Nature of interactions in mixed HCl-methanol-H_2O/NH_3 complexes. Evidence for existence of molecular proton wires

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Proton transfer reactions play a vital role in many biological, chemical and physical processes, for example creation of the ozone hole or aerobic generation of ATP. However, the conditions for proton transfer in different chemical complexes are still not fully understood. In this study, HCl ionization and proton sharing in mixed complexes were investigated. Specifically, hydrogen chloride-methanol-water and HCl-methanol-ammonia complexes were studied. The main tools used were molecular on-the-fly dynamics and density functional theory (DFT). Eight starting structures from molecular dynamics trajectories were heuristically chosen according to chemical intuition to search various region of potential energy surface (PES). The configurations were optimized using DFT with aug-cc-PVDZ basis sets. In order to determine their position on the PES, the IR spectra of all optimized structures were calculated. Two local minima and one transition state for both complexes were found. In all investigated complexes, both ionization of HCl and proton sharing between ion and CH3OH or two CH3OH molecules were observed. Moreover, the movement of a proton along methanol molecular chains was described.

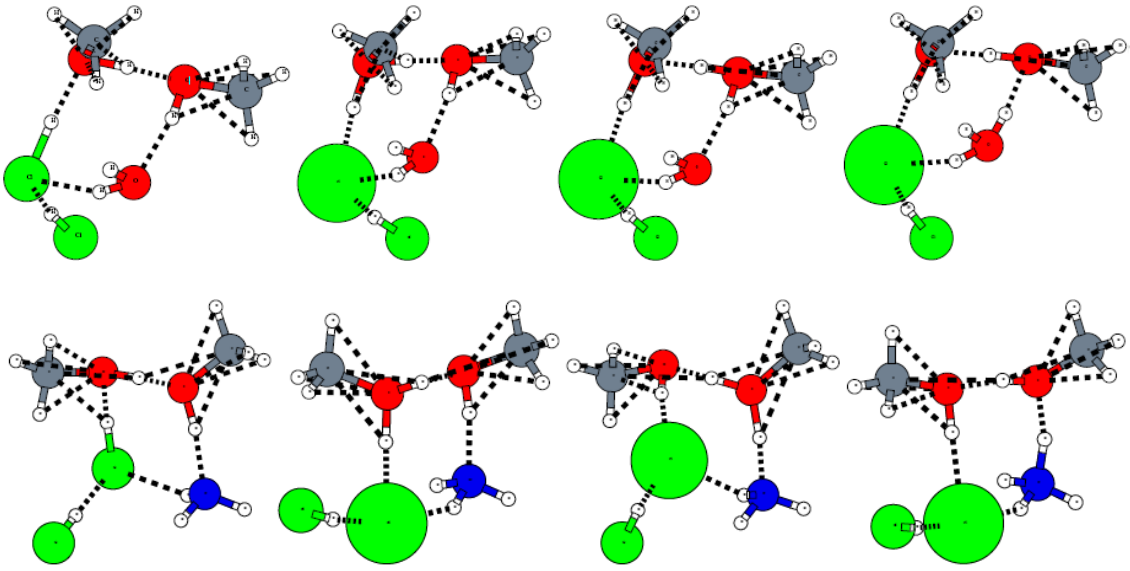

Fig. Trajectory snapshots at 100K for methanol-HCl-water complex (top), methanol-HCl-ammonia (bottom); red: oxygen, green: chlorine, gray: carbon, white: hydrogen. Expanded $Cl\text{-}Cl^-$ ion.