

Electron–methyl halides scattering. Total cross section measurements for methyl chloride and methyl fluoride

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Abstract. Electron transmission experiments have been carried out in CH_3F and CH_3Cl in the energy range between 0.3 and 250 eV. Absolute values for total cross sections are presented and compared with the available data of other groups. The present cross sections are found to be in good agreement with other experiments for CH_3F in the overlapping range of energies but deviate significantly from prior results in the case of CH_3Cl . Our present measurements, together with previous ones for CH_3Br and CH_3I , confirm the correlation between static electric dipole polarizability of investigated targets and total cross sections at intermediate energies.

1. Introduction

The interaction of electrons with methyl halides has been studied since the beginning of the thirties, when the first electron scattering experiments for these molecules—total cross section measurements—were done by Schmieder (1930) for CH_3F , and Holst and Holtmark (1931) for the CH_3Cl molecule.

For the CH_3Cl molecule, electron scattering processes have been the most intensively investigated at thermal energies. The application of many different experimental techniques was accompanied by marked discrepancies in the magnitude of the measured electron attachment rate constant and, consequently, of electron attachment cross section. Lee (1963), Blaunstein and Christophorou (1968), and recently Datskos *et al* (1990) applied swarm techniques, Wenworth *et al* (1968) used pulse sampling, Bansal and Fessenden (1972) employed microwave conductivity, Christodoulides *et al* (1975) and Schultes *et al* (1975) used the electron cyclotron resonance technique, and recently Kligler *et al* (1982) applied electron beam-controlled discharge.

Negative ion formation in resonance electron attachment to CH_3Cl has been studied experimentally by Dorman (1966), Scheunemann *et al* (1980), Chu and Burrow (1990), and Pearl and Burrow (1993) using the beam technique and by Petrović *et al* (1988), who employed a pulsed Townsend experiment. Some theoretical calculations were done by Fabrikant (1991, 1994).

Considerably less attention was paid to the investigation of the vibrational excitation of CH_3Cl molecules in collisions with electrons. The only experiment was performed by Shi *et al* (1992), while calculations connected with this phenomenon were carried out by Fabrikant (1991, 1994) and Gallup (1993).

Otwös and Stevenson (1956), Beran and Kevan (1969), and Deutsch and Schmidt (1984) investigated the total ionization cross section. Molecular orientation-dependent positive ion formation processes at 700 eV have recently been studied by Kasai *et al* (1993).

Many authors (Spence 1977, Hitchcock and Brion 1978a, b, Burrow *et al* 1982, Falcetta and Jordan 1990, Wan *et al* 1991, Guerra *et al* 1991, Shi *et al* 1992) have analysed electron transmission and/or inner-shell electron energy-loss spectra. Spence (1977) was looking for Feshbach resonances using the transmission technique.

Relatively less research of electron scattering deals with the CH_3F molecule. Investigations of the total ionization cross section were performed by Beran and Kevan (1969) (experimentally) and Deutsch and Schmidt (1984) (semi-empirically). Griffiths and Harris (1988) measured single- and double-ionization energies. Harshbarger *et al* (1972, 1973) studied Rydberg states using electron energy-loss spectroscopy and similar investigations were performed by Hitchcock and Brion (1978a) for inner-shell excitation. The electron transmission spectra at low energies have been studied both experimentally and theoretically by Modelli *et al* (1992).

Experimental absolute electron-scattering total cross sections for CH_3Cl (Holst and Holtsmark 1931, Benitez *et al* 1988, and Wan *et al* 1991) as well as for CH_3F (Schmieder 1930, and Benitez *et al* 1988) have hitherto been published for low energies only. Preliminary measurements in CH_3Cl for intermediate and high energies have just been performed by Karwasz (1994).

The work reported here is concerned with absolute total cross section measurements for electron scattering on CH_3F and CH_3Cl at low and intermediate impact energies. It is a continuation of earlier research involving methyl halides (CH_3I : Szmytkowski and Krzysztofowicz 1993 and CH_3Br : Krzysztofowicz and Szmytkowski 1994).

