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# Absolute elastic cross-sections for low-energy electron scattering from tetrahydrofuran

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**Abstract.** We present results for elastic electron collision cross-sections with tetrahydrofuran ($C_4H_8O$) in the energy range of 6.5–50 eV. The absolute cross-sections are determined from crossed beam measurements using the relative flow technique and cover the angular range between $10^\circ$ and $130^\circ$. Integral and momentum transfer cross-sections have also been derived from these results. The data, where possible, are compared to recent experimental results and theoretical calculations.

## Contents

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## 1. Introduction

Ionizing radiation is used widely in medicine as a probe in radio-diagnostic examinations and as a genotoxic agent in radiotherapy. It has been the commonly held belief that ballistic, high energy impacts were responsible for the bulk of cell and tissue damage when ionizing radiation enters the body. In recent years, experimental studies have indicated that secondary species generated by the primary ionizing particle can also play a significant role in radiation damage to DNA [1, 2].

Upon entering the body, high energy ionizing radiation quickly thermalizes through various scattering processes that liberate large numbers of low energy (0–20 eV) secondary electrons. These electrons then interact with bio-molecules such as water [3, 4], sugars [5] and DNA bases [6]–[11], and have been shown to cause significant damage to DNA through the process of dissociative attachment [12, 13]. This either directly leads to single or double DNA strand breaks, or results in the formation of free radicals, which can then chemically react with DNA to lead to strand breaking.

In this present experiment, we have investigated electron collisions with the tetrahydrofuran (THF) molecule using the crossed beam method. THF is a common organic solvent used in large amounts for a variety of industrial purposes [14]. There is also significant interest in THF as it presents a simple model for the deoxyribose building block of DNA. In particular, the backbone of DNA may be considered as a series of THF molecules held together by phosphate bonds to which the important bases are attached. The objective of the present study is to understand how electrons interact with this simple model of part of the DNA backbone. Such studies may help to understand the mechanism of dissociative electron attachment, and the measurement of absolute scattering information can be used to both test, and aid, the development of quantum scattering theory for such bio-molecules.

THF has previously been the subject of several theoretical and experimental studies. Early study by Le Page *et al* [15] was focused on differences in electron spectroscopy between the gas and solid phases. A resonance feature is reported for gaseous THF at 8.5 eV in the vibrational excitation of the C–H stretch modes, but is shifted about 1 eV lower for the solid-state measurements. Low-energy electron damage in the solid phase was reported by Breton *et al* [16], who discuss the production of aldehydes in terms of electron resonances, and also list previous investigations with gas, liquid and solid state THF.

Several absolute experimental scattering measurements in the gas phase have appeared more recently. Zecca *et al* [17] reported grand total cross-section (GTCS) measurements for both electrons and positrons at energies below 21 eV, while Mozejko *et al* [18] reported similar measurements, using electrons only, from 1–370 eV. Both groups observe a broad shape resonance centred around 6–8 eV in the GTCS. The first differential cross-sections (DCS) for elastic electron scattering were published by Milosavljevic *et al* [19] in the energy range 20–300 eV for scattering angles ranging from 10 to 110°. A recent publication also reports elastic DCS and vibrational excitation of the C–H stretch modes at 10 eV and for scattering angles from 20 to 180° [20].

