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Absolute cross sections for electron scattering from furan

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We report results of measurements and calculations of absolute cross sections for electron scattering from furan molecules (C_4H_4O). The experimental absolute differential cross sections (DCSs) for elastic electron scattering were obtained for the incident energies from 50 eV to 300 eV and for scattering angles from 20º to 110º, by using a crossed electron-target beam setup and the relative flow technique for calibration to the absolute scale. The calculations of the electron interaction cross sections are based on a corrected form of the independent-atom method, known as the screening corrected additivity rule (SCAR) procedure and using an improved quasifree absorption model. The latter calculations also account for rotational excitations in the approximation of a free electric dipole and were used to obtain elastic DCSs as well as total and integral elastic cross sections which are tabulated in the energy range from 10 to 10 000 eV. All SCAR calculated cross sections agree very well with both the present and previously published experimental results. Additionally, calculations based on the first Born approximation were performed to calculate both elastic and vibrationally inelastic DCSs for all the modes of furane, in the energy range from 50 eV to 300 eV. The ratios of the summed vibrational to elastic DCSs are presented and discussed. Finally, the present results for furan are compared with previously published elastic DCSs for the tetrahydrofuran molecule and discussed. © *2012 American Institute of Physics.* [http://dx.doi.org/10.1063/1.4742759]

I. INTRODUCTION

The motivation to study electron interactions with furan molecules (C_4H_4O) in recent years predominantly comes from radiation damage research, since its structure may be considered as a simple representative of the sugar component in the DNA backbone (see Fig. 1). Electron interactions with small biomolecules analogue to building blocks of large biological macromolecules (DNA, proteins) have been the subject of considerable interest, since it was discovered that low-energy electrons can cause significant DNA damage.[1,2] The primary, high-energy particle produces a large number of secondary low-energy electrons on its track in the biological medium; therefore, those electrons may play an important role in macroscopic radiation damage of living cells and tissues. Although it is usually considered that the dominant part of the secondary electrons are formed with rather low energies (below about 30 eV), the tail of their distributions can have a significant fraction of electrons with energies of the order of 10^2 eV.[3] Note also that an insight and accurate estimation of radiation damage produced by a specific type of high-energy particles represents an important part of research connected with cancer therapy.[4,5] For a better understanding and more accurate modeling of radiation damage, spectroscopic data and absolute cross sections for electron scattering from biomolecules are needed. With this motivation, a number of both theoretical and experimental studies on electron-molecule scattering have been reported in recent years. Particularly, our previous results include absolute differential cross sections for elastic electron scattering from several different molecules representing sub-units of either DNA (Refs. 6–9) or proteins.[10,11]

Furan is a five-member hydrocarbon ring containing an oxygen atom (see Fig. 1) and belonging to C_{2v} point symmetry group.[12] Its structure can, therefore, be considered to be relevant as the simplest representative of the sugar unit in the DNA backbone,[13] similar to the tetrahydrofuran molecule (THF) which has been intensively investigated in recent years with this motivation. Particularly, theoretical and experimental absolute differential cross sections (DCSs) for elastic electron scattering by THF have been reported by several groups.[6,14–20] However, it must be taken into account that, contrary to THF, the furan molecule is not saturated and an existence of π orbitals makes it chemically distinct from THF. For example, the process of dissociative electron attachment, which is considered to be particularly important in radiation damage research since it could lead to DNA strand breaks,[1,2] is very different for these.[21] On the other hand, although

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FIG. 1. Schematic drawing of furan, tetrahydrofuran (THF), and deoxyribose molecules.

being chemically very different, furan and THF have a similar structure with the difference being in only four H atoms, so they should also have similar cross sections for elastic electron scattering in the energy range of interest in the present work (above 50 eV), where the independent atom model (a molecular cross section is approximated by a sum over atomic cross sections) starts to be operative. This has been already shown by comparing the elastic DCSs of THF (an ether) and the furanose alcohols.[8] Nevertheless, although the furan and THF molecules are quite similar from a structural standpoint, THF has a significantly larger dipole moment (1.75 D) than that of furan (0.71 D).[22] Since for a molecule with a relatively high permanent dipole moment rotational excitations become more significant (see Ref. 23 and references therein), this could influence both the experimentally obtained elastic DCSs and theoretical elastic DCSs calculated by using the screening corrected additivity rule (SCAR) method. Indeed, the former cannot separate rotational and vibrational excitations due to a limited energy resolution, while the latter theoretical method ignores these processes. In the present work, additional calculations based on the first Born approximation have been performed to estimate an influence of both rotational and vibrational excitations to the pure elastic electron scattering that cannot be resolved experimentally. According to our knowledge, this is a unique study of vibrational to elastic DCS ratios in the present energy range, where these inelastic processes are usually considered to be negligible.

