Exploring the structural features of Glucose and Fructose with simulated ^{1}HNMR using JSPEC View (Jmol)

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1. INTRODUCTION

Carbohydrates are a class of naturally occurring organic compounds of carbon, hydrogen and oxygen which are primarily produced by plants. In the green plants, carbohydrates are produced by a process called photosynthesis. This process involves the conversion of simple compounds CO_2 and H_2O into glucose ($C_6H_{12}O_6$) and is catalyzed by green color pigment chlorophyll present in the leaves of plants in the presence of sunlight. **Glucose** is most common monosaccharide. It is known as Dextrose because it occurs in nature principally as optically dextrorotatory isomer. **Fructose** is another commonly known monosaccharide having the same molecular formula as glucose. It is levorotatory because it rotates plane polarized light towards the left. It is present abundantly in fruits. That is why it is called fruit-sugar also.

In this work we are going to explore the structural features of Glucose and Fructose with simulated ^{1}HNMR obtained from JSPEC view in Jmol.

2. OBJECTIVES

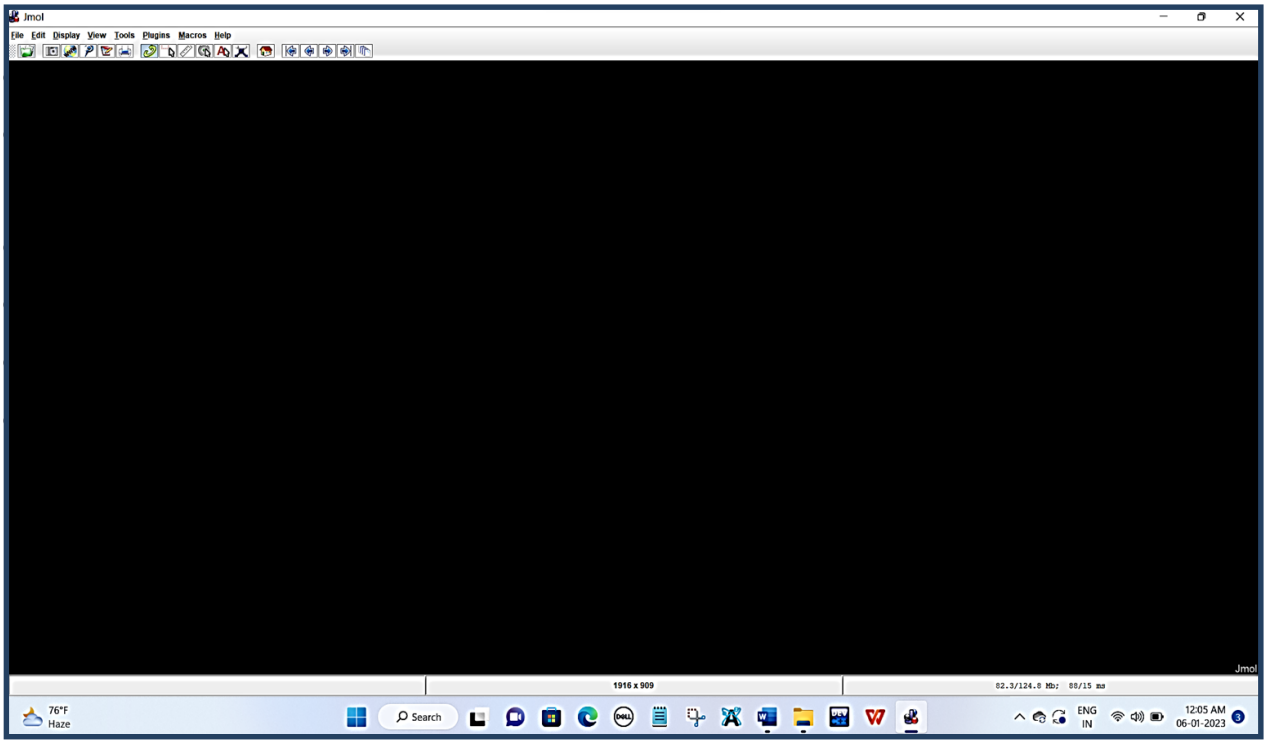
- To create 3D structure of Glucose and fructose in Jmol interface
- To obtain the simulated ^{1}HNMR for Glucose and Fructose in JSPEC view of Jmol
- To account for the existence of 6 carbon atoms in the Glucose and Fructose molecule
- To account for the existence of 5 hydroxyl groups in Glucose and Fructose
- To account for the existence and position of Aldehydic group in Glucose molecule
- Exploring the cyclic structures of Glucose and Fructose molecule

3. INSTALLATION OF Jmol

- Creating 3D molecular model
- Jmol is an open-source Java viewer for chemical structures and biomolecules in 3D
- It is free and open source software, written in Java, it runs on Windows, Mac OS X, Linux and Unix systems.

3.1. Procedure for installation of Jmol

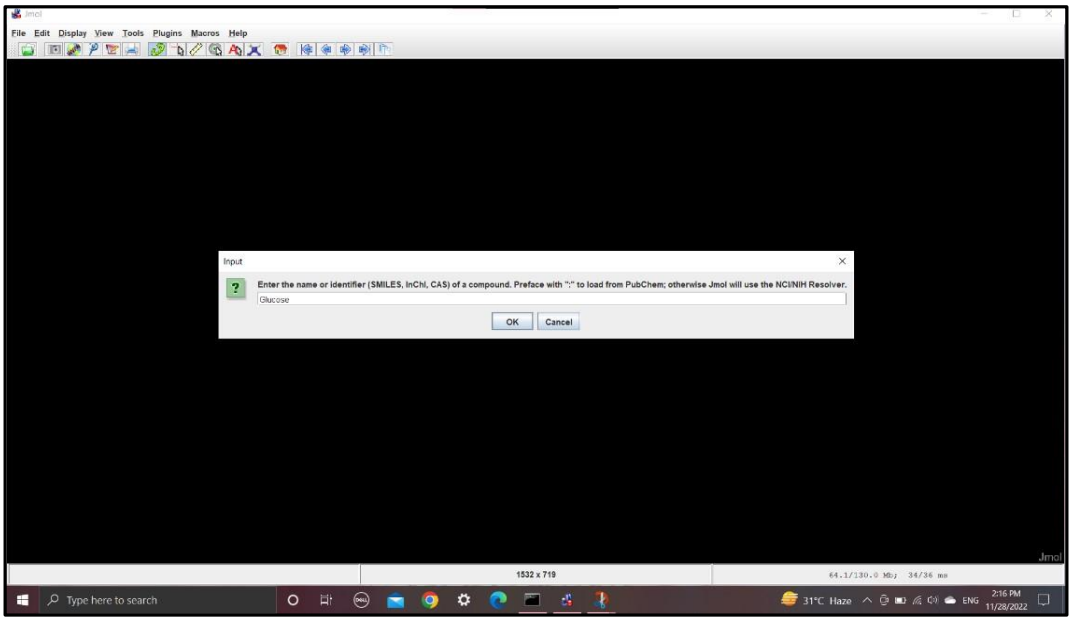
- The open source Jmol software needs JAVA application installed in your computer.



