

MEASUREMENT OF KINETIC ENERGY DISTRIBUTION OF POSITIVE IONS FROM ELECTRON INDUCED DISSOCIATION OF PYRIMIDINE MOLECULE

ALEKSANDAR R. MILOSAVLJEVIĆ^{1,*}, JELENA B. MALJKOVIĆ¹,
DRAGUTIN ŠEVIĆ¹, IZTOK ČADEŽ² and BRATISLAV P. MARINKOVIĆ¹

¹Laboratory for Atomic Collision Processes, Institute of Physics,
University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia

²Jožef Stefan Institute, Jamova cesta 39, SI-1000 Ljubljana, Slovenia

*E-mail: vraz@ipb.ac.rs

Abstract. We report preliminary results on measurements of kinetic energy distribution of positive ions formed upon electron induced dissociative ionization of gaseous pyrimidine molecule ($C_4H_4N_2$). The kinetic energy spectra were recorded without precedent mass/charge analysis, for different incident electron energies (50-250 eV) and different detection angles (40° - 90°) with respect to the incident beam direction. An influence of the residual gas background to the recorded distributions has been investigated.

1. INTRODUCTION

The investigation of electron interaction with molecules that may be used as a chemical or molecular model for the parts of large biomolecules has been mostly motivated in recent years by the radiation damage research. Pyrimidine (1,3-diazine), $C_4H_4N_2$, belongs to the group of dyazine ring molecules, which may represent a model for the single nucleosides (thymine, cytosine and uracil) in nucleic acids. The most recent work on pyrimidine includes the VUV photoionization (Vall-Ilosera et al. 2008, Schwell et al. 2008), electronic states resolved PEPICO spectroscopy (Plekan et al. 2008), measurements of absolute differential cross sections for elastic electron scattering (Maljković et al. 2009) and VUV photoabsorption and electron energy loss spectroscopy (Silva et al. 2010). The investigation of kinetic energy and angular distributions of positive ions formed upon electron ionization of biomolecules could be important in many aspects such as the input data for energy deposition modelling and estimation of by-product production following radiation damage, as well as for fundamental understanding of molecular structure and finding real appearance thresholds of ionic fragments.

The present contribution gives information on the kinetic energy distribution of all positive ions formed upon the ionization of pyrimidine molecule, without an analysis of ionic fragments by their mass/charge ratio. The used electron energy range (50-300 eV) is of interest regarding the inelastic scattering and stopping

power of electrons in an organic based tissue (Oller et al. 2006), as well as for accessing a possible influence of core shell excitations (K 1s carbon threshold at 284 eV) to fragment ion distributions. Furthermore, our previously reported results for tetrahydrofuran (C₄H₈O) and tetrahydrofurfuryl alcohol (C₅H₁₀O₂) (Milosavljević et al. 2006) have shown a strong dependence of the low-energy ions yield (close to 0 eV) on the incident electron energy and, especially, the detection angle with respect to the incident beam direction. This effect was considered to be an experimental artefact but further explanations were not possible to be given at the time. In the present work, possible limitations in experimental determination of ionic energy spectra, regarding the pressure, incident electron beam characteristics and experimental arrangement are investigated in detail.

2. EXPERIMENTAL SET-UP

The measurements were performed by using a crossed beams experimental set-up (Milosavljević et al. 2006a), with slight modifications of the detection scheme to allow an efficient detection of positive ions (Milosavljević et al. 2006). Briefly, an electron gun produces a well collimated incident electron beam, which is crossed perpendicularly by a molecular beam produced by a stainless still needle. The gun can be rotated around the needle in the angular range from -10° to 110° in the present case. The interaction volume defined by the crossing of the electron and molecular beams is in a field free region. The ions which enter through the first grounded electrode of a four-element cylindrical electrostatic lens are further focused and accelerated into a double cylindrical mirror analyzer (DCMA), followed by three-element focusing lens and a single channel electron multiplier. DCMA was set to work in the constant pass energy mode, so the positive ions kinetic energy distributions were measured by recording the count rates as a function of the negative potential that accelerates ions to pass through the analyzer. A high negative voltage (~ 2.5 kV) at the nose of the channeltron insures efficient detection of ions. The base pressure was about 4×10^{-7} mbar, while the working pressure was usually less than 5×10^{-6} mbar. The uncertainty of the incident energy scale was determined to be less than ± 0.4 eV, by observing a threshold for He⁺ ions yield. The energy resolution of the ions kinetic energy spectrum is limited only by the analyzer and a desired signal to noise ratio and was about 0.2 eV in the present case. The incident electron beam current was about 50 nA.