A considerable number of papers have been published concerning electron interaction with the furan molecule. Very recently, Khakoo *et al.*[13] have reported experimental and theoretical DCSs for elastic electron scattering by furan at incident energies from 1 eV to 50 eV and in the angular range between 10° and 130°. Szmytkowski *et al.*[24] reported absolute total cross sections, measured over energies from 0.6–400 eV using a linear electron transmission method; in the same paper the authors also reported calculated integral and ionization cross sections up to 4 keV, obtained by an additivity rule approximation and a binary-encounter-Bethe approach, respectively. Hargreaves *et al.*[25] reported measurements of DCSs for the vibrational excitation of furan, obtaining results for nine features spanning the electron energy loss range of 0–0.8 eV. The excitation spectrum of furan has been also measured by Giuliani and Hubin-Franskim,[26] using high resolution electron energy loss spectroscopy at 30 eV incident electron energy and scattering angles of 10° and 25°. Furthermore, Bettega and Lima[27] have reported calculated integral, differential, and momentum transfer cross sections for elastic scattering of low-energy electrons by furan using

the Schwinger multichannel method with pseudopotentials. Those computations were performed in the static-exchange and in the static-exchange plus polarization approximations. Also, Sulzer *et al.*[21] studied the dissociative electron attachment to furan, tetrahydrofuran, and fructose using a crossed electron–molecular beams experiment with mass spectrometric detection of the anions. Electron attachment by a series of molecules including furan has been investigated by Modelli and Burrow[28] through electron transmission spectroscopy. Finally, it should be noted that beside radiation damage research, the furan molecule is of general interest in chemical physics, since it represents one of the simplest non-saturated heterocyclic compounds. Also, this molecule attracts considerable attention in the life sciences. For example, furan and its derivates have been identified in small numbers of heat-treated food and since it is classified as possibly carcinogenic to humans, a great concern has been carried out to the analysis of this substance naturally occurring in food (by degradation of amino acids and reducing sugars).[29] Crews and Castle[30] have also examined furan in foods, its metabolism, and toxicity.

In the present paper, we report both experimental and theoretical absolute cross sections for electron scattering from furan. The experimental absolute elastic DCSs are obtained in the incident energy range from 50 eV to 300 eV and an angular range from 20° to 110°. The calculations of elastic DCSs, integral elastic (ICSs), and total cross sections (TCSs) are performed by using an improved independent atom method (IAM), denoted as SCAR procedure, with a quasifree absorption model potential, which includes relativistic and many-body effects. Moreover, the present SCAR calculations also take into account the rotational excitation cross section for a free electric dipole (SCARND procedure). Additionally, a separate set of calculated results has been obtained on the basis of the unitarized first Born approximation (UFBA) (Ref. 31) to estimate vibrationally inelastic cross sections, in the energy range used in measurements. In parallel, the elastic DCSs have also been calculated using the UFBA method and compared with the experimental results as well. Finally, we report tabulated results on experimental elastic DCSs in the energy range 50-300 eV, calculated ratios of vibrationally inelastic to elastic DCSs in the energy range 50–300 eV, and calculated integral elastic and total cross sections in the energy range from 10–10 000 eV. Also, both theoretical and experimental results for furan are compared to relevant recently published data[13,24] and previously reported results for the THF molecule[6] and discussed.

II. EXPERIMENT

Elastic electron scattering from the furan molecule has been studied using a cross electron-target beam apparatus, which has been described in detail in previous papers,[8,10,32] therefore only a brief description will be given here. The experimental setup consists of an electron gun, a double cylindrical mirror energy analyzer and a channel electron multiplier as a detector. All components are enclosed in a double μ-metal shielded vacuum chamber. The primary electron beam is formed by an electron gun (without monochromator)

with a hairpin thermo-electron source defining an energy resolution limit of around 0.5 eV. Scattered electrons are energy analyzed by a double cylindrical energy analyzer before being detected by a single channel electron multiplier. The base pressure of about 4×10^{-7} mbars was obtained by a turbomolecular pump, while the working pressure was usually kept in the range $(2–5) \times 10^{-6}$ mbars. The molecular beam is obtained by using a stainless steel needle and the electron gun can be rotated around it in the angular range from about $-40°$ to $110°$ (in the present experiment). The uncertainty of the incident electron energy scale has been previously determined to be less than ± 0.4 eV (Ref. 32) and we do not expect that contact potential effects for the present target may cause significant differences for the used incident energies and the obtained energy resolution. The angular resolution is better than $\pm 2°$.[32]

The anhydrous furan was purchased from Aldrich with a declared purity better than 99%. Before starting the measurements a few freeze-thaw-pump cycles under vacuum have been made. Furan is a liquid at room temperature and was introduced into the scattering region from a glass container via a gas line system. The furan molecule is characterized by a very high vapor pressure (493 mm Hg at 20 °C) and relatively low dipole moment (0.71 D). Therefore, it allows much more stable experimental conditions during gas phase measurements in comparison with previously studied "sticky" molecular targets with a much lower vapor pressure, such as THF and its derivates. In the present work, the gas-handling system (sample container, pipes, needle) was kept at the room temperature, still providing a stable driving pressure behind the needle and a high enough scattering electron signal.

