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Computational Study of D-glucose and its Differential Cognitive Effects on Well-being and Quality of Life

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Abstract

GAMESS computational chemistry package is a freeware available on the web. It has been successfully applied for the structure elucidation of the commonly available D-glucose. In the current research, IR and Raman spectra of D-glucose were theoretically calculated by utilizing the density functional theory (DFT), combined with B3LYP/3-21G basic set. IR and Raman activities were estimated through the GAMESS computational package. Moreover, the NMR spectrum was also obtained through the Gaussian 09 package. Theoretically calculated and experimentally calculated results were compared using the B3LYP/3-21G level of theory. The results of both calculations were nearly the same. The optimization of structure with the various levels of theory and Basis sets was studied and the best results were obtained using B3LYP/3-21G, and these results agreed considerably with the experimental results. The current computational analysis may be useful to predict complex carbohydrate precursors and other carbohydrate molecules.

Keywords: blood glucose, carbohydrates, D-glucose, dextrose, DFT, GAMESS, quantum mechanics

Introduction

Carbohydrates depict an exceptionally huge classification of compounds, characteristically of bio-related frameworks, which play a significant role in the various pathways essential for life. Glucose is a simple sugar and one of the three dietary monosaccharides with the molecular formula $C_6H_{12}O_6$ [1]. The foremost type of sugar found in the blood is glucose (dextrose). It is considered as a major energy source for the body's cells and it can be obtained through the process of glycolysis. It can be directly obtained from the food that we intake

or alternatively, it can be produced within the body from many other substances through the process of gluconeogenesis. The produced glucose is transported to other cells through the blood stream [2]. It can also be produced in plants during photosynthesis by utilizing carbon dioxide and water in the presence of daylight that acts as an energy source. The synthesized glucose is utilized in fabricating cellulose. Cellulose is considered as the most abundant carbohydrate inside the cell walls [3]. After digestion, glucose remains in the body as a polymer. In plants, it is mostly present in the form of amylopectin and it can be found as glycogen in all life-forms. In living organisms, glucose is present in blood as a necessary constituent. Normally, two types of glucose, that is, D-glucose and L-glucose have been delivered artificially in relatively limited quantities and have lesser significance [4].

Glucose is a kind of sugar that can be obtained from food. The body utilizes it as an energy source and for maintaining life. After the breakdown of food glucose moves into the circulatory system, so it is also known as blood glucose [4]. This movement of glucose from the blood towards cells is aided by a hormone known as insulin. It has been observed that diabetic patients have a higher amount of glucose in their blood as compared to the blood glucose level of a normal person [5]. Such patients need more insulin to regularize their cell functions and to decrease the amount of glucose within the blood [6]. High blood glucose levels for a long period of time can harm the eyes, kidneys and other related organs. A safe and effective prescription of glucose is crucial to maintain a healthy level of blood sugar [7]. Glucose works by quickly expanding the proportion of glucose/sugar in the blood stream. Glucose is administered to people debilitated by drinking a great deal of alcohol. It may be used to treat hyperkalemia (anomalous measures of potassium in blood).

Glucose originates from substances rich in sugar similar to bread, potatoes and organic products. After the intake of food, it moves down to the stomach. Here, acids and chemicals act on it and separate it into minor pieces [8]. This breakdown of food results in the discharge of glucose and it enters into the digestive organs for consumption. From that point onwards, glucose enters into the circulatory system. Once, the glucose enters into the blood stream a specific hormone, that is, insulin makes it a part of the cells. Body intends to keep the level of