2. Experimental

In the reported experiment a linear transmission technique has been applied. For detailed discussion of this technique the reader is referred to Bederson and Kieffer (1971). In the present experiments we have used the same apparatus as in our previous total cross section measurements (e.g. Szmytkowski *et al* 1992, Szmytkowski and Krzysztofowicz 1993, and Krzysztofowicz and Szmytkowski 1994), with minor improvements. A schematic diagram of the spectrometer employed is presented in figure 1. A thoriated tungsten hairpin filament (F) is used as the electron source. The electrostatic electron optics consists of an electron

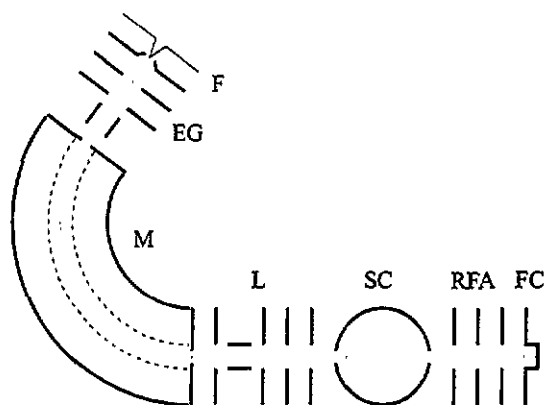


Figure 1. Schematic diagram of apparatus: F—filament, EG—electron gun, M—monochromator, L—system of focusing and deflecting electron lenses, SC—scattering cell, RFA—retarding field analyser and FC—Faraday cup.

gun (EG), a 127° electrostatic cylindrical deflector (M) producing a quasimonoenergetic beam of electrons ($\Delta E = 70$ meV, FWHM), a system of deflecting plates and electron zoom lenses (L), a field-free scattering cell (SC), and a retarding field analyser (RFA) followed by a Faraday cup (FC) collecting electrons at the end of their path. All parts of the electron optics are made of copper and surfaces exposed to electrons are coated with colloidal graphite. Helmholtz coils are applied to reduce external permanent magnetic fields in the electron optics region to a value lower than 1×10^{-7} T.

A beam of energy-selected electrons irradiates the investigated gas sample in the scattering chamber. Attenuation of intensity of the electron beam passing through the scattering volume is measured to derive the total cross section with the Bouguer-de Beer-Lambert law:

$$\sigma(E) = \frac{k\sqrt{T_i T_m}}{pL} \ln [I_0(E)/I_p(E)] \quad (1)$$

where E is electron impact energy, $I_0(E)$ and $I_p(E)$ are electron beam intensities in the absence and in the presence of the gas under study in the scattering cell, respectively. L is the length of the scattering volume, p is pressure of the investigated gas measured with a Baratron, $T_m = 322$ K is the temperature of the manometer head, T_i is temperature of the target gas, usually lower than T_m by some 9–14°; k is the Boltzmann constant. Equation (1) takes into consideration the thermal transpiration effect (Knudsen 1910).

Measurements at given energy were carried out in 2–12 series typically consisting of 10–20 single runs. It was established that the total cross sections obtained in different series at the same energy were independent, within the limits of statistical uncertainties, of applied sample pressures and electron beam intensities (≤ 10 pA). The final values of the total cross section at particular energies are weighted means of the average from different series of individual runs.

The energy calibration procedure was performed with reference to the oscillatory resonance structure in N_2 near 2.3 eV, using a mixture of the gas sample under study and nitrogen. Accuracy of the energy scale was estimated to be ± 70 meV.

A significant source of serious experimental error in transmission experiments is the inability to fully discriminate between unscattered and forwardly scattered electrons which leave the interaction volume through the exit orifice. Incomplete discrimination systematically lowers the measured total cross sections. The error associated with this effect increases at higher impact energies and is usually higher for targets with a permanent electric dipole moment. It also depends on angular resolution of the detector system.

