

Total cross-section measurements for electron collisions with α -tetrahydrofurfuryl alcohol ($C_5H_{10}O_2$)

Paweł Możejko*, Alicja Domaracka, Elżbieta Ptasińska-Denga, Czesław Szmytkowski

Atomic Physics Division, Department of Atomic Physics and Luminescence, Faculty of Applied Physics and Mathematics, Gdańsk University of Technology, 80-952 Gdańsk, Poland

Received 28 July 2006; in final form 11 August 2006

Available online 23 August 2006

Abstract

The absolute total cross-section (TCS) for electron scattering from α -tetrahydrofurfuryl alcohol ($C_5H_{10}O_2$; THFA) has been measured using the linear transmission technique for energies ranging from 1 to 370 eV. The obtained TCS function has the relatively high magnitude over the whole energy range studied. That is also characterized by the broad enhancement spanned between 3.5 and 15 eV superimposed with two distinct resonant-like structures. Additional weak structures can be distinguished below 3 eV while two other features are discernible above ionization threshold. The present TCS is compared with available experimental and theoretical cross section data.

© 2006 Elsevier B.V. All rights reserved.

1. Introduction

The knowledge of electron interaction with DNA and RNA and their molecular subunits is necessary to understand all events leading to damage of the living cell induced by ionizing radiation [1,2]. Such radiation produces a large quantity of the secondary species including a significant number of the low-energy (0–20 eV) electrons (LEE), which can induce single and double strand breaks in the DNA [3]. Since the DNA and/or RNA are large and complex polyatomic targets, the detailed description of the subsequent events induced by electron impact on these macromolecules needs the complete and reliable electron-scattering data for molecular DNA/RNA constituents and their analogues. Recent electron-scattering studies have shown that the damage to DNA induced by LEE can proceed via direct and/or reactive electron interaction within the DNA backbone i.e. with phosphate group and deoxyribose unit [4–6]. Moreover, the strand breaks men-

tioned above occur via scission of the C–O bond of the backbone [6]. Thus, it is evident that special attention should be devoted to the electron interaction with sugar-phosphate unit and/or its molecular analogues. For that reason, we have recently measured the absolute TCS for tetrahydrofuran (THF) molecule, the simplest analogue of the DNA deoxyribose [7]. The main objective of the present studies is to provide absolute TCS for tetrahydrofurfuryl alcohol (THFA) within wide impact electron energy range. THFA can be treated as a close analogue of deoxyribose unit of the DNA; its schematic structure is shown in Fig. 1.

Experimental and theoretical studies on the electron scattering from THFA have started quite recently, they are not very numerous as yet and can be summarized as follows. The molecular structure of THFA in the gas-phase has been studied by means of the electron diffraction method [8]. Electron-stimulated desorption of the H^- from condensed THFA has been investigated within 5–40 eV [9,10]. The elastic electron–THFA scattering cross-section has been computed [11] with the independent atom method (IAM) for intermediate collision energies (50–2000) eV. The cross section for electron-induced ionization of THFA

* Corresponding author.

E-mail address: paw@mif.pg.gda.pl (P. Możejko).

URL: <http://www.mif.pg.gda.pl/kfal/atom.html> (P. Możejko).

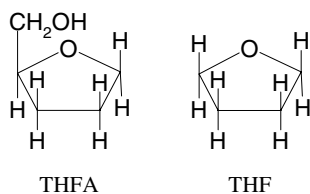


Fig. 1. The schematic structure of α -tetrahydrofurfuryl alcohol ($C_5H_{10}O_2$) molecule; for the comparison the structure of tetrahydrofuran (C_4H_8O) is presented.

has been derived within binary-encounter-Bethe (BEB) method for energies ranging from the threshold up to 4000 eV [11]. Very recently, elastic differential cross sections (DCS) have been measured with crossed beam method for incident electron energies from 40 to 300 eV and scattering angles ranging from 30° to 110° [12]. The same authors reported DCS, integral elastic and inelastic cross sections calculated with the screen-corrected additivity rule (SCAR) within 5–5000 eV energy range [12].

