Structural Properties, Theory Functional Calculations (DFT), Natural Bond N-(4-Hydroxy-cyclohexyl)-acetamide

Ali Rahmani, Meisam Rahmani, Pezhman Khalili

Young Researchers and Elite Club, Takestan Branch, Islamic Azad University, Takestan, Iran

ABSTRACT

In this paper, the optimized geometries and frequencies of the stationary point and the minimum-energy paths are calculated by using the DFT (B3LYP) methods with 6-311 basis sets. The geometries and normal modes of vibrations obtained from B3LYP6-311 calculations are in good agreement with the experimentally observed data. B3LYP6-311 calculation results indicated that some selected bond length and bond angles values for the N-(4-Hydroxy-cyclohexyl)-acetamide. In this theoretical study we used density functional theory to calculate the molecular structures of N-(4-Hydroxy-cyclohexyl)-acetamide.

INTRODUCTION

Any fundamental understanding of protein and peptide structure, dynamics, and function requires methods to measure protein secondary structure. X-ray crystallography and two-dimensional nuclear magnetic resonance (2-D NMR)(1-4) are the most incisive protein structural probes because they can provide highly accurate three-dimensional structures.

However, X-ray diffraction gives a static picture, and NMR gives only a limited amount of dynamical information [2,4]. In addition, these techniques are labor intensive and require protein samples that differ from the normally desired dilute aqueous solution phase. We report here a new methodology to determine dilute solution protein and peptide secondary structures, using UV resonance Raman spectroscopy (UVRSS) excited with a 206.5-nm CW laser directly into the amide π→π* transitions of the peptide bonds [5-11]. The resulting spectra are dominated by the amide vibrations, whose frequencies, Raman cross sections, and bandwidths depend sensitively on secondary structure [12-13].

Experimental:
Chemicals and reagents:
The optimized structural parameters were used in the vibrational frequency calculations at the DFT level to characterize all stationary points as minima. All computational are carried out using Gaussian 09w program. Harmonic vibrational frequencies (v) in cm⁻¹ and infrared intensities (int) in Kilometer per mole of all compounds were performed at the same level on the respective fully optimized geometries. Energy minimum molecular geometries were located by minimizing energy, with respect to all geometrical coordinates without imposing any symmetrical constraints.

NBO study on structures:
The structure of the compound has been optimized by using the DFT (B3LYP) method with the 6-311 basis sets, using the Gaussian 09w program. Density functional theory methods were employed to determine the optimized structure of C₇H₁₀O₂N₁. (Table 1, Figure 1) Natural Bond Orbital's (NBOs) are localized few-center orbitals that describe the Lewis-like molecular bonding pattern of electron pairs in optimally compact form. More precisely, NBOs are an orthonormal set of localized "maximum occupancy" orbitals whose leading N/2 members (or N members in the open-shell case) give the most accurate possible Lewis-like description of the total N-electron density. This analysis is carried out by examining all possible interactions between "filled" (donor) Lewis-type NBOs and "empty" (acceptor) non-Lewis NBOs, and estimating their energetic importance by 2nd-order perturbation theory.
Fig. 1: Optimized geometries of C₈H₁₀O₂N₁, at B3LYP/6-311G level of theory.

Table 1: Geometrical parameters optimized for C₈H₁₀O₂N₁ some selected bond lengths and angles.

<table>
<thead>
<tr>
<th>Method</th>
<th>Bond lengths</th>
<th>Bond angles</th>
</tr>
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<tbody>
<tr>
<td>B3LYP/6-311G</td>
<td>C₁-C₂ 1.3816</td>
<td>C₂-C₃ 1.408</td>
</tr>
<tr>
<td></td>
<td>C₃-O₁₆ 1.3797</td>
<td>C₄-O₁₆ 1.4199</td>
</tr>
<tr>
<td></td>
<td>O₁₆-H₁₇ 1.9738</td>
<td>C₁-C₁₋₋₁₋₋₁</td>
</tr>
<tr>
<td></td>
<td>118.8177</td>
<td>116.2315</td>
</tr>
<tr>
<td></td>
<td>125.3268</td>
<td>94.4168</td>
</tr>
<tr>
<td></td>
<td>111.6627</td>
<td>90.6177</td>
</tr>
</tbody>
</table>