To reduce the fraction of scattered electrons, which do not contribute to the attenuation of the transmitted current, we used the retarding field analyser at the entrance of the Faraday cup. However, the analyser discriminates only the inelastically scattered electrons. As angular distributions of electrons elastically scattered on CH_3Cl and CH_3F molecules are unavailable, no direct correction of the measured cross section due to small-angle scattering in the present experiment is possible. For a rough estimation of the error related to this effect, the elastic data for the H_2O molecule (Danjo and Nishimura 1985, Katase *et al* 1986, Johnstone and Newell 1991), which has the same dipole moment as CH_3Cl and CH_3F , have been used. Calculations indicate that, for the applied geometry of the detector system (acceptance angle ~ 1 msr), the error introduced in the total cross section from forward scattering is less than 2% over the entire energy range considered here, for both of the molecules investigated (see table 1).

The direct sum of all systematic uncertainties was estimated to be 10% below 1 eV, gradually decreasing to 5% in the range 10–30 eV, and increasing again up to 7% at 200 eV.

Table 1. Effect of main experimental errors on the measured total cross section (in per cent).

Source of error	Energy (eV)				
	< 0.7	1.25	6.5	30	200
Statistical	< 1				
Systematic:					
Forward scattering	1	0.5	< 0.4	< 0.4	1.5
Electron energy	3	0.4	0.3	< 0.1	< 0.1
Beam intensity	2.5	2.5	2	1.5	2.5
Inhomogeneity of target			0.4		
Scattering path			0.6		
Temperature determining and thermal transpiration effect	0.3				
Pressure determining	2	2	2	1.5	1.5
Sum of systematic (max. error)	10	7	6	5	7

Statistical uncertainties (one standard deviation of the weighted mean values) are always lower than 1%. The main sources and estimated values of uncertainties are presented in table 1.

Commercially available CH_3Cl (Merck-Schuchardt) and CH_3F (Matheson Gas Products) were used without further purification. A mass spectrometric analysis of the gas in the cylinder showed the purity of these samples to be better than guaranteed, i.e. 99.5% for CH_3Cl and 99% for CH_3F .

3. Results

Total cross sections for electron scattering from CH_3Cl and CH_3F molecules have been measured in the energy range from slightly below 0.5 up to 250 eV. Our results are presented in numerical form in table 2.

3.1. CH_3Cl

Our electron-methyl chloride molecule absolute total cross section versus impact energy is plotted in figure 2 and compared with results available in the literature: the pioneering experiment of Holst and Holtsmark (1931) and the more recent low-energy data of Benitez *et al* (1988) and Wan *et al* (1991). With regard to the general shapes, the present total cross section and the data of Benitez *et al* (1988) and Wan *et al* (1991) are quite similar. Our results are significantly higher than those measured by other groups, especially in the region of the minimum, where the discrepancy reaches 30%. However, the apparent discrepancies do not exceed the combined experimental error of the experiments compared.

For the lowest energies applied the total cross section sharply decreases from almost $50 \times 10^{-20} \text{ m}^2$ at 0.4 eV to about $32 \times 10^{-20} \text{ m}^2$ at 1.5 eV. To complement the present data, it is worth noting that for energies lower than those applied in our investigation the total cross section still drastically increases and its value obtained by Christodoulides *et al* (1975) from their electron-cyclotron resonance experiment is as high as $1790 \times 10^{-20} \text{ m}^2$ at about 0.05 eV. Such behaviour of the total cross section in the low-energy region is characteristic for polar molecules and might be explained in terms of direct processes (Christophorou *et al* 1982).

Table 2. Absolute total cross sections (TCS) measured for electron impact of CH₃F and CH₃Cl molecules in units of 10⁻²⁰ m².