Theoretical investigations concerning THF have also become more common in recent times. DCS for elastic electron scattering have been computed by Mozejko and Sanche [21] using the independent atom method (IAM) for collision energies in the range 50–2000 eV. They also calculated the cross-section for electron impact ionization of THF, from the ionization threshold up to energies of 4000 eV. Integral cross-sections, both elastic and electronically inelastic, have been calculated for THF by Bouchiha *et al* [22] using the R-matrix method, at collision energies from 1–10 eV. Although they did not observe a shape resonance, a few core-excited resonances are reported. Trevisan *et al* [23] completed calculations of DCS and momentum transfer cross-sections (MTCS) of elastic electron scattering by THF using the complex Kohn variational method, and report a broad shape resonance in the 8–10 eV energy range in the MTCS. Elastic integral cross-sections for both THF and phosphoric acid, which constitutes the remainder of the DNA backbone, have been computed by Tonzani and Greene [24], who also use a variation of the *R*-matrix method. Resonances for THF have been observed around 8.6 and 14.1 eV, but the authors indicate that their model usually predict resonances 1–2 eV higher than experiment due to the use of the static exchange approximation. Most recently Winstead and McKoy [25] published elastic integral, DCS and MTCS from deoxyribose and related molecules, including THF. Using the Schwinger multichannel method, shape resonances in the integral cross-section and MTCS of THF are reported at energies of 8.3 and 13.5 eV, after compensating for the static exchange approximation.

## 2. Experimental apparatus

Elastic electron scattering from THF has been studied using a crossed electron-target beam apparatus. The THF vapour has been obtained from a liquid sample of THF, which has a purity greater than 99% (Sigma–Aldrich Australia), and has been further purified by a number of freeze, pump and thaw cycles. It is admitted to the scattering system at a relatively low driving pressure via a temperature-controlled needle valve and gas-handling system. To prevent condensation, the needle valve and gas lines are heated to about 323 K and the beam-forming needle, by which the gas enters the collision region, is maintained near 348 K.

The monoenergetic (FWHM ∼70 meV) electron beam is obtained from a conventional electron monochromator, and scattered electrons are energy analysed before being detected by a channel electron multiplier. The absolute value of the incident energy was determined through calibration against the position of the negative ion resonance feature for electron scattering from helium at 19.365 eV [26]. The experimental apparatus has been described in detail in a number of previous publications (e.g. [27]).

To determine absolute cross-sections the relative flow technique is implemented. The technique involves measuring the relative electron scattering intensities for the gas under study and for a standard gas for which there is an accurate set of DCS, in our case THF and helium respectively. The variational calculations of Nesbet [28] for the He cross-section is used as the absolute calibration for energies below 20 eV, and the rational function fits of Boesten and Tanaka [29] to a range of helium cross-sections are used for the higher energy measurements. The driving pressures for both gases are determined such that the collisional mean free path in the beam-forming needle are the same, and thus the collision-dependent profile of the gas beams should be identical in the collision volume, which is situated just above the needle exit. Initially the hard sphere diameter for THF, from which the mean free path is calculated, was estimated using molecular bond lengths. However, this value was found to be similar to hard sphere diameters determined via both the Lennard–Jones model [30] and the equation of state. In order to test the effect that these different values might have on the DCS, we conducted measurements using different values for the hard sphere diameter, and thus different driving pressures for THF. These different operating conditions appeared to have no significant effect on the DCS in the region around the calculated values. Typical driving pressures used were 0.2 Torr for THF and 1.0 Torr for He.

**Table 1.** Experimentally determined DCS for elastic electron scattering by gas phase THF, in units of $10^{-16}$ cm$^2$ sr$^{-1}$, as a function of scattering angle and incident energy. Integral and MTCS in units of $10^{-16}$ cm$^2$ are shown at the foot of each column. Absolute errors are given in parentheses. The uncertainty in the integral cross-sections is estimated to be 20–25%.

