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Correlation of the total cross section for electron scattering by molecules with 10–22 electrons, and some molecular parameters at intermediate energies

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Abstract

Accurate experimental values of the total cross section (σ_T) for electron scattering by molecules (CH_4 , NH_3 , N_2 , CO and CO_2) in the energy range 0.5 to 5 keV have been analysed to obtain correlations with molecular properties. A formula for σ_T , as a function of the number of target electrons and molecular polarizabilities, has been deduced. This empirical expression reproduces to within 6% our experimental results for the abovementioned molecules and has been used to obtain results for other molecular targets with 10 to 22 electrons. Total cross sections show reasonable agreement with the experimental and theoretical data for this energy range. © 1997 Published by Elsevier Science B.V.

1. Introduction

Total cross section values for electron–molecule interactions (σ_T) are needed in many scientific and technological applications (astrophysics, atmosphere physics, nuclear fusion, etc.). For this reason, the number of related works published in recent years has increased, especially for electron energies above 500 eV, where experimental and theoretical data are scarce. Accurate measurements in this energy range require good angular and energy resolution to avoid effects due to forward scattered electrons. From the theoretical point of view, the variety of open channels at these energies demands the use of approaches based on complex optical potentials, giving results which could be strongly dependent on the potential chosen (see Ref. [1]).

The energy range considered in this work has a special interest in the search for systematic relations

between total cross sections and other molecular properties. Previous studies show that the molecular parameters involved seem to be the number of target electrons, the polarizability and the dipole moment [2,3]. However, the discrepancies in the available σ_T values have not allowed a clear relationship with these parameters to be defined. Our recent measurements [4–7] have yielded accurate σ_T values for electron–molecule scattering (CH_4 , NH_3 , N_2 , CO and CO_2) in the energy range from 0.5 to 5 keV due, among other things, to the good scattering geometry used. In addition, the influence of forward electron scattering for our experimental conditions has been checked by means of a Monte Carlo electron transport simulation [6] and found to be less than 0.5%, even at 5 keV. Moreover, Joshipura and Vinodkumar [8] have deduced from calculations [8,9] an energy dependence of the total cross sections which shows excellent agreement with that observed in our experi-

ments. These considerations have prompted the present work.

In this work, an analytical formula has been deduced to obtain total cross sections for electron scattering by molecules, in the energy range from 0.5 to 5 keV, as a function of the number of target electrons and the molecular polarizabilities. This formula reproduces our experimental results for CH₄, NH₃, N₂, CO and CO₂ to a good approximation and has been used to calculate σ_T values for other molecules, whose electron number ranges from 10 to 22. These results have been compared with experimental [10–13] and theoretical [1,2,8,9,14] data in the literature.

2. Procedure

The energy dependence of the total cross sections observed in our experiments [4–7] for electron-molecule scattering at energies ranging from 0.5 to 5 keV agrees with that calculated by Joshipura and Vinodkumar [8], who give the expression:

$$\frac{\sigma_T}{a_0^2} = A \left[\frac{E_0}{\text{keV}} \right]^{-B}, \quad (1)$$

where E_0 is the electron energy in keV, A and B are parameters which depend on the molecular properties of the targets and a_0 is the Bohr radius. Table 1 shows the values of these parameters obtained by fitting our experimental results [4–7] to Eq. (1). As may be seen in this Table, the ' B ' parameter takes a similar value for all the studied molecules. The average value of this parameter is 0.78 ± 0.02 , with a standard deviation which is not significant within the experimental errors. For this reason we have assumed this mean value for all the studied molecules, with an uncertainty of about 3%. How-

Table 1

Values of the parameters of Eq. (1), deduced from the experimental results of Refs. [4–7] when the energy is given in keV and σ_T in units of a_0^2

Parameter	CH ₄	NH ₃	N ₂	CO	CO ₂
A	6.57	5.99	7.63	7.67	11.2
B	0.778	0.777	0.819	0.758	0.777

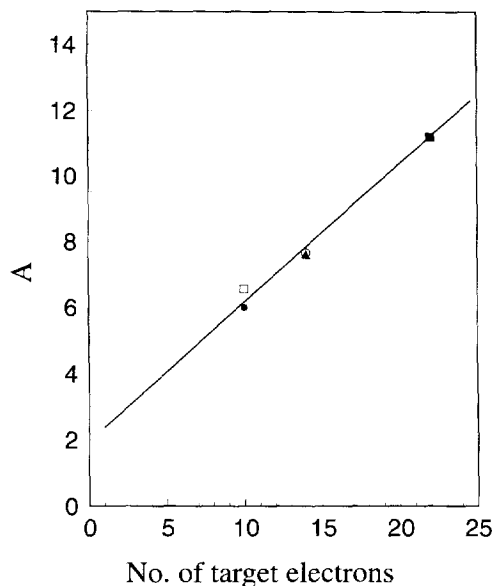


Fig. 1. Value of the A parameter of Eq. (1) as a function of the number of target electrons for: (●) NH₃, (□) CH₄, (▲) N₂, (○) CO and (■) CO₂.

ever, the ' A ' parameter is clearly different for each molecule, showing a quasi linear dependence with the number of target electrons (Z). In Fig. 1 the

