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Abstract: Differential cross sections (DCSs) for elastic scattering of electrons from alanine, have been measured using a crossed beam system for incident energies between 20 eV and 80 eV and scattering angles from  $10^{\circ}$  to  $150^{\circ}$ . The experimental data were placed upon an absolute scale by normalisation to calculated absolute integral cross sections obtained using the corrected independent atom method incorporating an improved quasifree absorption model. The calculated data-set includes DCSs and integral elastic and inelastic cross sections in the incident energy range between 1 eV and 10000 eV. These theoretical results are found to agree very well with the experimental data both in the shape and magnitude of DCSs except at the smallest scattering angles.

Dear Editor,

Please find attached the manuscript of our original scientific paper with the title:

**Elastic scattering of electrons from alanine**

By: B.P. Marinkovic, F. Blanco, D. Sevic, V. Pejcev, G. Garcia, D.M. Filipovic, D. Pavlovic, N. J. Mason

To be considered for publishing in Professor Eugen Illenberger Honour issue of IJMS.

Sincerely yours,

Bratislav Marinkovic

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All remarks and questions put by referees were accepted and treated adequately. We are indebted to the referees for their comments and suggestions that improved a quality of the paper.

The general quality of the figures was checked. Also the picture of alanine molecules was included in the manuscript. References were improved. The figure captions were made clearer. The Tables were checked and only at one point it was found the mismatch with the error value presented in Figure (this was value at 60 eV and 150 deg.). The error value in Table 1 was corrected.

The relation between the inelastic cross section shown in previous Figure 2 and now Figure 3 and the absorption potential contribution  $V_a(r)$  to the electron-atom interaction approximate optical potential was more clearly stated.

We defined more explicitly few physical quantities: the  $f_i(\theta)$  function of formula (4) & (6), and the dispersion functions evoked in the 2<sup>nd</sup> § of the page 5.

We discussed the dependence of the IAM approximation (p4) on the type of bond and on  $\pi$  delocalization of electrons.

In the experimental part we have explained the procedure used for the calibration of the electron energy scale.

We compared the absolute elastic cross sections of alanine to those of smaller organic systems such as THF and THFA.

# Elastic scattering of electrons from alanine

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## Abstract

Differential cross sections (DCSs) for elastic scattering of electrons from alanine, have been measured using a crossed beam system for incident energies between 20 eV and 80 eV and scattering angles from 10° to 150°. The experimental data were placed upon an absolute scale by normalisation to calculated absolute integral cross sections obtained using the corrected independent atom method incorporating an improved quasifree absorption model. The calculated data-set includes DCSs and integral elastic and inelastic cross sections in the incident energy range between 1 eV and 10000 eV. These theoretical results are found to agree very well with the experimental data both in the shape and magnitude of DCSs except at the smallest scattering angles.

*Key words:* elastic electron scattering, cross sections

*PACS:* 34.80.Bm Elastic scattering of electrons by atoms and molecules, 34.10.+x General theories and models of atomic and molecular collisions and interactions

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## 1 Introduction

The investigation of electron interactions with molecules that represent the main constituents of proteins has been motivated in recent years by a need to understand the processes that lead to radiation damage of a living cell. It is

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believed that processes driven by low-energy secondary electrons, which are produced in large quantities along the track of a primary high-energy particle, are of particular importance in a direct DNA damage [1,2]. Recently a large amount of experimental and theoretical work on electron interactions with DNA (or RNA) components, namely the bases (adenine, guanine, thymine, cytosine, uracil) and the backbone sugar deoxyribose (or analogue molecules: tetrahydrofuran (THF), tetrahydrofurfuryl alcohol (THFA) and 3-hydroxytetrahydrofuran (3hTHF)), has been reported, a comprehensive review of which can be found in the recent paper by Leon Sanche [3]. We have recently published elastic cross sections for THF [4] and THFA [5] and now wish to extend these to alanine. Alanine belongs to the simplest  $\alpha$ -amino acids and is often considered as a model system for properties of more complex systems. Its chemical formula is  $\text{HO}_2\text{CCH}(\text{NH}_2)\text{CH}_3$ . The  $\alpha$ -carbon atom of alanine is bound with a methyl group (see Figure 1). Dissociative electron attachment to gas phase alanine has been studied by Alfatooni et al. [6], Ptasińska et al [7] and Vasil'ev et al [8]. However, to our knowledge, no experimental results concerning electron scattering (neither elastic nor inelastic) with gaseous alanine molecules have been published other than our results [9,10].