2. Experimental

The present measurements of the absolute TCS for the electron scattering with THFA molecules have been carried out using the electron spectrometer working in the linear transmission configuration under single collision conditions. The spectrometer electron-optics assembly consists of an electron gun, a 127° cylindrical electrostatic condenser with a system of electrostatic lenses, a reaction cell and a retarding field analyzer (RFA) together with the Faraday cup (FC) detector. The monoenergetic electron beam ($\Delta E \approx 80$ meV) is directed into a scattering cell, which is filled with the studied target vapour. The electrons passing through the cell and getting across up to the exit orifice are energetically discriminated with the RFA unit and finally, the transmitted electrons are collected with the FC detector. The well-known Bouguer-de Beer–Lambert formula allows to determine the absolute total cross section, $Q(E)$, at each selected collision energy, E :

$$I_g(E) = I_0(E) \exp[-nLQ(E)].$$

$I_0(E)$ and $I_g(E)$ are the intensities of the electron beam transmitted across the scattering cell taken with and without the target in the cell, respectively, L ($=30.5$ mm) is a length of the reaction path and n is the number density of the target determined from the measurements of gas target pressure and temperatures of the cell and manometer head [13,14]. To ensure the absolute energy values, the experimental energy scale was calibrated against the resonant oscillatory structure around 2.3 eV in molecular nitrogen [15]; overall inaccuracy of the energy scale is about 0.1 eV. The α -tetrahydrofurfuryl alcohol vapour has been obtained from a liquid sample (Aldrich) of a quoted purity of 99.0%, which has been degassed with a number of freeze–pump–thaw cycles.

The other working conditions worth mentioning are:

- the electron spectrometer optics is maintained at a base pressure of 10^{-5} Pa;
- in the electron optics and interaction region the magnetic field is reduced by Helmholtz coils to the value below $0.1 \mu\text{T}$;
- the temperature of the scattering chamber (310–320 K) differs slightly from the temperature of the mks capacitance manometer head (322 K) thus the correction due to the thermal transpiration effect [13] does not exceed 2%;
- the sample supplying line and valve are maintained at about 315 K to establish the thermal conditions same as in the scattering region.

For the details of the measuring setup, experimental procedures and data processing the reference can be made to our earlier papers [16,17].

The final TCS value for each energy studied is an average of a large number of data measured in independent series (3–14) of individual runs (~ 10 in a series). Statistical uncertainties (one standard deviation of weighted mean values) are well below 1% over the entire energy range. The direct sum of all potential individual systematic errors, related to determination of quantities necessary to TCS derivation, has been estimated to be up to 10% at the lowest energies applied, decreasing gradually to about 5% between 10 and 100 eV, and increasing to 6% at the highest collision energies we operated. The reported data are not corrected for the forward-scattering effect, however, the potential maximum lowering of the TCS value due to that effect has been estimated based on data from Ref. [11] and it is included in the overall systematic error.

3. Results and discussion

Present experimental absolute electron-scattering TCS values for α -tetrahydrofurfuryl alcohol (THFA, $C_5H_{10}O_2$) molecule are reported in Table 1. In Fig. 2 the results for THFA are shown together with our recent TCS measurements for tetrahydrofuran (THF, C_4H_8O) [7]. There are two characteristic features of the e^- -THFA TCS energy-dependence. First, the TCS magnitude appears to be relatively high over the whole energy range investigated. Second, the TCS has very pronounced, broad, two-peak enhancement spanned between 3.5 and 15 eV. The maximum at 5.5–6.0 eV reaches the value of $69 \times 10^{-20} \text{ m}^2$ while the second one ($68 \times 10^{-20} \text{ m}^2$) peaks at 9.0–9.5 eV. At the lowest applied energies, below 1.4 eV, the TCS is nearly constant. Since THFA is the polar molecule (of estimated electric dipole moment $\mu \sim 2$ D) one may expect that towards zero energy the TCS should start to increase markedly. Between 1.5 and 3.5 eV two structures can be distinguished: more intensive maximum peaks around 2.1 eV and less visible structure is located near 2.7 eV. Above ionization threshold other two features are discernible on the descending slope of the TCS energy function; close to 18 eV and around 70 eV the TCS curve markedly changes its slope.

