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Total Cross Section Measurements of Electrons Scattered by Nitrogen and Carbon Dioxide in the Energy Range 500-3000 eV

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Abstract The experimental total cross sections for electrons scattered by carbon dioxide and nitrogen molecules in the energy range 500-3000 eV were measured by the transmission technique and are reported in this paper. The apparatus, experimental techniques and possible sources of error are discussed in details. Comparison of the present experimental data with the results obtained through the addition of the integral elastic cross section and the calculated semi-empirical ionization cross section is made and shows a good agreement. These are the first reported measurements of this kind for electron beam energies above 1600 eV for nitrogen and above 600 eV for carbon dioxide.

1. INTRODUCTION

The goal of this paper is to present measurements of the total cross section (elastic plus inelastic collision) of electrons scattered by nitrogen and carbon dioxide in the energy range between 500 and 3000 eV.

It is well know that experimental results are useful for testing theoretical formalisms. The total cross sections for electron--atom scattering in the intermediate and high energy range are particularly important to test the validity of the forward dispersion relation for electron-atom scattering proposed by Gerjuoy and Kraall. These aspects are discussed in detail by Blaauw *et al*[1,2].

Experimental results are important also in solving problems concerning applications in areas such as plasma physics and astrophysics, where the results should lead to a better understanding of atmospheric phenomena such as auroral processes and the atmospheres of other planets.

Most of the results described in the literature have been obtained for low energy electrons (up to a few hundred electron-volts).

The results obtained up to 1971 have been discussed in the review article by Bederson and Kieffer[3]. For the nitrogen molecule, Blaauw *et al*[2,4], obtained results for the total cross section (TCS) in the energy range between 15 and 750 eV. Another group[5] extended the energy range to 1600 eV. The apparatus is described by Dalba *et al*[6]. The results reported in the present paper extended the energy range of the TCS of nitrogen up to 3000 eV. For the carbon dioxide molecule, despite the interest in cross section data to understand atmospheric processes, there are no TCS measurements above 500 eV, and the present results are the first reported total cross section in the energy range considered

Regarding the theoret-ical aspects, the differential elastic cross sections, DECS, for the electron-molecule scattering has been successfully treated in the intermediate energy range by the incoherent renormalized multicentre potential model (IRMPM)[7-10]. On the other hand, the total inelastic cross sections (TICS) has been studied systematically by Inokuti *et al*[11] and Bonham[12], using Bethe's theory[13,14].

In the following section we describe briefly the experimental set-up, the various sources and the estimated magnitude of the experimental errors. Some theoretical aspects of total cross section, the results obtained and a discussion are also included.

2. EXPERIMENTAL

The electron scattering apparatus is housed in a single vacuum chamber pumped with a 6" oil diffusion pump with a liquid nitrogen trap. The ultimate pressure inside the apparatus[15,16] is around 5×10^{-6} torr.

In order to measure the total cross section the technique of the electron transmission through gases was used. An electron gun produces a stable beam of energy between 20 and 3000 eV. The primary electron beam current is measured by an electrometer and is approximately 10 nA over most of the energy range. The current becomes stable after three hours of operation. When the energy is changed, the electron gun is re-adjusted to give a maximum current.

To avoid deviations of the electron beam trajectory, a Helmholtz coil reduces the magnetic fields inside the chamber to less than 10 mGauss. The equipment is made of aluminium alloy and brass to avoid stray magnetic fields.

The collision chamber is a cylinder 80 mm in length and the entrance and exit apertures are both 0,8 mm in diameter. The acceptance angle is 0.57 degrees at the electron detector. The electron beam is collected in a Faraday cup after the exit slit.

The pressure in the collision chamber is measured by a Shulz--Phelps type sensor. The Shulz-Phelps gauge is calibrated against a capacitance manometer. The calibration measurements are made with the pressure between 0.015 and 0.07 torr. A plot of the values of the pressure read through the capacitance manometer measurements versus the values given by the Schulz-Phelps gauge results in a straight line.

When the primary electron beam is stable, the gas is introduced in the collision chamber and the transmitted current and pressure are measured. The total cross section is related with the measured quantities as:

$$I = I_0 \exp(-N\sigma \ell) \quad (1)$$

where σ is the total cross section, I is the transmitted current, N is the number density of particles (atoms or molecules) in the scattering volume, which is related to the pressure and ℓ is the length of the scattering chamber. I_0 is the primary electron beam current and since it is constant, the plot of log I against pressure (in torr) allows us to obtain the total cross section from the gradient of the straight line times a constant factor. Assuming the ideal gas behaviour, this constant factor is $-T/7730$, where T is the temperature in the absolute scale.