In the present paper, we report both theoretical and experimental elastic electron scattering cross sections for alanine. Absolute normalized DCSs are obtained over an incident energy range between 20 eV and 80 eV and over an angular range from  $10^\circ$  to  $150^\circ$ . Calculated DCSs and integral elastic and inelastic cross sections are based on the independent atom method (IAM) [11] using an improved quasifree absorption model potential, which includes relativistic and many-body effects, as well as non ionizing inelastic processes [12]. These theoretical results are found to agree very well with the experimental data.

## 2 Experiment

A detailed description of the experimental apparatus and a discussion of the measurement procedure for obtaining DCSs as a function of either scattering angle or incident electron energy has been reported recently [13].

Briefly, the apparatus used in this experiment, ESMA, is an electron spectrometer using hemispherical energy selectors as both the monochromator and analyzer. A molecular beam of alanine was formed by heating a powder sample (DL-alanine, Märk, 99% purity) in an oven with the nozzle of aspect ratio  $\gamma = 0.1$  at a temperature of 460 K. In order to avoid any decomposition of the sample the product effusive molecular beam was produced at the lowest possible temperature. No decomposition of the sample molecule was ob-

served in the energy-loss spectra, this is in accord with recent investigations on the relationship between chemical structure of amino acids and their thermal decomposition [15]. The molecular beam was crossed perpendicularly by the monoenergetic electron beam. The electron energy scale was calibrated against the  $3s3p\ ^1P_1$  excitation threshold of Mg at 4.346 eV using the same procedure explained in [14]. To the best of our knowledge absolute measurements of total, ionization, elastic integral or differential cross sections of alanine have not been reported before. Therefore our measured experimental data was normalized using the present theoretical data. This theoretical method has been shown to give reliable absolute integral cross sections (ICSs) and DCSs for elastic scattering of electrons from different polyatomic molecules, at medium incident electron energies and higher scattering angles above  $20^\circ$ .

The experimental results were therefore placed on an absolute scale using absolute theoretical ICS. Absolute experimental DCSs were then derived “backwards” after scaling the experimental ICS. Such scaling is easy to accomplish, because the shape of relative ICS is similar to the theoretically calculated ICS.

Errors in the relative DCSs measured as a function of scattering angle include statistical errors (0.1%-3%) evaluated according to Poisson’s distribution and short-term stability errors (1%-5%), arising from measured discrepancies in repeated measurements at the same incident energy and scattering angle. The errors due to uncertainties in the incident electron energy (3%) and true zero position function (0.5%) must also be taken into account. The final error must also include the uncertainty of the theoretical ICS value used for calibration to the absolute scale including errors arising from the DCS extrapolation towards forward and backward scattering angles and numerical integration, these are estimated at some (20%), the largest error in the present experiment.

### 3 Theoretical method

The present calculations of the electron molecular cross sections are based on a corrected form of the independent-atom method (IAM), known as the SCAR (Screen Corrected Additivity Rule) procedure. All the details for this procedure have been extensively described in previous works [12,16] where it has been applied to many other molecular species, so only a brief summary will be given here.

In the standard IAM approximation the electron-molecule collision is 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. At low energies, where atomic cross sections are not small compared to the 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 no longer negligible. These corrections have been shown to be important in many molecular systems [12,16–19].

It has been shown [12] that the energy range for which deviations from the IAM approximation are relevant depends on the size of the molecule: 10% or larger screening corrections take place for N<sub>2</sub> and CO up to 200 eV, for CO<sub>2</sub> up to 300 eV, and for benzene up to 600 eV.

