

Structural Rearrangements and Proton Transfer within Water Clusters of Atmospheric Relevance



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Presented by...

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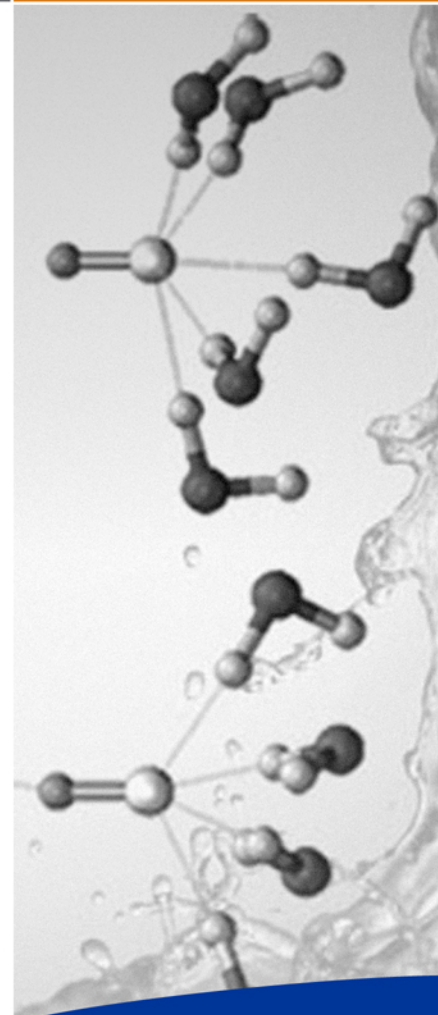


Abstract Hydrogen/deuterium exchange induced in reactions of various protonated or deprotonated water clusters, $(X)(Y)(H_2O)_n$ ($1 \leq n \leq 30$; containing ammonia, pyridine and/or hydrogen sulphate) with heavy water has been studied experimentally at near-thermal collision energies. The interpretation has been facilitated by quantum chemical calculations, including extensive Born-Oppenheimer molecular dynamics simulations. Lifetimes of the collision complexes have been estimated using RRKM theory. The experiments reveal unique and surprising details of the structure and dynamics of water clusters. For a given cluster size, both the total cross-section for isotope exchange and the relative amount of single and double substitution of H by D depend on the chemical properties of the core molecules X and Y. The experimental observations can be rationalized on the basis of the basicity and solubility of the core molecules X and Y. It appears that single H/D exchange is proton-catalyzed, while double substitution has contributions from this mechanism as well as from ligand exchange. The tendency for a proton to migrate within a water cluster is determined by a fine balance between the relative proton affinities of the various basic sites. Solute molecules may slow down proton migration by having high proton affinity. On the other hand, water solvation and local hydrogen bond patterns may modify the proton affinity of a given site significantly.

More info?

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Date: February 25

Location: EMSL
Auditorium

Time: 11:00 am