15. Structure and dynamics of proton solvation in water-acetone mixtures

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Proton transfer is an ubiquitous phenomena and it is of paramount relevance in solutions chemistry. In aqueos solution, proton diffusion is controlled by the well-known Grotthuss mechanism, which is intimately related with the dynamics of hydrogen bond. This mechanism considers not the individual diffusion of a tagged proton, but a translocation of the average position of the excess charge which requires succesive spatial rearrangements along chains of hydrogen bonds. In this poster, I will present an analysis of the modifications that take place in the solvation structure and in the proton transfer dynamics for different water-acetone mixtures, covering almost all of the concentration range. Our analysis will be based on results from MD experiments using a multistate empirical valence bond Hamiltonian model that naturally includes a proton translocation mechanism. Our results predict a stabilization of the solvated Eigen cation [$H_9O_4^+$] at lower water molar fractions, in detriment of the symmetric Zundel dimer [$H_5O_2^+$]. For every mixture studied, the average solvation structure in the close vicinity of the hydronium is characterizad by three hydrogen bonded, acceptor water molecules. Characteristic times for the proton translocation jumps have been computed using population relaxation time correlation functions. Compared to the pure water results, the rates at low water molar fractions fall down up to one order of magnitude. The proton diffusion is also drastically reduced, reaching values which are three times lower than those obtained for pure water.