3. SOURCES OF ERROR

In this section we will discuss various systematic and random statistical errors. However, the sistematic error introduced by the undiscrimination between the transmitted and scattered electrons at small angles is discussed separately in the section of the results.

The main sources of the experimental error are:

a) primary electron beam fluctuation. To minimize this, the electron gun is turned on three hours before starting the data acquisition. In our experiments the maximum fluctuation is around 2%;

b) pressure reading. For each measurement, the pressure inside the scattering chamber is kept stable and therefore the error contribution is due to the pressure reading. A digital multimeter connected to the pressure meter allows readings within a maximum accuracy of 0.5%;

c) temperature. The temperature reading is taken in two places, at the gas inlet tubulation and near the exit aperture of the collision chamber. For both cases the readings were always the same as the ambient temperature. For the various sets of experiments the temperature varies between 22^{o} to $28^{o}C$, nevertheless to obtain the total cross section in eq. (1), the value is assumed to be $25^{O}C$.

The combined standard deviation of the errors is estimated by the following expression:

$$\overline{d\sigma} = (\overline{d\sigma^2})^{1/2} = \left| \left(\sum_{i=1}^{M} \frac{\partial\sigma}{\partial\rho_i} \Delta\rho_i \right)^2 \right|^{1/2} \qquad (2)$$

where ρ_i and $\Delta\rho_i$ are the experimental parameters and the stanclard deviations respectively. The derivative $\partial\sigma/\partial\rho_i$ is analitically calculated by equation (1). The error in the total cross section is approximately 4.2%.

An additional error of 1.5% in the total cross section (TCS) has been estimated due to other sources of random errors such as the fluctuation on the primary beam energy, spurious magnetic field and delocalized gases. Therefore an overall estimated standard deviation is approximateiy 6%.

4. THEORY

The total cross section is defined as a sum of integralelastic cross section (IECS) and the total inelastic cross section (TICS). The IECS is obtained by integrating the differential elastic cross section (DECS) over all the scattering angles. The DECS values used are the calculated results by Lee and Freitas for electron-linear molecule scatteringusing the renormalizedmulti-centrepotential model[7,10]. The agreement verified between these theoretical values of DECS and experiment, for nitrogen[9,10] and carbon dioxide[17], is in general, within the experimental uncertainties.

The differential inelastic cross section is given by:

$$\frac{d\sigma^2}{d\Omega dE} = \left(\frac{d\sigma}{d\Omega}\right)_R f(E,K) \frac{k_n K^2}{kE} \tag{3}$$

where $d\sigma^2/(d\Omega dE)$ is the cross section relative to the energy loss E and observation solid angle R. The factor $f(E,K)$ is the generalized oscillator strength, k is the incident electron momentum, k_n is the scattered electron momentum and K is the inelastic momentum transfer. $(d\sigma/d\Omega)_R$ is the Rutherford cross section and in atomic units it is written as $4/K^4$,

$$K = (k^2 + k_n^2 - 2kk_n \cos\theta)^{1/2} \tag{4}$$

where θ is the scattering angle. Using Bethe theory[13], it is possible to write the TICS[11,12] as:

$$\sigma_{in}(k^2) = \frac{4\pi Z^2}{k^2} \left| M_{tot}^2 \log(4k^2\ C_{tot}) + \frac{\gamma_{tot}}{k^2} + \dots \right| \tag{5}$$

where Z is the atomic number. Inokuti et al[11] have calculated the quantities M_{tot}, C_{tot} and γ_{tot} for severa1 atoms and there are no calculations for the molecules under study. However, it is verified that experimental ionization cross sections have been determined by Rieke and Prepejkal[18] for energies above 0.1 MeV. These experimental values can be fitted to an expression similar to eq. (5) :

$$\sigma_{in} = 1.874 \times 10^{-20}\ (cm^2)\ C \left| \left(\frac{M^2}{C}\right) (\beta^2 \log|(\beta^2/(1-\beta^2)|-1) + \beta^{-2} \right| \tag{6}$$

where β is the incident electron velocity divided by the velocity of light. Consequently, the semi-empirical parameters M and C can be obtained for N_2 and CO_2 and they are respectively, $M^2=3.74$ and $C=34.84$; $M^2=5.75$ and $C=57.91$.

