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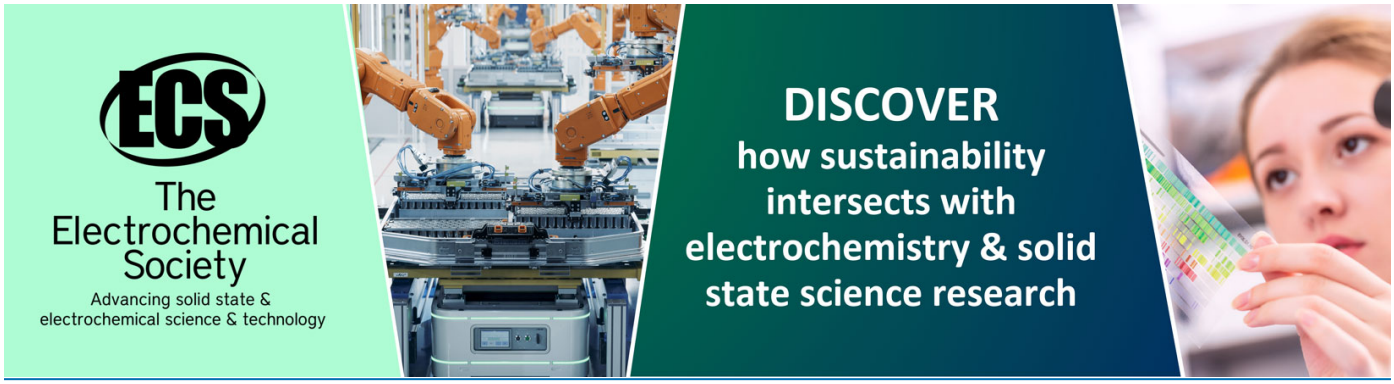

Charge dependence of fragmentation process induced by ion collisions with furan molecule

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Synopsis The goal of this work is to describe the system evolution after ion-molecule interaction. We combine different quantum chemistry and statistical mechanics approaches in order to give extended description of the process. Herein we report on a recent study of the fragmentation mechanism of neutral, singly- and doubly-ionized furan molecule in the gas phase.

Furan belongs to the family of ring structures often taken as an elementary analogue system of deoxyribose, fundamental component of the DNA backbone chain. Therefore, it can serve as a model system for track simulations in biological medium. Transfer of energy to the environment of the DNA initiates a sequence of events depending on the quantity of energy being transferred and electronic structure of the surrounding matter. Extensive theoretical and experimental research has already focused on understanding the fundamental reactions occurring in biological matter after irradiation. However, as the mechanism of formation of various products is still unclear, in this work we aim at extending and complementing previous studies.

In this communication, we present a merged approach of Density Functional Theory (DFT) quantum chemistry methods with statistical Monte Carlo technique. Firstly, we have performed molecular dynamics simulations using the Atom-Centered Density Matrix Propagation (ADMP) method [1] for the internal energy deposited to the system varying from 5 to 30 eV. Extensive statistical analysis of the obtained trajectories allowed us to identify most abundant dissociation channels. The dynamics of the neutral system is dominated by unimolecular opening of the furan ring and hydrogen transfer. In the case of singly-ionized furan the most abundant channels consist of production of formyl radical (CHO) and cyclopropenyl cation ($C_3H_3^+$) as well as $C_3H_4O^+$ cation and hydrogen atom for higher energies. Doubly-ionized furan fragmentation follows a dissociation path with one channel clearly distinguishable as most probable (67% of the trajectories for the energy of 14 eV). This channel leads to production of two fragments: formyl cation (CHO^+) and cyclopropenyl cation ($C_3H_3^+$) by direct cleavage of the furan ring.

Snapshots of the most probable reaction channel for singly- and doubly-ionized furan are shown in Fig. 1. Subsequently, in order to gain complementary energetic and structural information on the fragmentation mechanism, we have performed calculations of the critical points on the potential energy surface of the most apparent channels appearing in the dynamical calculations.

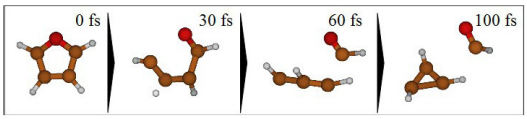

Figure 1. Mechanism of fragmentation to $C_3H_3^+$/CHO and $C_3H_3^+$/CHO^+ channels.

The statistical Microcanonical Metropolis Monte Carlo (M_3C) method [2,3] has been employed as an alternative approach to understanding the fragmentation process. The M_3C technique provides fragmentation probabilities as a function of the excitation energy. Comparison of our preliminary results with the experimental data [4] leads to the conclusion that M_3C method is a promising theoretical tool for reproducing the mass spectrum of the studied system.

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