

LETTER TO THE EDITOR

The total elastic cross section for electron scattering from SF₆Hyuck Cho[†], Robert J Gulley and Stephen J Buckman

Atomic and Molecular Physics Laboratories, Research School of Physical Sciences, Australian National University, Canberra, ACT, 0200, Australia

Received 3 March 2000

Abstract. Absolute differential cross sections for elastic scattering of electrons from SF₆ have been measured at 11 energies between 2.7 and 75 eV for scattering angles between 10 and 180°. The differential measurements use, for the first time, the magnetic angle-changing technique of Read and Channing in combination with the relative flow technique to obtain absolute elastic scattering cross sections at backward angles. These cross sections have been extrapolated in the forward direction to enable the integral elastic cross section to be calculated. The cross section derived from this process is in excellent agreement with that proposed recently by Christophorou *et al* and supports their hypothesis that several of the earlier measurements underestimate the integral elastic cross section between 5 and 75 eV.

1. Introduction

In a recent review of electron collision cross sections for SF₆, Christophorou *et al* (1999) noted a significant discrepancy between the existing experimental determinations of the total elastic cross section. Also, at low energies where the sum of total elastic and total vibrational excitation cross sections should be roughly equivalent to the (well known) grand total cross section, several of the total elastic determinations implied a value for the total vibrational cross section which was unrealistically large. That is, the total elastic cross sections seemed to be too small.

Each of these previous determinations of the total elastic cross section were made by extrapolating and integrating measured absolute differential cross sections. Srivastava *et al* (1976) measured differential cross sections (DCS) for elastic scattering at energies from 5 to 75 eV and scattering angles between 20 and 135°. These cross sections were later renormalized by Trajmar *et al* (1983). Rohr (1979) measured DCS at energies between 0.3 and 10 eV and angles in the range from 20–120°, establishing the absolute scale by comparing the scattering intensity to that of helium. Sakae *et al* (1989) measured absolute DCS between 75 and 700 eV at scattering angles between 5–135°. The absolute values were obtained by measuring the ratio of elastic scattering for SF₆ to that of helium in a flooded gas cell. Finally, Johnstone and Newell (1991) measured DCS between 5 and 75 eV at angles in the range 10–120°. They used the relative flow technique at a fixed angle of 90°, and the helium cross sections of Nesbet (1979) and Register *et al* (1980) to establish their absolute scale. As they are of relevance to the present discussion, we also note the grand total scattering measurements of Kennerly *et al* (1979), Ferch *et al* (1982), Dababneh *et al* (1988), Zecca *et al* (1992), Randell *et al* (1992) and Kasperski *et al* (1997), and the vibrational excitation cross section measurements of Rohr

[†] Permanent address: Chungnam National University, Taejeon, Korea.

(1977). From a theoretical perspective there is, to our knowledge, only one contemporary calculation, a close-coupling approach by Gianturco *et al* (1995).

When one compares these measurements, as has been done comprehensively by Christophorou *et al* (1999), a number of observations can be made. First, at low energies (< 10 eV) the total elastic cross section of Rohr (1979) is larger than the cross sections of both Trajmar *et al* (1983) and Johnstone and Newell (1991) but it is in reasonably good agreement at very low energies with that of Randell *et al* (1992). Second, at high energies (75 eV) the cross sections of Trajmar *et al* and Johnstone and Newell are substantially smaller (about a factor of two) than those predicted by Sakae *et al* (1989). Finally, at low energies (5 eV) the cross sections of Trajmar *et al* and Johnstone and Newell are not consistent with the values of the grand total cross section and the estimated vibrational excitation cross section (Christophorou *et al* 1999).

The derivation of integral elastic cross sections from differential measurements is fraught with difficulty, particularly in a case such as SF₆ where its high dipole polarizability (44 au) ensures that the scattering is strongly enhanced in the forward direction. One must extrapolate the DCS measurements to forward angles, which are inaccessible due to the primary electron beam, and to backward angles which are usually precluded from measurement due to mechanical constraints imposed by the physical size of the electron spectrometers. Thus there may be several reasons for this discrepancy in the total elastic cross section. It may be due to inaccuracies in the angular distribution measurements and/or the absolute normalization process, or it may be due to the extrapolation process itself which, in the absence of any reliable theoretical calculation, is usually 'eyeballed'. The purpose of the present work was to investigate both the differential and total elastic scattering cross sections for SF₆ with a view to resolving this discrepancy. The process has been aided by the use of a magnetic angle changing device, based on the novel design of Read and Channing (1996), which has enabled DCS measurements at energies below 15 eV to be extended to a scattering angle of 180°. This, we believe, is the first application of this technique in conjunction with the relative flow method in order to obtain absolute scattering cross sections. The present DCS results extend from 2.7 to 75 eV and cover the angular range from 10 to 180°. The bulk of the DCS data will be presented in a forthcoming article (Cho *et al* 2000).