While the detailed considerations leading to the SCAR expressions are somewhat involved, the final results are relatively simple. In the first place, for integrated (elastic or inelastic) cross sections, the usual additivity rule (AR) expressions are replaced by modified ones:

$$\sigma^{elast} = \sum_i s_i \sigma_i^{elast} \quad \text{and} \quad \sigma^{inelast} = \sum_i s_i \sigma_i^{inelast} . \quad (1)$$

Here we introduced screening coefficients ( $0 \leq s_i \leq 1$ ) reduce the contribution from each atom to the total cross section. Calculation of  $s_i$  coefficients requires only data on the position and the total cross section  $\sigma_i$  of each atom in the molecule. The explicit expressions for  $s_i$  are [12,16]:

$$\begin{aligned} \varepsilon_i^{(1)} &= 1, \\ \varepsilon_i^{(k)} &= \frac{N - k + 1}{N - 1} \sum_{j(\neq i)} \sigma_j \varepsilon_j^{(k-1)} / \alpha_{ij} \quad (k = 2, \dots, N), \end{aligned} \quad (2)$$

$$s_i = 1 - \varepsilon_i^{(2)}/2! + \varepsilon_i^{(3)}/3! - \varepsilon_i^{(4)}/4! + \dots \pm \varepsilon_i^{(N)}/N! . \quad (3)$$

Where  $N$  stands for the number of atoms in the molecule, the  $j$  index in sums  $\sum_{j(\neq i)}$  runs over all the  $N$  atoms except the  $i$  one,  $\alpha_{ij} = \max(4\pi r_{ij}^2, \sigma_i, \sigma_j)$ , and  $r_{ij}$  is the distance between centers of atoms  $i$  and  $j$ . The successive auxiliary  $\varepsilon_i^{(k)}$  contributions arise from overlapping  $k$ -atoms and so only  $\varepsilon_i^{(2)}$  exists for diatomics.

Secondly, for the elastic differential cross section, instead of the standard form

$$\frac{d\sigma^{elast}}{d\Omega} = \sum_{i,j} f_i(\theta) f_j^*(\theta) \frac{\sin qr_{ij}}{qr_{ij}} , \quad (4)$$

(where, as usual,  $q = 2K \sin \theta/2$  is the momentum transfer and  $f_i(\theta)$  is the scattering amplitude for  $i^{th}$  atom) now we have [16]

$$\begin{aligned} \frac{d\sigma^{elast}}{d\Omega} \cong & (1 - X_S) \frac{\sigma^{elast} - \sigma_D}{4\pi} + \\ & + [1 + X_S \left( \frac{\sigma^{elast}}{\sigma_D} - 1 \right)] \frac{d\sigma_D}{d\Omega} , \end{aligned} \quad (5)$$

where  $\sigma_D$ ,  $d\sigma_D/d\Omega$  and  $X_S$  are defined by:

$$\begin{aligned} \sigma_D &= \sum_i s_i^2 \sigma_i^{elast} , \\ \frac{d\sigma_D}{d\Omega} &= \sum_{ij} s_i s_j f_i(\theta) f_j^*(\theta) \frac{\sin qr_{ij}}{qr_{ij}} , \end{aligned} \quad (6)$$

$$X_S \approx \int_0^{45^\circ} \frac{d\sigma_D}{d\Omega} \sin \theta d\theta / \int_0^{180^\circ} \frac{d\sigma_D}{d\Omega} \sin \theta d\theta . \quad (7)$$

Expressions (5-7) result in [16] after an analysis of the angular distribution including redispersion processes inside the molecule, and after some estimation on the relevance of these contributions.

It must be noted that only atomic spatial coordinates are necessary for the calculation, with no consideration of the molecular symmetry or bond type, so the procedure can be easily applied to arbitrary species. Once the atomic cross sections and scattering amplitudes are known, the corrected molecular quantities are directly derived from the equations (1-3) and (5-7). Screening corrections become significant only at low energies, resulting in a reduction of total values and a smoothing of maxima and minima in differential cross sections.

The procedure used for calculation of the corresponding atomic cross sections has been extensively described elsewhere [20–22], so only a brief comment will be given here. For our purposes the electron-atom interaction is represented by the approximate *ab initio* optical potential  $V_{opt}(r) = V_s(r) + V_e(r) + V_p(r) + iV^a(r)$ . Here  $V_s(r)$  is the static potential calculated by using the charge density deduced from Hartree-Fock atomic wave functions including relativistic corrections,  $V_e(r)$  is the exchange potential for which the semiclassical energy-dependent formula derived by Riley and Truhlar [23] is used,  $V_p(r)$  represents the target polarization potential in the form given by Zhang et al. [24], and finally the absorption potential  $V^a(r)$  accounting for inelastic processes is based on the revised quasifree model [25].

