DELAYED FRAGMENTATION OF DOUBLY CHARGED ADENINE OBSERVED IN 100 keV PROTON COLLISION

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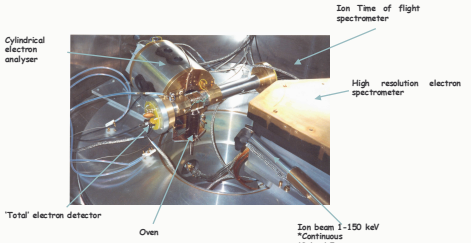
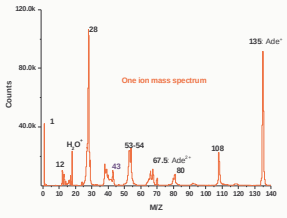
By using a multi correlation time of flight technique, we have investigated the fragmentation of the Adenine impacted by 100 keV protons. This latter energy corresponds to the maximum of the Linear Energy Transfer in biological medium resulting in the Bragg peak formation.

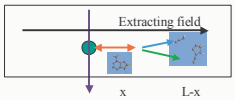
Experimental Method : (Electron spectroscopy) -Multistop time of flight



Fragmentation of singly charged Adenine

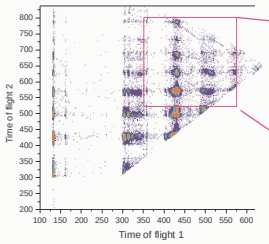


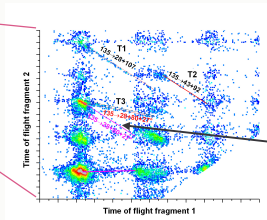
SIMULATION OF THE FRAGMENTATION PROCESS



AND INTENSITY ALONG THE TRACK

Fragmentation of doubly charged Adenine : 2D spectrum





Apart the islands (mass correlations), **we could distinguish some 'parasitic' structures** (noted T1, T2, T3) **that correspond to the fragmentation of the adenine molecule within the extraction field [1]**

FRAGMENTATION PATTERN and ACCESS TO THE LIFETIME

T3

$Ade^{2+} \xrightarrow{fast} 27^0 + 108^+ \xrightarrow{\tau} 27^0 + 28^+ + 80^+$

$Ade^{2+} \xrightarrow{\tau} 27^0 + 28^+ + 80^+$ in agreement with the experiment

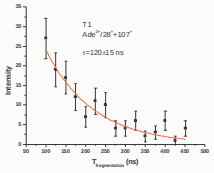
ADENINE^{2+}

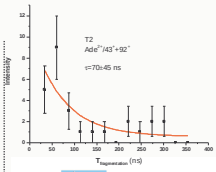
VERY LONG LIFETIMES OF 100 - 200 ns ARE OBSERVED !!

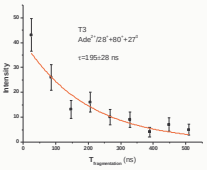
ORIGIN OF METASTABILITY ???

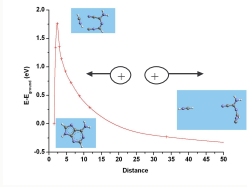
CAN BE UNDERSTOOD IN TERMS OF ACTIVATION BARRIERS [2] ALONG THE FRAGMENTATION PATHWAYS (TUNNEL EFFECT)

EVALUATIONS **ARE DONE WITH** ***ARGUSLAB [3]*** **or** ***MOPAC*** **CODES IN THE PM3 APPROXIMATION**

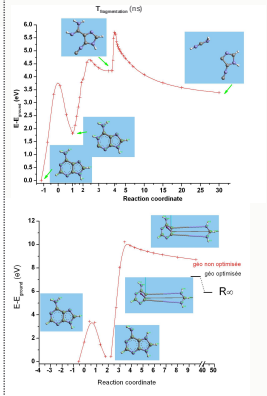




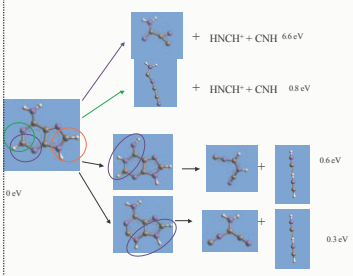




Emission of $[H\text{-}C\text{-}N\text{-}H]^+$



Formation of mass 43 : proton transfer



☞EVIDENCE OF LONG LIFETIMES FOR THE ADENINE^{2+} AGAINST FRAGEMNTATION IN THE GAS PHASE

☞WE NEED 'ELABORATE' THEORETICAL INVESTIGATIONS OF FRAGMENTATION PATTERNS

References:

[1]: H.Lebius et al, Phys.Scripta T80 (1999),197

[2]: F.Liu, Phys.Rev.Lett 59 (1987),2562

[3]: ArgusLab4.0.1 Mark A.Thompson, Planaria Software