Although the experimental values of the total ionization cross sections used in the fitting procedure were obtained for energies above 0.1 MeV, in this work eq. (6) with the given semi-empirical parameters is extended to the energy range of our interest in order to estimate σ_{in}. Besides, since the TICS is the sum of the ionization cross section and discrete excitation cross sections, the value obtained from eq. (6) is incomplete.

In the next section the values obtained by this procedure will be compared to the experimental data.

5. RESULTS AND DISCUSSION

For nitrogen and carbon dioxide molecules, the total cross sections have been reported using both, time-of-flight technique and electron transmission method. In general. the results obtained through the time-of-flight technique agree with the results of the transmission technique.

In the intermediate energy range there are results, for nitrogen, measured by Blaauw *et al*[1,2] at energies up to 750 eV, Dalba *et al*[6] up to 1600 eV and by Hoffman *et al*[19] up to 700 eV, using the transmission technique. For carbon dioxide, there are the experimental results reported by Kwan *et al*[20] up to 500 eV.

Table 1 shows our experimental dataof total cross section (TCS) for e^--nitrogen and e^--carbon dioxide interaction in comparison with the results of other authors. In the same table we also show the integral elastic cross section (IECS) for both gases. In figure 1 the experimental values of the TCS are displayed in comparison with thesemi -empirical values of TCS obtained through the addition of the IECS with σ_{in} calculated with eq. (6).

One notes that our experimental values of the total cross section for nitrogen between 500 and 1100 eV agree within 6% with the results obtained by Dalba *et al*[6]. Over 1100 eV the discrepancies are larger and Dalba's results lie always above. At 500 eV the sum of the theoretical integral elastic cross section (IECS) of Jain *et al*[10] and the σ_{in} value obtained using eq. (6) is 15% lower than the present results and also lower than other experimental values. At 800 eV the theoretical cross section is 6% lower.

For carbon dioxide, at 500 eV the present result agrses with the experimental result of Kwan *et al*[20]. When compared with the integral elastic cross section (IECS) calculated by Botelho *et al*[21] plus σ_{in} from equation (6), the discrepancy is around 4% at 500 eV and rising to 17% at 1500 eV. Using the experimental integral elastic crosssection (IECS) of Iga *et al*[22] and σ_{in} (eq. (6)), excellent agreements with the results of the present work at 500, 800 and 1000 eV are verifisd.

Table 1 - Absolute values of the total cross section (TCS) and of integral elastic cross section (IECS) for electrons scattered by molecular nitrogen and carbon dioxide (in Å^2).

	N_2					CO_2			
	TCS				IECS	TCS		IECS	
E (eV)	Present work	Dalba *et al*[5]	Blaauw *et al*[2]	Hoffmann *et al*[19]	Jain *et al*[10]	Present work	Kwan *et al*[20]	Iga *et al*[22]	Botelho *et al*[21]
500	4.01	3.75	3.69	3.46	2.29	5.31	5.16	2.98	2.98
600	3.44	3.39	3.19	3.10		4.66			
700	2.97	2.98	2.77	2.83		4.19			
800	2.57	2.62			1.63	3.72		2.31	2.04
900	2.29	2.33				3.43			
1000	2.07	2.12				3.24		1.92	1.61
1100	1.86	1.99				3.06			
1200	1.72	1.85				2.87			
1300	1.55	1.72				2.66			
1400	1.43	1.61				2.51			
1500	1.31	1.51				2.36			1.06
1600	1.20	1.42				2.23			
1700	1.12					2.11			
1800	1.03					2.00			
1900	0.957					1.93			
2000	0.915					1.85			
2100	0.864					1.75			
2200	0.821					1.66			
2300	0.791					1.59			
2400	0.763					1.52			
2500	0.735					1.45			
2600	0.700					1.34			
2700	0.670					1.27			
2800	0.650					1.21			
2900	0.631					1.13			
3000	0.622					1.07			

The discrepancies between the values of the present work and the experimental data of Dalba et *al*[6] for nitrogen can be attributed to the aperture size used in the scattering chamber. The finite size of the apertures of the apparatus causes the absence of electron attenuation at small angles and consequently the decrement of the measured total cross section. Therefore experimentally, the total cross section is defined when the limiting angle of acceptance of the detector iszero.