For each atom the corresponding radial scattering equation was numerically integrated, and the resulting complex partial wave phase shifts  $\delta_l$  were used to obtain the atomic scattering amplitudes and total cross sections [20–22]. In particular, the data used here for C, H, O and N atoms are exactly the

same as those used in references [12,25]. For each atom the total cross section resulting from the optical theorem includes inelastic contributions arising from the  $iV^a(r)$  imaginary potential, while total elastic cross section is obtained by integrating the differential elastic values. Total inelastic cross sections are the difference between total and integrated elastic values.

While it is difficult to estimate the accuracy of the calculated differential cross sections, errors are not expected to be larger than 25% in the 50-500 eV energy range for  $30^\circ$  to  $120^\circ$  angles. This is supported by the observed agreement of this kind of calculation with experimental results for molecules of similar size to alanine. ( $\text{CF}_4$  and  $\text{C}_3\text{F}_8$  in [16], or benzene,  $\text{C}_6\text{F}_6$  and  $\text{C}_4\text{H}_8\text{O}$  tetrahydrofuran in [26]).

## 4 Results and discussion

Absolute experimental DCSs as a function of the scattering angle have been obtained in  $10^\circ$  steps up to  $150^\circ$  and from  $30^\circ$  for 20 eV,  $20^\circ$  for 40 and 60 eV and  $10^\circ$  for 80 eV incident electron energies. At low energies DCSs cross section could not be measured at small scattering angles due to the influence of the primary electron beam. These relative angular dependences were converted to relative DCSs by introducing effective path-length correction factors. These correction factors account for the effective volume changes and were determined using the paper by Brinkmann and Trajmar [27] for effusive molecular beams using large total scattering cross sections, the present aspect ratio of the nozzle and with cone-defining apertures that ensured that no vignetting occurred. Extrapolation of experimental points toward zero scattering angle was made using the calculated angular dependences, but with gradually diminishing calculated DCS values according to the observed deviation from angles smaller than  $40^\circ$ .

Our results are presented in Table 1 and DCSs presented at selected incident energies in Figure 2. In general our theoretical results agree very well with the experiment in the shape of the DCS for all the measured energies. However, some deviations between calculated DCSs and experiment occur for scattering angles smaller than  $40^\circ$  although these become less pronounced as impact energy increases.

In Table 2 and Figure 3 the present calculated integral elastic, inelastic and total cross sections for electron scattering from alanine are shown. It is interesting to compare the absolute elastic cross sections of alanine with those of other smaller organic systems such as tetrahydrofuran and tetrahydrofurfuryl alcohol. Recent measurements of elastic differential cross sections for THFA [5] molecule show that the cross sections are similar both in shape and ab-

solute value. The same holds for the comparison between cross sections for alanine and THF molecule. The absolute values at 20 eV impact energy are almost identical in the range of scattering angles between  $40^\circ$  and  $90^\circ$ , while for smaller and larger angles the DCSs for THF are larger than those for alanine for a factor of 2. At higher impact energies the DCSs for alanine are smaller than those for THF by a factor of 1.4 to 1.3 (at  $50^\circ$ ), while at the highest investigated energy of 80 eV and scattering angles from  $100^\circ$  to  $140^\circ$  the present cross sections are smaller by a factor of 1.65. This behaviour is expected since THF molecule forms a ring structure with larger geometrical cross section.

The strongly forward peaked calculated DCSs for alanine lead to an over-estimation of the integral cross sections if they are derived from integration formula:

$$\sigma^{elast} = 2\pi \int_0^\pi \frac{d\sigma}{d\Omega} \sin \theta d\theta . \quad (8)$$

Therefore the angular dependence at small scattering angles should be closely looked at in the future.

## 5 Conclusion

Elastic scattering of electrons from alanine has been investigated both experimentally and theoretically. The measurements were performed using a cross-beam experiment for incident electron energies between 20 eV to 80 eV and scattering angles from  $10^\circ$  to  $150^\circ$ . Absolute cross sections were derived by normalising to theoretical results. These calculations were based on a corrected form of the independent-atom method, known as the Screen Corrected Additivity Rule procedure, using an approximate *ab initio* model potential known as the quasifree absorption model, which is improved to correct for many-body effects and nonionization processes.

The shape of the present experimental DCSs for elastic scattering from alanine, is very well reproduced by the present calculations. Therefore, at least over the angular range from about  $40^\circ$  to  $150^\circ$ , the latter can be used for reasonable and fast estimation of the DCSs for elastic scattering of electrons by alanine.