2. Experimental apparatus and techniques

The apparatus used for the present investigation has been well documented (e.g. Gibson *et al* 1999) and will not be described in any detail here. It consists of a pair of hemispherical electrostatic analysers for the production, energy analysis and detection of scattered electrons. The energy resolution for the present work was typically 50 meV and the electron beam current was in the range 1–5 nA. The substantive difference between this apparatus and that which we have described previously is the inclusion of the magnetic angle-changing device. The present device is based very closely on the innovative design of Read and Channing (1996). They demonstrated that by using two highly localized, coaxial magnetic fields surrounding the interaction volume one could effectively rotate the scattering geometry of an apparatus to enable measurements to be performed at large scattering angles. By carefully matching the magnetic fields, a strong deflecting force could be established to enable the incident beam direction to be rotated by, for example, 45°. The (elastically) scattered electrons undergo a similar rotation as they exit the field, resulting in a total change of scattering angle of 90°. This technique has been successfully used in a number of recent applications (Zubek *et al* 1996, 1999, Trantham *et al* 1997). In a departure from the Read and Channing design, we have enclosed the two magnetic field coils in a pair of μ -metal pole pieces. This, we have demonstrated by magnetic modelling

calculations (Trantham *et al* 1997), provides for even higher localization of the magnetic field. In practice there is no discernible effect on the operation of the electron spectrometer (beam current, energy resolution, etc) when the field coils are activated, other than rotating the incident beam direction by 45° . Thus, with the electron analyser positioned at the 'conventional' 90° position, we can record elastic scattering events at 180° . Such measurements have been carried out in the present case at incident energies up to 15 eV. Thermal limitations on the enamelled wire used for the field coils in the present device precluded safe operation above this energy. Details of the construction of this device will be provided in a forthcoming paper (Cho *et al* 2000). The absolute scale for the elastic DCS has been established using the relative flow technique with helium as a reference gas. The helium cross sections of Nesbet (1979) and Fursa and Bray (1997) were used for the normalization process.

3. Results and discussion

Absolute, differential elastic scattering cross sections have been measured at 11 energies between 2.7 and 75 eV. Integral cross sections (ICS) and elastic momentum transfer cross sections have been derived from these by extrapolating the DCS to 0° in the forward direction and where necessary (above 15 eV) to 180° , and then integrating the resulting cross section. These cross sections are given in table 1. Examples of the DCS at energies of 5 and 75 eV are given in figure 1 and the elastic integral and elastic momentum transfer cross sections are shown in figure 2. The absolute uncertainty on the elastic DCS is typically less than 10% and, with the removal of the uncertainty associated with the extrapolation to large scattering angles, we estimate the uncertainty on the total elastic cross section to be no larger than 20%.

Table 1. Integral elastic (Q_i) and elastic momentum transfer (Q_m) cross sections for SF₆, in units of Å².

Energy (eV)	Q_i	Q_m
2.7	18.73	16.10
5.0	20.15	14.14
7.0	24.29	15.47
8.5	24.60	14.49
10	24.45	15.09
12	26.81	17.62
15	25.51	14.86
20	24.73	15.65
30	29.72	13.18
50	22.13	8.09
75	18.02	7.28

In figure 1(a) we show the elastic DCS at an energy of 5 eV. Good agreement is found with the measurements of Rohr (1979) at all scattering angles. There are large discrepancies (a factor of 2) between the present measurements and those of both Srivastava *et al* (1976) and Johnstone and Newell (1991) at angles less than 60° . At larger scattering angles all of the measurements are in reasonably good accord and the present measurements show a cross section that decreases gradually at backward angles. The general features of the present cross section are well reproduced in the close coupling calculation of Gianturco *et al* (1995). At 75 eV, the highest energy for the present measurements, we can compare with the earlier measurements of Srivastava *et al* (1976), Sakae *et al* (1989), and Johnstone and Newell (1991), this is shown in figure 1(b). The agreement with the cross section of Sakae *et al* is excellent,

