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AF Moretto-Capelle, Patrick, Le Padellec, Arnaud, Briere, Guillaume, Massou, Sophie, Franceries, Frederic

TI Energetics and metastability of the adenine dication observed in proton-adenine collisions  
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ID ELECTRONIC-STRUCTURE; CROSS-SECTIONS; FRAGMENTATION; IONS; C-60; MOLECULES; THERAPY; SPACE

AB We present here a study that deals with the correlated fragmentation of a doubly charged adenine molecular target induced by a 100 keV proton beam. We have elucidated part of the dissociation dynamics for several channels and have obtained the corresponding kinetic energy released values. We have extracted activation energies by combining our experimental data with computations using the ab initio GAMESS code. We have observed metastability patterns against fragmentation, for which we have extracted the temporal mechanism (one or two steps). Subsequently, we have obtained lifetimes in the 100-200 ns range. In the simplest case of two-body fragmentation with the emission of mass 28, the determination of transition states and reaction paths has showed that emission of the H-C-N-H fragment is preferred to that of C-N-H-2. From the calculated activation barriers and lifetimes, we have deduced an equivalent temperature of the dication that we have compared with the existing models. (c) 2007 American Institute of Physics.

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