

**Ionization and Fragmentation of the Pyrimidine bases induced by 100 keV proton collisions.**



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Proton therapy is a non-ablative powerful method that enables to deliver the right radiation dose to a targeted tumor with minimal side effects. The growing needs in proton therapy makes it necessary to understand the damages caused by these radiations on a molecular level. We present in this poster results obtained on proton collision induced dissociation of isolated pyrimidine bases resulting from double ionization of these molecules.



	<b>Projectile :</b> 100 keV pulsed proton beam (maximum LET in water)	
	<b>Target :</b> Pyrimidine bases in vapor phase	
	<b>Detection :</b> All charged fragments by time of flight spectroscopy	
	<b>Results :</b> "one stop" spectra "two stop" spectra	

**Results on cytosine : two charged fragments :**

<table border="1"> <thead> <tr> <th></th> <th>Cytosine</th> <th>Uracil</th> <th>Thymine</th> </tr> </thead> <tbody> <tr> <td>I</td> <td>24.23 eV</td> <td>25.82 eV</td> <td>24.41 eV</td> </tr> <tr> <td>R</td> <td>-1.99 eV</td> <td>-0.92 eV</td> <td>-0.99 eV</td> </tr> <tr> <td>F</td> <td>-3.87 eV</td> <td>-6.11 eV</td> <td>4.68 eV</td> </tr> </tbody> </table>		Cytosine	Uracil	Thymine	I	24.23 eV	25.82 eV	24.41 eV	R	-1.99 eV	-0.92 eV	-0.99 eV	F	-3.87 eV	-6.11 eV	4.68 eV	
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DFT (B3LYP)- Gaussian 03 calculations 6-311G** Base (triple-split-valence+polarization)																	

**Results on cytosine : three or more fragments :  $i1i2n \rightarrow i1+i2n \rightarrow i1 + i2 + n$**

		<b>Slopes :</b> Theoretical / Exp i1i2 : -0.7 / -0.7 i1n : -0.3 / -0.3 i2n : 0.4 / NA		E1 = -55.431312 ua E2 = -113.346235 ua E1 + E2 = 168.777547 ua ΔE = 0.24293 ua ≅ 6.61 eV
		<b>Slopes :</b> i1i2 : -0.8 / -0.7 i1n : -0.2 / -0.3 i2n : 0.3 / 0.5		E1 = -93.651541 ua
		<b>Slopes :</b> i1i2 : -1 / -1.02 i1n : 0 / -0.02 i2n : 0 / -0.09		E = -169.020477 ua

**Results on Uracil and Thymine for M= 44 uma :**

Uracil					
Thymine					