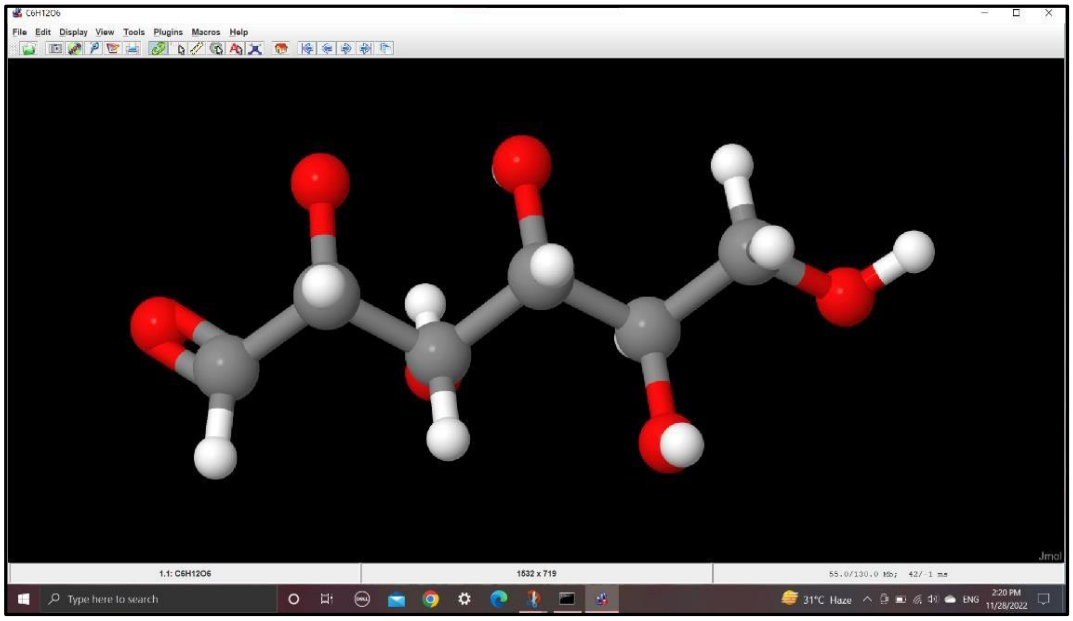
4. Structural elucidation of Glucose and Fructose

4.1. Procedure for creating the 3D Structures of Glucose and Fructose molecule in Jmol

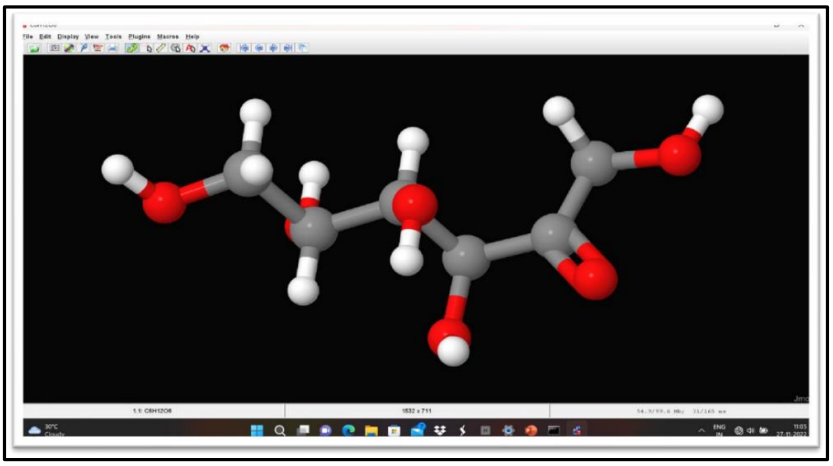
- We have built up glucose and fructose molecule in Jmol
- At first, we have to go to **file option** in **tool bar**.
- We have to choose **Get mol option.**
- Next, we have chosen Glucose and Fructose from their database.
- It looks like this: Glucose and Fructose



The 3D structure of Glucose molecule



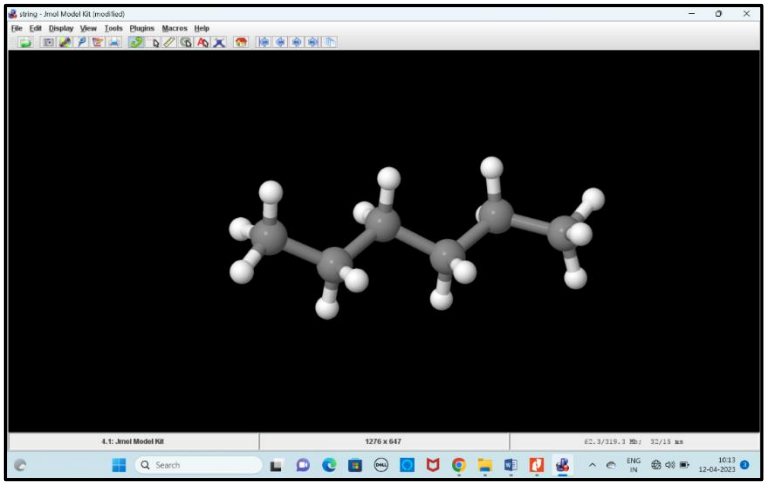
The 3D structure of Fructose molecule



4.2.Procedure for creating the 3D Structures of n-hexane molecule in Jmol

- We have built up n-hexane molecule in Jmol
- At first, we have to go to **file option** in **tool bar**.
- We have to choose **Get mol option.**
- Next, we have chosen n-hexane to import from their database.

The 3D structure of n-hexane molecule

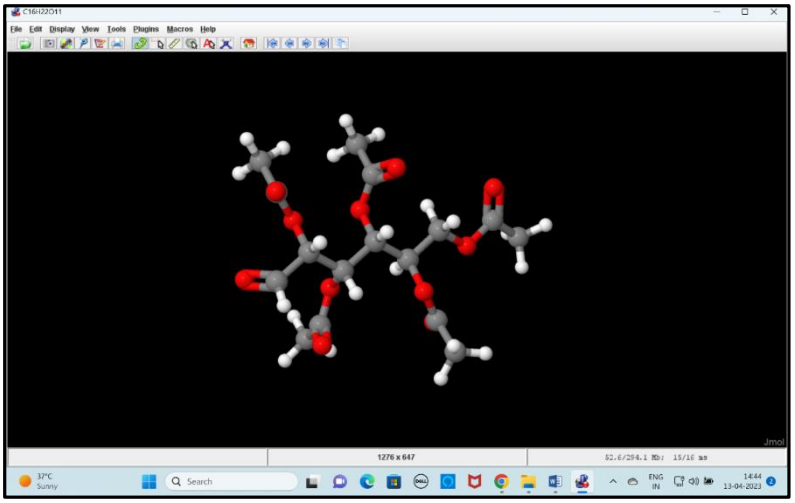


4.2.1. Procedure for obtaining simulated ^{1}HNMR of n-hexane molecule in JSPEC view of Jmol

- Open the Jmol interface window with the 3D structure of n-hexane
- In the menu bar go to “tool” menu click the spectra inside that choose ^{1}HNMR
- New JSPEC view dialogue box opens with ^{1}HNMRspectra of n- hexane

4.3. Procedure for creating the 3D Structures of glucose penta acetate molecule in Jmol

- We have built up glucose penta acetate molecule in Jmol
- At first, we have to go to **file option** in **tool bar**.
- We have to choose **Get mol option**
- Next, we have chosen glucose penta acetate to import from their database

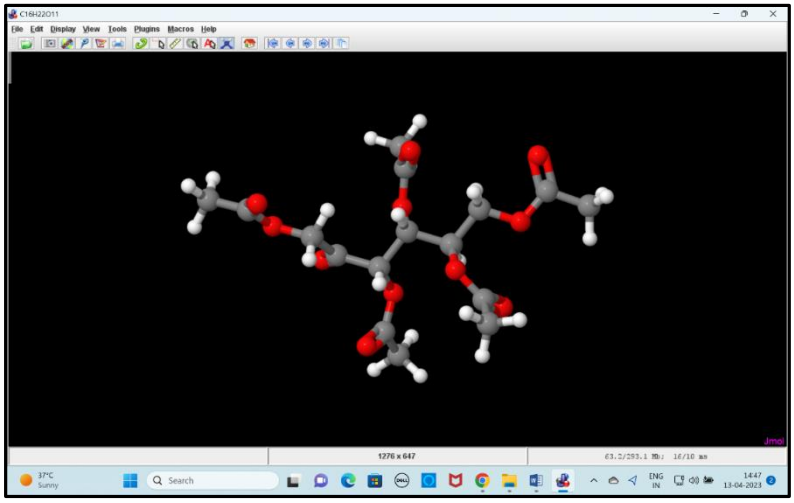


4.3.1. Procedure for obtaining simulated ^{1}HNMR of glucose penta acetate molecule in JSPEC view of Jmol

- Open the Jmol interface window with the 3D structure of glucose penta acetate
- In the menu bar go to “tool” menu click the spectra inside that choose 1HNMR
- New JSPEC view dialogue box opens with ^{1}HNMRspectra of glucose penta acetate

4.4.Procedure for creating the 3D Structures of fructose penta acetate molecule in Jmol

- We have built up fructose penta acetate molecule in Jmol
- At first, we have to go to **file option** in **tool bar**.
- We have to choose **Get mol option**
- Next, we have chosen fructose penta acetate to import from their database



