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Effect of hydration on the physical properties of glucose

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ABSTRACT

The effect of hydration on the electronic properties of glucose (Gl) is studied by quantum mechanics by using DFT procedures atB3LYP/6-31g(d,p). Total dipole moment, the highest and the lowest occupied molecular orbital (HOMO/LUMO band gap energy) and molecular electrostatic potentials (ESPs) are calculated at the same level of theory for all model molecules. The results indicated that there is an enhancement in the electronic properties of Gl where TDM of Gl is increased from2.5454Debye to 4.3157Debye while HOMO/LUMO band gap energy is decreased from 13.0994 eV to 3.2749 eV. Also, the calculated ESP results are indicated that the electro-negativity is increased due to hydration which means that the reactivity is increased and hence the electronic properties are improved.

Keywords: *DFT; Glucose; Hydration; TDM and ESP.*

1. INTRODUCTION

Carbohydrates are classified among the most important biomolecules which have key role in several important processes in the biological systems [1-3]. Among them located Glucose which is a simple monosaccharide sugar, it is considered as the source of energy in animals and plants [4]. It is one of the main products of photosynthesis and starts respiration. The natural form (D-glucose) is also referred to as dextrose, especially in the food industry [5]. Hydration of Glucose as well as other carbohydrates is considered among the important point of research[6-7]. On the other hand computational methods are utilized extensively to study the electronic; physical and chemical properties of many systems and molecules [8-10]. It could be also utilized to study the biomolecules with promising results supporting the experimental findings [11-13]. Different level of theories was early utilized to elucidate different properties of glucose as well as other carbohydrates. Ab initio quantum mechanical calculations were used to study the crystalline structures α-D-Glucose and β-D-Glucose monohydrate [14]. D-Glucose anomers were studied both in gas phase and solution with density functional theory DFT [15]. The study is further continued for conformational analyses with higher DFT level of the theory [16]. Studying such important biomolecules is not limited to theoretical approaches but also spectroscopic tools such as FTIR and FT-Raman could be used to elucidate the molecular structures of glucose and its derivatives as well as other carbohydrates [17-21]. Recently many researchers devoted their work to study the hydration and different functions of glucose [22-24]. Modeling materials with density functional theory level is not limited to biological molecules [25-27] but also covering many other emerging and new materials [28-30].

Based upon this consideration the present computational work is conducted with DFT to study the hydration of glucose. The geometrical parameters, total dipole moment (TDM), energy band gap and electrostatic potentials (ESP) are calculated at B3LYP/6-31g (d, p) level.

2. MATERIALS AND METHODS

Calculation details.

Density functional theory (DFT) is conducted to study the effect of hydration on the electronic properties of glucose (Gl). As a consequence, model molecules presenting Gl and hydrated Gl are subjected to optimization at B3LYP/6-31g (d,p) [31-33] using GAUSSIAN09 [34] program at Spectroscopy Department, National Research Centre, Egypt. In addition to the geometrical parameters (bond distances and angels). Physical parameters such as total dipole moment (TDM), energy gaps(HOMO/LUMO band gap energy) and electrostatic potentials (ESP) are also calculated using the same quantum mechanics. Furthermore, the calculated IR spectrum is also introduced for all studied structures at the same level of calculation.

3. RESULTS AND DISCUSSIONS

A model molecule for glucose (Gl) is built as indicated in figure 1 a, b. Glucose is studied at B3LYP/6-31g (d,p) then hydrated glucose is studied at the same level of theory. Glucose is proposed to interact with water molecules (W) through weak interaction as indicated in figure 1 c, d, e, f, g, and h, respectively. The hydrated glucose is following the scheme XW where X=1-6 units of water which are subjected to optimization using B3LYP/6-31g (d,p). As indicated in figure 1 there are 7 model molecules for glucose as well as hydrated glucose up to 6 water molecules.

The influence of hydration is recorded in terms of different physical properties including the electronic properties, total dipole moment (TDM) and band gap energy (HOMO/LUMO band gap energy). Electrostatic potentials are calculated as they considered the most important physical properties that depict the reactivity of the studied structures.

