Dynamics of Dissociative Electron Attachment to Furan and Pyridine

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Synopsis Dissociative electron attachment (DEA) of furan (C_4H_4O) and pyridine (C_5H_5N) is studied using a negative ion imaging spectrometer. The dissociation channels are analyzed using ion kinetic energies and angular distributions. E.g. for the dehydrogenation channel of furan the comparison with theory allows the identification of the negative ion resonance involved.

Dissociative electron attachment (DEA) was found to be an important process in the chemistry of biomolecules. The furan molecule (C_4H_4O) (Figure 1) comes close to glucose which is part of the DNA backbone. Also pyridine (C_5H_5N) has a wide occurrence in nature.

The experiments were carried out using the negative ion momentum imaging apparatus in Heidelberg [1]. The apparatus comprises a crossed beam configuration of a cold supersonic gas jet and a pulsed mono-energetic electron beam from a photoemission electron source. Anions produced in the interaction region are accelerated towards a microchannel plate detector by a pulsed electric field. Time of flight as well as impact position on the detector are recorded to reconstruct the fragment ion mass and momentum vector.

For furan our study concentrated on the electron impact energy around 6 eV where a previous study [2] found several negative fragmentation products for which we propose the following dissociation reactions:

$$C_4H_4O + e^- \rightarrow C_3H_3^- + CHO$$
 (1)

$$C_2HO^- + C_2H_2 + H$$
 (2)

$$C_4H + H + H_2O \qquad (3)$$

$$C_4 H_3 O^- + H \tag{4}$$

The identification of these pathways follows from established thermo-chemical data and our measurement of the ion kinetic energies as shown in Figure 2. E.g. for channel (3) water formation is required since otherwise C_4H^- cannot be formed energetically. In case of the two-body decay channels (1) and (4) the total kinetic energy release (KER) spectra show maxima at non-zero energies and as result the angular distribution of the ions can be analyzed.

For the furanide anion $FN-H^-$ (C₄H₃O⁻) in channel (4) an anisotropic angular emission pattern is observed which is in rather good agreement with

results from *ab initio* complex Kohn calculations [3]. Thus, we can conclude on hydrogen abstraction from the C3 atom following electron attachment in a Feshbach resonance of A_2 symmetry.

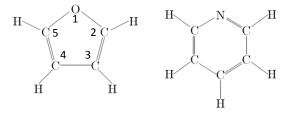


Figure 1. Chemical structure of furan (left) and pyridine (right).

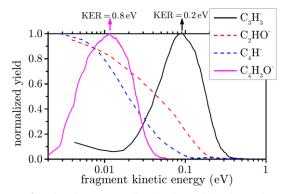


Figure 2. Kinetic energy distribution of the investigated fragments of furan.

For pyridine our observations include a symmetric dissociation process forming NH_2^- . More detailed results will be discussed at the conference.

References

- [1] T. N. Rescigno et al. 2016 Phys. Rev. A 93 052704
- [2] P. Sulzer et al 2006 J. Chem. Phys. 125, 44304
- [3] S. F dos Santos *et al.* 2016 47th APS DAMOP meeting, Providence, Rhode Island.

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