| | $E_0$ (eV) | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| $\theta$ (°) | 6.5 | 8 | 10 | 15 | 20 | 30 | 40 | 50 |
| 10 | – | – | – | – | – | – | – | 69.0(5.48) |
| 20 | – | – | 17.4(2.87) | 16.1(3.52) | 21.4(2.07) | 23.7(2.76) | 15.3(1.26) | 11.1(0.84) |
| 25 | 9.62(0.86) | 10.4(1.78) | – | – | – | – | – | – |
| 30 | 6.16(0.65) | 6.34(0.72) | 7.66(0.60) | 7.00(0.73) | 5.09(0.38) | 3.80(0.31) | 2.36(0.18) | 1.79(0.14) |
| 40 | 3.34(0.28) | 3.29(0.38) | 3.17(0.25) | 2.38(0.20) | 2.07(0.16) | 1.69(0.12) | 1.32(0.10) | 1.08(0.08) |
| 50 | 2.47(0.28) | 2.33(0.19) | 2.27(0.18) | 1.86(0.16) | 1.65(0.12) | 1.21(0.10) | 0.90(0.07) | 0.75(0.05) |
| 60 | 2.13(0.17) | 1.83(0.15) | 1.82(0.14) | 1.50(0.11) | 1.31(0.12) | 0.91(0.07) | 0.67(0.05) | 0.49(0.04) |
| 70 | 1.57(0.15) | 1.45(0.13) | 1.51(0.11) | 1.32(0.10) | 1.14(0.11) | 0.71(0.06) | 0.45(0.04) | 0.31(0.03) |
| 80 | 1.27(0.11) | 1.49(0.11) | 1.48(0.11) | 1.27(0.10) | 1.02(0.10) | 0.55(0.05) | 0.34(0.03) | 0.27(0.02) |
| 90 | 1.43(0.12) | 1.74(0.13) | 1.63(0.12) | 1.26(0.11) | 0.92(0.10) | 0.47(0.05) | 0.33(0.04) | 0.25(0.02) |
| 100 | 1.89(0.15) | 2.03(0.15) | 1.79(0.14) | 1.35(0.11) | 0.89(0.10) | 0.51(0.06) | 0.38(0.05) | 0.24(0.02) |
| 110 | 2.45(0.19) | 2.30(0.17) | 1.97(0.16) | 1.45(0.13) | 0.99(0.12) | 0.66(0.09) | 0.53(0.08) | 0.32(0.02) |
| 120 | 2.79(0.23) | 2.57(0.19) | 2.24(0.18) | 1.54(0.16) | 1.11(0.14) | 0.94(0.11) | 0.82(0.14) | 0.49(0.05) |
| 130 | 2.93(0.27) | 2.63(0.20) | 2.42(0.18) | 1.57(0.15) | 1.30(0.16) | 1.26(0.16) | 1.22(0.23) | 0.74(0.08) |
| $Q_i$ | 41.01 | 38.18 | 40.97 | 36.93 | 37.71 | 33.38 | 27.81 | 22.95 |
| $Q_m$ | 29.31 | 28.26 | 29.72 | 20.46 | 19.20 | 14.82 | 14.02 | 7.71 |

## 3. Results and discussion

Absolute DCS for electron scattering from the THF molecule at eight incident energies between 6.5 and 50 eV are presented in table 1. They are also shown in figures 1 and 2, together with other available experimental and theoretical cross-sections. The energy dependences of the elastic scattering cross-section for scattering angles of 60, 90 and 120° are also shown in figure 3. The elastic integral and MTCS are presented at the foot of each column of DCS data in table 1 and are shown in figure 4. The experimental uncertainties on the present DCS vary typically from 7 to 10%, and in a few cases are as high as 20%. The estimated errors on the derived elastic integral and MTCS are 15–20%.

In figures 1 and 2, a comparison is made at selected energies between the present data, the theoretical calculations of Trevisan *et al* [23] and Winstead and McKoy [25] and the experimental DCS of Milosavljevic *et al* [17, 18] and Dampe *et al* [31]. At both 6.5 and 8 eV (figures 1(a) and (b)) the present values are in excellent agreement with both of the theoretical calculations across the entire angular range. Note that in figure1(a) the calculation of Trevisan *et al* is at the slightly different energy of 6 eV. We also note that at this energy the cross-section is quite large, being everywhere greater than $1 \times 10^{-16}$ cm$^2$ sr$^{-1}$. At 10 eV, once again the agreement between the two theoretical calculations and the present experiment is excellent across the entire, common angular range. At 15 eV (figure 1(d)) in addition to comparison with the theoretical calculations, we can also compare with the recent results of Dampe *et al*. The level of agreement between