Table 1
Absolute total cross section (TCS) for electron scattering from α -tetrahydrofurfuryl alcohol ($C_5H_{10}O_2$) in units of $10^{-20} m^2$

Energy	TCS	Energy	TCS	Energy	TCS
1.0	58.6	5.0	67.3	30	52.0
1.1	58.4	5.5	69.2	35	50.4
1.2	58.2	6.0	69.1	40	49.7
1.3	58.1	6.5	67.7	45	48.6
1.4	58.1	7.0	67.0	50	48.0
1.5	58.6	7.5	66.8	60	46.8
1.6	58.6	8.0	67.0	70	45.7
1.7	58.7	8.5	67.9	80	44.0
1.8	59.5	9.0	68.3	90	42.5
1.9	60.1	9.5	68.2	100	40.2
2.0	60.6	10.0	67.3	110	38.4
2.1	60.7	10.5	66.9	120	37.2
2.2	60.5	11.0	64.8	140	34.1
2.4	60.0	12.0	63.5	160	32.1
2.5	60.0	13.0	61.3	180	30.0
2.7	60.4	15.0	58.6	200	28.1
3.0	60.2	17.0	57.0	220	25.8
3.3	60.3	19.0	56.9	250	23.5
3.5	60.6	21.0	55.8	270	21.9
3.7	61.5	23.5	54.6	300	20.1
4.0	62.8	26.0	53.3	350	18.2
4.5	64.9	28.5	52.4	370	16.7

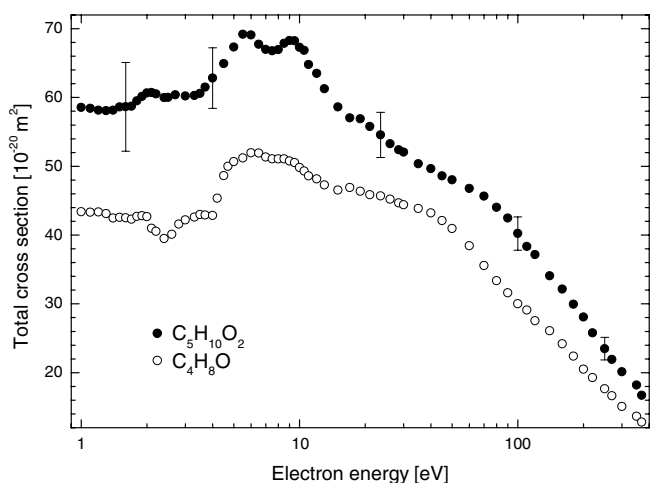


Fig. 2. Absolute TCS for $e^-C_5H_{10}O_2$ collisions: ●, present results. The error bars in selected points represent the total (systematic plus statistical) experimental uncertainties. For comparison the TCS for $e^-C_4H_8O$ collision (○) [7] is included.

Due to lack of data for particular electron-scattering processes in gaseous THFA, the description of the observed TCS features may be based only upon the results obtained for solid-phase THFA or for molecules of similar structure. Fig. 2 clearly shows that the TCS for $C_5H_{10}O_2$ is generally similar in the shape to that for its counterpart C_4H_8O [7] while they are distinctly different in magnitude. The main difference in the structure of both compared molecules (see Fig. 1) lies in the fact that hydrogen atom at α -carbon position in a heterocyclic furan ring is replaced with a CH_2OH group; thus the molecular size of THFA is larger than that for THF what reflects in the higher TCS values

for THFA. Surprisingly, the presence of the additional CH_2OH group does not create any new structure in the TCS curve. Both TCS energy functions exhibit two weak structures for energies below 4 eV, two-peaked broad enhancement spanned between 4 and 14 eV and two humps above ionization threshold. The low-energy TCS structures for THFA and THF slightly differ in energy positions due to differences between the respective energy levels. The maxima near 6.5 and 9 eV can be explained as a result of a superposition of several short-lived resonances formed in the vicinity of these energies. The resonances are likely to be responsible for the resonant vibrational excitation of C–H stretching and/or CH_2 scissoring modes of molecules ([7] and references therein). Indeed, such resonances have been already observed in the vibrational spectra for other ring molecules [18]. It is also worth noting in Fig. 2 that some structures observed for THFA appear to be more distinct than in the case of THF. The higher intensity of the 6.5 and 9 eV maxima for THFA may be related to the increased number of C–H bonds at α -carbon due to the presence of CH_2OH group.