DCSs for elastic electron scattering from furan have been measured at selected incident electron energies, from 50 to 300 eV (in 50 eV steps), and at scattering angles from $20°$ to $110°$ (in $5°$ steps). At a given electron energy, the relative cross section has been derived as a function of scattering angle by measuring the elastic scattering intensity at the maximum of the elastic peak. The angular response of the apparatus has been checked for each set of measurements (and for different incident electron energies) by recording the relative angular dependence of the elastic DCS for Ar or Kr, under the same experimental conditions. The background contributions of the elastic electron intensities have been measured by directing the molecular beam through the side leak and were subtracted from the measured electron yields. The background contributions were around 15% at low incident energies and scattering angles, and around 10% at higher energies. The relative angle dependent cross sections were further normalized to the absolute points obtained at several scattering angles ($40°$, $80°$, or $90°$) using the relative flow technique[33–35] and Ar as a reference gas with its known DCSs published by Williams and Willis.[36] Our procedure of the relative flow measurements and the schematic of the experimental setup have been given in our previous papers.[8,10] Briefly, in the relative flow method the scattered electron signal from a target gas (with unknown DCSs) is compared to the signal from a standard gas (Ar in the present case), at the same incident electron energy and the same scattering angle, under the same experimental conditions (meaning that the beam profiles for the both gases are

the same).[33–35] In the present experiment, the ratio of the pressures behind the gas needle forming the molecular beam was adjusted to be around 2 (P_{Ar}/P_{furan}), according to the available gas kinetic diameter for furan of 5.24 Å.[13] Also, the pressure of furan behind the needle was maintained below 0.2 mbars. Finally, it is worth pointing out that the absolute values of the cross sections did not depend crucially on the pressure ratios (within the uncertainties in the measured cross sections). The relative flow rate has been determined by closing an outlet to the chamber, admitting target gases into a closed constant volume and then measuring the pressure increase in time (measured by a MKS baratron).[8,10] The influence of adsorption on surfaces to the relative flow measurements[37] is reduced in the present case, because the furan molecule has a very high vapor pressure and a small dipole moment (see also Ref. 37).

The final set of experimental absolute DCSs is consistent with respect to independently measured relative DCS as a function of the scattering angle at fixed incident energy (and vice versa) and absolute DCSs (obtained by relative flow method) data. All these independent datasets were cross checked for possible disagreements, thus checking the experimental procedure and possible inconsistencies of the reference cross sections. The errors for the relative DCSs measured as a function of the scattering angle include statistical and short term stability errors. In the present case statistical errors, according to Poisson's distribution were around 0.3%–3.5% and short term stability errors were 1%–5%, according to the spread in repeated measurements at the same incident energy and scattering angle. The errors for the absolute DCSs include the error for reference DCSs for Ar[36] as well as errors of measured signal intensities and flow rates. In the present case, due to stable experimental conditions and high signal to background ratios, the uncertainty of the signal intensities and obtained flow rates are small and the overall error is largely defined by the error on the reference absolute DCSs for Ar which we assume to be about 20%. The later thus dominantly defines a minimal uncertainty on our results and the overall error of the present absolute elastic DCSs for furan is typically up to 25% and up to 30% for small scattering angles.

III. CALCULATIONS

A. Screening corrected additivity rule

Present calculations of elastic molecular DCSs, as well as integral elastic and total cross sections, were based on a corrected form of the IAM, known as the SCAR procedure,[38,39] with an improved quasifree absorption model potential, which includes relativistic and many-body effects, as well as inelastic processes. The same theoretical method has been already used in our previous works on deoxyribose analogue molecules,[7,8] a pyrimidine base analogue,[9] and peptide bond analogues[10,11] where an excellent agreement with experimental results has been obtained.

The SCAR procedure has been described in detail previously.[7,23,39,40] Briefly, the role of the SCAR correction to the standard IAM procedure is reducing the values obtained from the standard additivity rule to account for

geometrical overlapping of the atomic cross sections. The standard IAM approximation is based on reducing the problem of an electron/molecule collision to collisions 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. In this approach, the molecular scattering amplitude is derived from the sum of all the relevant atomic amplitudes, including the phase coefficients, which lead to DCSs for the molecules of interest. Integral cross sections (ICS) can then be determined by integrating those DCS. The sum of the elastic ICS and the absorption ICS then provides the TCSs. Alternatively, the ICSs for the molecule can also be derived from the relevant atomic ICSs in conjunction with the optical theorem.[38] Unfortunately, in its original form, we found an inherent contradiction between the ICSs derived from those two approaches, which suggested that the optical theorem was being violated.[9] This problem, however, has been resolved[9] by employing a normalization during the computation of the DCSs, so that the ICSs derived from the two approaches are now entirely consistent.[9] At low energies, where atomic cross sections are not small compared to (squared) interatomic distances in the molecule, the IAM approximation fails because the atoms can no longer be considered as independent scatterers and multiple scattering within the molecule is not negligible (note that the energy range for which deviations from the IAM approximation is relevant depends on the molecule in question). To account for this, screening coefficients are introduced in the present SCAR method, resulting in a corrected cross section, at a given incident energy, calculated from the atomic cross sections.[7]

The SCAR method ignores the rotational and vibrational excitations and considers only inelastic processes arising from electronic excitations and ionization. Although this restriction is not significant in general for relatively high energies (as used in the present work) in the case of molecules with a relatively high permanent dipole moment, rotational excitation becomes more important.[23] Therefore, the SCARND procedure is introduced to account for this effect. This method consists of the calculation of the rotational excitation cross section for a free electric dipole by assuming that the energy transferred is low enough, in comparison with the incident energy, and therefore the first Born approximation (FBA) is expected to be valid.[41] The most important effect of this correction is the increase of the absolute value of the cross section, which is significant at low incident energies and small scattering angles.

