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Electron and positron collisions with polar molecules: studies with the benchmark water molecule

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Abstract
It is difficult to measure low-energy cross sections for collisions of charged particles with strongly dipolar systems since the magnitude of such cross sections is completely dominated by collisions in the forward direction. Theoretically, it is possible to account for the strong forward scattering using the Born approximation but the procedure for combining Born 'top-up' with the more sophisticated treatments required to treat the scattering in other directions is not unique. This comment describes recent progress in describing both electron and positron collisions with polar molecules taking the important water molecule as a benchmark. Previous calculations on electron water at collision energies below 7 eV are compared with new experiments. Positron water studies up to 10 eV are re-analysed based on given experimental acceptance profiles, which depend on the details of the apparatus and method used in the measurements. It is suggested that theory is capable of giving reliable results for elastic and rotationally inelastic electron/positron collisions with strongly dipolar species.

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(Some figures in this article are in colour only in the electronic version.)

1. Introduction

Collisions of electrons and positrons with polar molecules play a very important role in many situations including technological plasmas, astrophysics and radiation damage processes in biological physics and elsewhere. However, there is a particular difficulty in measuring cross sections for collisions between charged particles and strongly dipolar molecules since such collisions are very heavily peaked in the forward direction. This means that, given the necessarily finite width of any electron (positron) beam, many collisions do not deflect particles outside this beam. The use of magnetic angle changing devices (Read and Channing 1996) has greatly extended the angular range over which backward scattering can be measured (Cho *et al* 2003, Cho *et al* 2004) but has not solved the problem for scattering in the forward direction.

Electron and positron collisions with water are important in their own right as the water molecule is prominent atmospherically, common astrophysically and the major component of living systems. Such collisions can thus be assumed to be important in medical procedures such as positron emission tomography (PET) scans. Water has also become something of a benchmark system for collision physics and it is in this guise that we consider it here. In particular, recent electron collision studies successfully extrapolated measurements to lower angles using calculations based on the Born approximation (Khakoo *et al* 2008b, Silva *et al* 2008), leading to the claim (Silva *et al* 2008) that these new measurements disagree significantly with previous evaluations and as a consequence the results given in the recent tabulation of electron–water cross sections (Itikawa and Mason 2005) should be modified accordingly. Furthermore,

Čurík *et al* (2006) have recently made a variety of measurements for ultralow energy collisions which should be the hardest to reproduce theoretically.

Positron collisions are more difficult to study experimentally because of the significantly reduced fluxes that one has to work with. However, there have been several attempts to measure elastic collision cross sections between positrons and water (Beale *et al* 2006, Kimura *et al* 2000, Sueoka *et al* 1986, Sueoka *et al* 1987, Zecca *et al* 2006), although there remains little agreement between these measurements, particularly at lower energies. Almost certainly this problem is caused by different acceptance angles in the experiments to which, given the strong forward peaking of the cross section, the results are particularly sensitive. As could be expected, recent calculations by two of us (Baluja *et al* 2007) gives higher integral cross section (ICS) than the three measurements (Sueoka *et al* 1986, Zecca *et al* 2006, Beale *et al* 2006) which did not correct for loss of flux due to low angle scattering. However, our calculations, which agree well with those of Gianturco *et al* (2001), suggest that the results of Kimura *et al* (2000), who corrected earlier measurements (Sueoka *et al* 1987) to allow for the acceptance angle problem, significantly overestimate the forward scattering contribution at low energies for positron–water collision.

Theoretical studies of collisions with strongly polar molecules are also less straightforward than corresponding calculations on apolar systems. This is because the long-range nature of the dipole potential means that it is necessary to include a large number of partial waves in any scattering calculation. However, this is still not sufficient as performing such calculations but neglecting the rotational motions of the target molecules leads to an overestimate of the cross section. This is because the effect of rotational motion is to wash out the asymptotic potential due to the permanent dipole and its neglect leads to unphysical cross sections which diverge at low energy. Procedures to deal with this problem based on use of the dipole Born approximation are well documented (Gianturco and Jain 1986, Lane 1980, Morrison 1988, Padial and Norcross 1981). Although, as discussed below, this methodology is not without technical problems.

A number of calculations on the elastic and rotationally inelastic cross sections for electron water (Čurík *et al* 2006, Faure *et al* 2004a, 2004b, Gianturco *et al* 1998, Khakoo *et al* 2008b, Varello *et al* 1999) and positron water (Baluja *et al* 2007, Gianturco *et al* 2001) collisions have been reported. Where these studies considered the same energy ranges, they generally show reasonable agreement between them.