Energy (eV)	TCS		Energy (eV)	TCS	
	CH ₃ F	CH ₃ Cl		CH ₃ F	CH ₃ Cl
0.25		58.2	12	21.8	32.0
0.35	38.8	51.4	14	21.0	30.9
0.45	36.2	46.0	16	19.8	29.7
0.55	33.8	41.2	18	18.9	28.6
0.65	31.8	38.4	20	18.4	28.0
0.75	30.4	36.5	22	18.1	27.4
0.85	27.8	35.4	25	17.6	26.1
1.05	25.0	33.5	27	17.4	24.9
1.25	23.1	32.5	30	16.8	24.4
1.35		32.2	35	16.1	23.3
1.45	21.8	31.7	40	15.7	22.5
1.7	19.7	31.6	45	15.2	22.0
2.0	19.3	31.7	50	14.7	20.6
2.2	19.3	32.0	60	14.2	19.3
2.5	19.3	32.6	70	13.8	18.1
3.0	19.6	33.4	80	12.8	17.0
3.5	20.6	34.3	90	12.5	16.3
4.0	21.2	34.7	100	11.8	15.5
4.5	22.6	34.6	110	11.4	14.4
5.0	23.1	34.5	120	11.2	14.1
5.5	23.7	34.6	140	10.2	12.8
6.5	24.5	35.3	160	9.21	11.9
7.5	24.4	35.4	180	8.69	11.0
8.5	23.6	35.1	200	8.07	10.2
9.5	23.0	33.6	220	7.66	9.4
10.5	22.8	32.4	250	6.67	8.45

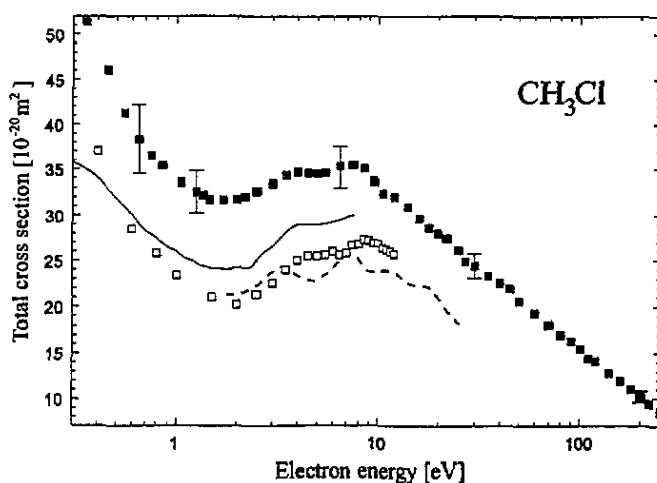


Figure 2. Absolute electron-CH₃Cl scattering total cross sections: (■) present; (---) Holst and Holtsmark (1931); (—) Benitez *et al* (1988); (□) Wan *et al* (1991). The error bars represent overall experimental uncertainties at selected energies.

In the dissociative electron attachment cross section some peaks are observed in the very low-energy range. However, authors disagree about the magnitude of the peaks, as well as their position at the energy scale. Chu and Burrow (1990) found two peaks: one close to 0 eV, with the magnitude of $8.5 \times 10^{-25} \text{ m}^2$ and the other at 0.8 eV with a magnitude of $2.1 \times 10^{-24} \text{ m}^2$. Petrović *et al* (1989), apart from the zero energy peak, found a $5 \times 10^{-24} \text{ m}^2$ peak at 0.18 eV. The observed discrepancies are most probably connected with contaminants which are difficult to remove.

All the results published so far show that the electron attachment processes for CH_3Cl have only a negligible contribution to the scattering process at the impact energies studied in this work.

In the higher energy range we can observe a shallow minimum of the total cross section around 1.5 eV and then its very slow increase. A wide weak maximum of $35 \times 10^{-20} \text{ m}^2$ is visible in the range 6–8 eV. On the low-energy side of the maximum there is a noticeable change in the slope of the total cross section energy dependence near 4 eV. A similar effect has been observed in earlier experiments.

Close to 3.45 eV, Burrow *et al* (1982) found a resonant feature in their derivative of transmitted current and assigned it to the lowest C–Cl σ^* orbital of a_1 -symmetry ($8a_1$, 2A_1). Some structure near 4 eV was also seen in the Benitez *et al* (1988) results. The resonance at 4 eV was analysed theoretically by Falcetta and Jordan (1990) and Guerra *et al* (1991). A controversy connected with the possible assignment of the e -symmetry state to that resonance (Wan *et al* 1991) has recently been resolved by Shi *et al* (1992) following their analysis of the electron impact vibrational excitation spectra for this state, in favour of the a_1 assignment. At the same time, a resonance of e -symmetry was localized near 5 eV. The presence of the 3.5 eV resonance of a_1 -symmetry has also been confirmed in the latest *R-matrix* calculations of Fabrikant (1994).