The error caused by this factor has been studied in our previous paper[16] for electron-argon scattering. In that study we had verified that the forward scattering is energy dependent and contributes from 3 to 17% when the impact energies vary from 500 to 3000 eV. Assuming that the behaviour of nitrogen and carbon dioxide is closely the

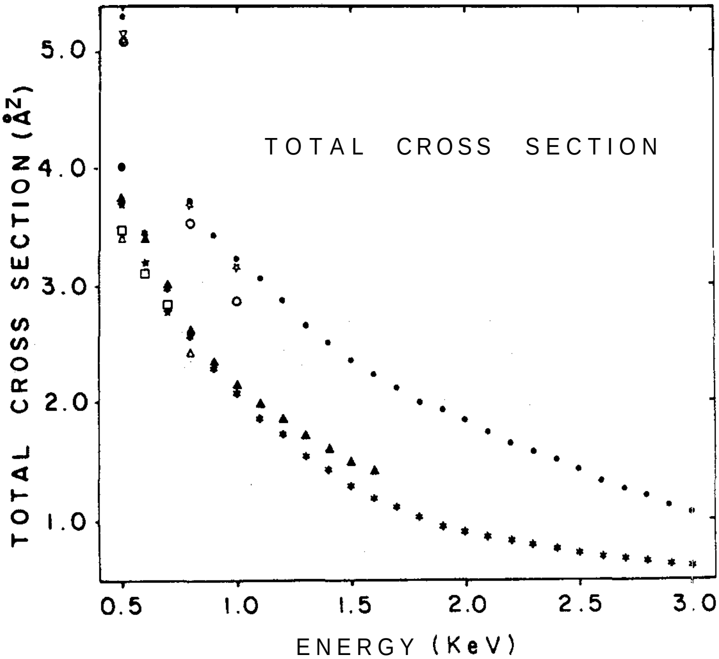

Fig. 1 - Absolute values of the total cross section for electrons scattered by molecular nitrogen: ✱ the present work; Δ Dalba *et al*[6]; ★ Blaauw *et al*[2]; □ Hoffman *et al*[19]; ▲ Jain *et al*[10] + σ_{in}. Carbon dioxide: ● the present work; ▽ Kwan *et al*[20]; ✡ Iga *et al*[22] + σ_{in} and O Botelho *et al*[21] + σ_{in}.

same as argon, the maximum contribution of this systematic error is estimated to be 17% for all energies, therefore the maximum overall experimental error becomes 23%.

At high energies the total elastic cross section can be obtained using the Born Approximation and can be written as[23]:

$$\sigma_{el} = \pi k^{-2} |A - Z^2 k^{-2} + \dots| \tag{7}$$

$$A = 8 \int_0^{\infty} (Z - F(s))^2 \, s^{-3} \, ds \tag{8}$$

where k is the incident electron momentum and s is the magnitude of the momentum transfer vector, Z is the atomic number and $F(s)$ is the atomic X-ray form factor. Adding equation (5) to equation (7) and neglecting terms $O(k^{-4})$, the total cross section can be written as:

$$k^2 \sigma_{tot} = A \log k^2 + B \qquad (9)$$

The graph of $k^2 \sigma_{tot}$ versus $\log k^2$ with our experimental values is a straight line and a least square fit gives $A=-48.655$ and $B = 799.48$ for nitrogen, and $A = 110.38$ and $B = 227.82$ for carbon dioxide, where k^2 is in Å^{-2} and σ_{tot} in Å^2.

6. CONCLUSION

In this paper experimental measurements of the total cross section of electrons scattered by molecular nitrogen and carbon díoxide are presented for energies from 500-3000 eV. For energies above 1600 for N_2 and above 600 for CO_2 the values of TCS are reported by the first time to our knowledge.

There is a systematic error arising from the finite angular resolution and this error is quoted to be 17% for all impact energies and the maximum overall experimental error is 23%. Since the effect due to the forward scattering is energy dependent and increases with the increment of the energy, the above quoted errors might be overestimated at the lower impact energies.

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Resumo

Foram medidas as Secções de Choque Total (SCT) para o espalhamento de elétrons de energias entre 500 a 3000 eV transmitidos através de nitrogênio e dióxido de carbono. É descrito o aparelho utilizado na obtenção dos resultados experimentais, a técnica utilizada e possíveis fontes de erros. Os dados experimentais da Secção de Choque Total são comparados com resultados teóricos obtidos a partir da soma da secção de choque diferencial elástica integrada aos valores semi-empíricos da secção de choque total de ionização e com valores experimentais da SCT disponíveis. Para o nitrogênio, acima de 1600 eV e para o dióxido de carbono, acima de 500 eV. estes são os primeiros resultados reportados na literatura.