The estimation of the speed of ultrasound in liquids is the fundamental requirement for investigating the transport properties of liquid and solid systems. The standard mathematical methods of measuring the ultrasonic velocity may be classified into three types. They are (i) Wavelength method, (ii) Brillouin scattering and (iii) Propagation time measurement approach. Of the above methods, the wavelength method includes Optical method, Pulse technique and Interferometric method. In the present study, interferometric method is planned for experimental measurement of ultrasound velocity. In the present proposal, the speed of ultrasound waves of aqueous solutions of Polyethylene Glycol (PEG) 200 has been computed for different concentrations (2%, 4%, 6%, 8% & 10%) at 303K and these experimental values compared with theoretical values obtained by using various mathematical methods like Nomotto’s Relation, Vandeal and Vangeal Relation, Impedance Relation, and Rao’s specific sound velocity. The most reliable method that matches with experimental method is identified and analysed in this paper (Ref: Gayathri A, Venugopal T. Analysis of speed of acoustic waves in binary liquid systems through mathematical and experimental methods. *Indian Journal of Science*, 2015, 13(36), 1-4), (Image: www.pi2.uni-stuttgart.de/).
ANALYSIS

MATHEMATICS

Analysis of speed of acoustic waves in binary liquid systems through mathematical and experimental methods
Gayathri A, Venugopal T

The estimation of the speed of ultrasound in liquids is the fundamental requirement for investigating the transport properties of liquid and solid systems. The standard mathematical methods of measuring the ultrasonic velocity may be classified into three types. They are (i) Wavelength method, (ii) Brillouin scattering and (iii) Propagation time measurement approach. Of the above methods, the wavelength method includes Optical method, Pulse technique and Interferometric method. In the present study, interferometric method is planned for experimental measurement of ultrasound velocity. In the present proposal, the speed of ultrasound waves of aqueous solutions of Polyethylene Glycol (PEG) 200 has been computed for different concentrations (2%, 4%, 6%, 8% & 10%) at 303K and these experimental values compared with theoretical values obtained by using various mathematical methods like Nomoto’s Relation, Vandeal and Vangeal Relation, Impedance Relation, and Rao’s specific sound velocity. The most reliable method that matches with experimental method is identified and analysed in this paper.

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PHYSICS

Highest occupied molecular orbital and lowest unoccupied molecular orbital study of 1-Phenyl-2-propanamine using Density Functional Theory method
Kurinjinathan P, Lavanya J, Rajalakshmi K

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-2propaniamine 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 \(\Delta E = 5.63\) 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.

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PHYSICS

Spectroscopic and Computational insights into the structure of Chlorthalidone using HF and DFT methods
Latha B, Gunasekaran S, Srinivasan S, Ramkumaar GR

This study deals with the identification of the title compound, Chlorthalidone by means of quantum chemical calculations. Molecular geometry, vibrational wave numbers and thermodynamic properties were carried out by Hatree-Fock (HF) and DFT levels of theory using 6-31G(d,p) basis set. A detailed interpretation of the vibrational spectra of this compound has been made on the basis of the calculated Potential Energy Distribution (PED). The vibrational frequencies were calculated in these methods and were compared with the experimental frequencies which yields good agreement between observed and calculated frequencies. The study is extended to calculate the HOMO – LUMO energy gap, ionization potential, global hardness, chemical potential and global electrophilicity. \(^1\)H and \(^{13}\)C NMR spectra were recorded and resonance chemical shifts of the molecule were calculated. UV–Visible spectrum of the compound was recorded in the region 200–600 nm and the electronic properties were calculated by TD-HF approach. The geometrical parameters, harmonic vibrational frequencies, IR intensities and absorption wavelengths were compared with experimental and theoretical data of the molecule.

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