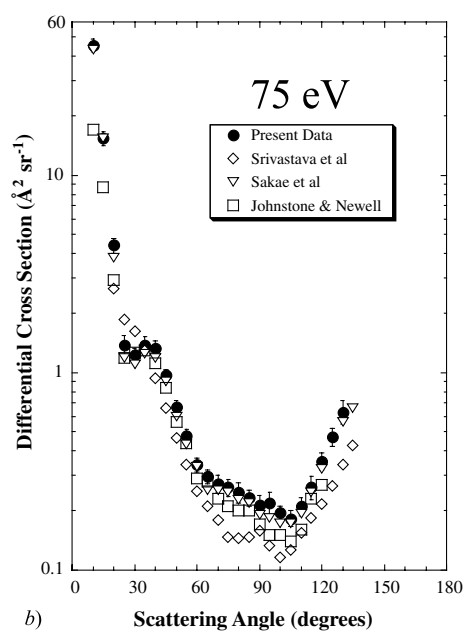
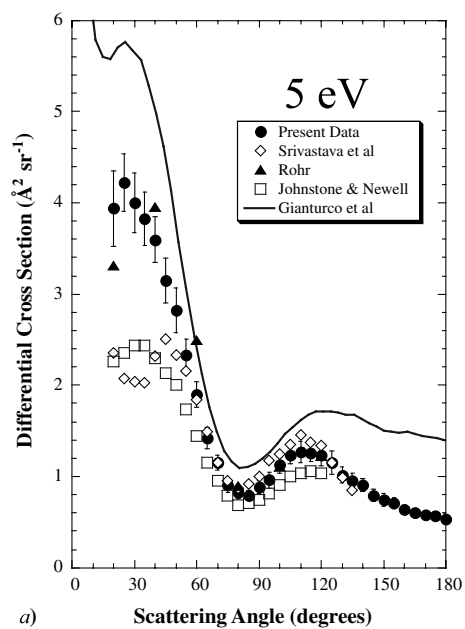


Figure 1. (a) Elastic differential cross section for electron scattering from SF_6 at 5 eV. (b) Elastic differential cross section for electron scattering from SF_6 at 75 eV.

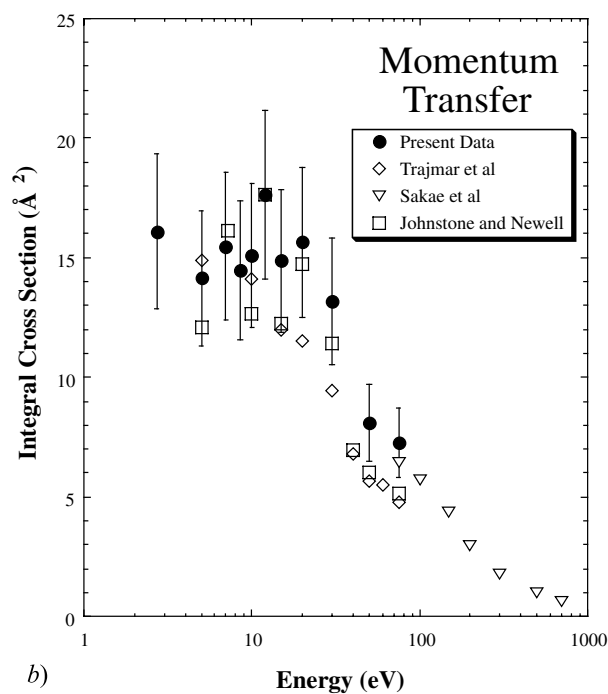
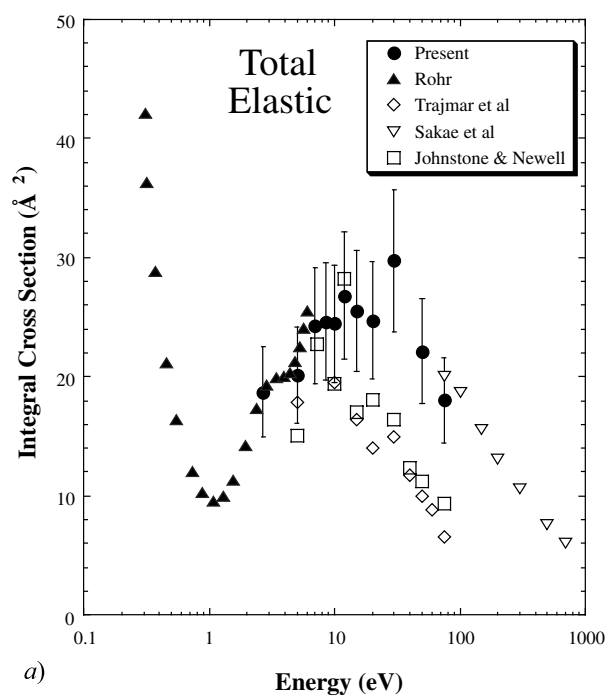


Figure 2. (a) The total elastic cross section for SF_6 . (b) The elastic momentum transfer cross section for SF_6 .

with the two sets of data lying well within the bounds of the stated uncertainties at all scattering angles. The agreement with the cross section of Johnstone and Newell is also very good at all but the smallest of scattering angles ($<20^\circ$). The cross section of Srivastava *et al* shows the same general shape as the other three measurements but is lower than all at most scattering angles and does not predict the shallow minimum at forward scattering angles ($\sim 30^\circ$).