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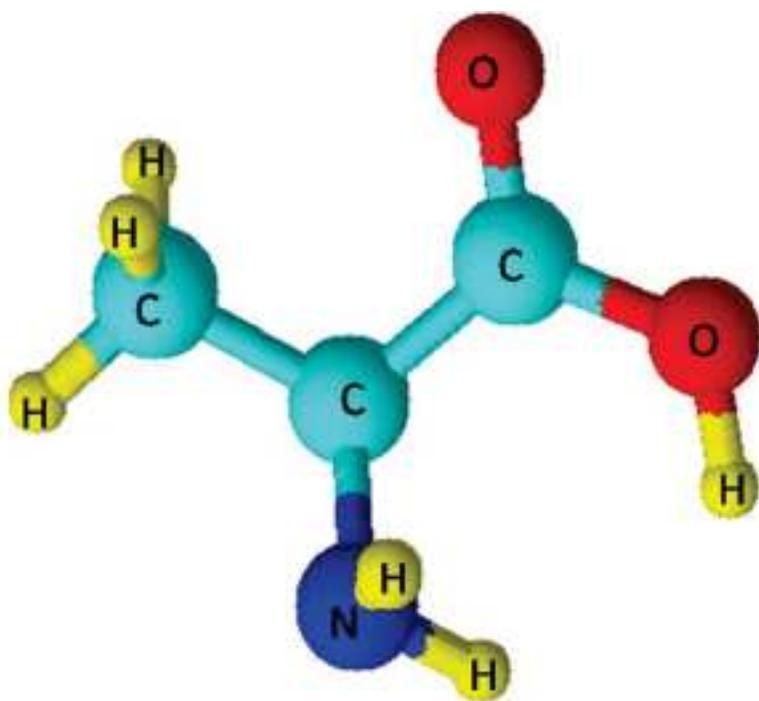


