Elementary reactions of water clusters

Professor Einar Uggerud

Mass Spectrometry Laboratory and
Centre for Theoretical and Computational Chemistry
Department of Chemistry
University of Oslo
P.O. Box 1033 Blindern,
0315 Oslo

The physics and chemistry of water is not only relevant to our existence and daily life, but is truly fascinating in its own right. The many well-known anomalies of water in its liquid and solid phases continue to puzzle the minds of scientists, and despite the apparent simplicity of the isolated H_2O molecule, the factors governing the properties of water in its condensed states are highly complex and incompletely understood. In order to expand the limits of knowledge and to bridge the gap between the gaseous and condensed phases water clusters are ideal model systems. However, water clusters are also interesting by themselves, and are particular relevant to the vital atmospheric processes that regulate cloud formation, and are thereby linked to the earth's radiation balance and precipitation patterns. By necessity, cloud particle development starts by the formation of small water containing clusters. Consequently, the quest for better knowledge of the physical and chemical properties of nanoscale clusters poses a challenge to scientists in an era with many worries about our future climate.

The talk will consist of three parts, each reflecting on one elementary reaction type associated with water.

- In the first part we will report on water cluster evaporation, determination of activation free energies of water molecule elimination, cluster structures and magic numbers.
- The second part will be devoted to proton transfer and proton mobility within water, including experimental data from H/D exchange experiments and the outcome of computational modelling.
- Finally, in the third part, we will reveal details of the chemical reactions that occur when high-energy water clusters pass through caesium vapour. It turns out that this initiates a series of events resembling the spontaneous and vigorous oxidation-reduction reactions that take place when a piece of an alkali metal is thrown into water.