In Fig. 3 the present experimental TCS is compared with available theoretical cross sections. It is evident that the sum of the ionization and elastic cross sections computed by Mozejko and Sanche [11] reproduces the shape of the measured TCS quite well for energies above 80 eV. However, the total cross section computed this way is higher than the experimental TCS by about 4% between 100 and 300 eV and by about 10% at higher impact energies. The summed cross-section (elastic + inelastic) derived by Milosavljević et al. [12] agree well with the general shape of our measured TCS for energies above 20 eV. Comparing to the experiment, their cross section is lower by about 10% between 20 and 100 eV; for higher energies the disagreement becomes smaller and at 300 eV both cross sec-

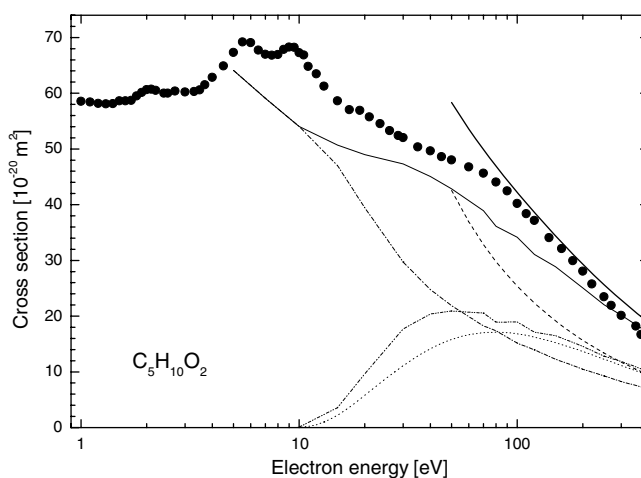


Fig. 3. Comparison of experimental and theoretical cross sections for electron collision with tetrahydrofurfuryl alcohol. Experimental: ●, present absolute TCS results. Theoretical cross sections: —, sum of elastic and ionization from Ref. [11]; —, sum of elastic and inelastic (SCAR), [12]; - - -, elastic, [11]; · · ·, elastic, [12]; - · · ·, inelastic, [12]; · · ·, ionization [11].

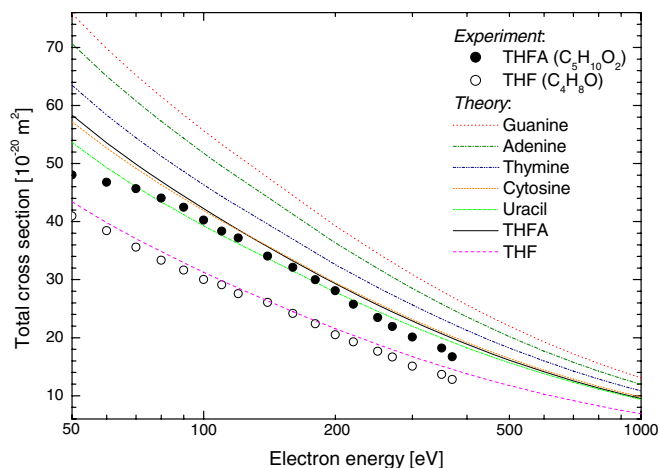


Fig. 4. Comparison of absolute e^- - $C_5H_{10}O_2$ TCS with cross sections evaluated for DNA and RNA bases and for THF.

tions merge in the value. From both theoretical results it is also evident that the weak, broad hump observed in the experimental TCS around 70 eV is associated with relatively high maximum in the ionization cross-section.

Since the sum of the calculated elastic and ionization cross sections [11] reproduces quite well the shape and values of the present intermediate-energy TCS for THFA, we have also evaluated the summed cross sections for other subunits of the DNA and RNA using theoretical data for elastic and ionization channels [11,20] computed with independent atom and binary-encounter-Bethe methods, respectively. It is worth noting that total cross sections (elastic + ionization) computed this way satisfactorily reproduce the intermediate energy experimental data for some other molecules (e.g. NF_3 [21], SF_4 [22], SO_2ClF [23], SO_2Cl_2 [24] and C_4H_8O [7]). In Fig. 4 the summed cross sections for electron collision with guanine ($C_5H_5N_5O$), adenine ($C_5H_5N_5$), thymine ($C_5H_6N_2O_2$), cytosine ($C_4H_5N_3O$), uracil ($C_4H_4N_2O_2$), THFA and THF are compared for collision energies from 50 to 1000 eV. In that energy range cross-section functions for all investigated targets monotonically decrease with the increasing energy. Within the whole energy range studied the magnitude of TCS for THF is the lowest, while electron-collisional processes are the most efficient for guanine and adenine. The calculated cross-section for THFA is higher than that for THF by about 40% in the 50–1000 eV energy range.

