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AF Lopez-Tarifa, Pablo; du Penhoat, Marie-Anne Herve; Vuilleumier, Rodophe; Gaigeot, Marie-Pierre; Rothlisberger, Ursula; Tavernelli, Ivano; Le Padellec, Arnaud; Champeaux, Jean-Philippe; Alcami, Manuel; Moretto-Capelle, Patrick; Martin, Fernando; Politis, Marie-Francoise
TI Time-dependent density functional theory molecular dynamics simulation of doubly charged uracil in gas phase
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DE uracil; proton collision; nonadiabatic dynamics; biological damage
ID BIOLOGICALLY RELEVANT MOLECULES; ELECTRONIC-STRUCTURE; AQUEOUS-SOLUTION; LIQUID WATER; FRAGMENTATION; MECHANISMS; COLLISIONS; RADIATION; RADICALS; DAMAGE
AB We use time-dependent density functional theory and Born-Oppenheimer molecular dynamics methods to investigate the fragmentation of doubly ionized uracil in gas phase. Different initial electronic excited states of the dication are obtained by removing electrons from different inner-shell orbitals of the neutral species. We show that shape-equivalent orbitals lead to very different fragmentation patterns revealing the importance of the intramolecular chemical environment. The results are in good agreement with ionion coincidence measurements of uracil collision with 100 keV protons.
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