Total absolute cross section measurements for electron scattering on CS$_2$ molecules

Czesław Szmytkowski
Department of Physics, Technical University of Gdańsk, 80-952 Gdańsk, Poland

Received 7 July 1987

Abstract. The absolute total electron scattering cross section for CS$_2$ was measured from 0.4 to 80 eV using a linear transmission method. A minimum cross section ($17 \times 10^{-20}$ m$^2$) occurs near 0.8 eV followed by a very broad maximum ($53 \times 10^{-20}$ m$^2$) around 9 eV, with a monotonic decrease at higher energies. Comparison is made with existing experimental and theoretical integrated cross sections.


The results of absolute measurements of the total electron scattering cross sections for CS$_2$ are presented in this paper. The measurements were made with a linear transmission spectrometer (see, e.g., Szmytkowski et al 1984) and cover an energy range 0.4-80 eV. Preliminary results between 1 and 20 eV were reported by Szmytkowski (1983).

The experimental procedure is based on the relation between the attenuation of electron current and total cross section $\sigma(E)$. If the electron beam of primary intensity $I_0$ travels a distance $L$ in the homogeneous target of density $n$ particles per unit volume, then the output current $I_s$ is given by the Beer-Lambert relation

$$I_s(E) = I_0(E) \exp[-n\sigma(E)]$$

where $E$ is the electron energy.

In the present experiment the electron beam, before entering a 30.5 mm long scattering chamber was energy selected by a 127° electrostatic cylindrical deflector.
The electrons which left the scattering region through the exit orifice of the chamber were detected by a Faraday cup. The absolute electron energy scale was determined with an accuracy of ±80 meV in relation to the resonance structure in the transmitted electron current around 2.3 eV in molecular nitrogen. The number density $n$ of the target vapour was determined from the ideal gas law ($p = nkT$). The absolute pressure $p$ in the scattering volume was measured with a capacitance manometer and was in the range of 0.04-0.2 Pa, while the pressure outside the scattering cell was typically three orders of magnitude lower. The manometer head was kept at a temperature of $322 \pm 1$ K whilst the scattering cell temperature was sustained between 316 and 322 K. The gas pressure readings have been corrected for the thermal transpiration effect (Knudsen 1910). The target vapour was let alternately into the scattering cell and outer vacuum volume in such a way that the electron optics was exposed to the same partial pressure of the vapour in both modes of operation (with and without the target in the scattering cell).

The measurements were carried out at a given energy for a series of runs using a range of target pressures and different sets of electron-beam-controlling parameters. The final results are the weighted means of the mean cross sections obtained in different series of individual runs.

The statistical uncertainties (one standard deviation of weighted mean values) over the entire energy range were lower than 2%. The overall systematic error was calculated as the direct sum of all single contributions. This error is equal to 9% below 4 eV decreasing to 6% at higher energies.

Vapour of CS$_2$ was obtained from the liquid of Analar purity (a stated boiling point range of 319-319.5 K). It was used without further purification other than repeated freeze–pump–thaw cycles to remove dissolved gases.

The measured total cross section values (at selected energies) are presented in table 1 and compared with integrated elastic cross sections calculated by Lynch et al (1979) and experimental integrated normalised total (elastic+vibrational) cross sections of Sohn et al (1987) in figure 1. The agreement of the reported cross sections with the data of Sohn et al (1987) with respect to the shape is good but the results of Sohn et al are, on average, about 25% lower in magnitude. The disagreement is slightly outside the combined uncertainties of both experiments. The total cross sections of Sohn et al (1987) include integral normalised elastic and vibrational cross sections for excitation of fundamental modes only. At the same time their measurements show that the cross 

### Table 1. Total absolute cross sections for electron-CS$_2$ scattering in units of 10$^{-20}$ m$^2$ (for selected energies). 

<table>
<thead>
<tr>
<th>Energy (eV)</th>
<th>Cross section</th>
<th>Energy (eV)</th>
<th>Cross section</th>
<th>Energy (eV)</th>
<th>Cross section</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.4</td>
<td>22.4</td>
<td>3.5</td>
<td>47.3</td>
<td>20</td>
<td>45.9</td>
</tr>
<tr>
<td>0.6</td>
<td>18.5</td>
<td>4.0</td>
<td>50.6</td>
<td>25</td>
<td>39.0</td>
</tr>
<tr>
<td>0.8</td>
<td>17.2</td>
<td>5.0</td>
<td>52.0</td>
<td>30</td>
<td>35.2</td>
</tr>
<tr>
<td>1.0</td>
<td>19.4</td>
<td>6.0</td>
<td>51.6</td>
<td>35</td>
<td>32.7</td>
</tr>
<tr>
<td>1.4</td>
<td>25.2</td>
<td>7.0</td>
<td>53.1</td>
<td>40</td>
<td>31.0</td>
</tr>
<tr>
<td>1.8</td>
<td>31.8</td>
<td>8.0</td>
<td>52.2</td>
<td>45</td>
<td>30.0</td>
</tr>
<tr>
<td>2.0</td>
<td>33.1</td>
<td>9.0</td>
<td>53.0</td>
<td>50</td>
<td>27.8</td>
</tr>
<tr>
<td>2.2</td>
<td>35.7</td>
<td>10.0</td>
<td>51.6</td>
<td>60</td>
<td>25.3</td>
</tr>
<tr>
<td>2.5</td>
<td>37.8</td>
<td>12.0</td>
<td>51.6</td>
<td>70</td>
<td>23.4</td>
</tr>
<tr>
<td>3.0</td>
<td>41.6</td>
<td>16.0</td>
<td>49.7</td>
<td>80</td>
<td>22.0</td>
</tr>
</tbody>
</table>
Electron scattering on $CS_2$ molecules