glucose steady in the blood stream. Glucose level is checked at regular intervals by beta cells present in the pancreas [9]. After the intake of food, the glucose level increases and beta cells actively allow the discharge of insulin in the blood stream to balance the glucose level up to normal. Insulin plays a key role in opening muscles, fats, and liver cells so that glucose can find the way inside them. A large portion of cells in the body use glucose alongside amino acids and fats for vitality. Regardless, it is considered as an essential wellspring of fuel for the cerebrum [10]. After the utilization of the vitality by the body that it needs, extra glucose is stored in the form of glycogen both in the liver and muscles [11]. The body has the ability to store enough fuel for about a day. If there is no intake of food for a couple of hours, it results into a drop of the blood glucose level and pancreas stop the production of insulin [12]. Many processes and substrates need glycolysis in collaboration with starch. The current examination reports the IR scope of D-glucose detached from the aromatic framework [13] and its dependence on thickness of quantum estimations united with the scaled quantum mechanical system [14]. Raman and infrared activities related to spectroscopic examinations were employed for a portion of vibrational gatherings to express the security expands, edge turns, and coupled movement [15]. Glucose levels directly relate to the psychological processing of the emotionally charged material [16].

2. Computational Studies

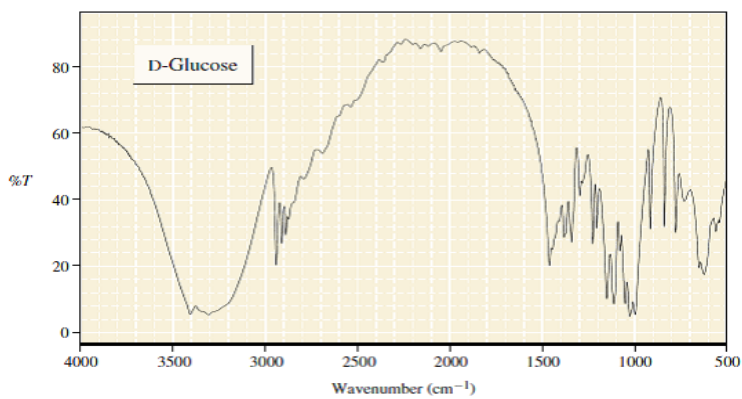

Figure 1. Experimental IR spectrum of D-glucose

IR and Raman activities of D-glucose were measured ranging from 3710-201 cm^{-1} with an accurate resolution of about 0.4 cm^{-1}. No thermo-decomposition with the range of 381-411 K was observed.

Thereby, QCM was employed for estimating both the total force of subatomic shafts as well as the grid to test the proportion (M/S) 28. The investigation of the exploratory spectra was aided as we smooth them up to an equal goal of 1.6-3.6 cm^{-1} with no impact on pinnacle powers in our obtained spectra. An enormous number of fundamentals, besides the conjunction of a few conformers, resulted in many covering ingestion bands in the obtained IR spectra. All spectra were run and collected in a range lying between 4000-400 cm^{-1}.

3. Computational Details

Computational investigation of the vibrational parameters of the D-glucose were carried out through a typical core i7 5^{th} generation machine with 4 giga bite of random-access memory (RAM) was used in the system. Avogadro version 1.2 was used for drawing the structure. Universal force field was applied for the optimization of geometry and KnowItAll Informatics System was operated for computing the obtained results. GAMESS with two modes was used to calculate the IR spectra [17]. Single point energy and frequency in the basic set of B3LYP and Pople type basis B3LYP/3-21G were exercised. It not only shortened the time of computation but also provided better results.

Vibrational frequencies were differentiated and infrared and Raman spectra of D-glucose were obtained. They revealed that D-glucose possesses strong crystalline structure due to coupled vibrations. Basic set-up was taken to calculate the frequency of the various modes of the nuclear vibrational motion within the same molecule with 3-21G in the presence of the gas phase using the number of the diffused heavy atom polarization function 1 to calculate the run type optimization-geometry. Optimization was designed for mathematical problems which provided a way by which r-vector value corresponding to E(r) at the local minimum, that is, the derivatization of the energy-term to the position-vector r of atoms, $\partial E/\partial r$ [14]. Computational model providing tentative E(r) may be used related to the quantum mechanics. As Hessian matrix is the double derivative of the energy functional, the algorithm used for geometry optimization in Gaussian was based on Hessian matrix. Hessian determined the local curvature of a function. In the case of computational chemistry, this function is potential energy surface [15]. Generally, Hessian is used for determining the extreme of a function. After optimization, to find that the stationary state on potential energy surface, or saddle point there

was needed to calculate Hessian since sign of its eigen values showed the character of stationary point. DFT, being a computational quantum mechanical modeling method, has been used in various fields including chemistry and material science for investigating the electron cloud or the nuclei motion of characteristic many-body systems, particularly molecules, atoms and condensed matter phases [14]. In this method, "Restricted Hartree-Fock(RHF) and Self Consistent Field(SCF) computed" was opted for only change in Fock Matrix to run the GAMESS calculation.