The other resonant effects, of the Feshbach type, were observed by Spence (1977) in the range of the total cross section maximum at 7.50, 8.96 and 9.65 eV. These very weak and sharp features could not be observed in our experiment. Resonances were also observed in dissociative attachment spectra as peaks near 3.3 and 7.4 eV by Chu and Burrow (1990).

Taking into account the higher impact energies, we can notice that, starting with the maximum, the total cross section decreases monotonically to the value of about $8 \times 10^{-20} \text{ m}^2$ at 250 eV. In this energy region the ionization phenomena play an increasingly important role in the electron scattering processes. The total ionization cross section at 75 eV, as measured earlier, constitutes from about one third (Otvös and Stevenson 1956) to about a half (Lampe *et al* 1957 and Beran and Kevan 1969) of the grand total cross section.

3.2. CH_3F

Figure 3 compares the present CH_3F absolute total cross section with the early results of Schmieder (1930) and with the more recent low-energy measurements of Benitez *et al* (1988). The results agree well within the limits of combined experimental uncertainties.

The shape of energy dependence of the $e^-/\text{CH}_3\text{F}$ total cross section is very similar to that for CH_3Cl . The cross section increases rapidly when energy decreases to very low values, has a wide, very shallow minimum of $19 \times 10^{-20} \text{ m}^2$ in the range of 1.8–3.5 eV, a maximum of $24 \times 10^{-20} \text{ m}^2$ around 5–8 eV, and decreases again beyond these energies.

A very broad feature around 6 eV can be seen in Benitez *et al* (1988) results, but it was not mentioned by the authors. It was observed by Modelli *et al* (1992) close to 5.3 eV and suggested to be of potential rather than resonant nature. Employing bound and continuum multiple scattering $X\alpha$ calculations they found no temporary anion state at such a

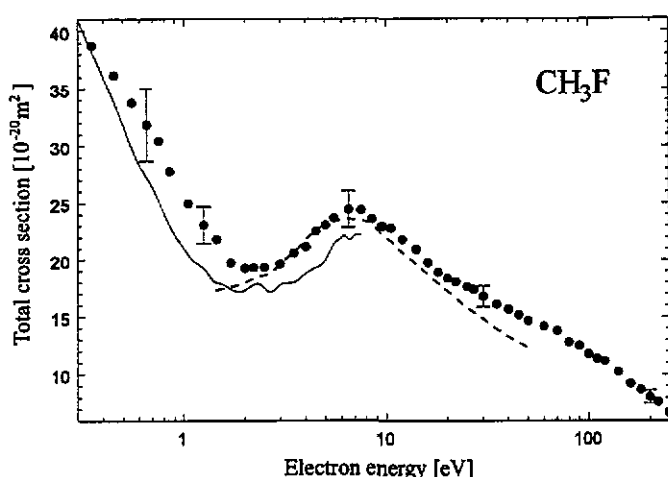


Figure 3. Absolute electron-CH₃F scattering total cross sections: (●) present; (---) Schmieder (1930); (—) Benitez *et al* (1988). The error bars correspond to overall experimental uncertainties estimated at some selected points.

low energy. In turn, the resonance about 10 eV predicted by calculations was not observed.

For CH₃F the total ionization cross section was investigated in more detail than that of CH₃Cl; it constitutes about 10% of the total cross section at 20 eV, about 25% at 30 eV, and almost 75% at 75 eV (Beran and Kevan 1969).