In figure 2(a) it is immediately obvious that the present total elastic cross section is in good agreement with both the low energy data of Rohr (1979) and the 75 eV cross section of Sakae *et al* (1989). The agreement with the cross sections derived from the (renormalized) DCS measurements of Srivastava *et al* (1976) or Johnstone and Newell (1991) is not as good. It is apparent that the present measurements predict a total elastic cross section at intermediate energies (10–50 eV) which is substantially higher than either of these measurements. These observations are consistent with the level of agreement found for the DCS measurements. They are also entirely consistent with the findings of Christophorou *et al* (1999) who proposed a recommended total elastic cross section that is very similar to the present results. It is not particularly easy to speculate on the cause of this discrepancy although we note that at those energies where the present ICS is larger than that of Srivastava *et al* or Johnstone and Newell, the present DCS is also larger. Thus the problem most likely arises from the absolute normalization of these data sets and not necessarily in the backward angle extrapolation process. This hypothesis is further supported by the elastic momentum transfer cross section shown in figure 2(b). Here the differences between the present and previous results are substantially smaller due to the smaller weighting that this cross section gives to forward scattering.

In conclusion, the present results provide an ideal demonstration of the utility of the magnetic angle-changing technique of Read and Channing (1996). In combination with the relative flow technique it has the potential to provide much needed information on absolute back-scattering cross sections, and to reduce the uncertainties that result on the integral elastic and elastic momentum transfer cross sections that are derived from them.

Acknowledgments

It is a pleasure to acknowledge fruitful discussions and numerous communications with James Olthoff and Loucas Christophorou who appraised us of the situation in SF₆ regarding the discrepancies in the integral elastic cross section and encouraged our measurements. We are most grateful to Dmitry Fursa and Igor Bray for the provision of tabulated helium cross sections. HC thanks the Australian Research Council for the provision of an International Fellowship as does RJG for a Postdoctoral Fellowship.

References

- Cho H, Gulley R J, Trantham K W, Uhlmann L J, Dedman C J and Buckman S J 2000 *J. Phys. B: At. Mol. Opt. Phys.* submitted
- Christophorou L, Olthoff J, Siegel R, Hayashi M and Nakamura Y 1999 *Bull. Am. Phys. Soc.* **44** 20 and private communication
- Dababneh M S, Hsieh Y-F, Kauppila W E, Kwan C K, Smith S J, Stein T S and Uddin M N 1988 *Phys. Rev. A* **38** 1207
- Ferch J, Raith W and Schröder K 1982 *J. Phys. B: At. Mol. Phys.* **15** L175
- Fursa D V and Bray I 1997 *J. Phys. B: At. Mol. Opt. Phys.* **30** 757
- Gianturco F A, Lucchese R R and Sanna N 1995 *J. Chem. Phys.* **102** 5743
- Gibson J C, Green M A, Trantham K W, Buckman S J, Teubner P J O and Brunger M J 1999 *J. Phys. B: At. Mol. Opt. Phys.* **32** 213
- Johnstone W M and Newell W R 1991 *J. Phys. B: At. Mol. Opt. Phys.* **24** 473
- Kasperski G, Mozejko P and Szymkowski Cz 1997 *Z. Phys. D* **42** 187

- Kennerly R E, Bonham R A and McMillan M 1979 *J. Chem. Phys.* **70** 2039
- Nesbet R K 1979 *Phys. Rev. A* **20** 58
- Randell J, Field D, Lunt S L, Mrotzek G and Ziesel J P 1992 *J. Phys. B: At. Mol. Opt. Phys.* **25** 2899
- Read F H and Channing J M 1996 *Rev. Sci. Instrum.* **67** 2372
- Register D F, Trajmar S and Srivastava S K 1980 *Phys. Rev. A* **21** 1134
- Rohr K 1977 *J. Phys. B: At. Mol. Phys.* **10** 1175
- 1979 *J. Phys. B: At. Mol. Phys.* **12** L185
- Sakae T, Sumiyoshi S, Murakami E, Matsumoto Y, Ishibashi K and Katase A 1989 *J. Phys. B: At. Mol. Opt. Phys.* **22** 1385
- Srivastava S K, Trajmar S, Chutjian A and Williams W 1976 *J. Chem. Phys.* **64** 2767
- Trajmar S, Register D F and Chutjian A 1983 *Phys. Rep.* **97** 216
- Trantham K T, Dedman C J, Gibson J C and Buckman S J 1997 *Bull. Am. Phys. Soc.* **42** 1727
- Zecca A, Karwasz G and Brusa R S 1992 *Chem. Phys. Lett.* **199** 423
- Zubek M, Gulley N, King G C and Read F H 1996 *J. Phys. B: At. Mol. Opt. Phys.* **29** L239
- Zubek M, Mielewska B, Channing J, King G C and Read F H 1999 *J. Phys. B: At. Mol. Opt. Phys.* **32** 1351