

Figure 2. According to obtained results the mass and surface area has most important role on krafft temperature.

Reference

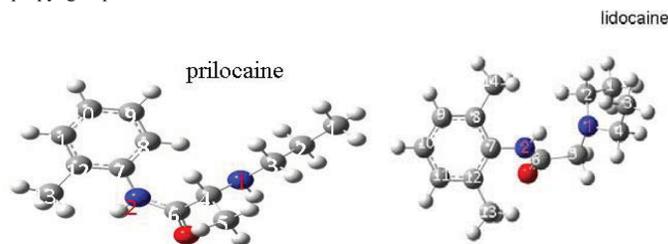
[1]sateesh Krishna chand chundra thesis submitted to the department of chemistry Eastren MichiganUniversity in Partial fulfillment of the requirements for degree of MASTER OF SCIENCE in chemistry.

Structure and conformation of lidocaine and Prilocaine. A DFT study

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Local anesthetics like lidocaine (N-(2,6-dimethylphenyl)-N2,N2-diethylglycinamide) and prilocaine ((RS) N-(2-methylphenyl)N-propylalaninamide) are amide local anesthetic and lidocaine is used typically to relieve itching, burning andpain from skin inflammations, injected as a dental anesthetic or as alocal anesthetic for minor surgery. Prilocaine is applied in dentistry and is a sodium channel blocker. Their common forms are salts and insoluble in water which have less toxic effects. Mass spectrometric methods are most commonly used. Unfortunately, these methods are destructive and the sample is no longer available for re-analysis by other laboratories. IR and Raman spectroscopy provide alternatives for non-invasively analyzing drug crystals. Furthermore, these methods are accurate and high sensitive for lower amounts of these materials [2]. The Raman and IR spectra of the titled compound are obtained and by using quantum chemistry calculations the frequencies are assigned to the normal modes [1]. The aim of this study is investigation on the structure, stable conformer, and vibrational spectroscopy in solid, CCl4 and CH3CN solutions of Prilocaine and lidocaine with using DFT calculations at B3LYP/6-31G** level of theory. 4 different stable conformers were obtained for Lidocaine and Prilocaine. The structures of the most stability of these conformers and atom numbering of the system are shown in Fig 1. The relative stabilities of the lidocaine conformers are in the range of 3.5-4.97 kcal/mol and those for prilocaine are in 3.5-5.1 kcal/mol range, with respect to the most stable conformer. Dihedral angle between Ph ring and N2C6 for prilocaine conformers is about 40-60° and more than those in lidocaine, so there is no resonance between them that it confirmed with calculated N-Ph bond length. The dihedral angles of O=C-CH-N1 in prilocaine and lidocaine are 77.25° and 154.37°, respectively. The difference is due to the presence of two ethyl groups bounded to N1 in Lidocaine while there is only one n-propyl group bounded to N1.



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IR and Raman spectrophotometric studies on the effects of pH and temperature on structural stability of human serum albumin(HSA)

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Human serum albumin is the most abundant protein in human blood plasma. Albumin is a soluble, monomeric protein which comprises about one-half of the blood serum protein. Albumin is essential for maintaining the osmotic pressure needed for proper distribution of body fluids between intravascular compartments and body tissues. It also acts as a plasma carrier by non-specifically binding several hydrophobicsteroid hormones and as a transport protein for heme and fatty acids(1) In this paper, we decided to determine the structural kinetic stability of human serum albumin by different factors such as pH and temperature(2). How these factors affected the protein stability, were shown by IR spectrums. In acidic or alkaline environment, the number and type of hydrogen bands varied due to the



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variation in OH-stretching and OH-bonding areas. Shift of the spectrum from 3400cm⁻¹ to 4000cm⁻¹ represents breakage of different strong and weak hydrogen bands and construction of concurrent new hydrogen bands. This events meant the obvious change in second structure of protein. In the area of 1800-2000cm⁻¹, some changes happened. In the area of 1660cm⁻¹ and 1584cm⁻¹, the peaks were weakened and in 1730cm⁻¹, the peak shifted in higher frequencies because of the variation in OH-bonding in intramolecular structure of water. In inert condition, we met no event.

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Investigating LDA and GGA approximations in Density-functional theory study of Physisorption of molecular hydrogen on graphene layer

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Molecular hydrogen is well-known for its weak van der Waals potential. Storage of hydrogen in carbon materials, with its potential application in hydrogen-fueled transportation system, has attracted much attention recently, and there are growing interests in the interactions between H₂ and hosts in solid lattices. For the interaction between a hydrogen molecule and a solid surface such as graphene, Density-functional theory, (DFT) [1], calculations are often needed. Many approximations have been put forward to calculate the exchange and correlation energies which have been broadly divided into two main categories. The local density approximation (LDA) assumes that the exchange and correlation energies are a function of the electron density at the point of evaluation only. The generalized gradient approximation (GGA), however, takes into account the gradient of the electron density at the point of evaluation. Typically, the adsorption energy is overestimated and the equilibrium distance is too short for results obtained within LDA. On the other hand, the adsorption energy is underestimated and the distance is too long when GGA are added to the functional. Bond lengths are measured as 0.75 and 1.42 Å for H-H and sp² carbon bonds, respectively, which compare well with the experimental values of 0.74 Å for H-H [2] and 1.41 Å for C-C bonds [3], by the GGA functional. Physisorption of H₂ on graphene layer is characterized by a shallow well of; 0.08 eV, and an equilibrium distance between H₂ and the surface around 2.7 Å [4], by the LDA functional calculations. Several adsorption sites were studied with the axis of the hydrogen molecule aligned parallel, or perpendicular, to the graphene layer. H₂ is placed above, or as close to, the center of the graphene plate to avoid edge effects on the hydrogen-graphene binding energies. Calculations were performed using the PWSCF package [5] in a plane-wave supercell approach using ultrasoft (Vanderbilt) pseudopotentials.

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Investigating the Properties of Bi-Carbon Nanotubes Combined by Peptide Linkages: A Computational Study

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PURPOSE: In this study, we have investigated the combinations of carbon nanotubes (CNTs) through peptide linkages. To this aim, density functional theory (DFT) calculations have been performed to understanding the effects of peptide linkages on the properties of the resulted bi-CNTs. Moreover, to better understanding the properties of the investigated structures, the parameters of nuclear magnetic resonance (NMR) spectroscopy have been also computed for the bi-CNTs. **RESEARCH METHODS:** The calculations have performed at the level of B3LYP DFT method and 6-31G* standard basis set employing the Gaussian 98 package. **CONCLUSIONS:** In this work, we have investigated the properties of bi-CNTs by the DFT computed NMR parameters. Our results have indicated that the properties of the bi-CNTs structures are significantly different from the properties of single CNTs. As a final remark, the existence of peptide linkage plays a dominant role in determining the properties of bi-CNTs.

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Electronic structure analysis of interaction of platinum nanoclusters with molecular oxygen by QTAIM method

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In the present work, the interaction between molecular oxygen and platinum nanosheets are studied and several values for multiplicity were considered. The charge transfer between oxygen and nanosheets are calculated to estimate donation-acceptation in the systems. Up