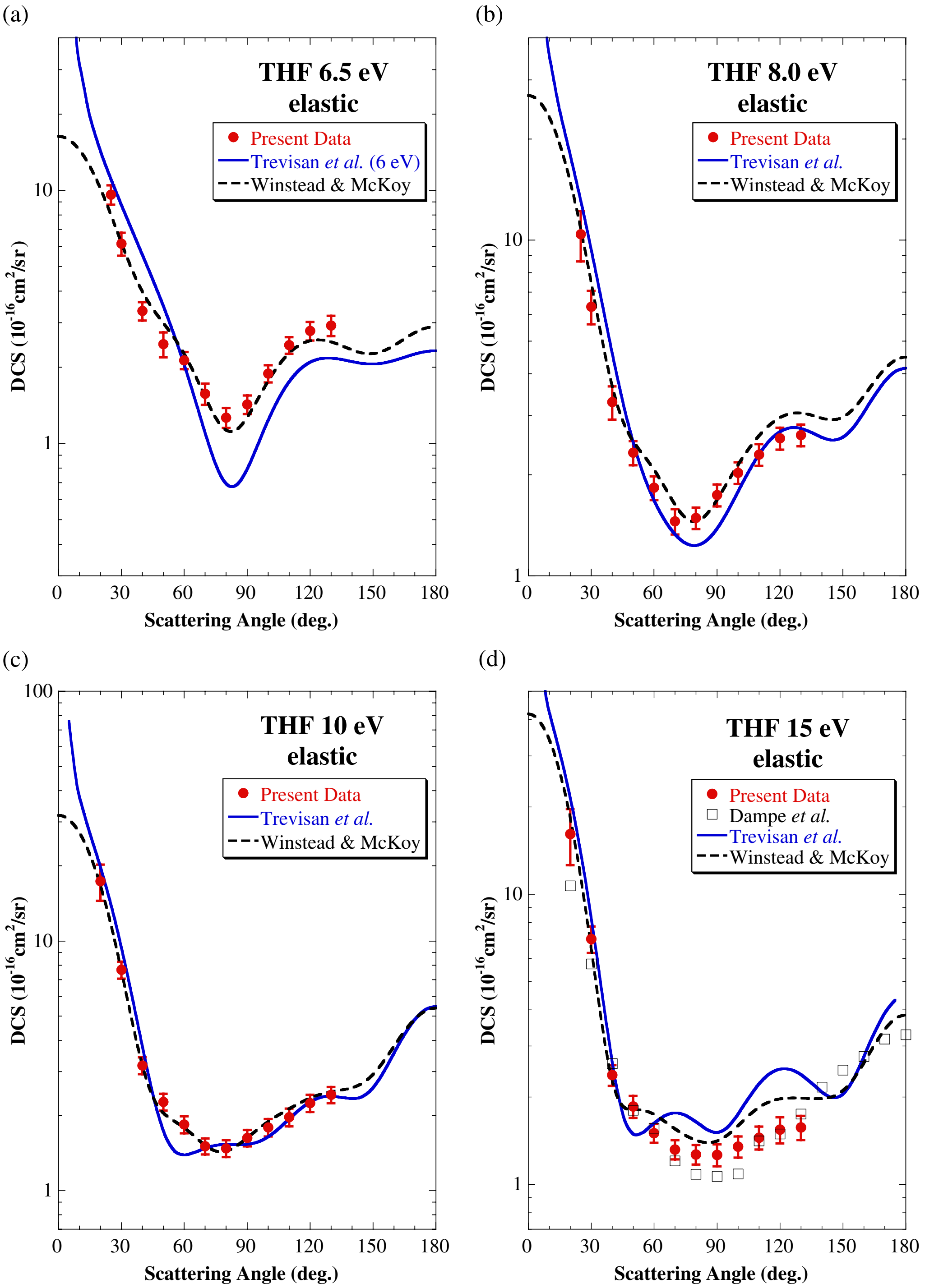

**Figure 1.** Absolute DCS (in units of $10^{-16}$ cm sr$^{-1}$) for electron scattering from THF at energies of (a) 6.5 eV, (b) 8.0 eV, (c) 10 eV and (d) 15 eV. The key to the data is shown on each plot.

