AU Lopez-Tarifa, P, du Penhoat, MAH, Vuilleumier, R, Gaigeot, MP, Tavernelli, I, Le Padellec, A, Champeaux, JP, Alcami, M, Moretto-Capelle, P, Martin, F, Politis, MF
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TI Ultrafast Nonadiabatic Fragmentation Dynamics of Doubly Charged Uracil in a Gas Phase
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DT Article
ID DENSITY-FUNCTIONAL THEORY; BIOLOGICALLY RELEVANT MOLECULES; IONIZATION; COLLISIONS; PROTONS
AB A combination of time-dependent density functional theory and Born-Oppenheimer molecular dynamics methods is used to investigate fragmentation of doubly charged gas-phase uracil in collisions with 100 keV protons. The results are in good agreement with ion-ion coincidence measurements. Orbitals of similar energy and/or localized in similar bonds lead to very different fragmentation patterns, thus showing the importance of intramolecular chemical environment. In general, the observed fragments do not correspond to the energetically most favorable dissociation path, which is due to dynamical effects occurring in the first few femtoseconds after electron removal.
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