4. Summary and conclusion

In this paper we have reported our experimental data for the electron-CH₃F and CH₃Cl scattering. Present total cross sections are generally higher than other available measurements (CH₃Cl: Holst and Holtmark 1931, Benitez *et al* 1988, Wan *et al* 1991, CH₃F: Schmieder 1930, Benitez *et al* 1988). The difference is especially clear in the case of the CH₃Cl molecule. It is noteworthy that in the case of the latest measurements for CH₃I (Szmytkowski and Krzysztofowicz 1993) our results were lower than the data of Benitez *et al* (1988) while for CH₃Br (Krzysztofowicz and Szmytkowski 1994) results from both laboratories were nearly the same.

The apparent discrepancies may be due to considerable systematic errors of experiments from other laboratories. Results of Benitez *et al* (1988) and Wan *et al* (1991), having originated in the same laboratory, differ from each other by nearly 15%, and their overall errors are close to 40% at 0.5 eV, and about 30% above 1 eV. Moreover, the results from the twenties and thirties obtained with the Ramsauer technique are well known to be on average 25% lower than recent measurements for the same targets taken with other methods.

So great experimental uncertainties are mainly attributable to effects related to the use of external magnetic fields for guiding of the electron beam and the resulting serious difficulties in a correct assessment of the electron path in the scattering region, as well as insufficient discrimination of forwardly scattered electrons (Golden 1978). Discrepancies between experiments with and without a magnetic field similar to the above have already been observed for other targets in the energy range examined in this paper (cf Szmytkowski *et al* 1989, 1992). At the same time, there has been notable consistency among results obtained in various laboratories by the linear transmission method, i.e. without magnetic

field.

While comparing the results for methyl halides it can be seen that the total cross section functions are similar in shape but their magnitude decreases as follows: $\sigma(\text{CH}_3\text{I}) > \sigma(\text{CH}_3\text{Br}) > \sigma(\text{CH}_3\text{Cl}) > \sigma(\text{CH}_3\text{F})$. The character of the energy dependences of the total cross sections is typical for polar molecules. In general, cross sections decrease with the increase of impact energy. However, at about 7 eV all of them have a weak maximum which probably results from overlapping of many weak resonant effects and direct processes possible in this energy range (Lynch *et al* 1979). Taking into account the impact energies above 50 eV for CH_3X ($\text{X} = \text{F}, \text{Cl}, \text{Br}, \text{I}$) molecules, which are characterized by relatively

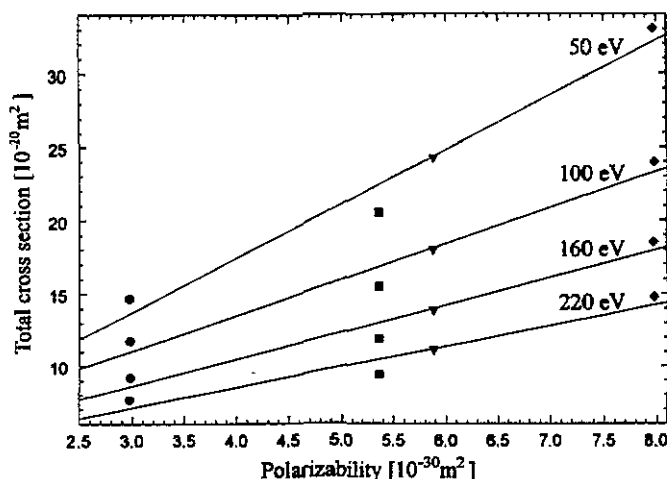


Figure 4. Our total cross sections versus electric dipole polarizability of target molecules (Miller 1993, 1994) at selected impact energies. (●) CH_3F , present; (■) CH_3Cl , present; (▼) CH_3Br , Krzysztofowicz and Szmytkowski (1994); (◆) CH_3I , Szmytkowski and Krzysztofowicz (1993). Regression lines have been traced for clarity.