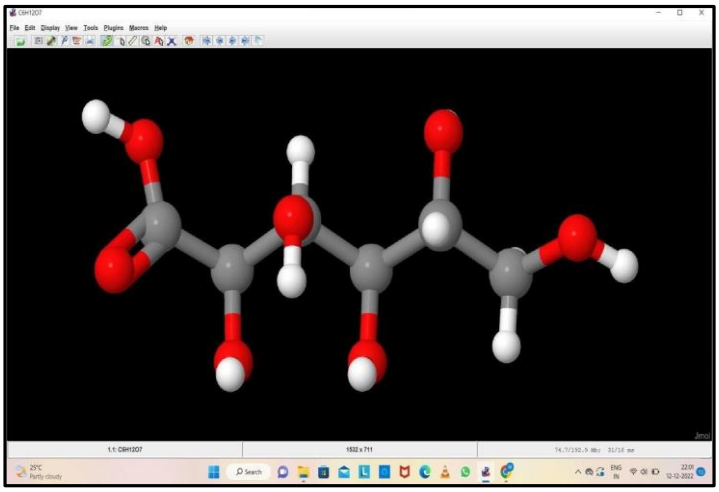
4.4.1. Procedure for obtaining simulated ^{1}HNMR of fructose penta acetate molecule in JSPEC view of Jmol

- Open the Jmol interface window with the 3D structure of fructose penta acetate
- In the menu bar go to “tool” menu click the spectra inside that choose ^{1}HNMR
- New JSPEC view dialogue box opens with ^{1}HNMRspectra of fructose penta acetate

4.5.Procedure for creating the 3D Structures of gluconic acid molecule in Jmol

- We have built up gluconic acid molecule in Jmol
- At first, we have to go to **file option** in **tool bar**.
- We have to choose **Get mol option**
- Next, we have chosen gluconic acid to import from their database

The 3D structure of gluconic acid

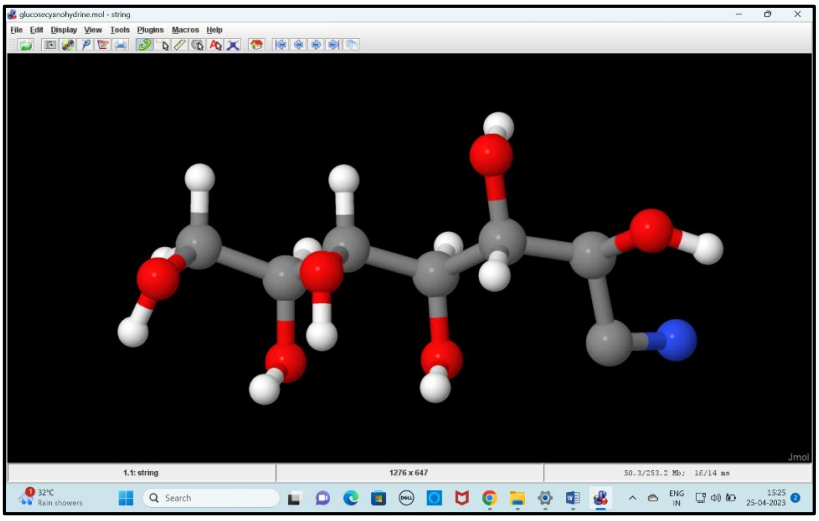


4.5.1. Procedure for obtaining simulated ^{1}HNMR of gluconic acid molecule in JSPEC view of Jmol

- Open the Jmol interface window with the 3D structure of gluconic acid
- In the menu bar go to “tool” menu click the spectra inside that choose ^{1}HNMR
- New JSPEC view dialogue box opens with ^{1}HNMRspectra of gluconic acid

4.6. Procedure for creating the 3D Structures of glucose cyanohydrin molecule in Jmol

- The 3D structure of glucose was imported from the database by clicking the Get MOL option in file menu
- Then the glucose structure was edited using model kit menu in Jmol interface
- The -CN group was introduced in the 6TH carbon, 1st carbon was edited to have CH_2OH.



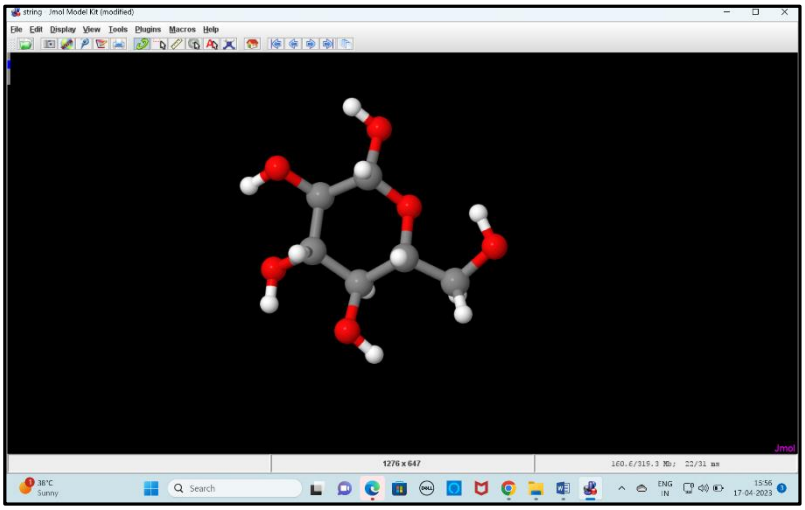
4.6.1. Procedure for obtaining simulated ^{1}HNMR of glucose cyanohydrin molecule in JSPEC view of Jmol

- Open the Jmol interface window with the 3D structure of glucose cyanohydrin
- In the menu bar go to “tool” menu click the spectra inside that choose ^{1}HNMR
- New JSPEC view dialogue box opens with ^{1}HNMRspectra of glucose cyanohydrin

4.7. Procedure for creating the 3D cyclic structure of Glucose molecule in Jmol

- We have built up cyclic structure glucose molecule in Jmol
- At first, we have to go to **file option** in **tool bar**.
- We have to choose **Get mol option**
- Next, we have chosen cyclic structure of glucose to import from their database

The 3D cyclic structure of Glucose molecule

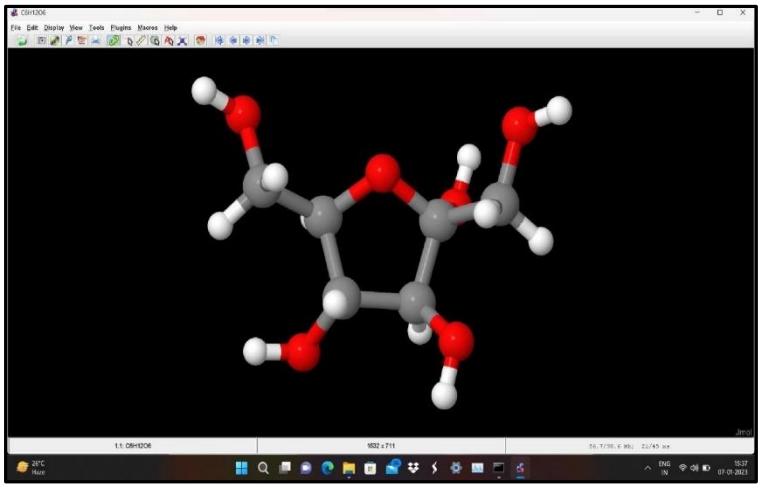


4.7.1. Procedure for obtaining simulated ^{1}HNMR of cyclic structure of Glucose molecule in JSPEC view of Jmol

- Open the Jmol interface window with the 3D cyclic structure of glucose
- In the menu bar go to “tool” menu click the spectra inside that choose ^{1}HNMR
- New JSPEC view dialogue box opens with ^{1}HNMRspectra of cyclic structure glucose

4.8.Procedure for creating the 3D Structures of cyclic structure of Fructose molecule in Jmol

- We have built up cyclic structure fructose molecule in Jmol
- At first, we have to go to **file option** in **tool bar**.
- We have to choose **Get mol option**
- Next, we have chosen cyclic structure of fructose to import from their database



