

Effects of the environment on the uracil molecule ionization induced by $^{12}\text{C}^{4+}$ ion beam

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Effects of the environment on the uracil molecule ionization induced by $^{12}\text{C}^{4+}$ ion beam

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Synopsis In this study the fragmentation of isolated uracil molecules, uracil clusters and hydrated uracil clusters induced by $^{12}\text{C}^{4+}$ ions at 36 keV energy has been investigated. The mass spectra obtained by a TOF mass spectrometer are analyzed and compared to each other in order to see how the environment affects the fragmentation dynamics. The main differences between the mass spectra are highlighted and possible fragmentation pathways are proposed.

The studies of ionization induced by heavy charged particles are particularly important to understand the processes occurring during hadron therapy for cancer treatment. Gas phase studies allow to characterize the radiation damage of biomolecules, like DNA/RNA bases for example, at the molecular level. However, in a real biological system, the biomolecule is incorporated in a complex environment, which certainly affects its properties and behavior.

To unravel the role of the environment in the fragmentation of uracil, we have measured and compared the mass spectra of isolated uracil molecules and uracil clusters (Fig. 1). Even though the two spectra are very similar, differences can be observed in the intensity of different fragments and in the opening/closing of fragmentation channels.

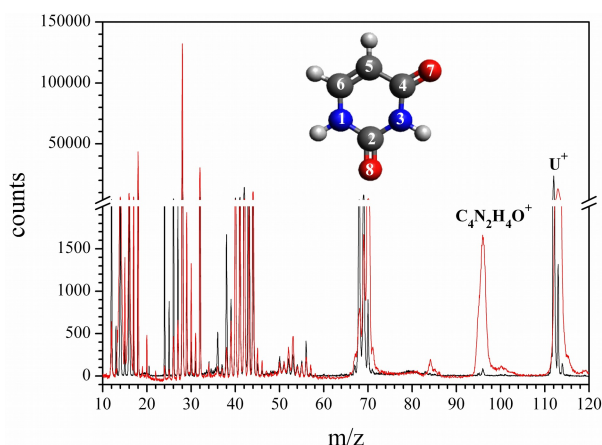


Figure 1. Comparison between isolated uracil molecules (black line) and uracil clusters (red line). The spectra are normalized to the same total area in the region up to the monomer.

For example, in the mass spectrum of uracil clusters a broad feature can be observed at $m/z=96$, attributed to the formation of $\text{C}_4\text{N}_2\text{H}_4\text{O}$ fragment ion due to the loss of an OH group by the parent ion. This fragment, which is almost negligible in the uracil molecules mass spectrum, indicates that O atoms may have weaker bonds within the clusters as a result of the hydrogen bridge bonds.

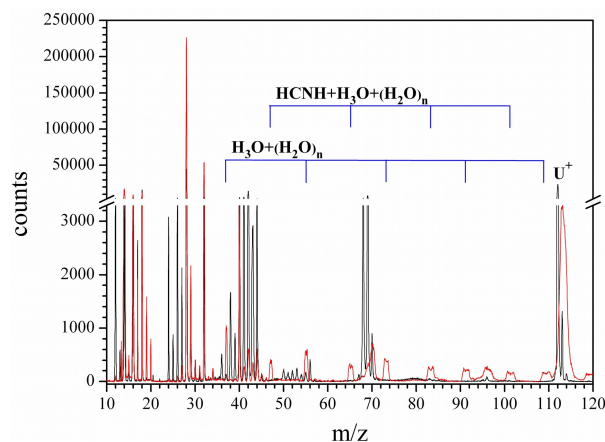


Figure 2. Comparison between isolated uracil molecules (black line) and hydrated uracil clusters (red line).

Many fragments observed in the mass spectra of the isolated uracil molecules and uracil clusters cannot be found in case of hydrated clusters (Fig. 2), confirming that the presence of the water molecule has a protecting effect on the nucleobases [1]. Nevertheless, in the case of the hydrated uracil clusters a series of hydrated fragments is observed.

References

- [1] S. Maclot *et al* 2011 *ChemPhysChem*. **12** 930

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