Finally, it seems to be interesting that the sum of the TCSs for THF and for methanol (CH_3OH) [19] is in reasonable agreement with TCS for THFA at energies above 80 eV. That means the electron-scattering TCS for complex targets at intermediate energies may be roughly but quite credibly estimated with the sum of TCSs for their subunits.

Acknowledgement

This work is a part of a research program sponsored by the Polish Ministry of Education and Science (MNiSzW).

References

- [1] L. Sanche, *Mass Spectrom. Rev.* 21 (2002) 349.
- [2] L. Sanche, *Eur. Phys. J. D* 35 (2005) 367.
- [3] B. Boudaïffa, P. Cloutier, D. Hunting, M.A. Huels, L. Sanche, *Science* 287 (2000) 1658.
- [4] X. Pan, P. Cloutier, D. Hunting, L. Sanche, *Phys. Rev. Lett.* 90 (2003) 208102.
- [5] X. Pan, L. Sanche, *Phys. Rev. Lett.* 94 (2005) 198104.
- [6] X. Pan, L. Sanche, *Chem. Phys. Lett.* 421 (2006) 404.
- [7] P. Mozejko, E. Ptasńska-Denga, A. Domaracka, Cz. Szmytkowski, *Phys. Rev. A* 74 (2006) 012708.
- [8] K.B. Borisenko, S. Samdal, I.F. Shishkov, L.V. Vilkov, *J. Mol. Struct.* 448 (1998) 29.
- [9] D. Antic, L. Parenteau, M. Lepage, L. Sanche, *J. Phys. Chem. B* 103 (1999) 6611.
- [10] D. Antic, L. Parenteau, L. Sanche, *J. Phys. Chem. B* 104 (2000) 4711.
- [11] P. Mozejko, L. Sanche, *Radiat. Phys. Chem.* 73 (2005) 77.
- [12] A.R. Milosavljević, F. Blanco, D. Šević, G. García, B.P. Marinković, *Eur. Phys. J. D* (2006) in press, doi:10.1140/epjd/e2006-00138-7.
- [13] M. Knudsen, *Ann. Phys. Lpz.* 31 (1910) 205.
- [14] K.F. Poulter, M.J. Rodgers, P.J. Nash, T.J. Thompson, M.P. Perkin, *Vacuum* 33 (1983) 311.
- [15] Cz. Szmytkowski, K. Macia, G. Karwasz, *Phys. Scripta* 54 (1996) 271.
- [16] Cz. Szmytkowski, P. Mozejko, G. Kasperski, *J. Phys. B* 31 (1998) 3917.
- [17] Cz. Szmytkowski, P. Mozejko, *Vacuum* 63 (2001) 549.
- [18] M. Allan, L. Andrić, *J. Chem. Phys.* 105 (1996) 3559.
- [19] Cz. Szmytkowski, A.M. Krzysztofowicz, *J. Phys. B* 28 (1995) 4291.
- [20] P. Mozejko, L. Sanche, *Radiat. Environ. Biophys.* 42 (2003) 201.
- [21] Cz. Szmytkowski, A. Domaracka, P. Mozejko, E. Ptasńska-Denga, L. Kłosowski, M. Piotrowicz, G. Kasperski, *Phys. Rev. A* 70 (2004) 032707.
- [22] Cz. Szmytkowski, A. Domaracka, P. Mozejko, E. Ptasńska-Denga, S. Kwitniewski, *J. Phys. B* 38 (2005) 745.
- [23] Cz. Szmytkowski, P. Mozejko, S. Kwitniewski, E. Ptasńska-Denga, A. Domaracka, *J. Phys. B* 38 (2005) 2945.
- [24] Cz. Szmytkowski, P. Mozejko, S. Kwitniewski, A. Domaracka, E. Ptasńska-Denga, *J. Phys. B* 39 (2006) 2571.