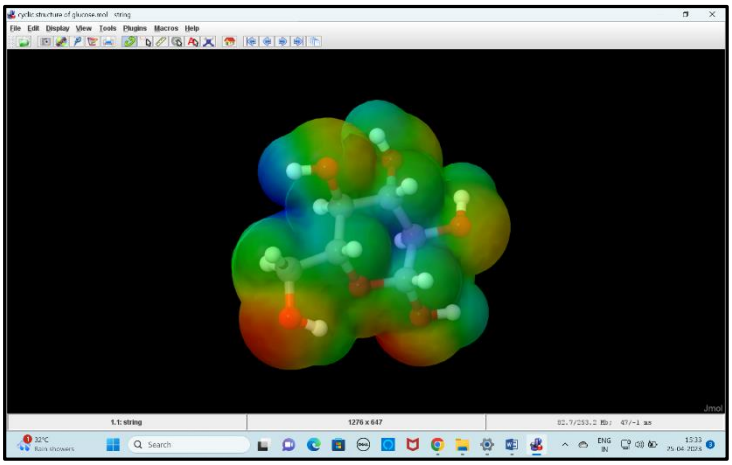
4.8.1. Procedure for obtaining simulated ^{1}HNMR of cyclic structure of Fructose molecule in JSPEC view of Jmol

- Open the Jmol interface window with the 3D cyclic structure of fructose
- In the menu bar go to “tool” menu click the spectra inside that choose ^{1}HNMR
- New JSPEC view dialogue box opens with ^{1}HNMRspectra of cyclic structure fructose

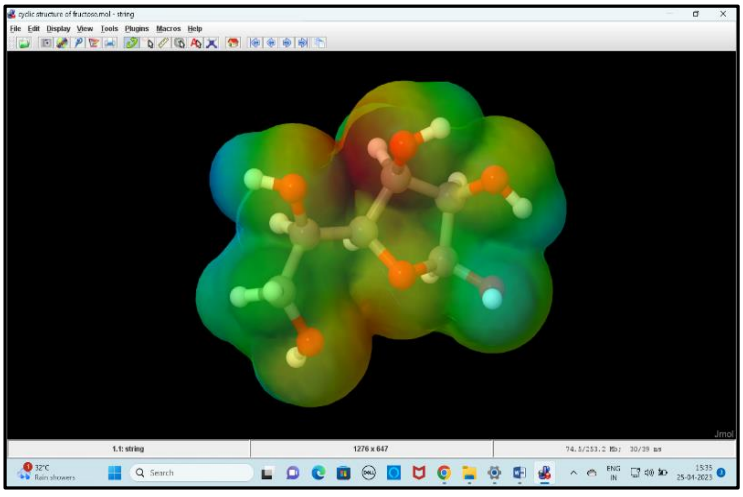
4.9. Procedure for getting the electrostatic surfaces for the molecules Glucose and Fructose in Jmol interface

- Get the cyclic structure of glucose/fructose molecule in the Jmol interface, Exit from the model kit
- Then right click on the molecule – will get a dialogue box; select “surfaces”.
- In surfaces menu select Molecular Electrostatic Potential –all range
- Now the molecule will appear like below

Molecular Electrostatic potential of the molecule Glucose



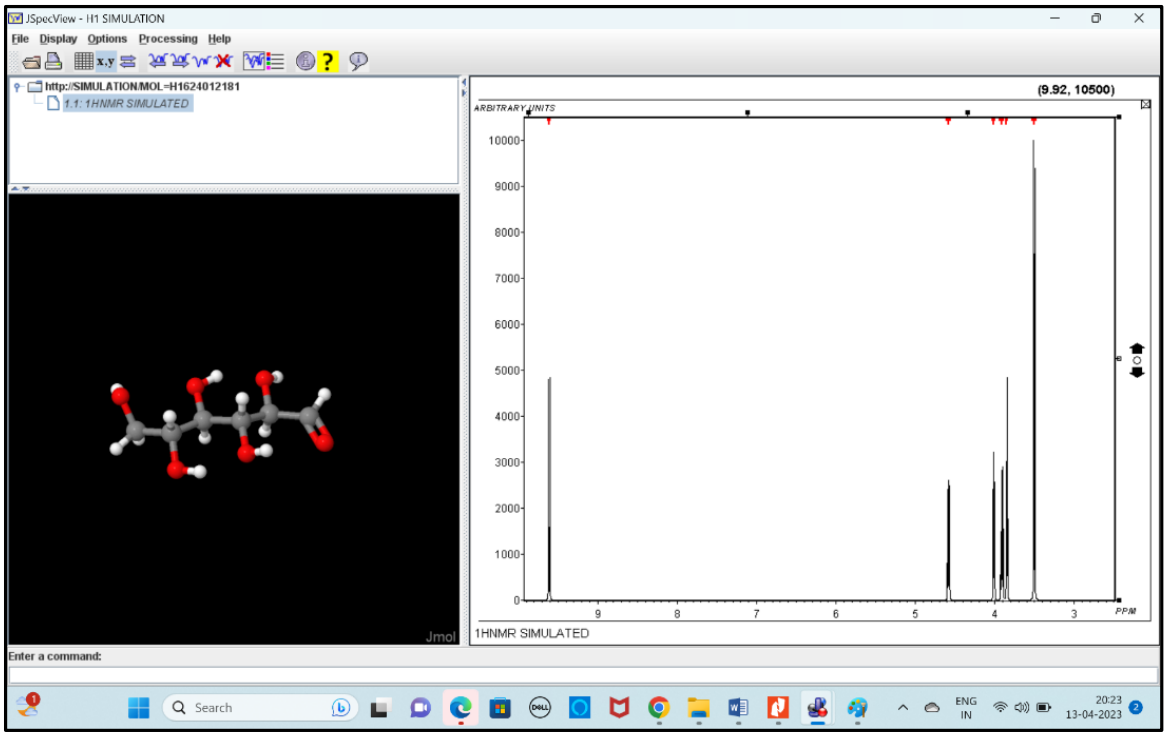
Molecular Electrostatic potential of the molecule Fructose

