

# Influence of H-Bonds on Acidity of Deoxy- Hexose Sugars

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## Abstract

The unusual monosaccharaides such as Deoxy-hexose sugars, including methyl-pentose and aldo-pentose are promising and important sugars in life science, which have enormous chemotherapeutic and pharmaceutical applications. However, little research on H-bond interactions in these systems has been reported. The aldo-pentose has a proton instead of the CH<sub>2</sub>OH group on C5; conversely, methyl-pentose has a CH<sub>3</sub> group on C5. The aim of the present study is to investigate the role and nature of intramolecular H-bonds on acidity of CH<sub>3</sub>-pentose sugars (L-fucose and L-rhamnose) and aldo-pentose sugars (D-xylose, L-lyxose, D-ribose and L-arabinose) using B3LYP/6-311++G(d,p) level. The calculated acidity values ([?]*H*acid) of these Dexoy-hexose were found to be from 343 to 369 kcal.mol<sup>-1</sup>, indicating they are stronger acid than ethanol and 2-propanol with the acidity values of 378.3 and 375.1 kcal.mol<sup>-1</sup>, respectively. This is related to the stabilization of the conjugate bases of these sugar through intramolecular H-bonds, which were analyzed in this study using AIM and NBO methods.

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