medical College, Patiala in 1984 and 1991, respectively. His research interest is mainly in clinical application especially cancer and drug de-addiction.

Publication of speakers:

1. Anil Batta Biochemical diagnosis of acute appendicitis
International Journal of Medical and Health
2. Anil Batta Burnout Syndrome in Medical Fraternity
3. Anil Batta Vitamin B12 and Depression Saudi Journal of Medicine
Scholars Middle East Publishers, Dubai, United Arab Emirates
4. Anil Batta Depression, Anxiety and Distress in Patients of Cancer Starting
Chemotherapy Scholars International Journal of Biochemistry Abbreviated Key
5. Anil Batta Biochemical Diagnosis of Dupuytren's Disease

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