Hydration of carbohydrate molecules

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Carbohydrates are among the most essential biomolecules that play principal roles in several biological processes such as molecular recognition, and structural stabilization and modification of proteins and nucleic acids that can act as cryoprotective molecules for living cells. Additionally, they play a significant role in many industrial applications related to, e.g., food, biotech, and cosmetics industries. [1] Although carbohydrates are generally considered hydrophilic compounds, they have substantial hydrophobicity that varies with their structure. In the gas phase, the energetically most stable conformations are the ones where hydroxyl groups form a well-defined intramolecular H-bonded pattern. [2] The competition of these intramolecular H-bonds with the intermolecular ones, which are formed between the carbohydrate ring oxygen and the water molecules, along with the hydrophobic interactions, determine the solvation shell of these molecules.

In this presentation, we consider four simple sugars, α-D-glucose, α-D-glucose, α-D-galactose, and α-D-mannose, whose molecular structures are very similar, yet their solubilities in water are rather different. We calculated different properties that characterize the hydration of carbohydrate molecules and reveal the differences between them. These include, among others the average number of acceptor and donor H-bonds, the average length of acceptor and donor H-bonds, and the properties of three and four-coordinated water molecules around carbohydrate molecules.

Using classical and ab initio molecular dynamics simulations provides a very strong base for our results. Thus, in the next step applying these tools, we investigated the hydration shell (hydrophobic and hydrophilic) of more systems, namely the cyclodextrin family. These molecules are cyclic oligosaccharides composed of D-glucose units which are linked through α−1,4 glycosidic bonds. Cyclodextrins have a hollow truncated cone shape with a hydrophobic inner and hydrophilic outer surface. It is a widely spread, although not properly proven, statement that water molecules in the cavity of CD molecules interact mainly with the central molecule by hydrophobic interaction. For a proper description of this interaction, we applied state-of-the-art correlation methods and energy decomposition analyses. Additionally, the strengths of intramolecular hydrogen bonds on the upper and lower rims of CDs have been analyzed using several quantum chemical descriptors.

REFERENCES

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