Dissociation of furan-2-carboxylic acid by low energy electrons

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Synopsis Electron attachment to molecular target can lead to a variety of negative fragment ions. We experimentally probe the main dissociative electron attachment channels in furan-2-carboxylic acid ($C_3H_3O_2 - COOH$) - a molecular target composed of two important structural units: a furan ring and a carboxylic group. In our studies we utilise nearly mono-energetic electrons at electron energies from 0 eV up to 15 eV. Our detection setup is based on extraction lens system and quadrupole mass spectrometer, that enables measurement of the energy dependent mass-selected yields of newly formed stable anions.

Many investigations have been focused on the understanding of physico-chemical processes of molecular complexes containing different heterocyclic rings [**?**]. Such compounds have important applications in many disciplines including medicine, biology, chemistry, pharmacology and material science, which place these molecular systems in a very interesting point of view. On the other hand molecular complexes containing carboxylic group are interesting due to the ease of forming double-hydrogen-bonded complexes [**?**].

The replacement of the adjacent to single C–O bond hydrogen atom in the furan ring by a carboxylic group results in formation of the furan-2-carboxylic acid molecule (F2CA) - see Fig. 1. Effectively, the molecular structure consists of a five-membered aromatic ring and a carboxylic group connected via single C–C bond.

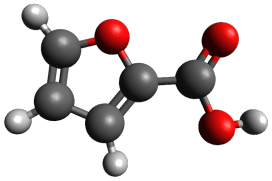

Figure 1. Ball-and-stick model of the structure of F2CA.

In our studies we collide low-energy electrons with the target gas molecules in the collision chamber, and our detection system is used for analysing negative ions created in the dissociative electron attachment (DEA) process [**?**]. We experimentally probe the main DEA channels in F2CA. Electron attachment to F2CA leads to a variety of negative fragment ions. Detailed energetics of formation of the DEA channels will be discussed. The example of such molecular fragmentation is shown in Eq. **??**:

$$e^- + \overbrace{\underbrace{C_4H_3O_2}_{\text{ring}}\,\underbrace{COOH}_{\text{carboxyl}}}^{\text{M}} \xrightarrow{M^{\#-}} \underbrace{(C_4H_3O_2\,COO)^-}_{(M-H)^-} + H\,, \tag{1}$$

where $M^{\#-}$ denotes a transient negative anion.

Dominant fragments arise from the cleavage of a single bond. Other fragments can be described using more complex fragmentation reactions. The DEA processes show one prominent resonance at 1.2 eV and three distinct energy bands in the region of 5–10 eV. The dissociation channel via C_2H^- anion is especially interesting as the theoretical and experimental results reveal the possible hydrogen migration between a ring and carboxylic structure prior to dissociation.

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