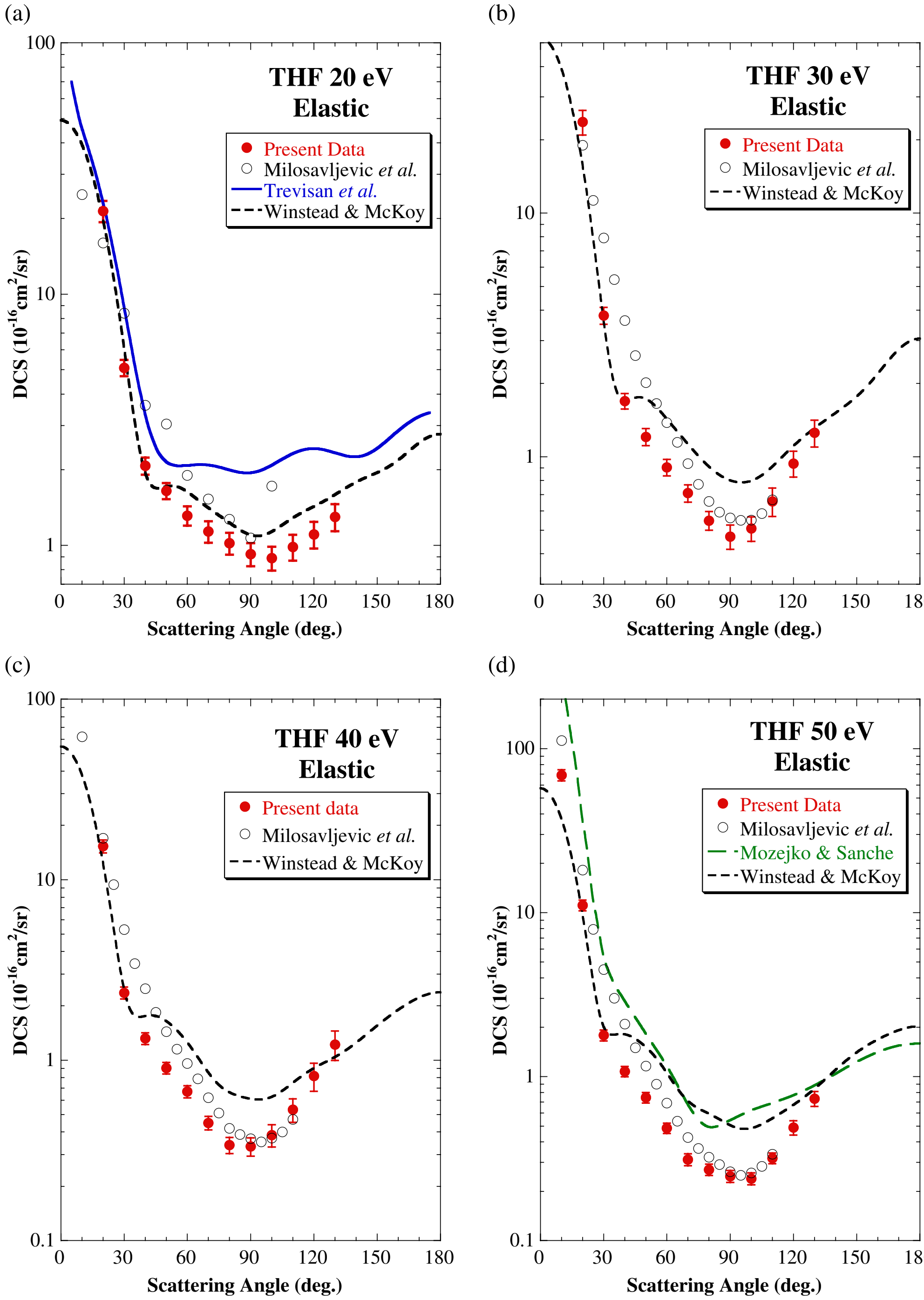

**Figure 2.** Absolute DCS (in units of $10^{-16}$ cm$^2$ sr$^{-1}$) for electron scattering from THF at energies of (a) 20 eV, (b) 30 eV, (c) 40 eV and (d) 50 eV. The key to the data is shown on each plot.

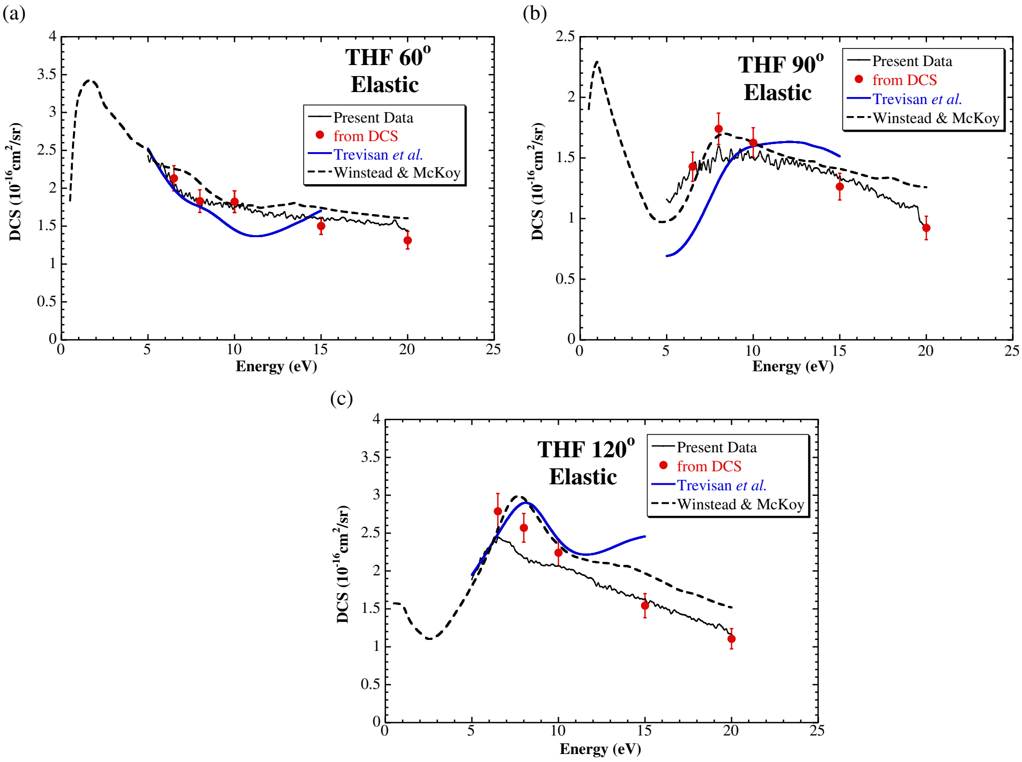

**Figure 3.** Absolute excitation functions (in units of $10^{-16}\,\mathrm{cm}^2\,\mathrm{sr}^{-1}$) for elastic scattering from THF at (a) 60°, (b) 90° and (c) 120°. The key to the data is shown on each plot.

the two experimental cross-sections is very good at all angles, and once again there is generally good accord with the two theoretical calculations, in particular that of Winstead and McKoy.