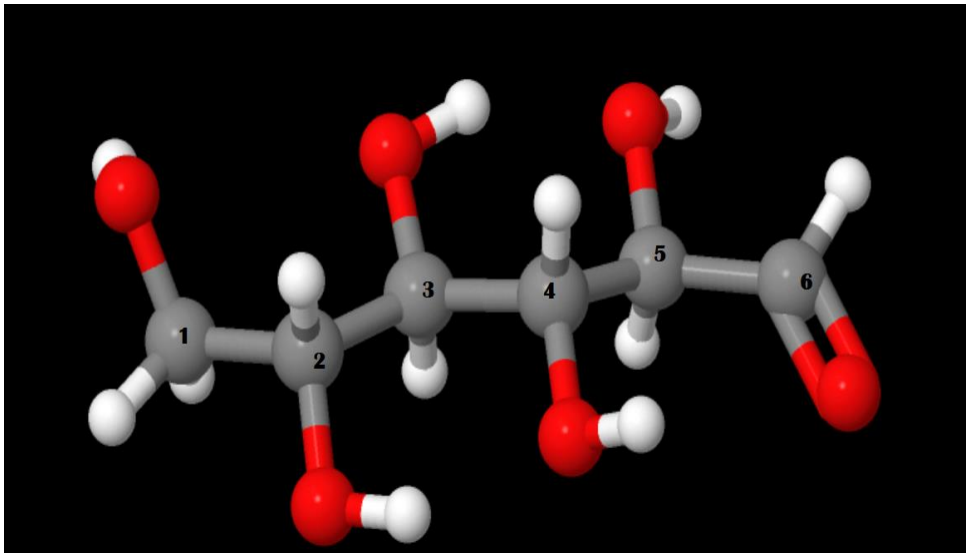


5. Result and Discussion

5.1. Simulated ^{1}HNMR spectra of Glucose and Fructose molecule obtained from JSPEC view of Jmol

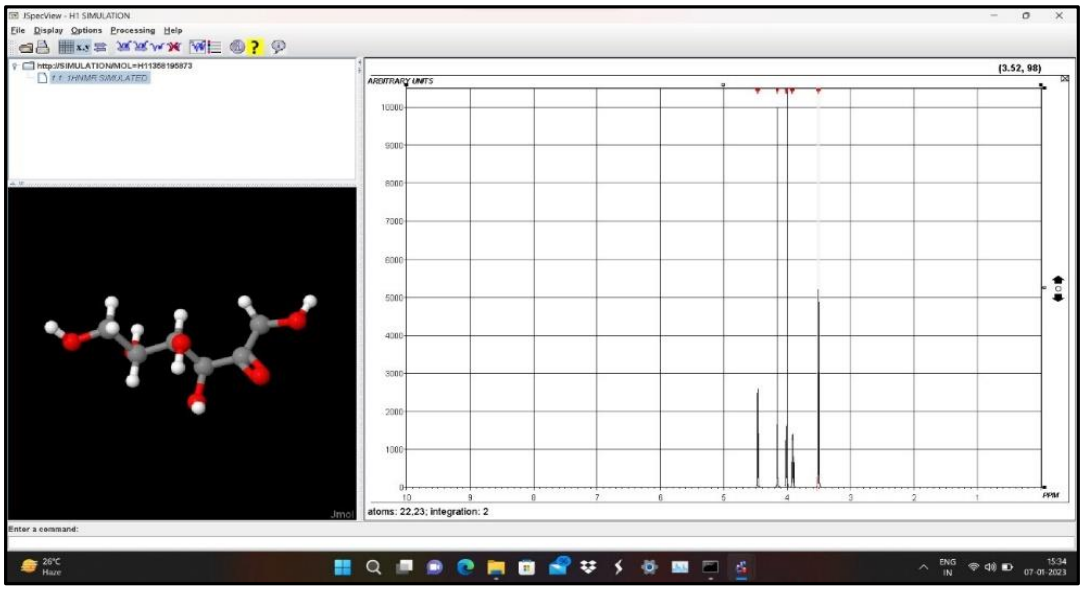
Simulated ^{1}HNMR spectra of Glucose molecule

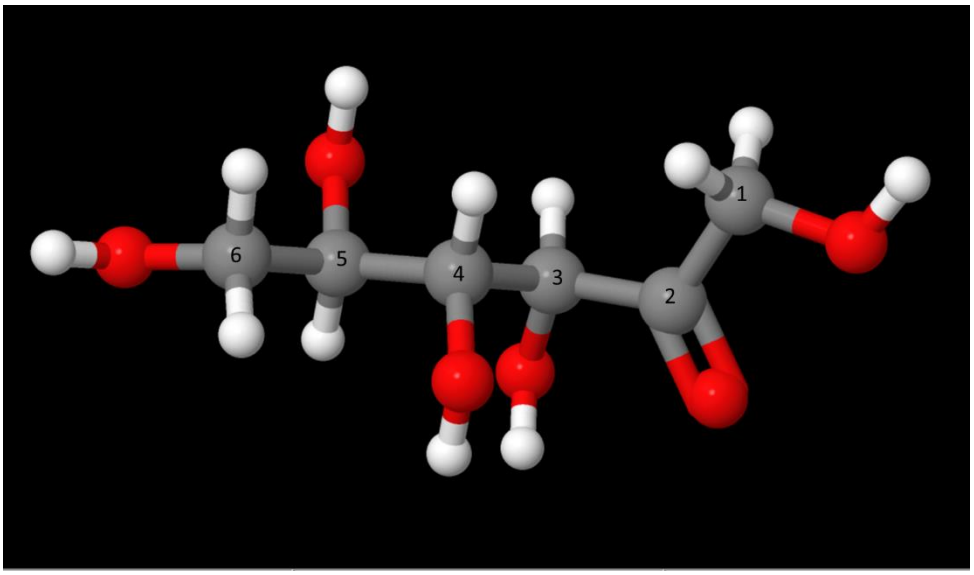




- The doublet peak at 9.63 PPM corresponds to the –OH proton attached to a C1 carbon at the end of the molecule, this is the most deshielded proton
- The doublet peak at 3.5 corresponds to the protons at carbon 1
- The multiplet at 4.6 PPM corresponds to the proton in the carbon 2

Simulated ^{1}HNMR spectra of Fructose molecule

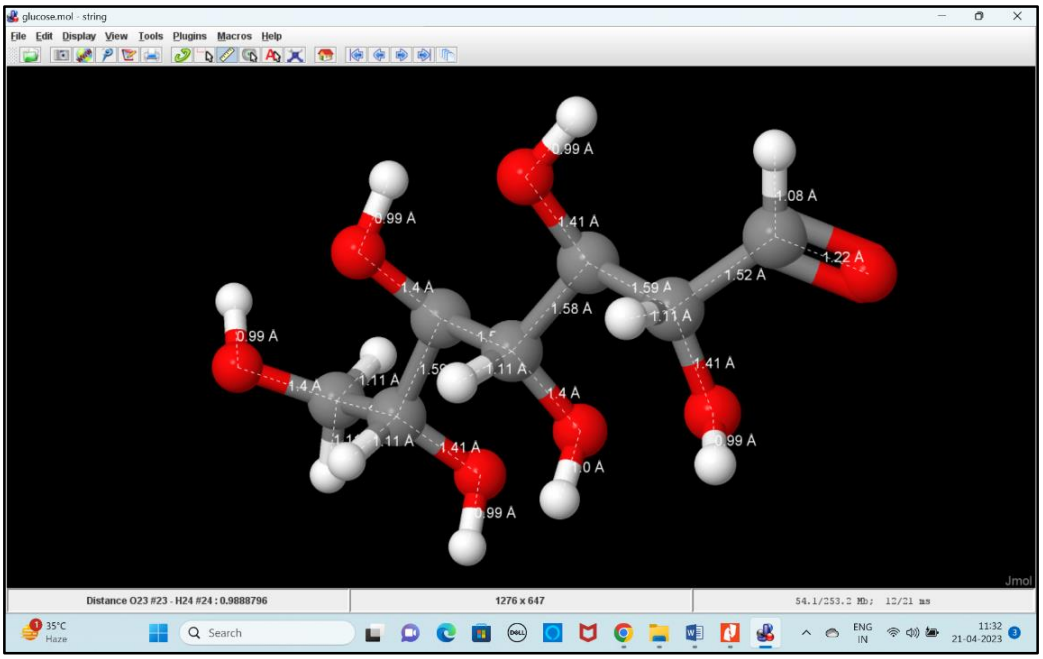




- The doublet at 4.46 PPM corresponds to the proton carbon 3
- The singlet at 4.1 PPM corresponds to the two protons carbon 1
- The doublet at 3.5 PPM corresponds to the proton at the carbon 6

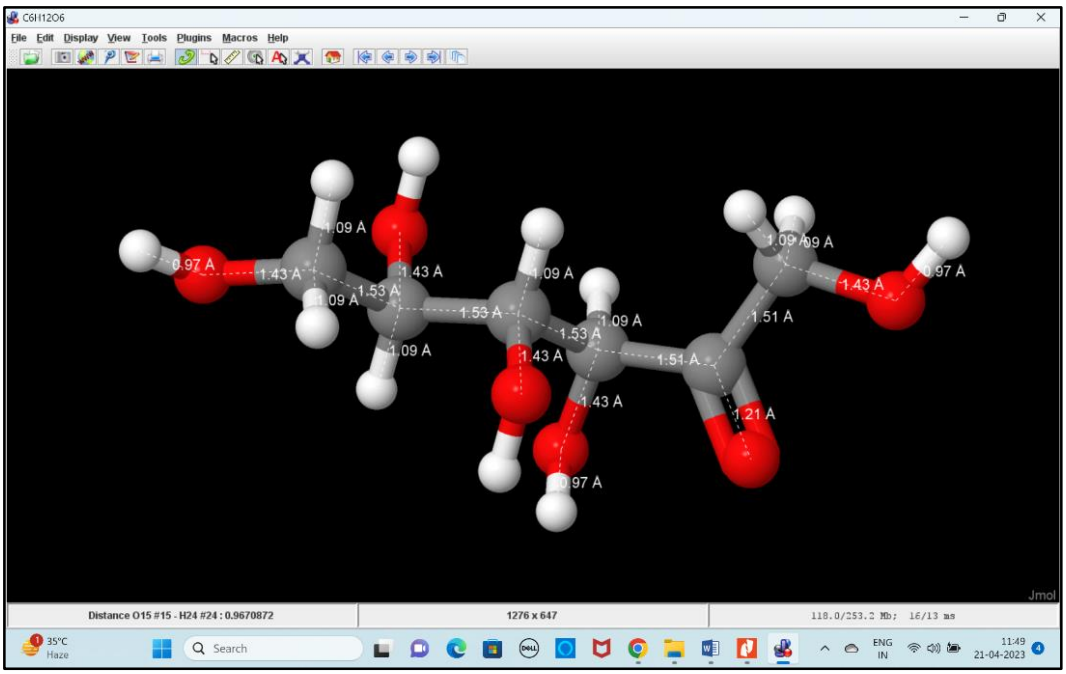
From the above observations in both glucose and fructose molecule the peaks obtained from stimulated 1HNMR shows the presence of 6-OH groups, each –OH group attached to different carbon attoms. The peak at 9.96 PPM appeared in glucose molecule is not seen in frunctose molecule which infers the presence of aldehydic group in glucose and presence of ketonic group in fructose at 2 position.

