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Low energy electron attachment to the uracil molecule

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Using a recently constructed high resolution crossed beams apparatus involving a hemispherical electron monochromator [1] we have studied electron attachment to the $C_4H_4N_2O_2$ molecule, better known as uracil.

The experimental set-up consists of a hemispherical electron monochromator, a supersonic nozzle expansion source and a quadrupole mass spectrometer. With this electron monochromator we can achieve an electron energy resolution of up to 30meV FWHM. Two different electron attachment studies one producing Cl^- from CCl_4 for the dissociative attachment processes and the other producing SF_6^- out of SF_6 was used to test the set-up and to determine the electron energy resolution. For the present measurements the determination of the electron energy distribution mainly was done by producing Cl^- from CCl_4 . This process was additionally used to calibrate the energy scale. The electron energy range investigated was in the region between 0 and 12eV.

Because uracil at room temperature is a white powder we used a modified C_{60} oven to introduce evaporated uracil into the apparatus. The most important point in modifying this oven was to attach an about 7cm long copper pipe to the open side of the oven. This helped us to guide the evaporated uracil directly into the collision chamber. The inside diameter of this pipe is about 0.8 mm. A typical temperature range of the oven during operation of the measurements is 180 to 185°C. Approximately 2mm further the crossing of uracil and the monochromatized electron beam occurs. The ions produced are extracted by a weak electric field either produced by one part of the collision chamber or by the entrance cone optics of the quadrupole mass spectrometer. After passing the mass spectrometer the ions are deflected and counted in single ion count mode with a channeltron.

In addition to series of electron impact ionization studies (in order to determine the mass spectrum and to obtain appearance energies) we did measurements on electron attachment to the uracil molecule $C_4H_4N_2O_2$. It is the first such study concerning the attachment of free electrons to the uracil molecule (see also the pioneering study about bound electron attachment to uracil by Schermann and co-workers [3]). The only comparable measurements have been carried out at the Berlin Laboratory of Illenberger and co-workers [2] where they investigated electron attachment to the 5-bromouracil molecule.

The main interest of this work is to find out what will happen when slow electrons are colliding with the cellular RNA compound uracil. It is generally considered that the types of primary damage in DNA by ionizing radiation (electrons, photons, ions) leads to the most significant biological effects [4]. These effects are known as double-strand breaks (DSB) and clustered lesions. These types of lesions have the greatest relevance of cellular effects underlying both human cancer risk from radiation exposure and the cell killing action of radiation used in radiotherapy.

In the present measurements the following anion fragments of uracil have been detected within our detection limit ($C_4H_3N_2O_2^-$), OCN^- , $(H_2C_3NO)^-$, CN^- , O^- . The most important result is that we cannot observe within our detection efficiency any traces of the parent anion (this has been confirmed by careful measurements of neighboring isotope peaks). The most intense fragment anion appears on a mass to charge ratio of 111 amu. Mass 111 corresponds to a uracil molecule missing one hydrogen. Moreover, the electron attachment spectrum for this

anion exhibits in the energy range from 0 to 3eV (see Fig.1) a number of resonant structures. The zero energy resonance is probably due to an s-wave attachment process. Other observed resonances appear at 0.68, 1.0, 1.44, 1.7, and 1.92eV. The error bars for these peak energy values are in the region of about ± 40 meV.

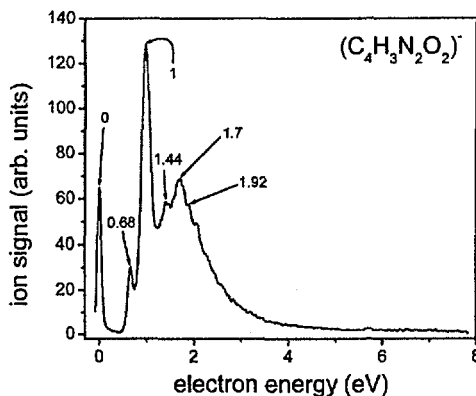


Fig. 1: Electron attachment spectrum for uracil producing the anion fragment $C_4H_3N_2O_2^-$.

It is interesting to note that this result, i.e. the missing of the parent anion is in contrast to recent observations by Schermann and co-workers [3], who observed the occurrence of the uracil parent anion when studying Rydberg electron attachment to gas phase isolated uracil molecules [3] and also in contrast to free electron attachment studies to bromouracil by Illenberger [2] who observed in these studies the parent bromouracil anion to be the major anion produced.

Another interesting observation is whereas the parent minus H anion is observed at zero electron energy, all other fragments do not appear in the zero energy range. The two most intense fragment anion species appear at mass 42 identified as OCN^- and at mass 68 identified as $(H_2C_3NO)^-$, the same fragment anions are also observed in [2]. In contrast to the measurements of Illenberger and co-workers [2] on the bromouracil, however, we see in addition the fragments CN^- and O^- . The intensity of these fragment anions is at least one order of magnitude lower than OCN^- yield. The onset of the first resonance for these anions appears at the relatively high electron energy of about 5eV for CN^- and at 9eV for the O^- , followed by two resonances with the maxima at approximately 7eV and 10eV for CN^- and in the case of the O^- production only one resonance at 10.2eV.

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