At an energy of 20 eV (figure 2(a)) the present experimental DCS can be compared with that of Milosavljevic *et al* [17, 18] and we see relatively good agreement in both shape and magnitude of the DCS. The present cross-section is also in excellent agreement with the calculated values of Winstead *et al* but is about a factor of two lower than the Kohn variational calculation above about 60°. At 30 eV (figure 2(b)) the present cross-section is slightly lower than that of Milosavljevic *et al* at most angles less than 90° and, while it is in good agreement with the Schwinger variational calculation at forward and backward angles, it lies about 30–40% below the theory between 50–110°. Very similar trends between the two experimental data sets, and between experiment and theory, are seen at energies of 40 and 50 eV (figures 2(c) and (d) respectively). At 50 eV it is also possible to compare with the independent atom model calculation of Mozejko and Sanche which predicts the shape of the cross-section rather well but is larger than experiment at all angles by between 10 and 50%. We note also that at this and other energies at forward angles, the Schwinger variational calculation is significantly lower in magnitude than the experimental cross-sections, principally because there is no explicit inclusion of the long-range dipole interaction through a Born-type approach.

In addition to the angular DCS determinations, measurements of the energy dependence of the elastic cross-section at a number of fixed scattering angles (elastic 'excitation functions' or EF)

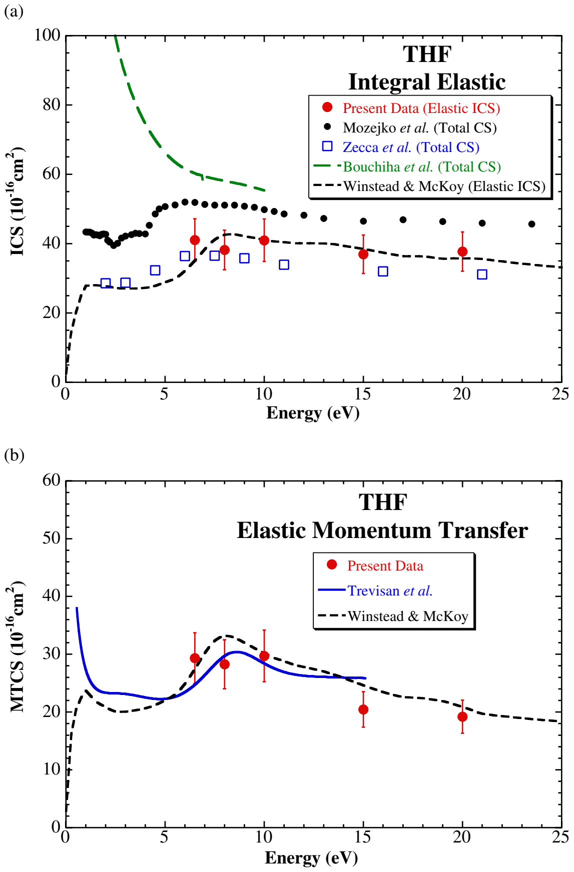

**Figure 4.** (a) Integral elastic and (b) elastic MTCS for electron scattering from THF in units of $10^{-16}$ cm.

have been performed. A comparison of these EF, at scattering angles of 60, 90 and 120°, with the Kohn variational and Schwinger variational calculations is made in figures 3(a)–(c). The data from the angular DCS measurements are also shown where applicable and, in general, these are in very good agreement with the EF results. At a scattering angle of 60° (figure 3(a)) the energy dependence and magnitude of all the cross-sections are in good agreement, and each indicate the (weak) presence of a shape resonance around 6–8 eV. At 90° (figure 3(b)) the EF measurement and DCS data are in excellent agreement with the calculation of Winstead and McKoy, while the Kohn variational calculation shows a similar energy dependence but the features are shifted about 2 eV higher in energy relative to the experiment. At 120° (figure 3(c)) the broad shape resonance is observed to be quite strongly present in both of the theoretical calculations at around 8 eV, whilst in the present measurement it is observed at around 6.5 eV. Consistent with the theoretical calculations however, its presence in the experimental cross-section is much more dominant at higher angles. Our preliminary investigations into the vibrational excitation of C–H stretching modes for THF have also indicated the presence of a negative ion resonance at ∼6.5 eV. The small structure observed in each of the EF at approximately 19.4 eV is due to the $He^-$ resonance, which appears as a consequence of the normalization process against helium.

