

Bifurcated hydrogen bonding in carbohydrate sugars

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Abstract

The eight aldohexoses series of carbohydrate sugars namely, β -D -allose, altrose, gulose, idose, talose, glucose, galactose and mannose, are stereoisomers, they differ by only the orientation of the hydroxyl group at the C2-C4 positions. *Ab initio* calculations based on density functional theory (DFT) using B3LYP/6-31G* have been performed to investigate intra-hydrogen bond characteristics of hydroxyl groups in aldohexose sugars. The atoms in molecules (AIM) approach and natural bond orbital analysis (NBO) are used to measure strength and energy intramolecular hydrogen bonding in aldohexoses. It has been found that all aldohexose sugars display regular intra-hydrogen bond (two-centered), except idose sugar displays bifurcated acceptor (three-centered) intramolecular hydrogen bonds. Maximum energy regular intramolecular hydrogen bonding are measured approximately 11.73 kcal/mol, while it is for bifurcated hydrogen bonds in idose is between 58% and 45% of regular hydrogen bonds. A theoretical point of view in intra-molecular hydrogen bond in carbohydrate aldohexoses would provide further insight into the monosaccharides structural maintenance and properties.

Keywords: Aldohexose, Bifurcated Hydrogen bonding, Hydroxyl group, DFT, AIM, NBO

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