B. Unitarized first Born approximation

Present calculations of the vibrationally inelastic cross sections (and also for the elastic cross sections) are based on the UFBA. The UFBA represents the FBA of a K-matrix (instead of T-matrix used usually in the FBA). In this way the approximated Hermitian K-matrix leads to a unitary S-matrix and therefore conservation of the scattering flux, which is not the case for the FBA. The usefulness of this approach was first demonstrated by Itikawa,[42] and it has been later noted that the

UFBA often yields results for scattering cross sections that are significantly more accurate than those obtained in the FBA.[43]

In the present case two channels, vibrationally elastic and inelastic, were included into the model. We considered a two-channel approximation by using only the vibrational ground state ν_0 and the first excited state ν_1. The two-channel FBA K-matrix describing the scattering event, with incoming k-vector $\vec{k}_{in}$ and outgoing k-vector $\vec{k}_{out}$ can be written as (we use the plane-wave normalization instead of the more common energy normalization)

$$\langle \nu_i \, \vec{k}_{out} | K | \nu_j \, \vec{k}_{in} \rangle \approx -\pi \langle \nu_i \, \vec{k}_{out} | V | \nu_j \, \vec{k}_{in} \rangle, \ \ i, j = 0, \, 1. \tag{1}$$

Vibrational modes ν_0 and ν_1 are considered harmonic. The interaction potential V is a sum of the static and exact exchange parts. Details about the *ab initio* evaluation of coupling between the vibrational modes and the continuum represented here by the plane waves can be found in Ref. 44. The unitarized first Born T-matrix is then obtained by the well-known expression that connects the transition matrix $\boldsymbol{T}_U$ and the reactance matrix $\boldsymbol{K}$:

$$\pi \, T_U = -K(1 - iK)^{-1}. \tag{2}$$

Elastic and inelastic scattering amplitudes are then directly proportional to the parts of the $\boldsymbol{T}_U$:

$$\begin{aligned} f_{ela}(\nu_0 \, \vec{k}_{out} \leftarrow \nu_0 \, \vec{k}_{in}) &= -4\pi^2 \langle \nu_0 \, \vec{k}_{out} | T_U | \nu_0 \, \vec{k}_{in} \rangle \\ f_{inela}(\nu_1 \, \vec{k}_{out} \leftarrow \nu_0 \, \vec{k}_{in}) &= -4\pi^2 \langle \nu_1 \, \vec{k}_{out} | T_U | \nu_0 \, \vec{k}_{in} \rangle \end{aligned}. \tag{3}$$

It should be pointed out that the UFBA is an approximation using a full static-exchange potential and it should not be confused with the (first) dipole Born approximation used in the literature, as the latter employs only a dipole potential that predicts zero cross sections for non-infrared modes. In the present case, the interaction potential that enters the above equations is assumed to be described by a static-exchange model[44] as we expect correlation-polarization forces to be negligible at the considered collision energies.

IV. RESULTS AND DISCUSSION

The experimentally obtained absolute DCSs for elastic electron scattering from the furan molecule, at the incident electron energies of 50, 100, 150, 200, 250, and 300 eV are tabulated in Table I and presented in Fig. 2 (circles). The DCS points directly measured at a specific incident energy and scattering angle (40°, 80°, or 90°) by relative flow method, and used to normalize the relative DCSs to the absolute scale, are presented as well (stars). It should be noted a good agreement between these two independently measured sets of data (relative and absolute DCSs), confirming the reliability of our experimental procedure. The experimental absolute elastic DCSs are in Fig. 2 compared with the present theoretical results. The full line represents the SCARND calculations, which include rotational excitations assuming a free dipole model as well as a normalization procedure to ensure the consistency of the derived ICSs with the optical theorem (see Sect. III A). However, note that the SCARND results basically overlap with the SCAR calculations for the present molecule,

TABLE I. Experimentally obtained differential cross sections for elastic electron scattering from furan, in units of 10^{-20} m^2 sr^{-1}, as a function of scattering angle and incident electron energy. The absolute errors of relative cross sections (statistical, short-term stability and uncertainty of the effective scattering volume) in the last significant digits are given in parentheses. The errors of the absolute cross sections are estimated to be typically up to 25% and up to 30% at scattering angles below 40°.