The present experimental system has been recently upgraded to allow measurements of absolute differential cross sections for electron/atom(molecule) scattering by using relative flow technique (Milosavljević et al. 2008). This system was used presently to investigate an influence of the residual gas background to the angular and the electron energy dependence of recorded kinetic energy distributions of fragment ions. The kinetic energy distributions were recorded when target gas is flown either through the needle or through the side leak, under the otherwise same experimental conditions.

3. RESULTS

The exemplary kinetic energy distributions of positive ions upon 100 eV electrons induced ionization of pyrimidine molecule, for two different detection angles with respect to the incident beam direction, are shown in Fig. 1. Since the exact calibration of the ion kinetic energy has not been performed yet, the distributions were presented as a function of the acceleration voltage. The kinetic energy of 0 eV corresponds to an acceleration voltage of about -5.7 V. The near 0 eV peak corresponds to a thermal distribution of both the parent ion and heavy fragments, which is additionally broadened due to a finite energy resolution. In addition, the spectra clearly show intensive bands corresponding to fragments with higher energies of several eVs, which are released in a dissociative ionization process.

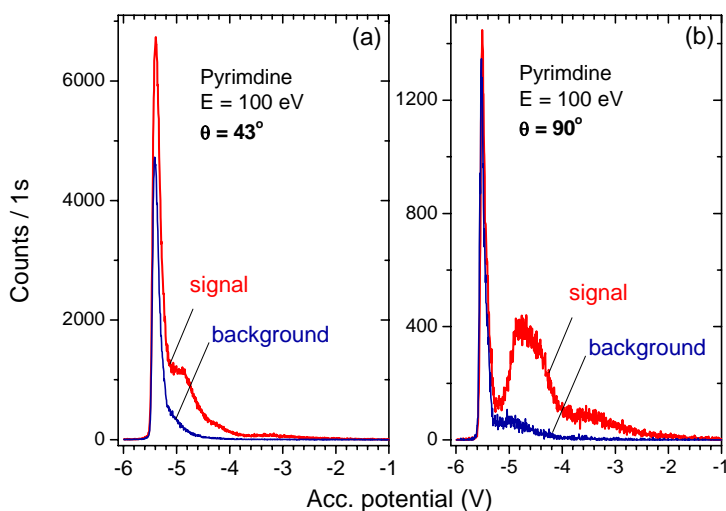


Figure 1: Kinetic energy distributions of positive ions upon 100 eV electrons induced ionization of pyrimidine molecule, for the detection angles with respect to the incident beam direction of 43° (a) and 90° (b).

The near 0 eV ions yield of practically the same intensity is measured when no gas is flown through the needle, suggesting a strong contribution of the residual background gas to the detection of thermal ions. Note also that the signal of thermal ions increases with decreasing the detection angle due to higher overlap between the incident electron beam and the detector view cone. Fig. 2 shows measured kinetic distributions of more energetic fragments for different detection angles and incident electron energies.

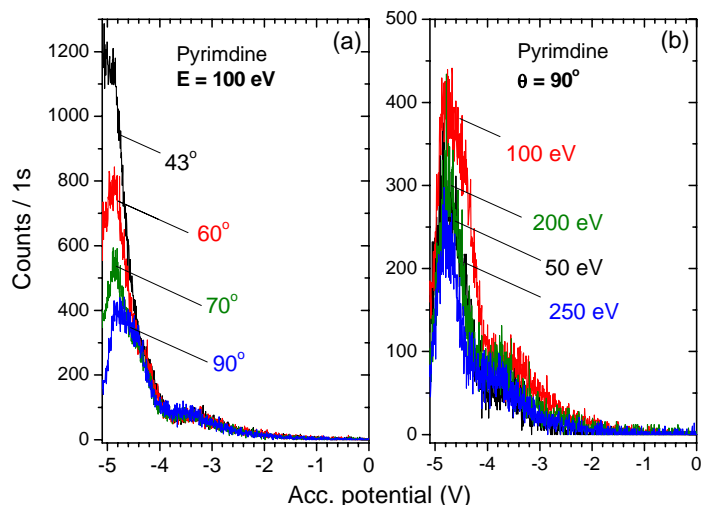


Figure 3: Kinetic energy distributions of positive ions upon electron induced ionization of pyrimidine molecule.

In conclusion, present results show an existence of energetic ionic fragments upon electron induced dissociative ionization of small molecules representing DNA building blocks. Further improvement of the experimental system is planned in order to perform more detailed investigations of angular dependence of distributions, for desired mass selected fragments.

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