Since these interactions lead to donation of occupancy from the localized NBOs of the idealized Lewis structure into the empty non-Lewis orbitals (and thus, to departures from the idealized Lewis structure description), they (Table are referred to as "delocalization" corrections to the zeroth-order natural Lewis structure. Natural charges have been computed using natural bond orbital (NBO) module implemented in Gaussian09w. The NBO Calculated Hybridizations are significant parameters for our investigation. These quantities are derived from the NBO population analysis. The former provides an orbital picture that is closer to the classical Lewis structure. The NBO analysis involving hybridizations of selected bonds are calculated at B3LYP methods and 6-311 level of theory. These data shows the hyper conjugation of electrons between ligand atoms with central metal atom. These conjugations stand on the base of p-d π-bonding.

The NBO calculated hybridization for C₈H₁₀O₂N₁ shows that all of compounds have SPX hybridization and non planar configurations. The total hybridization of these molecules are SPX that confirmed by structural. The amount of bond hybridization showed the inequality between central atoms angles (Table 2) shown distortion from normal VSEPR structures and confirmed deviation from VSEPR structures. (Figure 2). Some thermodynamic parameters Frequencies for C₈H₁₀O₂N₁ Zero-point Energy, correction Energy, Enthalpy lengths, Gibbs free Energy are calculated and confirmed with other published theoretical data (Table 4).

Fig. 2: The atomic orbital of the frontier molecular orbital for C₈H₁₀O₂N₁ at B3LYP/6-311G level of theory.
electron excitation from the highest occupied molecular orbitals (HOMOs) and lowest unoccupied molecular orbitals (LUMOs) are shown in Figure 2. The HOMO energy is directly related to the electron affinity. Energy difference between HOMO and LUMO as an electronic absorption corresponds to the transition from the ground to the excited state and is mainly described by one electron excitation from the highest occupied molecular orbital (LUMO). Therefore, while the energy of the HOMO is directly related to the ionization potential, LUMO energy is directly related to the electron affinity. Energy difference between HOMO and LUMO orbital is called as energy gap that is an important stability for structures. In addition, 3D plots of highest occupied molecular orbitals (HOMOs) and lowest unoccupied molecular orbitals (LUMOs) are shown in Figure 2. The HOMO–LUMO energies were also calculated at the LanL2DZ and the values are listed in Figure 2, respectively.

Frontier molecular orbital:
Both the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) are the main orbital take part in chemical stability. The HOMO represents the ability to donate an electron, LUMO as an electron acceptor represents the ability to obtain an electron. The HOMO and LUMO energy were calculated by B3LYP/6-311 method. This electronic absorption corresponds to the transition from the ground to the first excited state and is mainly described by one electron excitation from the highest occupied molecular orbital (LUMO). Therefore, while the energy of the HOMO is directly related to the ionization potential, LUMO energy is directly related to the electron affinity. Energy difference between HOMO and LUMO orbital is called as energy gap that is an important stability for structures. In addition, 3D plots of highest occupied molecular orbitals (HOMOs) and lowest unoccupied molecular orbitals (LUMOs) are shown in Figure 2. The HOMO–LUMO energies were also calculated at the LanL2DZ and the values are listed in Figure 2, respectively.

Conclusion:
In this research we are interested and studied on two fluorocarbon compounds were chosen to theoretical studies. The optimized geometries and frequencies of the stationary point and the minimum-energy paths are calculated by using the DFT (B3LYP) methods with 6-311 basis sets. B3LYP/LanL2DZ calculation results indicated that some selected bond length and bond angles values for the C_{10}H_{16}O_{2}N_{1}.

ACKNOWLEDGEMENTS

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REFERENCES