5.1.1. Measurement of bond length of Glucose and Fructose molecule obtained from in Jmol interface



The bond lengths were measured after drawing the 3D structure of the glucose molecule:

- The bond length of C-C bonds were around 1.5A
- The bond length of C-H bonds were around 1.1A
- The bond length of O-H bonds were around 0.99A
- The bond length of C=O was aroung 1.22 A

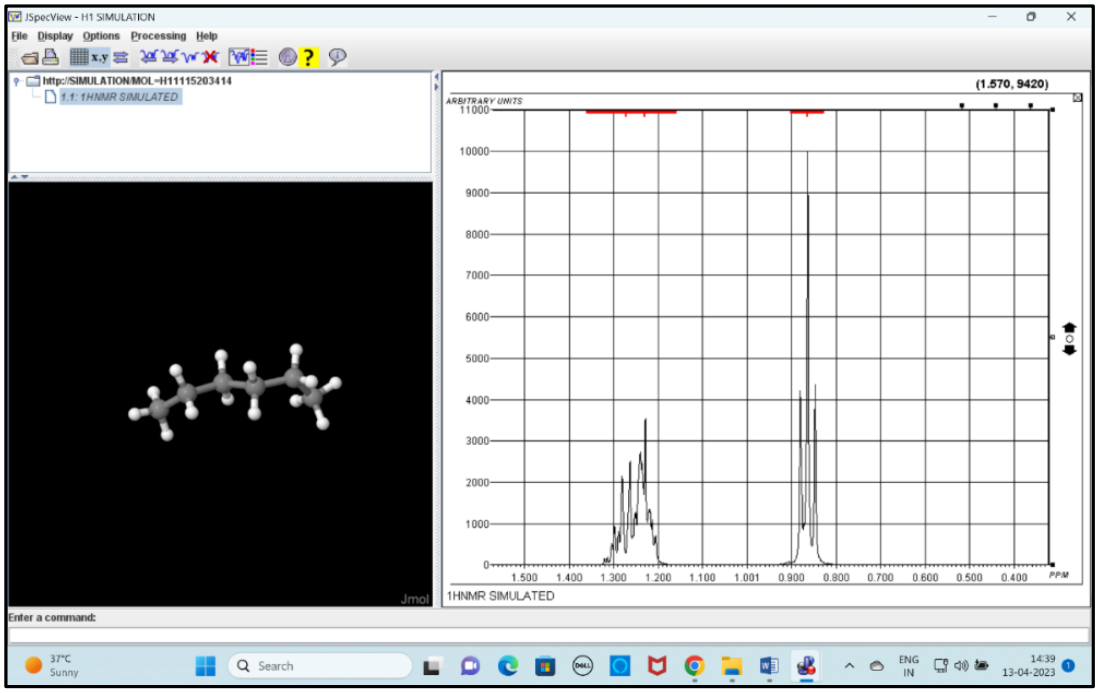


The bond lengths were measured after drawing the 3D structure of the fructose molecule:

- The bond length of C-C bonds were around 1.5A
- The bond length of C-H bonds were around 1.1A
- The bond length of O-H bonds were around 0.99A
- The bond length of C=O was around 1.21A

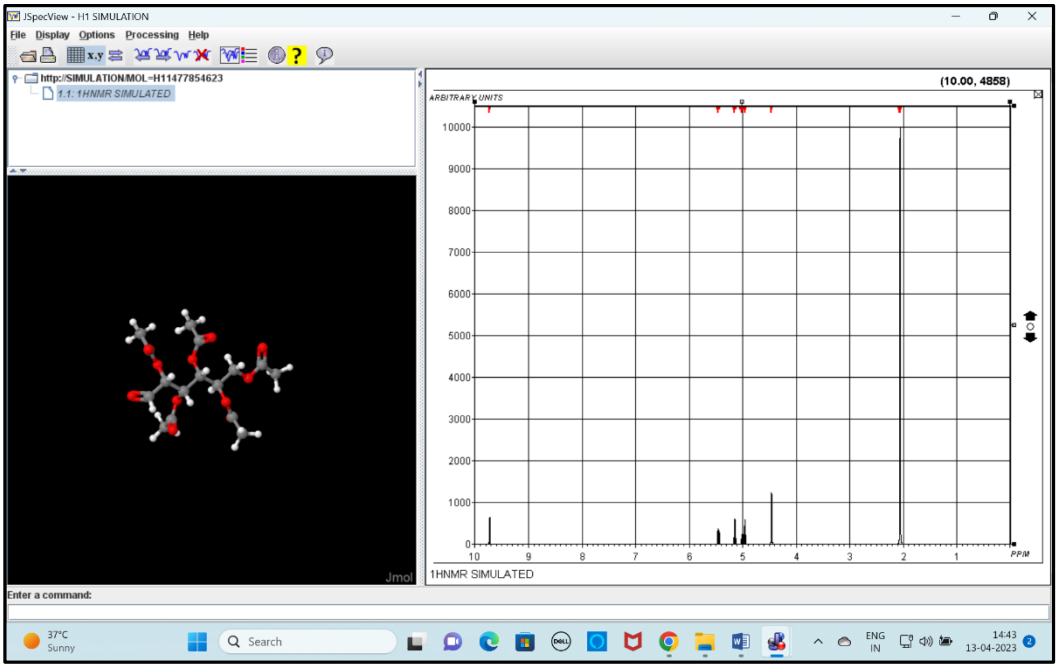
From the above observations in both glucose and fructose molecule the bond lengths were found to be similar which infers that the glucose and fructose were structural isomers and differs only in the fuctional group.

5.2. Simulated ^{1}HNMR spectra of n-Hexane molecule obtained from JSPEC view of Jmol



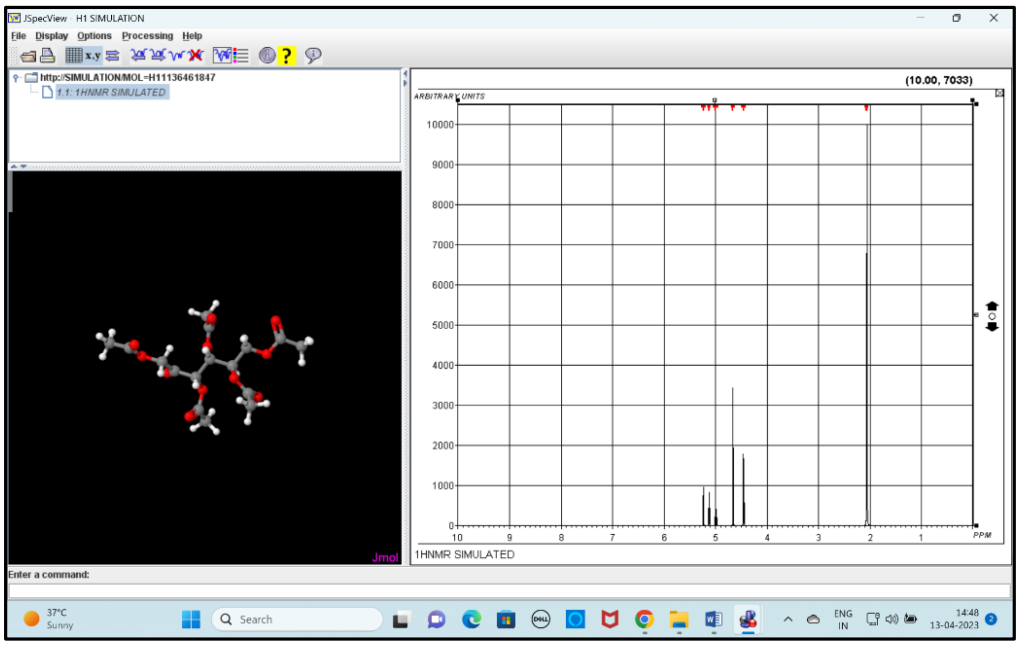
- The reduction of glucose and fructose with red phosphorus and HI gives n-hexane, which shows that the six carbon atoms in the glucose and fructose molecules were in a straight chain
- The simulated ^{1}HNMR for hexane shows a triplet peak at 0.864 PPM corresponds to the three protons at the edges of the hexane molecule and the crowded multiplet peaks from 1.2 to 1.3 corresponds to the protons in remaining carbon atoms