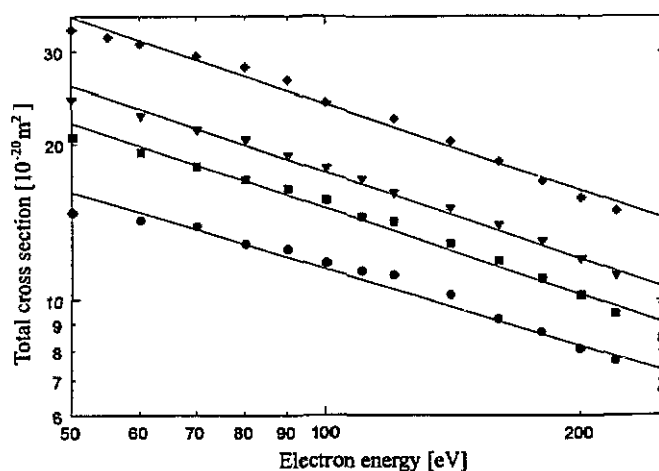


Figure 5. Energy dependence of total cross sections for CH_3X molecules. (●) CH_3F , present; (■) CH_3Cl , present; (▼) CH_3Br , Krzysztofowicz and Szmytkowski (1994); (◆) CH_3I , Szmytkowski and Krzysztofowicz (1993). Regression lines have been traced.

high and very similar permanent electric dipole moment ($\mu_{\text{CH}_3\text{F}} = 1.86$ D, $\mu_{\text{CH}_3\text{Cl}} = 1.82$ D, $\mu_{\text{CH}_3\text{Br}} = 1.89$ D, and $\mu_{\text{CH}_3\text{I}} = 1.62$ D, Lide 1993, 1994), we observe a strong correlation between the magnitude of the total cross section and the static electric dipole polarizability α of the target molecule (see figure 4). This dependence is nearly of the $\alpha^{0.5}$ -type and confirms previous observations (Szymkowski 1989). In the upper range of the studied energies the cross section versus energy dependence is similar for all investigated molecules and is of the $E^{-0.5}$ -type (see figure 5). Such behaviour of the cross section is analogous to the classical result for a pure asymptotic polarization potential (Vogt and Wannier 1954). It suggests that at intermediate energies the total cross section is, within a good approximation, proportional to the time the colliding electron spends in the vicinity of the molecule.

