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Dissociation of 2-oxopropanoic 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 (DEA) channels in 2-oxopropanoic acid ($\text{CH}_3 - \text{CO} - \text{COOH}$) - an important trace component in the Earth's atmosphere. In our studies we utilise nearly mono-energetic electrons at electron energies from 0 eV up to 15 eV.

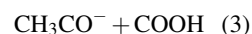
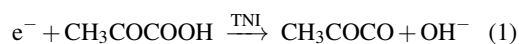
Atmospheric gases directly influence the global radiative balance by interaction and scattering of incoming radiation. 2-oxopropanoic acid² is a substantial atmospheric organic compound that originates from oxidation of isoprene emitted from trees. Apart from a tree-covered environment, pyruvic acid also comes from biomass burning, metabolism of animals and plants. However, in urban environment the primary origin of pyruvic acid comes from vehicular emissions [1, 2].

Dissociation of pyruvic acid by photon impact has been already studied in detail [3]. However, there is a lack of experimental studies dealing with interactions of electrons with pyruvic acid molecule, in particular concerning dissociative electron attachment. Free electrons are abundant species in the upper atmospheres and therefore interactions of electrons with pyruvic acid may play an important role in the atmospheric chemistry. Particularly, the dissociative attachment process, which is effective in bond breaking at subexcitation energies.

In our studies we used the mass spectrometer with trochoidal electron monochromator (MS-TEM). The MS-TEM consist of an electron beam of well defined incident energy, a target chamber where electrons collide with the target gas molecules, and quadrupole filter for analysing ions created in the dissociative attachment process [4].

Electron attachment to pyruvic acid 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 Fig. 1.

The most dominant main DEA channels for pyruvic acid (Eqs. 1-3):



These fragments OH^- , CH_3^- , CH_3CO^- arise from the cleavage of a single bond and corresponding resonances are observed within 3-8 eV. Other fragments can be described using more complex fragmentation reactions. Additionally, the evidence of dimers formation is also reported. Particularly, presence of dimers in the sample lead to a completely different behaviour of the dehydrogenated $(\text{M}-\text{H})^-$ anion. The fragmentation pattern and the energy range completely change upon the formation of hydrogen bonding. Dramatic energy shift towards lower energies (near 0 eV) is assigned to spontaneous proton transfer along the hydrogen bond during the electron attachment to the dimer.

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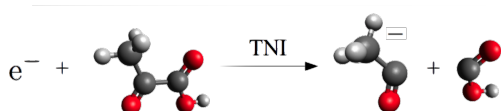


Figure 1. An example of fragmentation via possible DEA channel; with TNI being the transient anion formed upon resonant free electron attachment.

We experimentally probe the main dissociative electron attachment (DEA) channels in pyruvic acid.

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