Table 1 illustrates the change in TDM (as Debye) and HOMO/LUMO band gap energy (as eV) for glucose and glucose hydrated with water molecules up to 6 units. From the table, one can see that the calculated TDM of glucose structureis2.5454 Debye which increases to2.7878, 4.2224, 4.2540 and 4.3157 Debye for Gl- 1W, Gl- 2W, Gl-3W and GL- 4W respectively. TDMof the studied structure decreases again to 2.3866 Debye for hydration with 5 units of water. For hydration of glucose with 6 units of water, TDM increased again to 3.4471 Debye. HOMO/LUMO band gap energy \also shows a big change due to hydration where it is highly decreased from 13.0994 eV to 3.4877, 3.4812 and 3.4227 eV for Gl- 1W, Gl- 2W and Gl-3W respectively. For GL- 4W, Gl- 5W and Gl- 6W 3.2749, the TDM started to increase slightly to3.2749, 3.2847 and 3.5585 eV respectively.

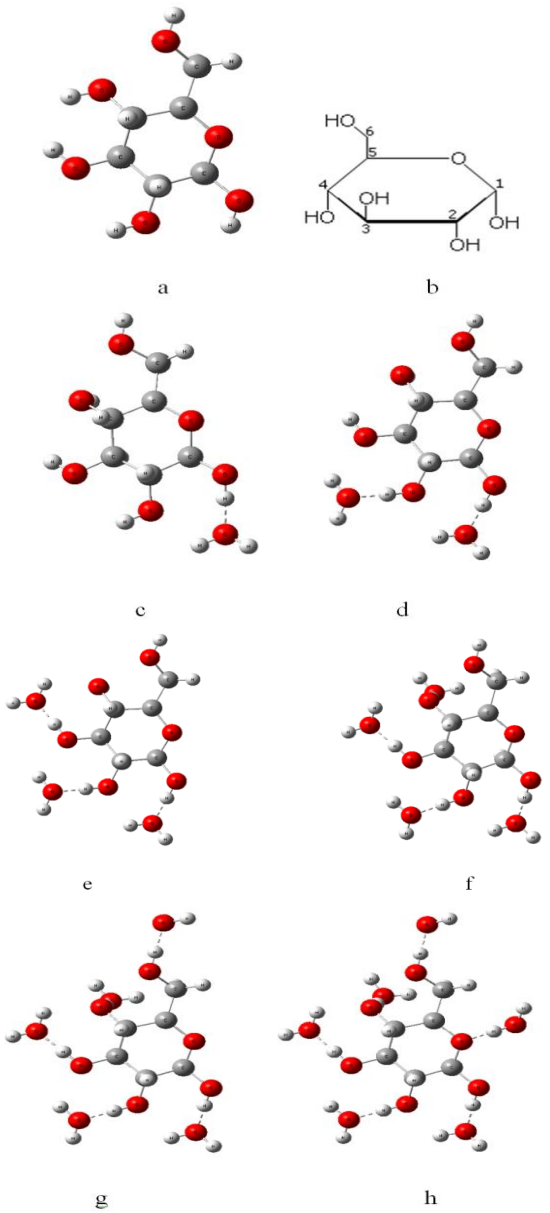

Figure 1. a) Model molecule for Glucose structure; b) schematic structure of the glucose. Hydrated glucose in case of c) one water molecule through OH, d) two water molecules throughout OH, e) three water molecules throughout OH, f) four water molecules throughout OH, g) five water molecules throughout OH, h) five water molecules throughout OH and one from O-linkage.

It is stated early that TDM and HOMO/LUMO band gap energy are together good indications for the reactivity of a given chemical structures. As the total dipole is increased and the band gap has decreased the reactivity is also increased [35-3630].

