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Spectroscopic and DFT insights of Ophthalmic Acid

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Spectroscopic and DFT insights of Ophthalmic Acid

Primary author: Amar Jyoti Saikia*1,2
Co-author: Lakhi Nath Borah3, Bhargab Borah4
Presenter: Amar Jyoti Saikia
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1 Department of Physics, Dhemaji College, Dhemaji
2 Department of Physics, Madhabdev University
3 Department of Physics, Madhabdev University
4 Department of Physics, DDR College, Chabua

*Corresponding Author: amasaik@gmail.com

Abstract: The current study is aimed at elucidating the structural, quantum chemical, and vibrational properties of ophthalmic acid employing the B3LYP/6-311++G(d,p) level of theory under the framework of DFT. The optimization followed by frequency calculation of the entitled molecule is performed using ORCA 6.0. The dipole moment, HOMO-LUMO energy gap, electrophilicity index, electron affinity, and ionization potential of ophthalmic acid are reported for the first time. The computed vibrational frequencies, i.e., Raman and IR, indicate the stability of the molecule with a total energy of -6.56×10ˆ5 kcal/mol. The NH_2 and O-H wave wavenumbers are observed around 3000-3500 cm^{-1}, while the C=O stretching modes are assigned around 1700 cm^{-1} with a maximum PED distribution of 85%.

Keywords: Ophthalmic acid, DFT, HOMO–LUMO, IR, Raman

Author: SAIKIA, Amar Jyoti (1 Department of Physics, Dhemaji College 2 Department of Physics, Madhabdev University)

Presenter: SAIKIA, Amar Jyoti (1 Department of Physics, Dhemaji College 2 Department of Physics, Madhabdev University)

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