4. Results and Discussion

After the completion of calculations, the following results were obtained;

Figure 1 and 2 shows IR spectrum and Raman spectrum of glucose.

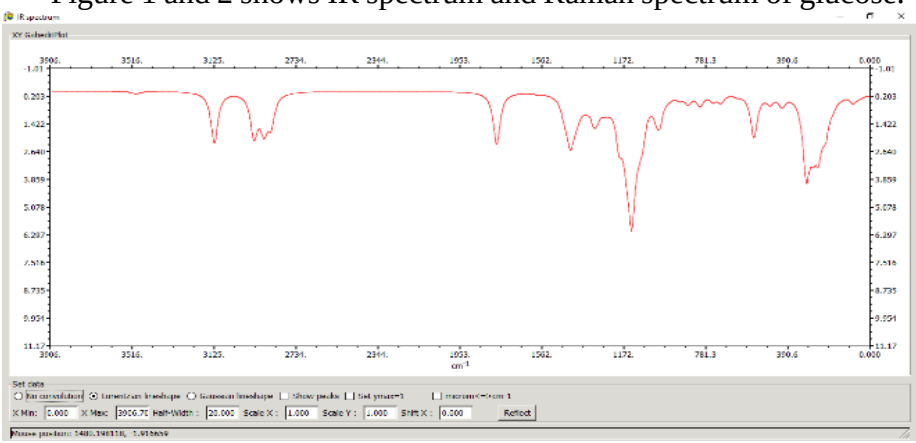

Figure 2. IR spectrum of glucose

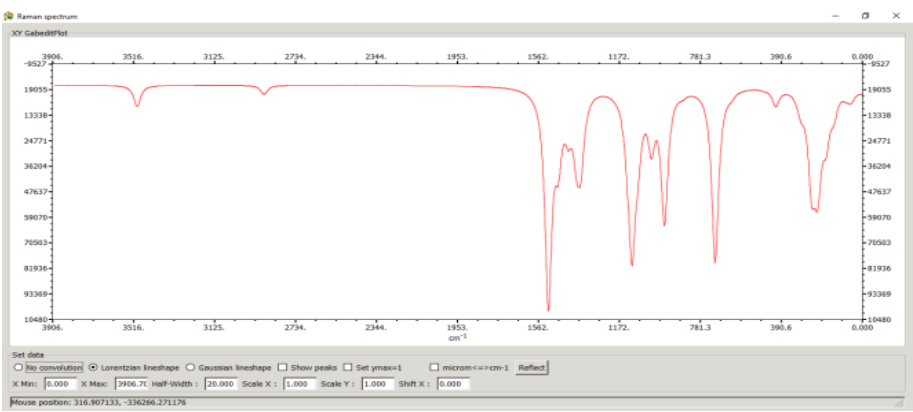

Figure 3. Raman spectrum of glucose

In Gaussian calculations, same parameters and basis sets were used with only a small change in B3LYP/6-31G. The shared processor 4 created the file running the Gaussian after the completion of the calculation and determined the spectrum on the Gaussian (Figure 4).

