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Positive-Ion/Negative-Ion Coincidence (PINICO) Experiments on Water

Water seems like a very common and ordinary molecule, due to how accustomed we are to seeing it in almost every aspect of our lives. However, it displays several unique or rare properties that are still very hard to understand in spite of the considerable amount of research performed about them. One of the very powerful methods used to investigate its properties and dissociation dynamics is Time-of-Flight Mass Spectroscopy (TOFMS).

TOFMS relies on four key steps: ionization, acceleration, drifting and detection. In this work, the ionization energy is provided by synchrotron light. This ionization is usually followed by dissociation of the excited molecule, producing fragments of various size and charge. An electric potential applied across the region in which the molecules and the light interact is then used to separate and accelerate the ions. In the drift section, temporal separation of the ions is achieved, depending on the speed they acquired from the electric potential. And finally, detection at the exit of the drift tube is used to categorize and quantify the ions based on the time of detection.

Performing TOFMS may be compared to using a hammer to smash a mechanical watch in order to understand how it works. The scattered pieces of the destroyed watch are then sorted and counted, which provides a better understanding of the properties of the watch. However, this metaphor does not do justice to a number of important features of TOFMS. The chemical properties and structure of molecules cannot be studied directly, contrary to a mechanical watch that can be carefully opened, and its machinery observed in operation. Brutally taking apart molecules is actually one of the best methods available in order to understand how they work. Also, this metaphor leaves out one very important detail concerning the sorting and counting of the pieces: usually, TOFMS only counts positive ions. Yet among the produced fragments are electrons, positive ions, negative ions, photons and neutral fragments. It's the equivalent of counting exclusively the cogs of the broken mechanical watch, disregarding any springs, wheels or screws. This creates additional loss of information in TOFMS, as it is difficult to collect all the particles created.

In order to obtain complementary information about fragmentation, different spectroscopy techniques have been developed based on coincidence detection of different fragmentation products. It is mostly used to detect two products in coincidence, but it can be extended to multiple coincidences as well. This coincidence detection can be used to obtain more precise information about the molecular fragmentation process occurring when the molecules are "smashed". Also, the least common fragments can carry information not seen with more common fragments. Indeed, just as with the watch, a rare fragment may only be produced by a specific smashing method, or it could only occur in a specific type of watch. Based on this observation, this work attempts at implementing coincidence spectroscopy of very common fragmentation products, positive ions, with much rarer products, negative ions. More specifically, time-of-flight mass coincidence spectroscopy of positive ions

and negative ions is performed in order to study the dissociation pathways occurring in the gaseous water molecule.

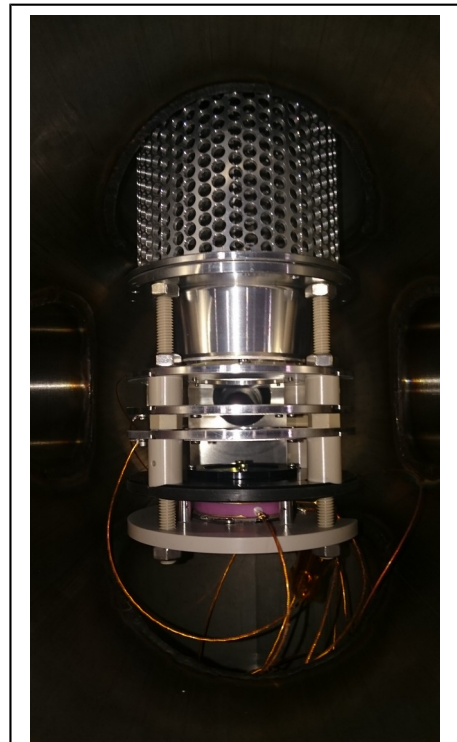
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