

Fragmentation Dynamics Of Methane Induced By Femtosecond

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fragmentation can occur. In the present work, we investigate theoretically, through ab-initio molecular dynamics simulations, the chemical reaction of dissociation of methane induced by intense femtosecond IR pulses. An alternative mechanism based on the

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Instantaneous (laser-field-dependent) potential energy curves leading to neutral fragmentations of methane were calculated at several laser intensities from 1.4×10^{13} to 1.2×10^{14} W/cm² (from 1.0×10^{10} to 3.0×10^{10} V/m) using ab initio molecular orbital (MO) methods to validate the observation of neutral fragmentations induced by intense femtosecond IR pulses (Kong et al. J. Chem. Phys. 2006, 125, 133320).

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The fragmentation of CH₄⁽²⁺⁾ dications following 55 eV, 75 eV, and 100 eV electron impact double ionization of methane was studied using a cold target recoil-ion momentum spectroscopy. From the measured momentum of each recoil ion, the momentum of the neutral particles has been deduced and the kinetic energy release distribution for the different fragmentation channels has been obtained.

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Abstract. The fragmentation pattern of CH₄²⁺ was experimentally studied at an intensity of approximately 10^{14} W/cm² with laser durations varying from 8 to 110 fs. When the laser duration was 8 fs, only the primarily fragmental CH₃⁺ ion was observed in addition to the parent CH₄⁺ ion. When the laser duration was 30 fs, small fragmental CH₂⁺ and H⁺ ions appeared. When the laser duration was ...

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the fragmentation of the methane molecule, which has attracted a lot of attention due to the tetrahedral structure of its ground state. In particular, the fragmentation has been induced by electrons [1]–[4], protons [5], atoms [6]–[8], synchrotron radiation [9]–[13] and lasers [14, 15].

[The role of the methyl ion in the fragmentation of](#)

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