Investigate the effect of OH group's orientation in Natural and Rare Sugars: DFT-AIM-NBO Study

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Monosaccharide carbohydrates play in many biological processes. β-D (glucose, galactose, mannose) are sugars that occur large amounts in nature. Rare sugars such as β-D (allose, altrose, gulose, idose and talose) which are numerous but only present naturally in small amounts. These sugars are stereoisomer and differ by only the orientation of the hydroxyl group at the C2-C4 positions. Ab initio calculations based on density functional theory using B3LYP/6-31G* have been performed to investigate the effect of hydroxyl group's orientation to the nature of hydrogen bonds and its strength in these sugars. The atoms in molecules (AIM) analysis confirm the existence of regular intra-molecular hydrogen bond paths, so that gulose and glucose display single bond critical points, and allose, galactose, and mannose display two bond critical points, talose,and altrose display three bond critical points,except idose displays bifurcated acceptor intra -molecular hydrogen bond at critical points. According to the Laplacian signs and total energy electron density in the appropriate critical point (3,-1) intra-molecular hydrogen bonds: (i) atrose and mannose should be assigned to a weak; (ii) gulose and glucose should be assigned medium; (iii) talose, galactose, allose and idose with different bonds are categorized on weak and medium intra-molecular hydrogen bond closed shells of interaction. Maximum energy regular intra-molecular hydrogen bonding is measured approximately 11.73kcal/mol, while it is for bifurcated hydrogen bonds in idose is between 58% and 45% of regular hydrogen bonds. From NBO analysis, the formation of intra-molecular hydrogen bonds in monosaccharide sugars implies that certain electronic charges are transferred from the lone pair to the anti-bonding orbital. These types of sugars have different applications in the Pharmaceutical field (Chemotherapeutic), foods industry, cosmetic, treatment for skin cancer, etc. Therefore, theoretical point of view of nature hydrogen bond in these carbohydrates would provide further insight into the monosaccharaides structural maintenance and properties.

Keywords: Natural and Rare sugars, Hydrogen bonding, AIM, NBO.

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