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HOMO-LUMO, NBO and Vibrational analysis of Sitagliptin by using DFT calculations and Experimental Study (FT-IR, FT-Raman and UV-Visible Spectroscopies)

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 vibrational spectra analysis of Sitagliptin was calculated using density functional theory method(B3LYP) by employing 6-31G (d, p) basis set, compared with experimental FT-IR and FT-Raman spectra in the region of 4000-400 cm^{-1} and 4000-100 cm^{-1}. The electronic properties like Homo-Lumo energies and molecular electrostatic potential (MEP) have been computed. The experimental FT-IR and FT-Raman spectra were compared with theoretical spectrograms. The Mullikan atomic charges were also calculated. The inter and intramolecular interactions of title molecule has been visualized using NBO analysis. Electronic stability of the title compound arising from hyper conjugative interactions and charge delocalization were also investigated based on NBO analysis.
Keywords : Sitagliptin, UV-Vis, NBO,FT-IR, FT-Raman.

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