Scattering angle (deg)	Electron energy (eV)					
	50	100	150	200	250	300
20	...	3.69(74)	...	1.89(39)	2.32(47)	1.74(35)
25	...	2.23(45)	...	1.45(30)	1.36(27)	0.93(19)
30	2.02(41)	1.49(30)	1.39(28)	0.94(19)	0.83(17)	0.651(14)
35	1.37(28)	0.98(20)	0.82(17)	0.554(28)	0.5267(73)	0.530(11)
40	0.990(41)	0.5715(72)	0.528(22)	0.456(94)	0.4181(59)	0.3170(69)
45	0.900(38)	0.4341(56)	0.400(82)	0.357(74)	0.2692(41)	0.1768(40)
50	0.747(31)	0.3593(48)	0.302(62)	0.227(47)	0.1545(26)	0.1187(29)
55	0.581(24)	0.3185(43)	0.208(43)	0.1642(88)	0.1150(21)	0.1115(27)
60	0.442(19)	0.2629(36)	0.175(36)	0.1324(74)	0.1045(19)	0.1016(25)
65	0.376(16)	0.2119(30)	0.148(30)	0.0992(56)	0.1023(19)	0.0874(22)
70	0.330(14)	0.1763(26)	0.1273(61)	0.1063(59)	0.0914(18)	0.0688(18)
75	0.309(13)	0.1490(23)	0.1146(56)	0.1059(59)	0.0778(16)	0.0574(16)
80	0.292(12)	0.1234(20)	0.108(22)	0.1037(58)	0.0655(14)	0.0467(14)
85	0.275(12)	0.1077(18)	0.100(21)	0.0868(49)	0.063(13)	0.0391(12)
90	0.264(11)	0.1020(17)	0.107(22)	0.0829(47)	0.054(11)	0.0326(11)
95	0.265(11)	0.1100(18)	0.120(25)	0.086(18)	0.0476(96)	0.0339(11)
100	0.278(12)	0.1191(19)	0.1167(57)	0.082(17)	0.0402(81)	0.0314(10)
105	0.304(13)	0.1284(21)	0.1203(58)	0.076(16)	0.03803(99)	0.0319(10)
110	0.324(14)	0.1403(22)	0.1225(59)	0.063(13)	0.0395(10)	0.0274(94)

at all presented incident energies and in the whole angular range (except close to 0°), showing that the contribution of rotational excitations to the DCSs for the furan molecule (having a relatively low permanent dipole moment) is practically negligible for the present energy range; therefore, only SCARND is plotted in Fig. 2. The present SCARND calculations of the elastic DCSs for the furan molecule agree very well with the experimental results, both in shape and
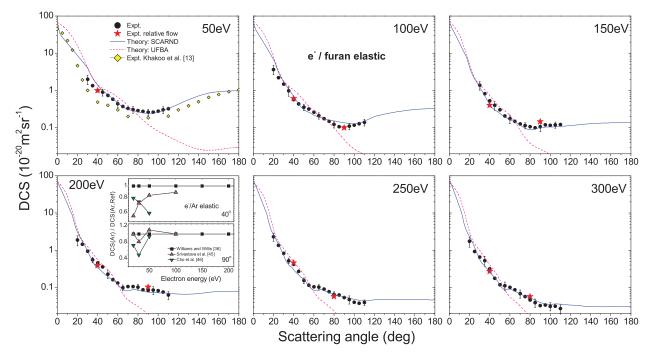

FIG. 2. Angular dependence of the absolute differential cross sections (DCSs) for elastic electron scattering from furan at different incident energies. Full circles represent the final absolute experimental differential cross sections; full stars represent absolute values obtained by the relative flow measurements; the calculations are presented by a full line (SCARND) and a dashed line (UFBA); diamonds represent the experimental points reported by Khakoo *et al.* [13] The inset shows the ratio of different reported absolute DCSs for elastic electron scattering from Ar to the reference DCS for this work published by Williams and Willis,[36] as a function of incident electron energy and at the scattering angles of 40° and 90°: squares Williams and Willis;[36] up triangles Srivastava *et al.*,[45] and down triangles Cho *et al.*[46]

on the absolute scale, as already confirmed previously for other molecules.[7–11] A small disagreement, outside of the error bars, can be seen only at the smallest measured scattering angles, for a few incident electron energies. This is also noted in our most recent papers and discussed that it could be due to both experimental and theoretical deviations in the low angular range.[11]

The theoretical DCSs calculated by using the UFBA method are presented in Fig. 2 as well. The reliability of calculations based on the first Born approximation (UFBA) is expected to increase with decreasing interaction potential in reference to the incident electron energy. Indeed, the agreement of the UFBA elastic DCSs with both the experiment and the SCARND theory is good for the present incident energy range and in the low angular range below about 60°. Nevertheless, the UFBA DCS curves significantly deviate at larger scattering angles where the impact parameters are generally smaller, therefore scattered electrons experience the more significant interaction potential which is not negligible (within the frame of the Born approximation) for the elastic scattering process in the present incident energy range. Still, the UFBA calculations reproduce well the present experimental DCSs in the low-angular range and this agreement increases with increasing the incident energy from 50 eV to 300 eV, as expected.

