Title:	Structure and simulation of a Zundel ion stabilized by 8-hydroxyquinoline-5, 7 disulphonic acid
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Abstract:	8-hydroxyquinoline-5, 7 disulphonic was synthesized and recrystallized 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 H7O3+ structure. This transition state structure de-solvated 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.
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