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# **CEPAS 2014**

## **CONTRIBUTED PAPER**

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#### ABSOLUTE CROSS SECTIONS FOR ELASTIC ELECTRON SCATTERING FROM FURAN AND THF MOLECULES

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The results of experimental and theoretical investigation of electron interaction with molecules that are analogue to deoxyribose in DNA are reported for 50 eV and 100 eV incident electron energie. Molecules used as targets are furan, tetrahydrofuran (THF) and 3-hydroksytetrahydrofuran (3hthf). The measurements were performed using a crossed beam technique, for scattering angles from 20° to 110°. The calculations of electron interaction cross sections are based on a corrected form of the independent-atom method, known as the SCAR (Screen Corrected Additivity Rule) procedure, using an improved quasifree absorption model. Calculated results agree very well with the experiment.

#### **1. Introduction**

The investigation of electron interaction with the molecules that are analogue to some parts of DNA has been motivated in recent years by research of radiation damage in biomaterial. Recently, group of Leon Sanche [1] has established that low energy electrons induce damage of single and double strand breaks in DNA. Molecules presented in this paper are furan ( $C_4H_4O$ ), tetrahydrofuran (THF,  $C_4H_8O$ ) and 3hydroxytetrahydrofuran (3hthf,  $C_4H_8O_2$ ), that may be considered as analogue to deoxyribose sugar in DNA. Experimental and theoretical results for these molecules [2-4] are compared on the absolute scale. Furan is a five-member unsaturated hydrocarbon ring, belonging to  $C_{2v}$  point symetry group. It different in only four H atoms from THF and in H<sub>4</sub>O from 3hthf. Therefore, according to the independent atom model (IAM) approximation [5,6] (see below) at high incident electron energies, the elastic differential cross sections for these molecules should be very similar on the absolute scale. on the other hand, although furan, THF and 3hthf are similar from the structual standpoint, furan posseses a significaly different dipol moment (0.71 D for furan, 1.75 D for THF and 1.67 D for 3hthf). Since for the molecule with high permanent dipol moment rotational excitations become more significant [5,6], this could influence the experimentaly and theoreticaly obtained absolute DCSs.

#### 2. Experimental set up and theory

The measurements of relative and absolute differential cross sections were performed using cross beam experimental setup, described previously [7]. Briefly, an electron gun produces a well collimated electron beam, which is crossed perpendicularly with molecular beam produced from a stainless steel needle. Electrons, formed in the interaction volume, are retard and focused by a four element electrostatic lens into a double mirror analyzer. Electrons are further guided by a three-element lens into the single channel electron multiplier. All these components are enclosed in a double  $\mu$ -metal shielded vacuum chamber. The base pressure was about  $4 \times 10^{-7}$  mbar, obtained by a turbo molecular pump. Working pressure was about  $2 \times 10^{-6}$ . Angular resolution was better than  $\pm 2^{\circ}$ . Experimental results were compared with previous once at the incident electron energy where a referent gas (here Ar) has deep minima [8]. The energy resolution

was about 0,4 eV, limited by a thermal spread of primary electrons. Experimental procedure included measurements of both relative and absolute differential cross sections (DCSs). Relative differential cross sections are normalized to the absolute scale according to the points obtained by the relative flow method [9,10]. Present calculations of molecular cross sections are based on a corrected form of the independent atom method, known as the screen corrected additivity rule (SCAR) procedure [5,6], with an improved quasifree absorption model potential, which includes relativistic and many body effects, as well as inelastic processes. The standard IAM approximation is based on reducing the problem of electron – molecule collisions to collisions with individual atoms by assuming that each atom of the molecule scatters independently. The role of SCAR correction to the standard IAM procedure is reducing the values obtained from the standard additivity rule to account for geometrical overlapping of atomic cross sections.

#### **3. Results**

Results of experimental and theoretical absolute differential cross sections for elastic electron scattering from furan, THF and 3hthf molecules, which are analogue to deoxyribose in DNA, has been shown in the Fig 1. In the present contribution, the results for furan, THF and 3hthf are compared and discussed for 50eV and 100eV. As expected, absolute DCSs show similar redistribution of scattered electrons from target molecules and cross sections are very close on the absolute scale for both energies. The agreement depends on both the incident energy and the scattering angle. At 100 eV DCSs for THF and 3hthf are slightly higher than the absolute points for furan and this difference is even more pronounced at 50eV at small scattering angles. This effect could be due to very different dipole moment of furan compared to THF and 3hthf. Absolute calibration for all three molecules was different. Relative flow method with Ar as the referent gas was used for furan [2], N<sub>2</sub> for THF and Kr for for 3hthf [4]. The absolute DCSs for 3hthf should be the biggest on the absolute scale, considering the size of molecule. However, a precise comparison is difficult to perform with the present experimental accuracy Also, 3hthf molecule has a low vapour pressure, so the heating was needed, which can include presence of isomers, so DCSs can be different from the expected ones.



Fig. 1. Comparison of differential cross sections for furan [2], THF [3] and 3HTHF [4] molecule.

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