

Investigations of Clusters of Cellobiose -Acid - (H₂O)_n

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The interactions between cellobiose and acids of different strengths, from very strong (H₂SO₄) to very weak (HCOOH), are studied in clusters of the type cellobiose-acid-(H₂O)_n. Ab initio molecular dynamics (DFT / BLYP with dispersion) is used to analyze the interaction between cellobiose and the micro-hydrated acids, in the gas phase, at room temperature. We compare these in terms of the probability for proton transfer (determined from Mulliken charges), to the active sugar site, as well as in terms of complete acid ionization. Initial findings show that in the case of cellobiose-HCl-(H₂O)_n, the sugar does not facilitate complete acid ionization as compared with the acid in pure water. The sugar, however does affect the pH of the acid. Detailed information on the preferred protonation site of cellobiose and the competition between the sugar and water protonation are presented. Differences in the ionization behaviour of different acids in complex with the sugar are discussed.