5.3. Simulated ^{1}HNMR spectra of glucose penta acetate molecule obtained from JSPEC view of Jmol



- The doublet peak at 9.73 PPM corresponds to the aldehydic proton in the glucose penta acetate
- The peaks from 4.9- 5.5 PPM corresponds to the –C-H protons
- The peaks at 2.06 and 2.05 PPM corresponds to the methyl protons ($–CH_3$)

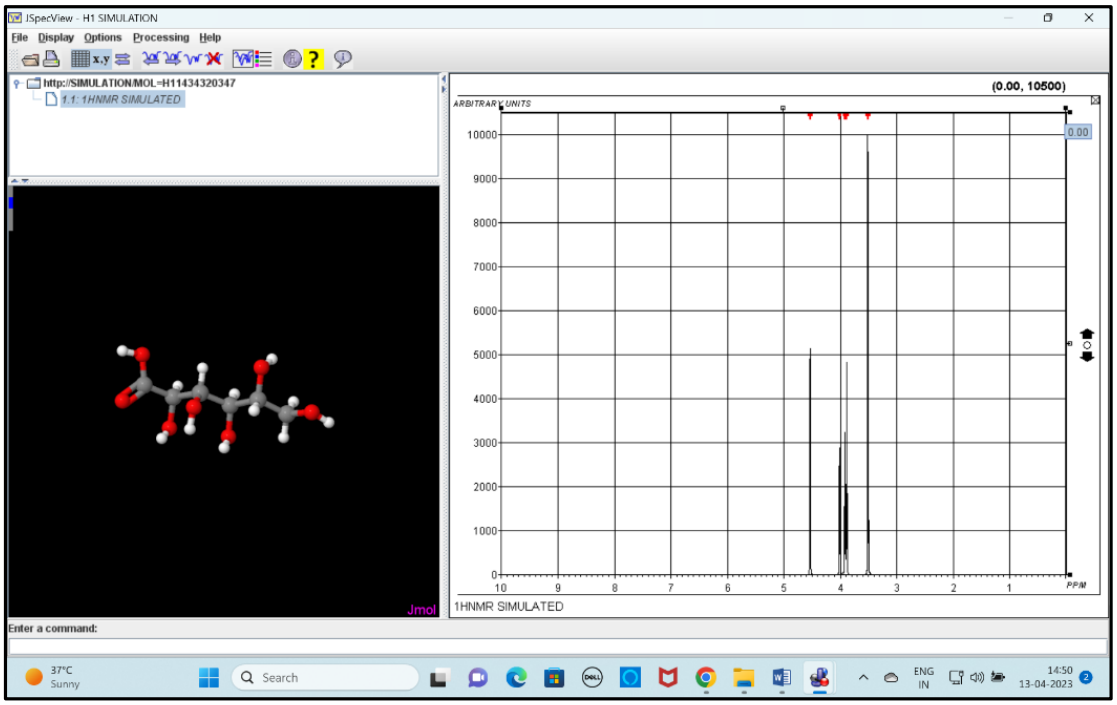
5.3.1. Simulated ^{1}HNMR spectra of fructose penta acetate molecule obtained from JSPEC view of Jmol



- The peaks from 4.9- 5.5 PPM corresponds to the –C-H protons, similar to that of the glucose penta acetate
- The doublet peak at 9.73 PPM of glucose penta acetate, is not seen in fructose penta acetate as it corresponds to aldehydic functional group
- A singlet peak at 4.66 PPM and a doublet at 4.45 PPM corresponds to $–CH_2$ protons next to the –C=O group

From the above observation we can conclude that both Glucose and Fructose on treatment with acetic anhydride gives glucose penta acetate and fructose penta acetate, which shows the presence of five hydroxyl group in the glucose and fructose molecule.

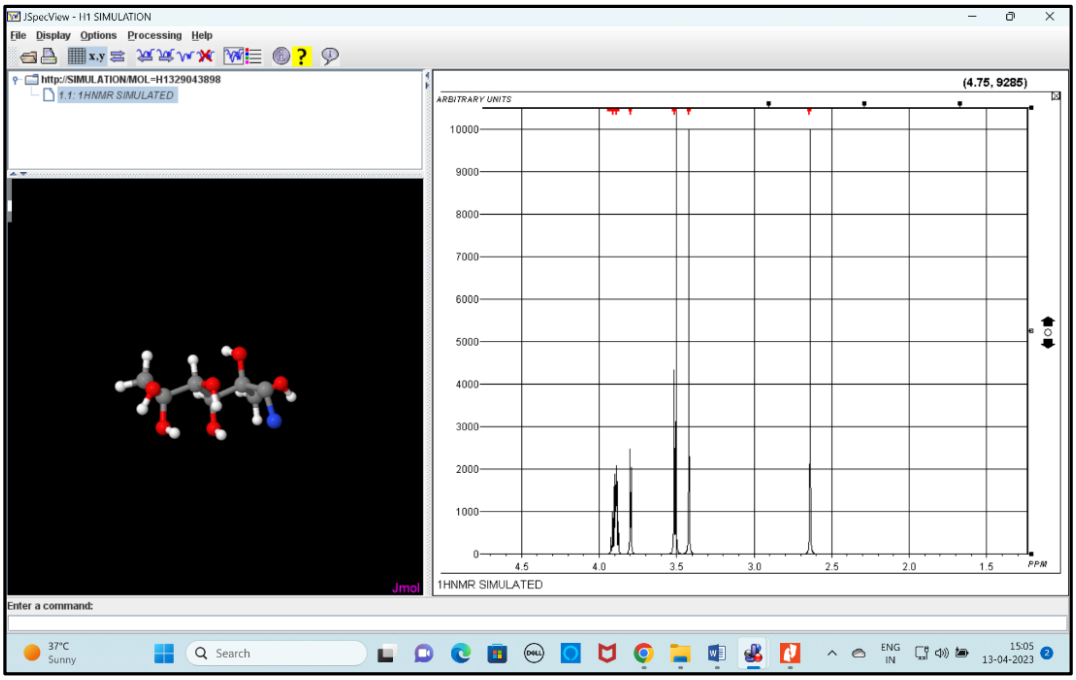
5.4. Simulated ^{1}HNMR spectra of gluconic acid molecule obtained from JSPEC view of Jmol



- The doublet peak at 9.63 PPM corresponds to the –OH proton of the glucose molecule was not seen in the simulated ^{1}HNMR spectra of gluconic acid , which confirms the oxidation of $–CH_2OH$ group to –COOH group in the glucose molecule
- Glucose on mild oxidation with Br water, forms gluconic acid, a monocarboxylic acid with 6 carbon atoms which shows the existance of carbonyl group is an aldehydic group in the glucose molecule

- Fructose shows no reaction with Br water which means in fructose molecule there is no possibility for the existance of –CHO group
- Fructose on oxidation with nitric acid gives glycolic acid and tartaric acid with less number of carbon atom than fructose. It is also evident that the position of –C=O group is 2. That is point at which the molecule has broken to give glycolic acid and tartaric acid.