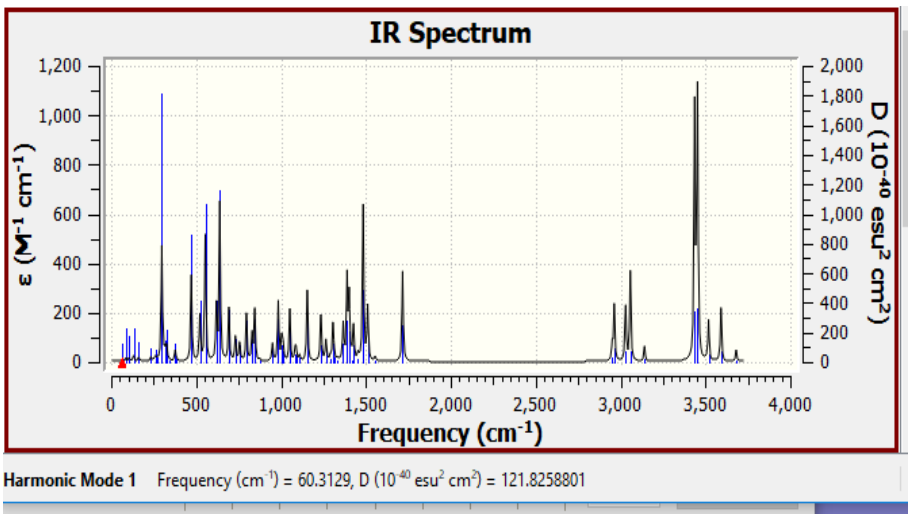

Figure 4A. IR spectrum of glucose in gaussian

For Raman calculations the same set of functionals was selected as for IR calculations in Gaussian software (Figure 5).

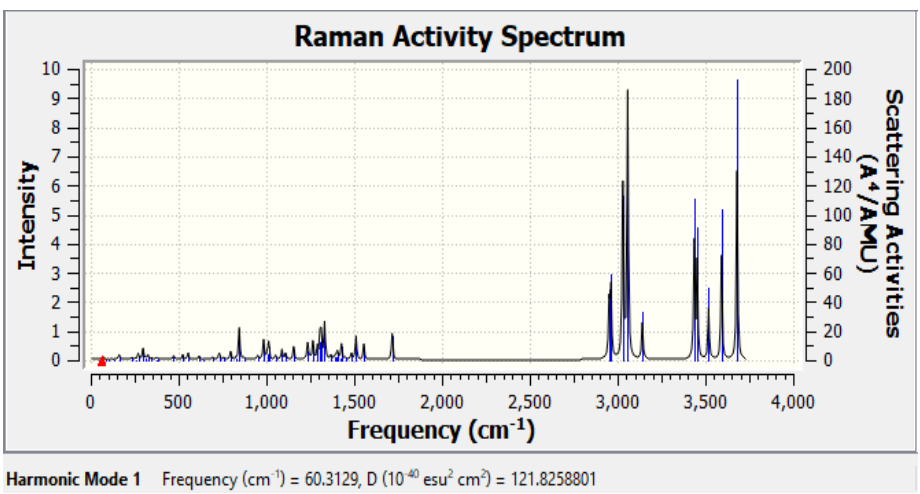

Figure 5. Raman spectrum of glucose in gaussian

For NMR spectra, we calculated the D-glucose in the Gaussian software (Figure 6).

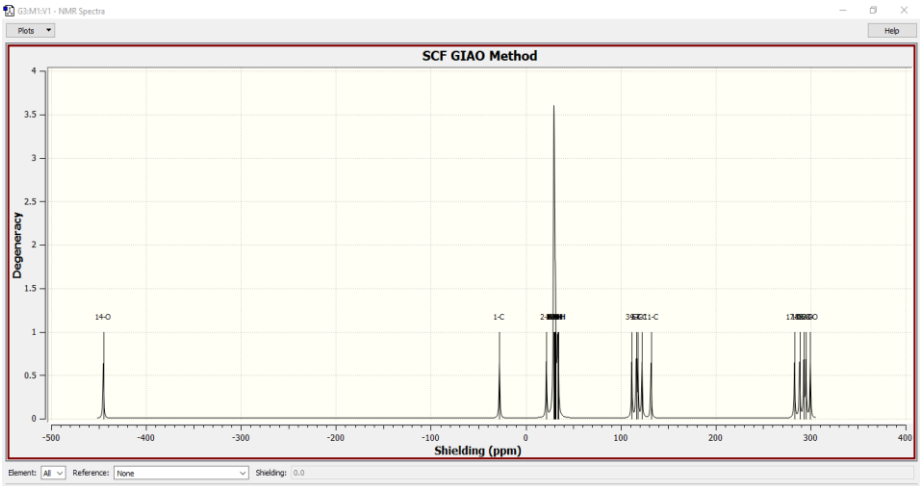

Figure 6. NMR spectrum of D-glucose in gaussian

For glucose, two carbohydrate molecules of low energy conformations were analyzed (Fig 7).Six conformations having low energy had been reported previously by conducting conformational studies using DFT related force-fields followed by calculation with DFT; the observed geometries provided information about the preliminary structures [18].

