Ionization and fragmentation of DNA-RNA bases induced by proton impact: experiment and calculations

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We present recent results gained on the fragmentation of (doubly) ionized DNA/ RNA components. The gas-phase bio-molecules are impacted with 100 keV protons, this energy corresponding to the maximum of dose deposition (Linear Energy Transfer) used for tumour treatments in medical applications. Molecular fragmentation is studied by mass spectrometry using a (correlated) time-of-flight technique [1]. Fragmentation of singly ionized as well as doubly ionized molecules has been investigated and in this latter case, the dication is unstable and decays by emission of two charged fragments (and subsequently neutrals). An example of correlation between charge fragments from initial Thymine^{2+} molecule is displayed in figure 1.

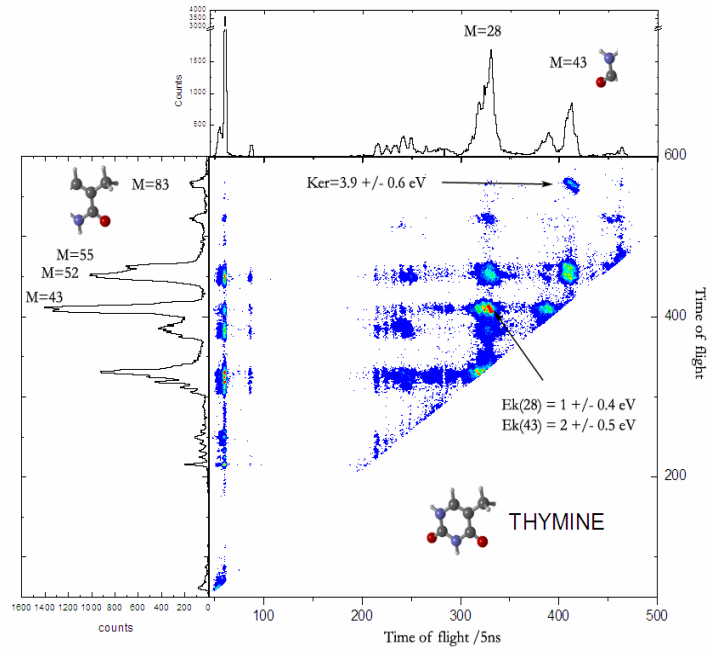

Figure 1: Correlations spectrum of Thymine $^{2+}$

From this spectrum, we can not only extract the branching ratios that correspond to the various fragmentation pathways, but also the Kinetic Energy Released in the fragmentation. Making use of the Gamess [2] or Mopac [3] codes, several reaction pathways have been investigated. Nature of the fragments, activation barriers as well as KER values can be inferred from calculations, and a valuable comparison between experiment and calculation data can be made. This will be presented at this conference.

[1] Patrick Moretto-Capelle et al J.Chem.Phys **127** (2007) 234311
[2] M.W.Schmidt et al J. Comput. Chem.,**14** (1993) 1347-1363.
[3] MOPAC2007, James J. P. Stewart, Stewart Computational Chemistry, Colorado Springs, CO, USA(2007).