Highest occupied molecular orbital and lowest unoccupied molecular orbital study of 1-Phenyl-2-propanamine using Density Functional Theory method

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ABSTRACT
1-phenyl-2-propanamine is a psychostimulant drug of the phenethylamine class used in the treatment of Attention Deficit Hyperactivity Disorder (ADHD). The molecular structure of 1-phenyl-2propanamine is shown in fig. The Fourier Transform infrared spectra of 1-phenyl-2-propanamine has been recorded in the region of 4000-400cm⁻¹. The structural bond parameters (bond lengths and bond angles) of the molecule have been calculated. Utilizing the observed FTIR data, a complete Vibrational assignment and analysis of the fundamental Vibrational modes of the compound were calculated at HF and DFT/B3LYP method with 631 G (d,p) basis sets. The energy gap between Highest Occupied molecular orbital (HOMO) and Lowest Unoccupied molecular orbital (LUMO) is found to be ΔE= 5.63 eV and it shows that 1-phenyl-2-propanamine is hard molecule. Moreover, it is clear from HOMO-LUMO analysis that charge transfer takes place within the molecule.

Keywords: 1-phenyl-2-propanamine; HF, DFT, B3LYP, FTIR, HOMO-LUMO.

1. INTRODUCTION
1-phenyl-2-propanamine (molecular formula C₉H₁₄CIN) is remains a widely abused drug throughout the world. It is also used therapeutically for weight loss, attention deficit disorder with hyperactivity (ADHD). ADHD has grown dramatically recently both in terms of diagnosis and treatment. Increasingly, older individuals are diagnosed and treated for ADHD.

2. EXPERIMENTAL DETAILS
Pure sample of 1-phenyl-2-propanamine is purchased from M/s Sigma Aldrich co., with the stated purity 99.99% and is used as such for spectral measurements.
3. COMPUTATIONAL METHODS
In the present work, the density functional method (DFT) using B3LYP levels at 631G(d,p) basis set has been employed with Becke's three parameter hybrid exchange functional with Lee-Yang-Parr functional using Gaussian09W package.

Figure: Geometry of 1-phenyl-2-propanamine optimized at DFT/B3LYP/631G level

4. HOMO-LUMO ANALYSIS
The molecular geometry of 1-phenyl-2-propanamine is shown in Fig.1. Both the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) are the two main orbitals that take part in chemical stability. The HOMO represents the ability to donate an electron, LUMO represents the ability to obtain an electron. The HOMO and LUMO energy calculated by DFT/B3LYP/6-31G method is shown in Fig.2. The positive phase is represented in red color and the negative phase is represented in green color. The energy gap of HOMO-LUMO explains the eventual charge transfer interaction within the molecule.

REFERENCES