International Journal of ChemTech Research
CODEN (USA): IJCRGG, ISSN: 0974-4290, ISSN(Online):2455-9555
Vol.11 No.10, pp 111-125, 2018

Vibrational and Molecular Structural Investigations of Pioglitazone – Combined Study of Experimental and Quantum Chemical Calculations (Density Functional Theory)

S.Rajesh[1]*, S. Gunasekaran[2], P.Rajesh[3]

[1] Department of Physics, St.Peter's University, Avadi, Chennai-600 054, India
[2] Research & Development, St.Peter's University, Avadi, Chennai-600 054, India.
[3]Department of Physics, Apollo Arts &Science College, Chennai-602105, India.

Abstract : The Fourier transform –Raman (FT-Raman) and Fourier transform infrared (FT-IR) spectra of (RS)-5-(4-[2-(5-ethylpyridin-2-yl) ethoxy] benzyl) thiazolidine-2,4-dione (pioglitazone) were studied in the region of 4000-100 cm^{-1} and 4000-400 cm^{-1}respectively. The theoretical spectral investigation of pioglitazone are also carried out by using density functional theory (DFT) with 6-31G (d,p) basis set. Experimental and theoretical values are compared. The entire vibrational assignments were carried out on the basis of the potential energy distribution (PED) of the vibrational modes using VEDA 4 program. The optimized geometry of the compound was calculated from the DFT-B3LYP. HOMO-LUMO energy gap has been calculated. The molecular geometry parameters like bond angle and bond length have been computed. The molecular stability arising from hyper conjugative interaction, charge delocalization has been analyzed using natural bond orbital (NBO) analysis. The Mullikan atomic charges have been computed. The molecular electrostatic potential (MEP) are also carried out to study the molecular interactions in the title molecule.
Key Words : Bond angle & Bond Length, MEP, HOMO-LUMO, Global descriptors.

S.Rajesh *et al* /International Journal of ChemTech Research, 2018,11(10): 111-125.

DOI= http://dx.doi.org/10.20902/IJCTR.2018.111015

*****