In this comment, we try to reconcile the various determinations of the cross sections for low-energy electron and positron collisions with the water molecule.

2. Theoretical background

A number of methods of treating the electron (positron) water collisions at short-range have been used, including single centre expansions (Gianturco *et al* 1998, Gianturco *et al* 2001), Schwinger variational calculations (Varelli *et al* 1999, Khakoo *et al* 2008b) and, our particular choice, the *R*-matrix method (Baluja *et al* 2007, Faure *et al* 2004a, 2004b). The latter two methods are based on the use of partial wave expansions within the fixed nuclei approximation. However, because of the long-range electron (positron)–dipole interaction, the partial-wave expansion does not converge in the fixed-nuclei approximation. Conversely for high partial waves the electron (positron) does not penetrate the wave function of the target molecule; under these circumstances calculations using the dipole Born approximation should be reliable. Since it is possible to compute analytically the contribution of all partial waves to the cross section both summed and individually using the Born approximation for a charged particle in a pure dipole potential (Cawford 1967), this has led to the widespread use of Born top-up procedures, within the adiabatic nuclei rotation (ANR) approximation (Lane 1980).

Within such Born top-up procedures, the cross sections are calculated in two parts. For the low-partial waves, cross sections are obtained using one of the sophisticated procedures mentioned above; these are necessary not only to allow correctly for short-range charge penetration effects but also to account for collisions that lead to changes in the rotational quantum number greater than one (Faure and Tennyson 2001). High partial waves are then accounted for by adding the total cross section calculated using the Born approximation and subtracting partial cross sections due to the low-partial waves already considered. In practice there are several ways of applying this procedure. One option is to adjust the differential cross section (DCS) by

$$\frac{\mathrm{d}\sigma^{\mathrm{total}}}{\mathrm{d}\Omega} = \frac{\mathrm{d}\sigma^{\mathrm{Born}}}{\mathrm{d}\Omega} + \sum_{L=0}^{L_{\max}} (A_L - A_L^{\mathrm{Born}}) P_L(\cos\theta), \qquad (1)$$

where the A_L coefficients are obtained as partial wave expansions up to some $l_{\max}$ (see, e.g. Itikawa 2000). This procedure was named the multipole extracted adiabatic nuclei (MEAN) method by Padial and Norcross (1981) who originally proposed it. The main problem with this is that one or more of the differences in the sum can become negative leading, potentially, to negative values of the DCS for certain angles. Negative cross sections are, of course, unphysical. It has therefore been suggested (Fliflet and McKoy 1980, Itikawa 2000, Rescigno *et al* 1992) that manipulating the scattering amplitude is a better procedure. However, while DCSs arising from the Born closure method for the scattering amplitude are always positive for all angles, they frequently show unphysical structures at angles where there is a change between the dominance of the scattering process by the dipole potential for forward scattering and short-range interactions dominating the potentials for sideways scattering, see Khakoo *et al* (2008a) for a recent example.

Our preferred approach is to use the MEAN method, as implemented in the program POLYDCS (Sanna and Gianturco 1998). Furthermore, we only consider transitions from the $J_{K_a K_c} = 0_{00}$ ground state of water. This is because Okamoto *et al* (1993) showed that the DCS does not depend on the initial rotational state of the target molecule unless the scattering angle is very close to 0°. This means that theoretical DCS can be computed for the target in its ground rotational state, independent of the (rotational) temperature of the corresponding experiment. It would only appear to

be necessary to average over a particular rotational state distribution at energies close to rotational thresholds, where the ANR approximation becomes invalid (Morrison 1988). We note, however, that ANR rotational cross sections are, in the present work, threshold-corrected using a simple kinematic ratio (Chandra and Temkin 1976).

So far discussion has concentrated on elastic and rotationally inelastic cross sections; however, for some applications momentum transfer cross sections are important. Momentum transfer cross sections are insensitive to forward collisions since these do not result in any change in the momentum of the colliding particles. They are therefore easier to determine experimentally. Previous studies have shown good agreement between theory (Faure *et al* 2004b) and experiment (Cho *et al* 2004, Johnstone and Newell 1991) for electron–water momentum transfer cross sections. So far there are no corresponding measurements for positron collisions, although it is likely that the calculated momentum transfer cross sections (Baluja *et al* 2007) will give agreement similar to that found for the electron case.