The present absolute DCSs are compared at 50 eV with recently published experimental result by Khakoo *et al.*[13] (it should be noted that the points below 15° and above 130° have been extrapolated by using the theory in Ref. 13) Although this DCS agrees very well in shape with the present experimental curve, it is somewhat lower in terms of the absolute scale. It is difficult to give a clear explanation for this discrepancy. Both experimental absolute DCSs have been obtained by using the relative flow method. Furthermore, as discussed in Sec. II, furan is not a very polar molecule and possesses a large vapor pressure, so the relative flow measurements can be obtained with a high accuracy. Additionally, the same gas kinetic diameter for furan was used. However, in the present case, Ar was used as the reference gas, while He was used in the previous experiment.[13] Helium is typically used as the reference gas in relative flow measurements due to several advantages, especially at low incident electron energies. For example, the cross sections for He are known very accurately and it has largely featureless cross sections, thus the small angular variations do not markedly affect the normalization. However, as explained earlier,[8] we prefer to use Ar or Kr because they possess similar gas-kinetic diameters as the target molecules (also resulting in more similar mass flow rates), which makes it easier to obtain similar experimental conditions and to perform more accurate measurements. Still, the accuracy of the final absolute DCSs, beside experimental challenges, also depends on the used reference cross section dataset. For the present case of Ar, we have used the elastic DCSs published by Williams and Willis[36] which is an independently obtained dataset covering the whole energy range of interest (50–300 eV), thus allowing one to have a consistent set of reference cross sections for all incident energies. In the lower energy range up to 100 eV, there exist several published independently measured elastic DCSs for Ar,[36,45,46] which are not always in a very good agreement,

unfortunately. As an illustration, the inset in Fig. 2 shows the ratio of absolute DCSs for elastic electron scattering from Ar published by different authors to that used in the present work as the reference set,[36] as a function of the incident electron energy and at the two scattering angles usually used in our relative flow measurements. It is important to note that, except for the DCS of Cho *et al.*[46] (at 50 eV, 40°), the discrepancy between the different sources strongly decreases with increasing incident energy and is not significant for the energy range of interest for the present work (above 50 eV). It can be also mentioned that the quite large disagreement between absolute DCSs for low energies at 40° might be due to a very steep angular dependence of the DCS for elastic electron/Ar scattering in this region,[32] so even for a very careful measurement a small angular shift could result in drastically different DCS values. Finally, considering the small shift on the absolute scale between the present and the previously published[13] absolute elastic DCS for furan at 50 eV, it could be partly a consequence of the used reference cross sections, especially that only one absolute point, at the scattering angle of 40°, was used for calibration in the present work at that energy. However, we do not expect that the present DCS at 50 eV is drastically shifted, which is also supported by the present SCARND calculations (note that integral elastic cross section calculated by using SCARND agrees very well with the previously measured result.[13]) Additionally, it should be also noted that our recently published experimental cross sections for the pyrimidine molecule,[9] obtained by the same procedure and with the same reference cross sections, practically overlap at 50 eV with the most recent experimental results by Palihawadana *et al.*[47]

The present measurements of elastic DCSs for furan were performed with an overall energy resolution of about 1 eV (full width at half maximum – FWHM of the elastic peak.[32]) Therefore, the rotationally and vibrationally inelastic processes in principle contribute to the present "elastic" DCSs, which could affect both their absolute value and shape, especially in the region around minima where the elastic cross section significantly decreases. A comparison between the SCAR and SCARND calculations (the latter accounting for the rotational excitations) shows absolutely negligible difference in the energy and angular range of the present experiment. However, neither the SCAR nor SCARND calculations account for the vibrational inelastic processes. It has been discussed previously that vibrational excitations should not affect significantly elastic DCSs in the present high-energy range.[6] Still, according to our knowledge, an explicit estimation of the absolute DCSs for vibrational excitation of similar molecules representing building blocks of large biopolymers, for the present incident energy range, has not been reported. Therefore, in the present paper, we have performed calculations based on the UFBA in order to explicitly obtain the ratio of the summed vibrational to elastic DCSs for the furan molecule, in the energy range from 50 eV to 300 eV. Furan belongs to a C_{2v} symmetry, therefore it has 21 non-degenerate vibrational modes and most of them are infrared active. The UFBA approximation should be valid enough for a good estimation of the vibrational DCSs in the present energy range (even though elastic DCSs were shown to be more reliable
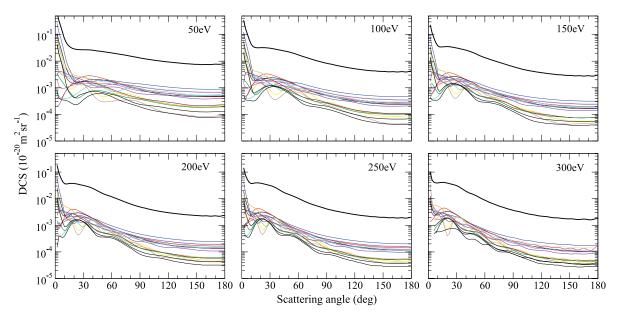
FIG. 3. Rotationally summed $0 \rightarrow 1$ vibrationally inelastic absolute differential cross sections for scattering of the electrons by furan molecules, calculated by UFBA method. All 21 excitation modes are plotted. Sum of all the vibrational excitation DCSs is displayed as a thick black curve.

only at small scattering angles), because the inelastic interaction is about two orders of magnitude weaker compared to the elastic (see the Sec. III B).

