Delayed fragmentation of doubly charged adenine observed in 100 keV proton collisions

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By means of a multi correlation time-of-flight technique, we did investigate the fragmentation of Adenine colliding with a 100 keV proton beam, energy that corresponds to the maximum LET in the biological medium. A "two stops" spectrum that displays the fragmentation of a doubly charged adenine molecule is shown in figure 1. Apart from the correlation islands (mass correlation), we could distinguish a bunch of 'parasitic' structures, noted T1, T2 and T3, which correspond to fragmentation patterns within the extraction field. From these tracks, it was then possible to evaluate lifetimes for excited states, i.e. metastable states, from which those structures originate. A plot for the T3 track is displayed in figure 2, and a sizeable lifetime of about 195 ns is been found. The origin of the metastability can be understood in terms of activation barriers along the fragmentation pathways. Indeed, by means of the Arguslab software -PM3 calculation- and for the two body break-up of the doubly charged Adenine in the T1 track -mass 28 and 107-, we did investigate the pathway -shown in figure 3- that leads to the $[H\text{-}C\text{-}N\text{-}H]^+$ emission. We anticipate, though this would have to be considered as a preliminary point, that a weak barrier of 1.8 eV has to be tunnelled in order to provoke the observed fragmentation pattern.

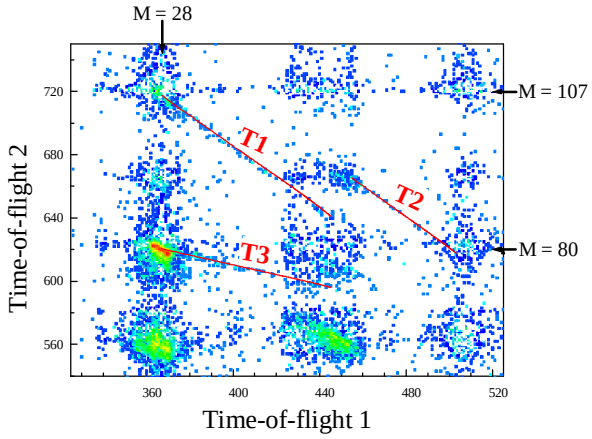

Figure 1 : two fragments ToF spectrum

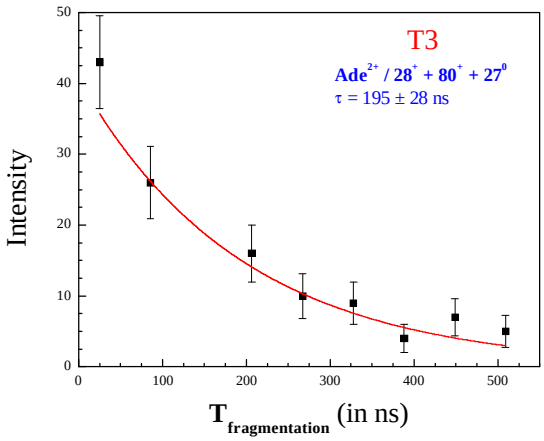

Figure 2 : lifetime

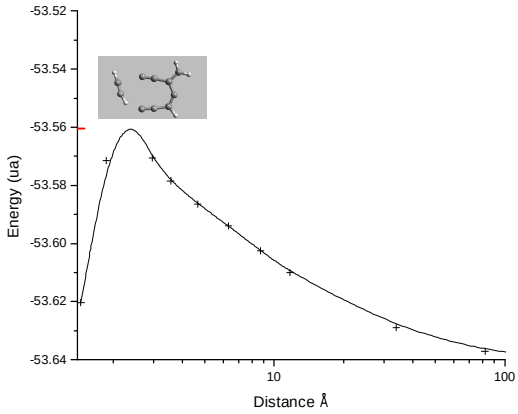

Figure 3 : reaction pathway for track T1