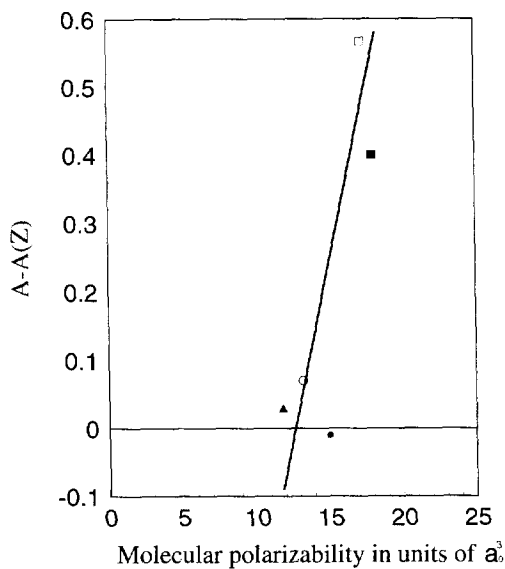


Fig. 2. Difference between the A parameter of Eq. (1) and that fitted by Eq. (2) ($A(Z)$) as a function of target polarizabilities for: (●) NH₃, (□) CH₄, (▲) N₂, (○) CO and (■) CO₂.

Table 2

Total cross sections in units of a_0^2 for electron scattering from molecules with Z ranging from 10 to 22 at 1 keV impact energy

Target	Z	α (a_0^3)	this work	Experimental		Theoretical		
				Refs.[4–7]	Refs.[10–13]	Refs.[8,9]	Ref.[14]	Refs.[1,2]
HF	10	5.6	5.26					4.63
H ₂ O	10	9.8	5.68		5.07	5.09		5.75
NH ₃	10	15.0	6.20	5.84	5.75	6.04		7.11
CH ₄	10	17.3	6.43	6.60	6.36	6.74	6.31	5.27
N ₂	14	11.8	7.48	7.49	7.33	7.21		8.44
CO	14	13.2	7.62	7.71	7.35	7.89		8.74
HCN	14	17	8.0					10.6
C ₂ H ₂	14	24	8.70					9.72
O ₂	16	10.7	8.17			7.93		9.88
H ₂ CO	16	17	8.80					
C ₂ H ₄	16	28	9.90				8.92	
HCl	18	18	9.70					11.5
CH ₃ F	18	18	9.70					
H ₂ S	18	25	10.4		10.0		7.85	8.59
CH ₃ OH	18	22	10.1					
CH ₃ NH ₂	18	27	10.6					
C ₂ H ₆	18	30	10.9					
CO ₂	22	18	11.3	11.3		11.9		15.0
N ₂ O	22	20	11.5			11.2		

values of the 'A' parameter are plotted against Z . As may be seen in this figure the points can be reasonably well fitted by a straight line. Thus, to a first approximation, we can represent the 'A' value by the following linear expression:

$$A(Z) = 0.40Z + 2. \quad (2)$$

By introducing these values of 'A' and 'B' in Eq. (1), the following expression of σ_T as a function of 'Z' can be obtained:

$$\frac{\sigma_T(Z)}{a_0^2} = (0.40Z + 2) \left[\frac{E_0}{\text{keV}} \right]^{-0.78}. \quad (3)$$

This formula reproduces our experimental values to within 10%. However, the accuracy of this approximation can be improved by taking into account the deviations of each 'A' value from the ones calculated by Eq. (2), for a given Z . In Fig. 2 we have plotted the differences ($A - A(Z)$) for the molecular targets studied in this work. As this figure shows, deviations from Eq. (2) can be fitted by the following straight line, as a function of the static molecular polarizability α in units of a_0^3 :

$$A - A(Z) = 0.1 \frac{\alpha}{a_0^3} - 1.3. \quad (4)$$

By combining this result with Eq. (2), the total cross sections can be represented as a function of Z and α by the empirical expression:

$$\frac{\sigma_T(Z, \alpha)}{a_0^2} = \left(0.40Z + 0.1 \frac{\alpha}{a_0^3} + 0.7 \right) \left[\frac{E_0}{\text{keV}} \right]^{-0.78}. \quad (5)$$

3. Results

As an example of the applicability of Eq. (5), Table 2 lists the total cross sections for electron scattering, obtained with this formula, for several molecules with Z ranging from 10 to 22 at 1 keV electron impact energy. The molecular polarizabilities used in these calculations were taken from Ref. [15]. As may be seen in this Table, the values obtained agree, to within 7%, with all the available experimental results [4–7,10–13] at this energy, except for H₂O which is about 12% higher. Theoretical data of Refs. [1,2], calculated from molecular optical potentials, are not consistent with the present values nor with the experimental ones, showing discrepancies of between 10 and 25%. However, the values

of Refs. [8] and [9], obtained by applying sum rules to atomic calculations with optical potentials agree to within 5% with those of the present work, except for H_2O (discrepancy about 11%). Similar calculations in Ref. [14] also show general agreement except for the H_2S molecule, whose calculated value is about 20% lower than the present value and the experimental one.

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