International Conference on
"Recent Trends in Structural Bioinformatics and Computer Aided Drug Design"
[ICSBCADD'2019]
11th - 13th December, 2019

Modeling Proton Hopping in 8-hydroxyquinoline-5, 7 disulphonic acid

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The hydrated proton H+ plays a fundamental role in chemical and bio-chemical processes occurring in both homogeneous and inhomogeneous aqueous environments, such as proton transport in bulk water and proton pumping through membrane proteins. The latter is an archetypical example for processes occurring in biological environments, where the proton is solvated and transferred in partially aqueous environments especially in reactive sites of enzymes. These biological environments are poorly represented by model systems in bulk water.

A variety of compounds have been synthesized in low water environments to understand and model the mechanism of proton hopping. Two main intermediates are seen during this process, the Zundel ion and the Eigen Ion.

We have synthesized 8-hydroxyquinoline-5, 7 disulphonic and recrystallized it in methanol to strip away molecules of water. The structure of the molecule revealed that Zundel ion was stabilized in the crystal. Ab-initio molecular dynamics simulation was then carried out to understand the dynamics of proton hopping in this complex. During the course of simulation, the Zundel ion coordinates with a water molecule to form an open H7O+3 structure. This transition state structure desolvated rapidly forming Zundel ion facilitating proton hopping in the first solvation shell. One of the sulphonic acid groups in the 5 or 7 position of the 8-hydroxyquinoline 5,7 disulphonic acid bonds with the Zundel ion favoring the proton to be transferred to the nearby water molecule through the formation of proton defects. The simulation results support the structural diffusion mechanism and that charged complex migrates through the hydrogen bond network.