The angular distributions have been used to derive elastic ICS and MTCS, at each incident energy, using the phase shift analysis technique of Campbell *et al* [32]. This technique removes some of the subjective nature of the alternative approach—an extrapolation by eye. For a molecule such as THF with a large dipole moment, the extrapolation to forward angles can be a highly uncertain process and the fitting of partial waves to the angular distribution helps yield more physically reasonable values for the forward and backward scattering angles.

In figure 4(a), a comparison of the present elastic ICS data is made with the total cross-section measurements of Zecca *et al* [17] and Mozejko *et al* [18], as well as with the *R*-matrix total cross-section calculation of Bouchiha *et al* [22] and the Schwinger variational calculation of Winstead and McKoy [25]. We see from the present measurements that the elastic ICS is quite constant in magnitude between 6.5 and 20 eV, and this is in excellent agreement with the Schwinger variational calculation. We also note that the shape resonance is only weakly present in the calculated elastic ICS and its appearance in the present measurements is not conclusive. A broad resonance-like feature is also observed in the total cross-section measurements of both Mozejko *et al* and Zecca *et al*. The present elastic scattering data is uniformly larger than the total cross-section of Zecca *et al*, which indicates that their measurement may well underestimate the total scattering cross-section. Zecca *et al* did not correct their results for forward angle scattering and the present measurements suggest that could be a serious limitation in their results. On the other hand the present measurement is consistent with the total cross-section of Mozejko *et al*, lying about 15–20% lower in magnitude and suggesting an appreciable contribution to the total cross-section comes from inelastic scattering. The present data is also compared to the *R*-matrix calculation of Bouchiha *et al* below 10 eV. They do not detect a shape resonance in their calculation but instead observe a rapidly rising cross-section at low energies and a few core-excited resonances around 8–9 eV.

The present results for the MTCS are shown in figure 4(b) and are compared to the theoretical efforts of Trevisan *et al* and Winstead and McKoy. These two calculations are in good agreement with one another and both show a strong resonant enhancement in the cross-section at around 8 eV. The present measurements are in good accord with the calculations and do not exclude the presence of a resonance in this region.

It is interesting to note that the shape resonance observed in both the present experiment, and the theoretical calculations, is relatively narrow in width (∼2 eV). In previous work (see for example Allan and Andric [33]) it has been observed that broad features in saturated, linear hydrocarbons become quite narrow when studied in the related cyclic compounds. A good example of this effect is seen in studies of *n*-propane and cyclopropane, and also in cyclopentane [33]. It may well be that the resonance observed in THF is of a similar character, although measurements of vibrational excitation should provide more detailed information.

## 4. Conclusion

This paper reports absolute DCS for elastic electron scattering from THF at energies from 5–50 eV, as well as integral and MTCS. The experimental cross-sections are in good agreement with the recent theoretical calculations of Trevisan *et al* and Winstead and McKoy. Measurements at energies between 10 and 50 eV are also shown to be in good agreement with results of Milosavljevic *et al* and Dampe *et al*. A broad shape resonance, predicted at around 8 eV by the calculations of Trevisan *et al* and Winstead and McKoy, and previously observed in the total cross-sections of Zecca *et al* and Mozejko *et al* is observed in the present study in the elastic channel at 6.5 eV and at a scattering angle of 120°. Preliminary investigations of the C–H stretch vibrational excitation channel have shown that a negative ion resonance also appears strongly at around 6.5 eV. Further investigations into vibrational excitation, and the role of resonant scattering, are currently being carried out.

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