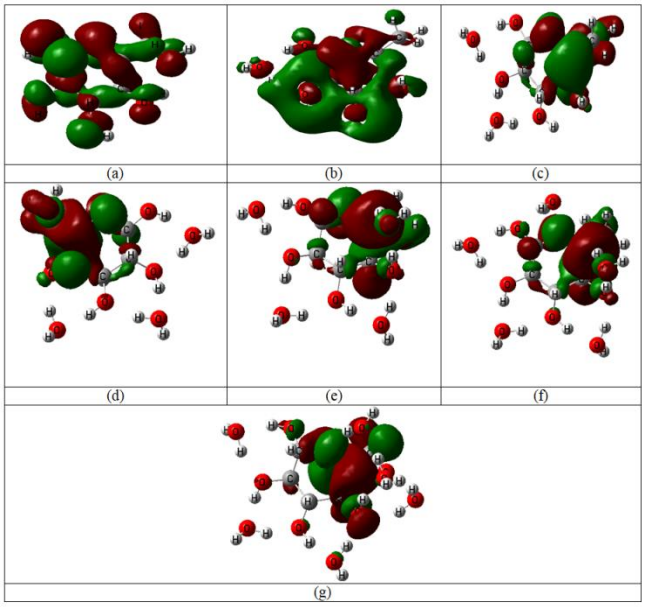

Figure 2. HOMO/LUMO band gap energy for a) Gl; b) Gl- 1W; c) Gl- 2W; d) Gl- 3W; e) Gl- 4W; f) Gl- 5W and g) Gl- 6W respectively which calculated at B3LYP/6-31g(d, p) level of theory.

Table1.TDM as Debye and HOMO/LUMO energies as eV for Gl and Gl-XW where X=1-6 which calculated at B3LYP/6-31g(d, p) level of theory.

Structure	TDM	E
Gl	2.5454	**13.0994**
Gl- 1W	2.7878	**3.4877**
Gl- 2W	4.2224	**3.4812**
Gl- 3W	4.2540	**3.4227**
Gl- 4W	4.3157	**3.2749**
Gl- 5W	2.3866	**3.2847**
Gl- 6W	3.4471	**3.5585**

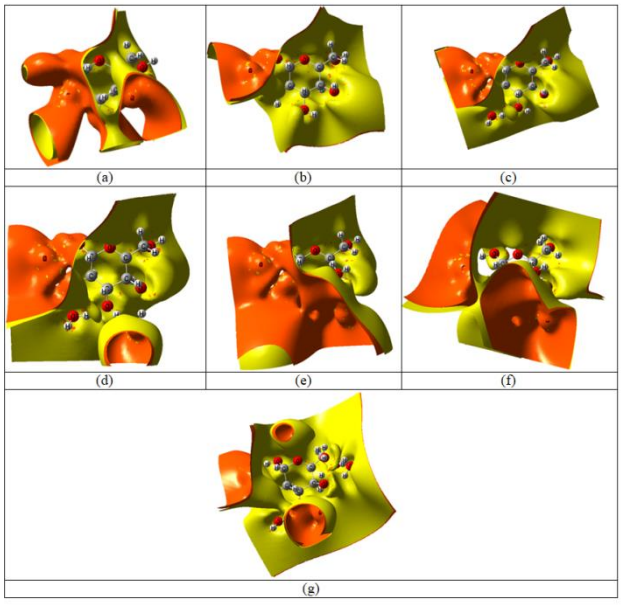

Figure 3. ESP as total surface area for a) Gl; b) Gl- 1W; c) Gl- 2W; d) Gl- 3W; e) Gl- 4W; f) Gl- 5W and g) Gl- 6W respectively which calculated at B3LYP/6-31g(d, p) level of theory.

Figure 2 shows the HOMO/LUMO band gap energy for glucose and hydrated glucose model molecules. Molecular electrostatic

potentials (ESPs) also can predict the reactivity of a given structure via the distribution of charges around the molecule where the distribution can be explained according to colors in the following sequence: red> orange> yellow>green> blue [37-38]. The red color means that the molecule is more reactive (the molecule is electro-negative) whereas the yellow color means that it is neutral and finally the blue color means that the molecule is positive. It is stated that ESPs is a good tool to represent active sites of biological as well as many other chemical structures [39].