Fig. 1. Chemical structure of L-alanine

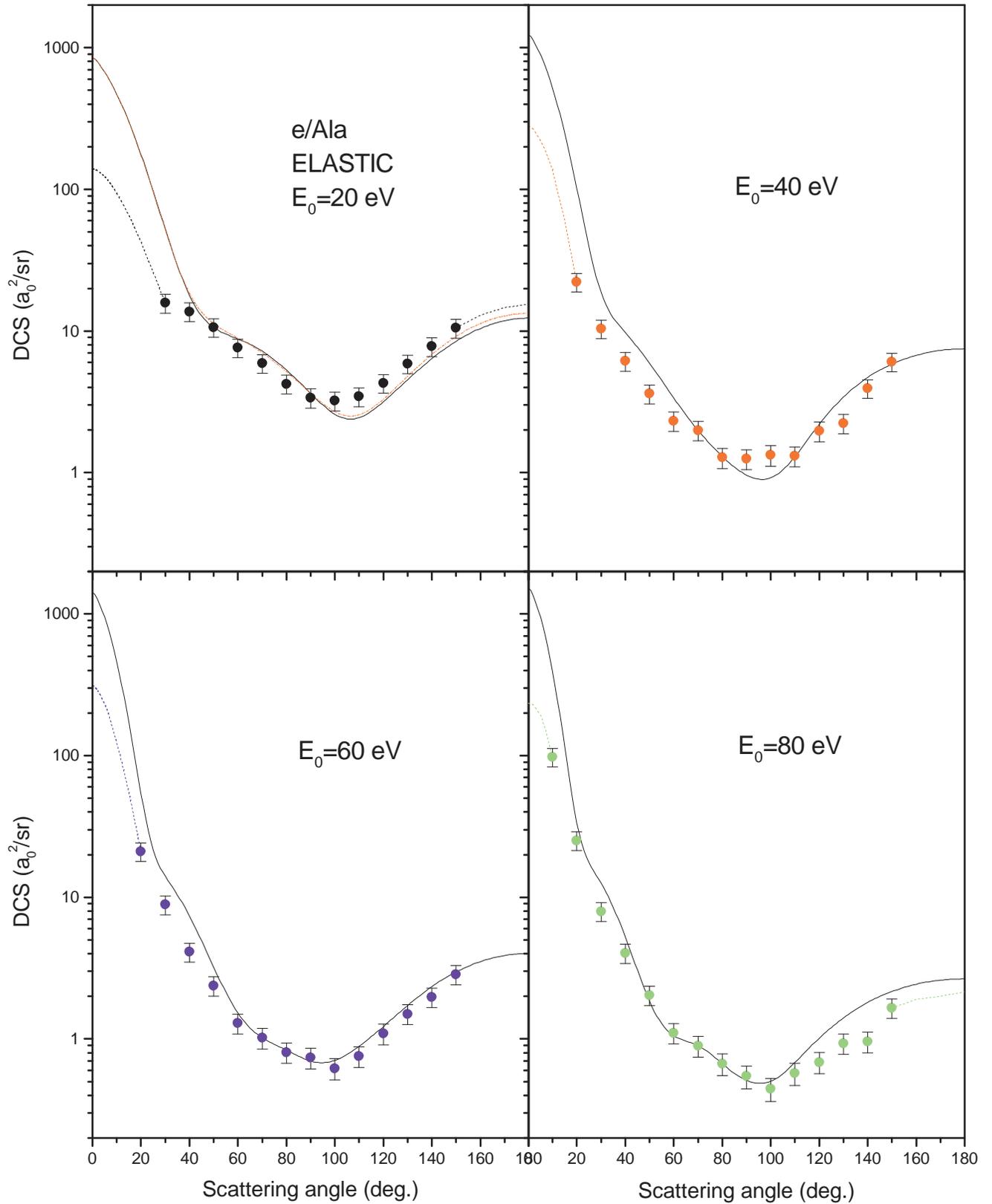


Fig. 2. Angular dependence of absolute DCSs for elastic electron scattering from alanine at different incident energies:  $\bullet$ , experiment;  $- -$ , extrapolated experiment;  $-$ , theory.

