RELATIVE ANGLE-DIFFERENTIAL CROSS SECTIONS FOR ELASTIC ELECTRON SCATTERING FROM PYRIMIDINE

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Abstract. Angle-differential cross sections for elastic scattering of electrons from pyrimidine are reported for the incident energies from 50-300 eV. Measurements were performed using a cross-beam technique, for scattering angles from 20° to 110°. Experimental relative elastic differential cross sections are compared with recent theoretical results for uracil, which is a pyrimidine base and a component of ribonucleic acid.

1. INTRODUCTION

The investigation of electron interaction with molecules which are analogue to DNA components has been motivated in recent years by the research of radiation damage in biomolecular systems (Boudaiffa et al. 2000). Since a large number of secondary low-energy electrons are formed on the track of primary high-energy ionizing particles they carry most of energy and play particulary important role in the final radiation damage, ascribed to the primary ionizing particle. To improve our understanding of the chain of the reactions leading to DNA and RNA damage (Hassan et al. 2000,Boudaiffa et al. 2000, Michael et al. 2000) and postulate new reaction models, spectroscopic data and cross section values for electron impact on DNA and RNA are needed. The pyrimidine (Py) molecule is akin to cytosine and thymine in DNA as well as uracil in RNA and therefore may serve as a model compound to investigate differential cross sections for elastic scattering of electrons from constituents of these biomolecules (Levesque et al. 2005). Pyrimidine ($C_4H_4N_2$) is a heterocyclic aromatic organic compound containing two nitrogen atoms at positions 1 and 3 of the six-member ring (Gilchrist 1997, see Figure 1). Three nucleobases found in nucleic acids, namely cytosine ($C_4H_5N_3O$), thymine ($C_5H_6N_2O_2$) and uracil ($C_4H_4N_2O_2$) are pyrimidine derivatives. Because of its similarity to nucleotide ring system, Py has been used as a simple theoretical model of the ring conformations in nucleotides (Lesyng et al. 1984, Herzyk et al. 1989,Berthier 1997). Levesque et al. 2005 have reported low-energy vibrational and electronic electron- energy-loss (EEL) spectra of pyrimidine condensed on a thin film of solid argon held at 18 K, for incident energy range of 2-12 eV. According to our knowledge, no theoretical results concerning elastic electron scattering from Py have been published. However, Možejko and Sanche 2003 have calculated differential cross
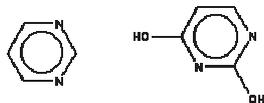
Figure 1: Structural formulae of pyrimidine (left) and uracil (right) molecules.

sections (DCSs) for elastic electron collisions with uracil, cytosine, guanine, adenine and thymine, using the independent atom method (IAM) with a static-polarization model potential, for incident energies ranging from 50-4000 eV. Total cross sections have also been calculated with the binary-encounter-Bethe model from the ionization threshold up to 5000 eV. The highest values of the elastic DCSs are obtained for the largest molecule (guanine) and the lowest for uracil which is smallest investigated molecule. Thus, the absolute elastic DCS value is connected with number of electrons in molecule and molecular size, while angular dependence of the elastic DCSs is related to molecular geometry.

In the present contribution, experimental results on elastic electron scattering from pyrimidine molecule have been reported. The experimental relative DCSs are obtained for 50, 100, 200 and 300 eV in the angular range from 20° to 110°. We have compared our results for pyrimidine ($C_4H_4N_2$) with calculations of Možejko and Sanche 2003 for the uracil molecule. Shapes of DCS curves show similarities at all impact energies.

2. EXPERIMENTAL

A detailed description of the present crossed-beam experimental set-up has been given elsewhere (Milosavljević et al. 2006). Briefly, an electron gun produces a nonmonochromated, 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 fr om about -40° to 120°. The scattered electrons are retarded and focused by a four-element cylindrical electrostatic len s into a double cylindrical mirror analyzer, followed by three-element focusing lens and a single channel electron multiplier. The base pressure of about 4×10^{-7} mbar was obtained by a turbo-molecular pump. The working pressure was usually less than 3×10^{-6} mbar and was checked for each experimental point. 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 best energy resolution is about 0.5 eV, limited by a thermal spread of primary electrons. The angular resolution was better than $\pm 2^o$. The experimental procedure was checked according to benchmark DCSs for elastic electron scattering by Ar. The anhydrous Py was purchased from Aldrich with declared purity better than 99 %.Py posses high vapor pressure, but the sample cointainer was still heated during a measurement at the temperature of about 50-60°C, because of system stability and further improvement of the signal. The temperature of the needle and pipes were around 70 ^{o}C and 60 ^{o}C, respectively. The background contributions, which were typically below 15 %, have been subtracted from the measured electron yields. The errors for the relative DCSs measured as a function of scattering angle include statistical errors (0.1-3 %) according to Poisson's distribution and short-term
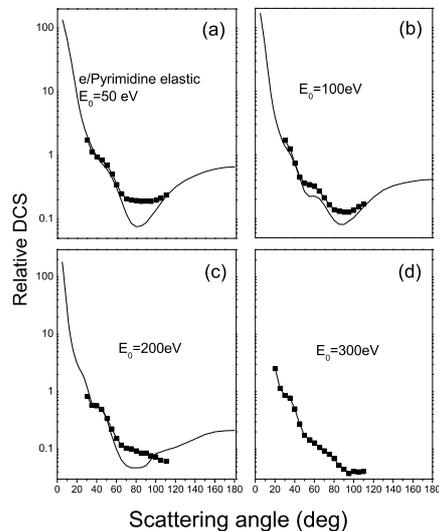
Figure 2: Angular dependence of relative DCSs for elastic electron scattering from Py molecule (∎, present experiment) and uracil (-, theory by Možejko and Sanche 2003). The DCSs are normalized at 40° for 50 eV, at 30° for 100 eV and at 50° for 200 eV.

stability errors (1-12 %), according to discrepancy of repeated measurements at the same incident energy and scattering angle.

3. RESULTS and DISCUSSION

The experimental relative DCSs are obtained for the incident electron energies of 50, 100, 200 and 300 eV, in the angular range from 20° to 110° (for 300 eV), and from 30° to 110° (for 50, 100 and 200 eV). The DCSs, experimental for pyrimidine and theoretical for uracil (Možejko and Sanche 2003), are normalized and presented in Figure 2. Theoretical results for uracil are based on the IAM approximation, where the electron-molecule collisions are reduced to the problem of collision with individual atoms by assuming that each atom of the molecule scatters independently and that redistribution of atomic electrons due to the molecular binding is unimportant. The theoretical DCSs for uracil are similar to experimental DCSs for pyrimidine for 50 eV and 100 eV, but at 200 eV DCSs do not seem to agree very well. The theoretical calculations for pyrimidine are under way (Garcia 2008). IAM technique gives more pronounced minima in the angular range from 60° to 100°, for all energies. The DCS at 100 eV is characterized by a minimum at about 90°, which disappears with increasing electron energy. At 300 eV the electron beam was better focused and experimental results exist down to 20°, but there are no calculations for uracil at this energy.

4. CONCLUSION

To conclude, the elastic scattering of electrons from Py has been investigated. The measurements were performed using cross-beam technique, for incident electron energies of 50, 100, 200 and 300 eV, and scattering angles from 20° to 110°. Experimental elastic differential cross sections are compared with recent theoretical results for similar molecule uracil ($C_4H_4N_2O_2$), available at 50, 100 and 200 eV. The shape of the present experimental DCSs for elastic electron-Py scattering shows resemblance with the calculations at 50 and 100 eV for uracil.

Acknowledgments

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