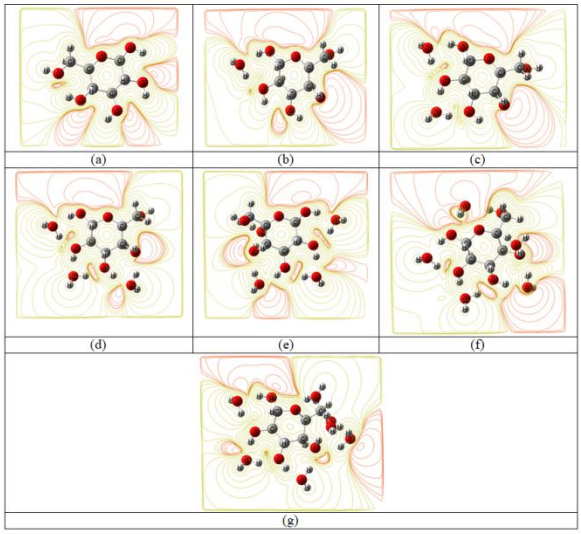

Figure 4. ESP as contour action for a) Gl; b) Gl- 1W; c) Gl- 2W; d) Gl- 3W; e) Gl- 4W; f) Gl- 5W and g) Gl- 6W respectively which calculated at B3LYP/6-31g(d, p) level of theory.

The most interesting point is to correlate activity with color scheme. The ESPs colors for the studied structures are shown in figures 3 and figure 4 for all the studied structures which present the change in ESP of glucose as a result of hydration. Figure 3 shows ESPs of glucose as a result of hydration as a total surface area while figure 4 shows ESPs of glucose as a result of hydration as a contour. From figure 3and figure 4, one can see that the red color is increased with increasing the number of water molecules, the electro-negativity is increased and hence the reactivity is also increased.

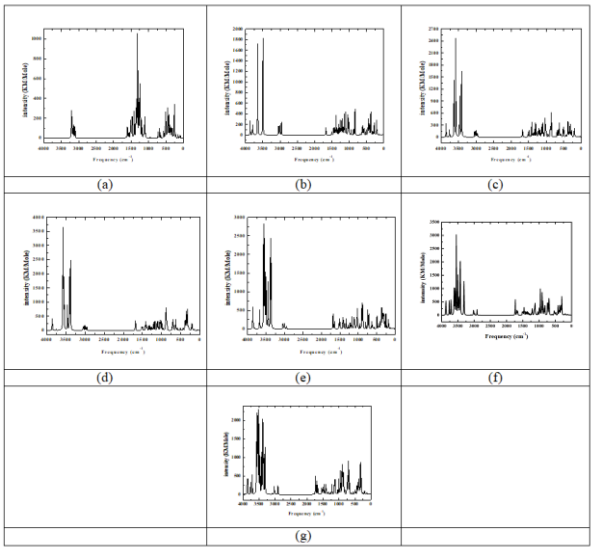

Figure 5. Infrared spectra for a) Gl; b) Gl- 1W; c) Gl- 2W; d) Gl- 3W; e) Gl- 4W; f) Gl- 5W and g) Gl- 6W respectively which calculated at B3LYP/6-31g(d, p) level of theory.

Figure 5 represented the calculated IR spectrum for all studied structures at the same level of theory. The assignments of the glucose are already carried out before and are not the scope of the present work.

As indicated in the spectra no negative frequencies are obtained which indicate that the studied structures are corresponding to the energy minimum and all are optimized structures.

4. CONCLUSIONS

The calculated parameters indicated that, from the electronic point of view, glucose is approximately insulator material where it possesses TDM of 2.5454 Debye and HOMO/LUMO energy of 13.0994 eV. As a result of hydration, the properties of glucose are enhanced where the TDM is increased to 4.3157 Debye while the HOMO/LUMO energy decreased to 3.2749 eV for hydration with 4 units of water. Furthermore, the electrostatic potential result also is indicated that the reactivity of glucose is increased upon hydration. Although the calculated spectra are not physical changes it is calculated to confirm that the studied structures are real and corresponding to optimized structures. This is indicated by the positive frequencies for all the studied structures. The obtained data confirms the suitability of DFT for studying biological and natural molecules such as glucose.

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