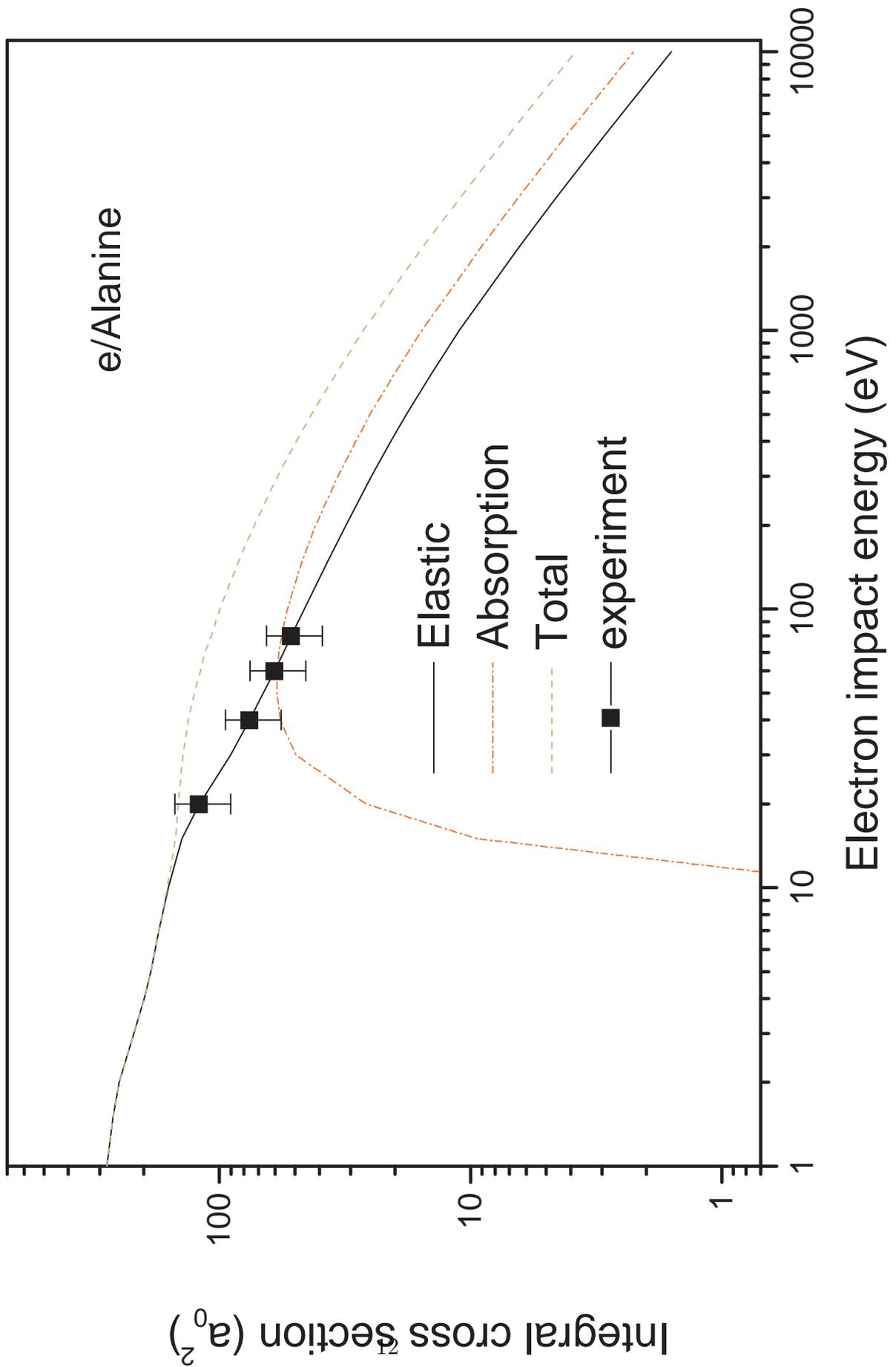


Fig. 3. Integral elastic cross sections (—■—, present experiment normalized to the

Table 1

Experimentally obtained differential cross sections for elastic electron scattering from alanine in units of  $a_0^2$  as a function of scattering angle ( $\theta$ ) and incident energy ( $E_0$ ). The absolute errors (statistical, short-term stability, uncertainty of  $\theta$  and  $E_0$ , uncertainty of incident electron beam and transmission function) in the last significant digits are given in parentheses.

$\Theta$ ( $^\circ$ )	$E_0$ (eV)			
	20	40	60	80
10	-	-	-	97.55 (14.93)
20	-	22.17 (3.40)	20.99 (3.22)	25.14 (3.85)
30	15.80 (2.42)	10.37 (1.60)	8.86 (1.37)	7.95 (1.23)
40	13.74 (2.11)	6.14 (0.95)	4.11 (0.64)	4.03 (0.63)
50	10.60 (1.63)	3.61 (0.57)	2.38 (0.38)	2.04 (0.33)
60	7.62 (1.17)	2.32 (0.37)	1.29 (0.21)	1.10 (0.19)
70	5.91 (0.91)	1.99 (0.32)	1.02 (0.17)	0.89 (0.15)
80	4.23 (0.66)	1.28 (0.21)	0.81 (0.14)	0.67 (0.12)
90	3.38 (0.53)	1.25 (0.21)	0.74 (0.12)	0.55 (0.10)
100	3.22 (0.50)	1.34 (0.22)	0.62 (0.11)	0.44 (0.08)
110	3.45 (0.54)	1.31 (0.22)	0.76 (0.13)	0.57 (0.10)
120	4.29 (0.66)	1.97 (0.32)	1.09 (0.18)	0.68 (0.12)
130	5.88 (0.91)	2.23 (0.36)	1.50 (0.24)	0.93 (0.16)
140	7.80 (1.20)	3.94 (0.62)	1.98 (0.31)	0.96 (0.16)
150	10.51 (1.61)	6.03 (0.93)	2.85 (0.44)	1.66 (0.27)

Table 2

Calculated integral elastic and inelastic and total cross sections for electron scattering from alanine in units of  $a_0^2$  as a function of incident energy ( $E_0$ ).

$E_0$ (eV)	Elastic	Absorption	Total
1	281	0	281
1.5	265	0	265
2	251	0	251
3	219	0	219
4	199	0	199
5	188	0	188
7	174	0	174
10	160	0.205	161
15	141	09.49	150
20	120	26	146
30	90.2	49.7	140
40	75.8	57.3	133
50	66.8	59.1	126
60	60.4	59.1	119
70	55.6	58	114
80	51.8	56.5	108
100	45.9	53.6	99.6
150	36.9	46.7	83.6
200	31.4	41.4	72.8
300	24.8	33.8	58.7
400	20.8	28.7	49.5
500	18	25.1	43.1
700	14.3	20.1	34.4
1000	11.1	15.6	26.7
2000	6.41	9.07	15.5
3000	4.57	6.46	11
5000	2.94	4.16	7.09
10000	1.59	2.24	3.83