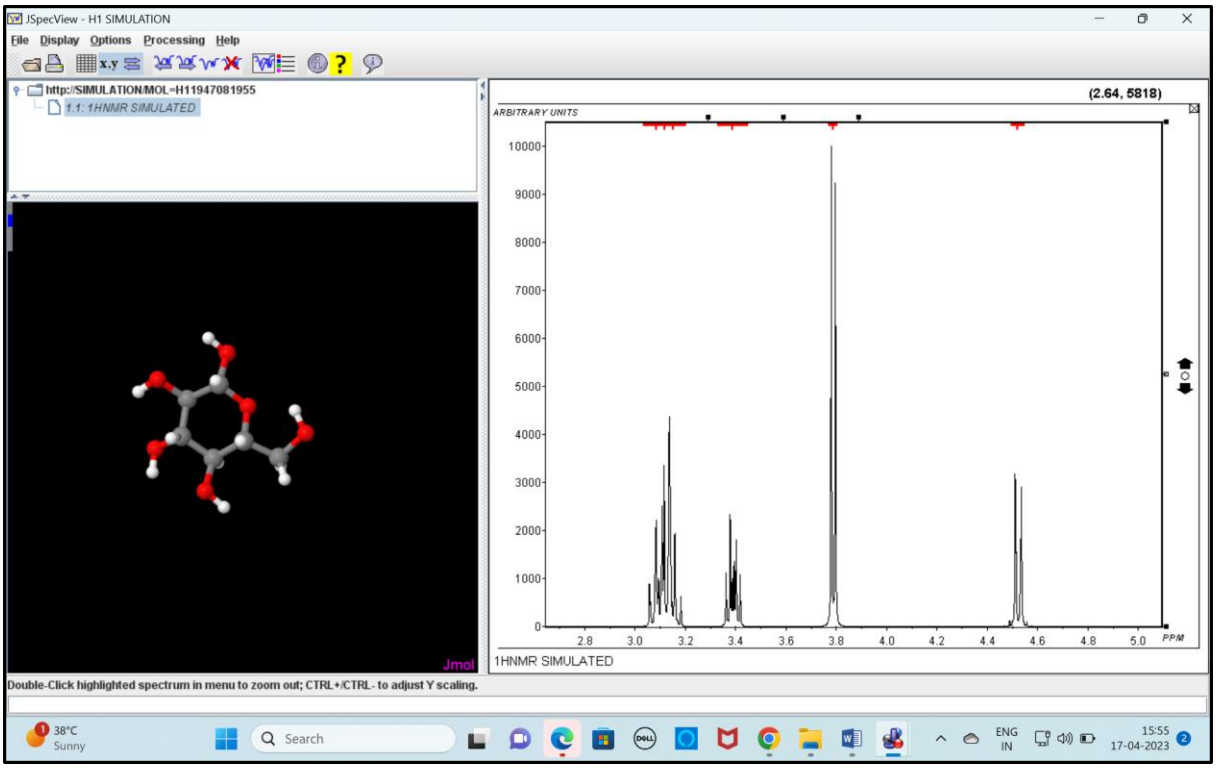
5.5. Simulated ^{1}HNMR spectra of Glucose cyanohydrin molecule obtained from JSPEC view of Jmol



- Similar to the aldehydes the glucose molecule also form cyanohydrin, which confirms the existance of –CHO group in glucose molecule
- The absence of the peak at 9.63 PPM in glucose cyanohydrin confirms the addition reaction undergone by the –CHO group of glucose molecule with HCN to form cyanohydrin

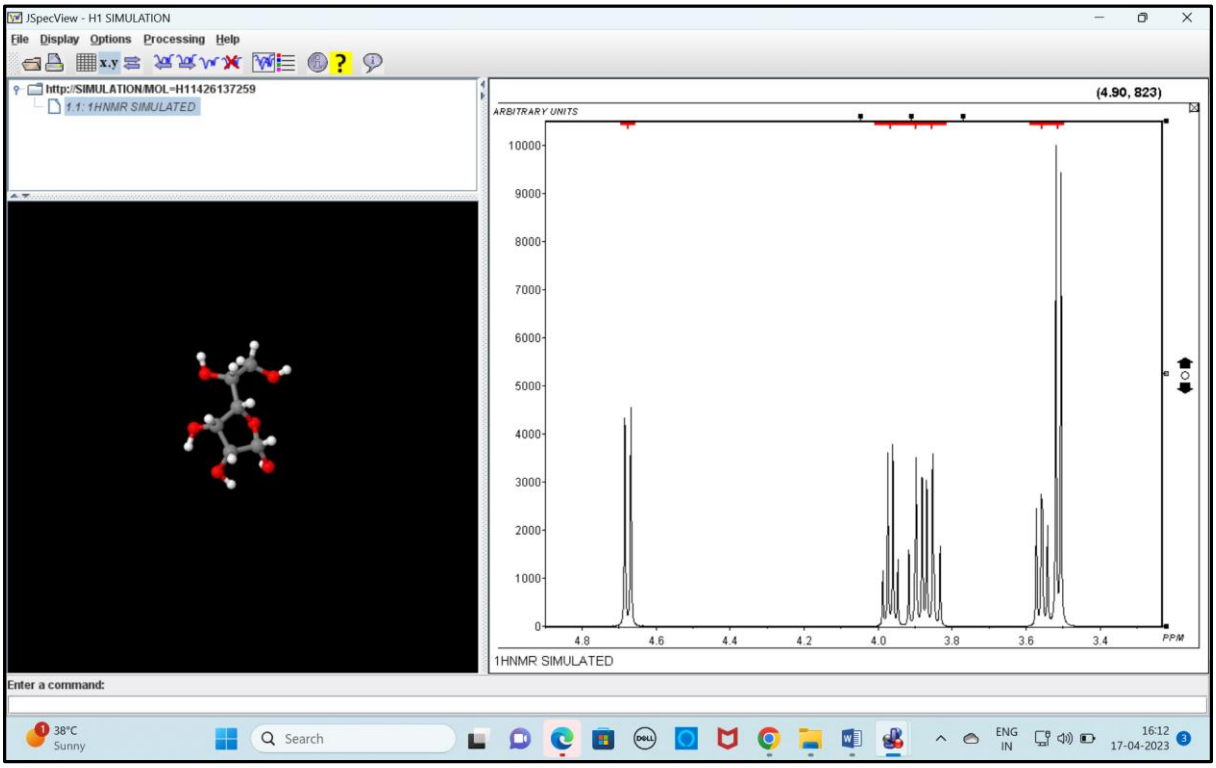
5.6. Simulated ^{1}HNMR spectra of cyclic structure of glucose and fructose molecule obtained from JSPEC view of Jmol

Simulated ^{1}HNMR spectra of cyclic structure of glucose molecule



- The doublet peak at 4.53 PPM corresponds to the –CH proton in the ring
- The doublet peak at 3.7 PPM corresponds to the $–CH_2$ proton outside of the ring
- The multiplet at 3.3 PPM corresponds to the –CH proton in the ring which is connected with the $–CH_2OH$ group outside the ring
- The cluster of multiplets from 3.0 to 3.2 PPM corresponds to the –CH protons in the ring structure

Simulated ^{1}HNMR spectra of cyclic structure of glucose molecule



- The doublet peak at 4.6 PPM corresponds to the –CH proton in the ring similar to that of the cyclic glucose structure
- The doublet peak at 3.96 PPM corresponds to the –CH proton bonded with –OH group, outside of the ring, which is not seen in the cyclic glucose structure
- The double at 3.5 PPM corresponds to the $–CH_2OH$ proton outside the ring bonded with –CHOH group outside the ring
- The cluster of multiplets from 3.8 to 3.9 PPM corresponds to the –CH protons in the ring structure
- The difference in the multiplet structure peak position of cyclic glucose and cyclic fructose is because of the number of carbon atoms in the ring, the glucose forms a six membered ring with 5-carbon atoms and 1-oxygen atom; fructose forms a 5 membered ring with 4-carbon atom and 1-oxygen atom

6. Conclusion

- The simulated ^{1}HNMR spectra obtained from JSPEC view of Jmol for glucose and fructose were compared, it was concluded that both the molecule differ only in their functional group
- The bond lengths of both the molecules were measured in Jmol interface and compared, it reveals that they are strutural isomers
- The formation of hexane by both of them reveals they have 6 carbon atoms in a straight line
- The formation of penta acetate by both the molecules reveals that they have 5-OH groups in 5 different carbon atoms
- The oxidation of glucose results in the formation of gluconic acid reveals that the aldehydic group in the terminal position of the molecule
- The fructose is not oxidised similar to glucose which means it is not having an aldehydic group
- The formation of addition compound cyanohydrin by glucose again confirms the presence of aldehydic group
- The glucose forms a 6 membered cyclic structure and fructose forms a five membered cyclic structured.

Acknowledgement

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