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References

- Bansal K M and Fessenden R W 1972 *Chem. Phys. Lett.* **15** 21–3
Bederson B and Kieffer L J 1971 *Rev. Mod. Phys.* **43** 601–40
Benitez A, Moore J H and Tossell J A 1988 *J. Chem. Phys.* **88** 6691–8
Beran A and Kevan L 1969 *J. Phys. Chem.* **73** 3866–76
Blaunstein R P and Christophorou L G 1968 *J. Chem. Phys.* **49** 1526–31
Burrow P D, Modelli A, Chiu N S and Jordan K D 1982 *J. Chem. Phys.* **77** 2699–701
Christodoulides A A, Schumacher R and Schindler R N 1975 *J. Phys. Chem.* **79** 1904–11
Christophorou L G and Christodoulides A A 1969 *J. Phys. B: At. Mol. Phys.* **2** 71–85
Christophorou L G, James D R and Pai R Y 1982 *Applied Atomic Collision Physics vol 3 Special topics* ed H S W Massey, E W McDaniell and B Bederson (New York: Academic) pp 87–167
Chu S C and Burrow P D 1990 *Chem. Phys. Lett.* **172** 17–22
Danjo A and Nishimura H 1985 *J. Phys. Soc. Japan* **54** 1224–7
Datskos P G, Christophorou L G and Carter J G 1990 *Chem. Phys. Lett.* **168** 324–9
Deutsch H and Schmidt M 1984 *Beitr. Plasmaphys.* **24** 475–86
Dorman F H 1966 *J. Chem. Phys.* **44** 3856–63
Fabrikant I I 1991 *J. Phys. B: At. Mol. Opt. Phys.* **24** 2213–25
—1994 *J. Phys. B: At. Mol. Opt. Phys.* **27** 4325–36
Falcetta M F and Jordan K D 1990 *J. Phys. Chem.* **94** 5666–9
Gallup G A 1993 *J. Phys. B: At. Mol. Opt. Phys.* **26** 759–74
Golden D E 1978 *Adv. At. Mol. Phys.* **14** 1–85
Griffiths W J and Harris F M 1978 *Int. J. Mass Spectrom. Ion Processes* **85** 69–79
Guerra M, Jones D, Distefano G, Scagnolari F and Modelli A 1991 *J. Chem. Phys.* **94** 484–90
Harshbarger W R, Robin M B and Lassette E N 1972, 1973 *J. Electron Spectrosc. Relat. Phenom.* **1** 319–32
Hitchcock A P and Brion C E 1978a *J. Electron Spectrosc. Relat. Phenom.* **13** 193–218
—1978b *J. Electron Spectrosc. Relat. Phenom.* **14** 417–41
Holst W and Holtsmark J 1931 *Det Kgl. Norske Videnskab. Selskabs* **4** 89–92
Johnstone W M and Newell W R 1991 *J. Phys. B: At. Mol. Opt. Phys.* **24** 3633–43
Karwasz G P 1994 Private communication
Kasai T, Matsunami T, Fukawa T, Ohoyama H and Kuwata K 1993 *Phys. Rev. Lett.* **70** 3864–7
Katase A, Ishibashi K, Matsumoto Y, Sakae T, Maezono S, Murakami E, Watanabe K and Maki H 1986 *J. Phys. B: At. Mol. Phys.* **19** 2715–34
Kligler D, Rozenberg Z and Rokni M 1982 *J. Chem. Phys.* **77** 3458–63
Krzysztofowicz A M and Szymkowski Cz 1994 *Chem. Phys. Lett.* **219** 86–90
Lampe F W, Franklin J L and Field F H 1957 *J. Am. Chem. Soc.* **79** 6129–32
Lee T G 1963 *J. Phys. Chem.* **67** 360–6
Lide D R 1993, 1994 *CRC Handbook of Chemistry and Physics* 74th edn (Boca Raton: CRC) p 9–42
Lynch M G, Dill D, Siegel J and Dehmer J L 1979 *J. Chem. Phys.* **71** 4249–54
Miller T M, 1993, 1994: *CRC Handbook of Chemistry and Physics* 74th edn (Boca Raton: CRC) p 10–199

- Modelli A, Scagnolari F, Distefano G, Jones D and Guerra M 1992 *J. Chem. Phys.* **96** 2061–70
- Otvös J W and Stevenson D P 1956 *J. Am. Chem. Soc.* **78** 546–51
- Pearl D M and Burrow P D 1993 *Chem. Phys. Lett.* **206** 483–7
- Petrović Z Lj, Wang W C and Lee L C 1989 *J. Chem. Phys.* **90** 3145–52
- Scheunemann H-U, Illenberger E and Baumgärtel H 1980 *Ber. Bunsenges. Phys. Chem.* **84** 580–5
- Schmieder F 1930 *Z. Elektrochem.* **36** 700–4
- Schultes E, Christodoulides A A and Schindler R N 1975 *Phys. Chem.* **8** 354–65
- Shi X, Stephen T M and Burrow P D 1992 *J. Chem. Phys.* **96** 4037–9
- Spence D 1977 *J. Chem. Phys.* **66** 669–74
- Szmytkowski Cz 1989 *Z. Phys.* **D 13** 69–73
- Szmytkowski Cz and Krzysztofowicz A M 1993 *Chem. Phys. Lett.* **209** 474–8
- Szmytkowski Cz, Krzysztofowicz A M, Janicki P and Rosenthal L 1992 *Chem. Phys. Lett.* **199** 191–7
- Szmytkowski Cz, Maciąg K, Karwasz G and Filipowicz D 1989 *J. Phys B: At. Mol. Phys.* **22** 525–30
- Vogt E and Wannier G H 1954 *Phys. Rev.* **95** 1190–8
- Wan H-X, Moore J H and Tossell J A 1991 *J. Chem. Phys.* **94** 1868–74
- Warman J M, Sennhauser E S and Armstrong D A 1979 *J. Chem. Phys.* **70** 995–9
- Wenworth W E, George R and Keith H 1968 *J. Chem. Phys.* **51** 1791–801