sections for vibrational excitation of overtones contribute a small fraction to the total scattering cross section. Also the dissociative attachment cross section in this energy range (Ziesel et al 1975) is at least two orders of magnitude lower than the total cross section. Taking the above facts into account the disagreement seems to be somewhat disturbing, especially because the results obtained in both laboratories for the OCS molecule (Sohn et al 1987, Szmytkowski et al 1984) are in much better agreement.

The calculations performed by Lynch et al (1979) show that, in general, the energy dependence of elastic cross sections for valence isoelectronic molecules $CO_2$, OCS and $CS_2$ is similar. In the case of the first two molecules calculations agree quite satisfactorily with the experiment (see, e.g., Szmytkowski et al 1984, 1987). For $CS_2$, however, certain significant differences are seen (figure 1) between the experimental results and the theoretical curve. The most visible difference is the presence of a sharp resonance maximum around 1.8 eV in the calculated cross section attributed to the formation of the $^2\pi_u$ $CS_2$ shape resonant state. The presence of a weak resonance band in this energy range has already been noted in transmission experiments of Burrow (unpublished, see Ziesel et al 1975) and Dressler et al (1987) as well as in threshold electron spectra by Dance et al (1978). A slight change of slope of the present cross section, seen around 1.8 eV, might be a demonstration of this resonance. However, the very recent experiment of Sohn et al (1987) did not confirm the presence of a resonant state of $^2\pi_u$ symmetry near the considered energy either in the elastic or vibrational channels. It should be noted that the calculations of Lynch et al (1979) do not include the motion of nuclei. Calculations performed for $CO_2$ (Lynch et al 1979) show that taking into consideration the vibrations leads to essential broadening.

Figure 1. Total $e^-CS_2$ scattering cross sections. Experimental: $\triangle$, Sohn et al (1987), normalised integrated (elastic + vibrational); $\bullet$, this work, absolute. Theoretical: full curve, Lynch et al (1979), integrated elastic. The error bars correspond to the overall experimental uncertainties at some selected points.
and lowering of the resonance peaks or even to a complete smearing out of weak resonances in the integrated cross section. A similar effect may, however, result in experiment from finite energy resolution. Another difference between experiment and the calculations of Lynch et al. (1979), common for CO$_2$, OCS and CS$_2$ molecules, is an overestimation of the calculated cross sections in the lowest-energy region.

The sharp increase of the total cross section above 0.8 eV may be partly due to the existence of a number of weak overlapping resonances. Their existence has been recently reported by Dressler et al. (1987). Further resonances, in addition to the 1.8 eV resonance, were also predicted in calculations of Lynch et al. (1979).

Above the first ionisation threshold (10.06 eV), an increasing role in the scattering process is played by ionisation phenomena. At 30 eV the cross section for ionisation (Ziesel et al. 1975) amounts to 22% of the total cross section and, by analogy with SO$_2$ and H$_2$S (triatomic molecules containing a sulphur atom), it probably increases up to about 40% at 80 eV.

Results of calculations of e$^-$–CS$_2$ scattering cross sections, performed using the variable-phase approach, will be published in a future article.

Acknowledgments

The author is grateful to K Maciag for his assistance in the preliminary stages of this work, to Dr M Zubek for valuable comments and to Professor H Ehrhardt for making his results available prior to publication. This work has been supported in part by the Polish Ministry of Science and Higher Education within Programme CPBP 01.06 under Project 3.01.

References

Foo V Y, Brion C E and Hasted J B 1971 Proc. R. Soc. A 322 555-54

— 1975 J. Electron Spectrosc. Relat. Phenom. 7 139-49
Kraus K 1961 Z. Naturf. a 16 1378-85
Szmytkowski Cz, Karwasz G and Maciąg K 1984 Chem. Phys. Lett. 107 481-4
Wilden D G and Comer J 1980 Chem. Phys. 53 77-84