384c The Role of Hydrogen Bonding Interactions in Acidic Sugar Degradation Pathways: an Ab Initio Molecular Dynamics Approach

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Our understanding of the roles that solvents play in chemical and biological reactions is very limited. We know that the sugar degradation pathways in acidic aqueous solutions are complex because of the multiple degradation products observed experimentally. In addition, the effects of reaction conditions such as temperature, cosolvents, and salts appear to affect the degradation products profoundly. Ab initio molecular dynamics simulations with explicit solvent water molecules were carried out to study the &beta-D-xylose and &beta-D-glucose degradation pathways under acidic conditions. It was found that water molecules actively participate in sugar degradation reactions due to hydrogen bonding interactions between the sugar molecules/reaction intermediates and the solvent molecules. The effects of water structure as a result of reaction conditions were investigated and will be discussed.