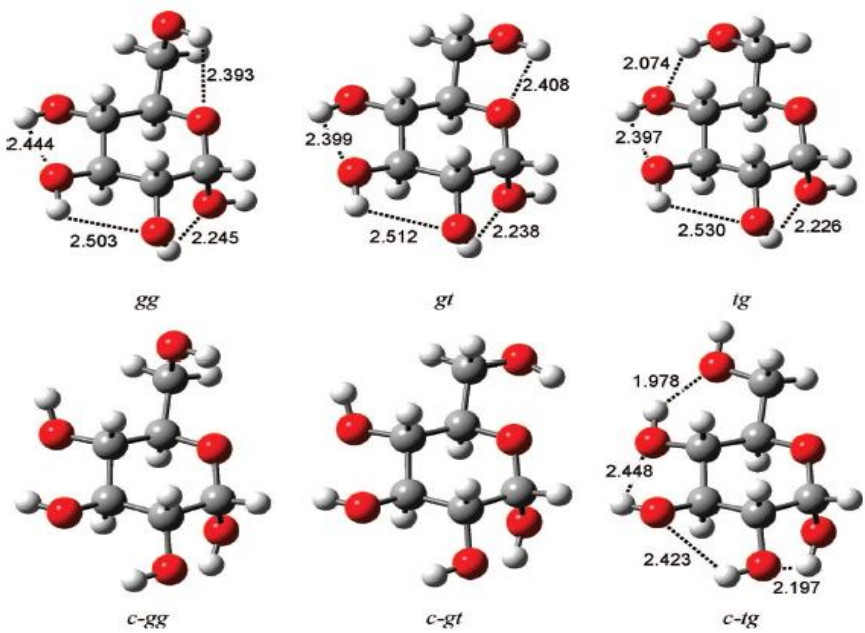

Figure 7. Characteristic conformers of R-D-glucose

Every glucose isomer is portrayed as a text related rotation isomerism. Inside the cyclic structure, rotation was found to occur at O6-C6-C5-O5 torsional angle called ω-angle, giving three staggered rotational conformers named as gauche-gauche (gg), gauche-trans (gt) and trans-gauche (tg). (Table 1 and 2)

Table 1. Characteristics of the Selected Fundamentals from the OH Stretching Region

Conformer	**Frequency cm^{-1}**	**Frequency cm^{-1}**
H Bond	**Calculated**	**Experimental**
Gg; O2-H...O1	3770	3580
Gt; O2-H...O1	3780	3580
Gt; O4-H...O3	3800	3610
Tg; O2-H...O1	3770	3580
Tg; O6-H...O4	3760	3570
C-tg; O4-H...O6	3740	3540

Table 2. Measured Lengths for Bonds Related to D-Glucose Optimized at the DFT Method B3LYP Level of Theory

Bond Distance	**B3LYP**
C-C(CH_2O)	1.537
C-C	1.538
C-H	1.121
O-H	0.985
C-O	1.455
C=O	1.235

5. Conclusion

IR, Raman and NMR spectra of D-glucose were obtained by the utilization of the quantum computational chemistry open source software package (GAMESS). High-level correlated quantum chemical calculations using the DFT method was selected for the conformations of D-glucose which indicated the evaluation capability of GAMESS as compared to the experimental results. These investigations reinforced the hypothetical assumption that D-glucose has gg, gt and ctg conformers as real parts of the compounds frequently used in the daily

life. This investigation was carried out to analyze the proof of the mental impacts of glucose and their effect on the feeling of prosperity and personal satisfaction.

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