The calculated UFBA rotationally summed $0 \rightarrow 1$ vibrationally inelastic differential cross sections for electron scattering from furan molecules are shown in Fig. 3. The ratio between the sum of the vibrationally inelastic and elastic theoretical DCSs calculated by the SCARND method are presented in Fig. 4. At low scattering angles (below 20°) the contribution of vibrational excitations to the elastic DCSs is clearly negligible, as expected, being of the order of 1% or

less. However, at higher scattering angles where the elastic DCSs attain small values, the contribution of the sum of vibrationally inelastic scattered electron current can increase to about 10%. The overall ratio does not depend strongly on the incident electron energy in the present range; however, in the high angular range the contribution of the vibrational DCSs increases with increasing incident energy, due to the decrease of the elastic DCSs for backward scattering (see Fig. 2). Finally, it is important to point out that even at energies and angles where the contribution of vibrationally inelastic processes is the most significant, it is still within the absolute
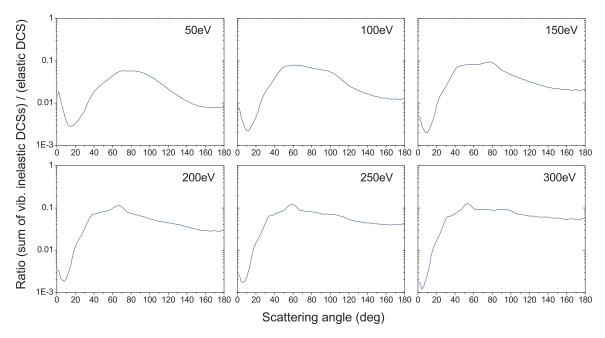

FIG. 4. Ratio between the sum of the vibrationally inelastic absolute differential cross sections (DCSs) calculated by using UFBA method (shown in Fig. 3) and the elastic DCSs calculated by using SCARND (shown in Fig. 2).
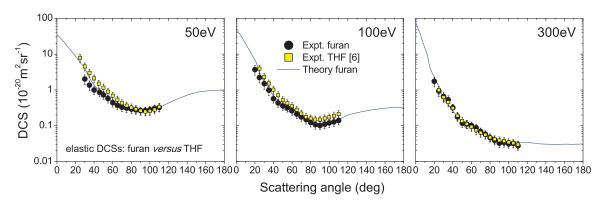
FIG. 5. Angular dependence of the absolute differential cross sections for elastic electron scattering from furan and tetrahydrofuran (THF) molecules at the incident energies of 50, 100, and 300 eV. The experimental results are presented by circles (furan) and squares (THF).[6] The furan theoretical results are presented by the solid line.

uncertainty of the present experimental absolute elastic DCSs, which was estimated to about 25% (see Sec. II). Therefore, the low-energy resolution experimental mode (see Ref. 32 for more details), which has been applied for the present incident energy range to measure elastic DCSs for furan, does not affect the reliability of the obtained results due to non-resolved vibrational processes. Also, an uncertainty of about 10% on the elastic DCSs is good enough to apply those data in the Monte Carlo simulations used to estimate energy deposition in the medium upon high-energy radiation.[48] Nevertheless, the present study reveals that, although the contribution of vibrationally inelastic processes strongly decreases with increasing incident energy at small scattering angles, as usually assumed, this contribution could increase to even above 10% at high scattering angles where the elastic DCSs attain small values. Therefore, it cannot be considered negligible if a highly precise study is needed.

In Fig. 5, the absolute elastic DCSs for furan are compared with our previously published results for THF (Ref. 6) at selected incident electron energies of 50, 100, and 300 eV. Although furan and THF are chemically distinct, they are structurally similar with the difference being in only four H atoms. Therefore, in the frame of the independent atom model approximation at high incident electron energies, the elastic DCSs for these two molecules should be very similar. Indeed, one could see that the experimental results confirm very similar DCS shapes. Both for furan and THF, the angular dependence of the DCSs show a broad minimum at around 90° at lower energies (50 eV and 100 eV), which disappears at higher energies (300 eV). The DCSs are also very close in value on the absolute scale. However, it is interesting to note that while the two sets of results for the different molecules literally overlap at the highest incident energy of 300 eV, there is a small discrepancy at lower energies. At 100 eV, the DCS of THF is slightly (but still within the experimental errors) shifted upwards on the absolute scale and the discrepancy is even more pronounced at 50 eV in the low angular range. A trivial explanation for this difference could be an experimental influence, since actually the absolute DCSs for THF have been obtained according to relative flow measurements at lower energies (see Ref. 6 for more details). Nevertheless, this effect can be also partly due to very

different permanent dipole moments of furan and THF (0.71 D and 1.75 D, respectively, see Sec. I). Consequently, even though the elastic DCSs are practically identical at high incident electron energies, the high permanent dipole moment of THF can more affect the electron scattering process at lower incident energies and scattering angles (see Ref. 23 and references therein). Furthermore, the significantly higher dipole moment of THF should result in more intensive rotationally inelastic processes, which cannot be resolved in the experiment, so this inelastic contribution can shift the DCS for THF upwards on the absolute scale.

