International Journal of ChemTech Research
CODEN (USA): IJCRGG, ISSN: 0974-4290, ISSN(Online):2455-9555
Vol.11 No.09, pp 147-154, 2018

Experimental and Computational approaches to the molecular structure of Myristicin - a biologically active compound of Nutmeg

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Abstract : Nutmeg (Myristica fragrans) is a spice plant belonging to Myristicaceae family. The main chemical components of Nutmeg are camphene, safrole, methyl eugenol and myristicin, which provide the spice its therapeutic properties. Myristicin (6-allyl-4-methoxy-1,3-benzodioxole) a crystalline phenolic ether $C_{11}H_{12}O_3$ is major active constituent of nutmeg which is reported to have the anti-inflammatory, antidiabetic, antihyperlipidemic, anti-diarrheal activity. The vibrational frequencies were calculated and compared with the experimental data by using the spectroscopic methods and Density Functional Theory (DFT) method with B3LYP6-311++G(d,p) basis set. Stability of the molecule arising from hyper conjugative interactions, charge delocalization has been analyzed using natural bond orbital (NBO) analysis. In addition, the calculated HOMO and LUMO energies and molecular electrostatic potential shows that charge transfer occurs in the molecule.

Key words : Density Functional Theory method (DFT),Natural bond orbital analysis (NBO),Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO).

J.Sherin Percy Prema Leela *et al* /International Journal of ChemTech Research**,** 2018,11(09): 147-154

DOI= http://dx.doi.org/10.20902/IJCTR.2018.110919

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