PHOTOINDUCED FRAGMENTATION OF ACETAMIDE CLUSTERS STUDIED BY MASS SPECTROSCOPY

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Large prebiotic molecules, such as acetamide, found in space, are of biological interest. Being the largest interstellar molecule known containing a peptide group, acetamide could be the source of larger peptides and therefore play a potential role in prebiotic chemistry. The clusterization of acetamide molecules can be considered as a simple model system to explore biologically important chemical proceses triggered by the solar radiation. We studied photofragmentation of small gas-phase acetamide clusters produced by supersonic expansion source using time-of-flight (TOF) ion mass spectroscopy combined with tunable vacuum-ultraviolet synchrotron radiation [1]. Fragmentation channels of acetamide clusters under vacuum-ultraviolet photoionization resulting in formation of the protonated and ammoniated cluster ions were identified with the discussion about the preceding intramolecular rearrangements. The influence of the photon energy on the stability of the clusters and their fragmentation channels was addressed. Also, the most stable arrangement of the acetamide dimer was identified. An important new result of this study was tracking the exact proton transfer path in protonation reactions with the help of deuterated sample, identifying that proton transfer from the amino group is a dominant transfer mechanism.

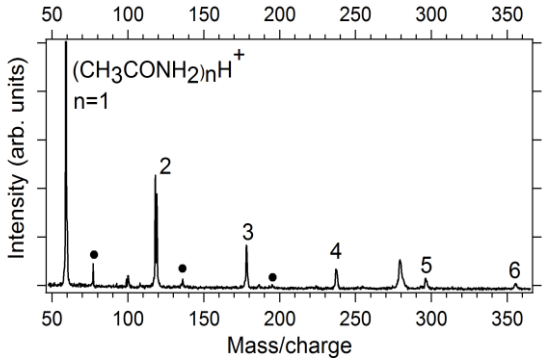

Fig.1 .TOF mass spectrum of acetamide clusters measured at 9.8 eV photon energy. The peaks labeled with numbers indicate protonated cluster ions $(CH_3CONH_2)_nH^+$. The bullets indicate ammoniated cluster ions $(CH_3CONH_2)_n(NH_3)H^+$.

References

1. M. Tarkanovskaja, K. Kooser, H. Levola, E. Nõmmiste, E. Kukk 2016, *The Journal of Chemical Physics, 145, 124313*.

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