The energy dependence of both ICSs and TCSs for electron collisions with furan molecules is presented in Fig. 6. The present TCS and ICS, calculated by using the SCARND method, are also tabulated in Table II, for the incident electron energy range from 10 to 10 000 eV. It is important to note a very good agreement of the present calculated results with recently published other experimentally obtained total
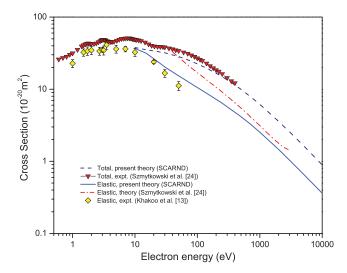

FIG. 6. Total cross sections (TCSs) and integral elastic cross sections (ICSs) for electron scattering from furan molecules. Full line: present ICS calculated by the SCARND method; dashed line: present TCS calculated by the SCARND method; diamonds: experimental ICS reported by Khakoo *et al.*;[13] triangles: experimental TCS reported by Szmytkowski *et al.*;[24] dashed-dotted line: theoretical results by Szmytkowski *et al.*[24]

TABLE II. Theoretical integral elastic and total cross sections for electron scattering from furan in units of 10^{-20} m^2, as a function of incident electron energy (E_0), calculated by using the SCARND method.

E_0 (eV)	Elastic	Total
10	36.68	37.80
15	31.64	35.28
20	26.54	33.88
30	20.38	31.92
40	17.33	29.96
50	15.32	28.28
70	12.77	25.56
75	12.29	24.98
100	10.56	22.48
150	8.484	19.01
200	7.252	16.60
250	6.384	14.87
300	5.712	13.44
400	4.788	11.40
500	4.144	9.940
700	3.304	7.952
1000	2.537	6.160
2000	1.462	3.584
3000	1.039	2.562
5000	0.6664	1.655
10 000	0.3612	0.8932

and integral elastic cross sections,[13,24] thus confirming the reliability of the used theoretical method. The present theoretical TCS fits almost perfectly the experimental points reported by Szmytkowski *et al.*[24] at higher electron energies, down to about 150 eV, while it is slightly below the experiment at lower energies. It should be noted that the SCAR calculations (not presented here), which do not account for the rotational excitations, produce a TCS that is somewhat lower on the absolute scale. Also, the present elastic ICS agrees very well with the experimental points reported by Khakoo *et al.*,[13] practically within the experimental errors, except for the last point at 50 eV which is somewhat lower on the absolute scale. Note that previously measured[13] DCS at 50 eV also appears to be somewhat below the present experimental DCS, which was discussed above in this section. The theoretical elastic ICS by Szmytkowski *et al.*[24] is relatively close to the present SCARND curve at higher energies (above about 500 eV), but generally overestimates the elastic ICS for furan, especially in the lower energy range. Both the elastic ICS and TCS for electron interaction with furan strongly decrease in the energy range above 10 eV. For example, from 10 eV (ICS = 36.68 × 10^{-20} m^2) to 10 000 eV (ICS = 0.36 × 10^{-20} m^2) the elastic ICS collapses by about two orders of magnitude.

V. CONCLUSION

The scattering of electrons from gaseous furan molecule has been investigated, both experimentally and theoretically. The DCSs for elastic electron scattering were measured by using a crossed electron-target beams setup and the relative flow method to normalize relative DCSs to the absolute scale. The absolute DCSs for elastic electron scattering by furan were calculated by using several theoretical approaches and compared to the experimental results. The SCARND calculations show an excellent agreement with the experiment, both in shape and on the absolute scale, as it was also reported previously for other molecular targets. Additionally, the SCARND method was used to calculate total and elastic integral cross sections for electron interaction with furan, which were tabulated in the range from 10 eV to 10 000 eV. Moreover, we also presented the theoretical elastic DCSs calculated on the basis of a simpler UFBA. The agreement of UFBA calculations with the experiment is good for the scattering angles smaller than about 60°, therefore, the present work shows that fully *ab initio* UFBA model can be used for a rather reasonable estimation of the absolute DCSs for elastic electron scattering from the furan in the present incident energy range and for smaller scattering angles. The present absolute elastic DCSs for the furan molecule are also compared with the previously published elastic DCSs for the THF molecule,[6] which are structurally very similar. The elastic DCSs for those two molecules basically overlap at 300 eV but some discrepancy is seen at lower energies, which might be partly due to their very different permanent dipole moments.

In the present work, we also used the first Born approximation to estimate the contribution of vibrationally inelastic DCSs for electron scattering from furan, since neither experimental measurement can resolve this contribution nor SCARND calculations account for these inelastic processes. The ratio of the sum of the vibrational to the elastic DCSs is presented as a function of the scattering angle at several fixed incident electron energies, showing the vibrationally inelastic contribution to be of the order of 1% at low scattering angles but increasing to even about 10% in the higher angular range.

The present both experimental and theoretical study on electron interaction with furan, as well as comparison with the results for the similar THF molecule, is important for a fundamental understanding of electron interaction with the furanose molecular systems and the results contribute to a fundamental understanding of electron interaction with biomolecules in the medium incident electron energy range. Moreover, the present results bring an extension to the existing absolute dataset for the furan molecule published in the lower energy range[13,24] and also complete up our previous work concerning the study on electron scattering from the molecules representing structural units of biological macromolecules work.[6–11] Finally, the present vibrational, elastic, and integral absolute cross sections for the furan can be important as starting parameters in Monte Carlo simulations used to model radiation damage.

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