**Mécanismes de fragmentation des bases ionisées d'ADN/ARN.**

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**Abstract**

The different fragmentation channels of three ADN and ARN bases, namely cytosine, adenine and guanine have been studied through DFT calculations. The energy dissociation and the fragmentation channels are all calculated from the most stable structure of each base. The elimination of a HNCO molecule is one major dissociation route for all bases, adenine excepted (That last one does not contain an oxygen atom in its structure). The elimination of a NH3 (or NH2) molecule is another route common for all the studied bases which contain an amino group. However, this last channel is relatively difficult, so that the corresponding peaks in the mass spectra are relatively weakly intense. The CO or HCN (HNC) loss is also investigated for most bases, either directly from the cationic bases or from primary fragments. First results were obtained for uracil [1], and are now completed for Cytosine, Adenine and Guanine [2].



Fig. 1. Fragmentation mechanisms of cytosine cation

**References**:

[1] L. Sadr Arani, P. Mignon, H. Abdoul-Carime, B. Farizon, M. Farizon, H. Chermette, Phys. Chem. Chem. Phys., 2012, 14, 9855–9870; Chemical Physics Letters 583 (2013) 165–169.

[2] L. Sadr Arani, P. Mignon, H. Abdoul-Carime, B. Farizon, M. Farizon, H. Chermette,  *submitted(2014)*.