3. Electron–water collisions

The calculations discussed below were all performed using the *R*-matrix method and H_2O wave functions developed by Gorfinkiel *et al* (2002) whose calculations considered partial waves up to *g* waves i.e. $l_{max} = 4$ and the 7 lowest electronic states of water in the close-coupling expansion. Gorfinkiel *et al* (2002) calculated cross sections for different molecular geometries, later extended to all geometries (Gorfinkiel *et al* 2005). Here, we only use the *R*-matrix calculations performed at the equilibrium geometry of H_2O using an *R*-matrix sphere of $10a_0$. This model gives a dipole moment of 1.864 D, which can be compared to the experimental value of 1.854 D (Clough *et al* 1973, Lodi *et al* 2008). DCS were calculated following the procedure implemented in the program POLYDCS (Sanna and Gianturco 1998).

The calculated DCS were summed over all final rotational states. As mentioned above, Okamoto *et al* (1993) have shown that these DCS do not depend on the initial rotational state of the target unless the scattering angle is very small (less than 1° for a collision energy of 1 eV). For this reason, DCS calculations performed with water in its ground rotational state are usually directly comparable to measurements done at room temperature (see, e.g. Faure *et al* (2004b)). However, as the collisional energy decreases, the critical angle increases (see equation (22) in Okamoto *et al* (1993)) and the neglect of temperature effects becomes questionable. In practice, we found these effects to remain mostly negligible at 300 K even for the lowest collisional energy presently measured (i.e. 18 meV). In the following, all the cross sections have therefore been calculated for the water molecule in its ground rotational state. A proper average over the experimental rotational distribution should prove crucial at very low energy only; this would correspond to the vicinity of the (dominant) rotational thresholds (a few meV) where the present approach becomes invalid.

We note that there has only been one attempt (Jung *et al* 1982) to measure electron impact rotational excitation cross sections for water over a range of energies. The limited data available in this study meant that such cross sections could only be obtained on the assumption that transitions with $\Delta J > 1$ could be neglected. Faure *et al* (2004a) show that this condition is not in fact obeyed well enough for the experiment to yield reliable rotationally resolved cross sections, although the rotationally summed cross sections obtained by Jung *et al* (1982) agree well with those calculated *ab initio*. At present it would appear that theory represents the only route to rotationally resolved cross sections and rates (Faure *et al* 2004a, Gianturco *et al* 1998); a similar conclusion was reached by Itikawa and Mason (2005). More recently, however, Čurík *et al* (2006) have measured ultralow energy cross sections for electron water collisions. This study yields cross sections integrated over all backward angles, *effective* ICSs.

Čurík *et al* (2006) also use a semi-empirical, quantum defect theory approach to calculate low-energy, state-to-state rotational excitation cross sections for water. Their approach involves tuning to the measured backward and effective ICSs given in the same paper. Their rotational excitation cross sections are in very good agreement with the *ab initio* results of Faure *et al* (2004a).

In order to compare our theoretical cross sections with those measured by Čurík *et al* (2006), one must account for the experimentally missed forward solid angle which depends on the position along the collision chamber. Effective ICSs were thus calculated by a numerical (trapezoidal) integration and then averaging the DCS over nine effective solid angles defined along the axis of the experiment. Backward cross sections were obtained by a numerical (trapezoidal) integration of the DCS over the backward 2π steradians. Note that integral and backward cross sections were computed both from our theoretical DCS (Faure *et al* 2004b) and the recent differential data of Khakoo *et al* (2008b). These latter were linearly interpolated at angles larger than 5° and additionally extrapolated at smaller angles using pure Born-dipole results.

As shown in figure 1, the agreement between the present theory and the experiment of Čurík *et al* (2006) is generally very good, particularly for the effective ICS. The small departure between theory and experiment below 40 meV might reflect non-adiabatic rotational effects which are not properly taken into account by our calculations. Including such effects really requires a close-coupling treatment of the rotational motion (Henry 1970). We note, however, that recent studies have shown the ANR to be surprisingly effective near threshold (Feure *et al* 2006). At energies above 1 eV, the experimental ICS also shows an enhancement which is not reproduced by our calculations. However, a rise in the pure elastic cross section was also observed above 3 eV (see Feure *et al* 2004b) and it was attributed to the Feshbach resonance of $^2B_1$ symmetry that lies just below the first excited electronic state at about 7 eV (Gorfinkiel *et al* 2002). As the position of this resonance depends strongly on the molecular geometry (Gorfinkiel *et al* 2002, Haxton *et al* 2004), inclusion of vibrational motion (in particular bending) is likely to have a strong effect on the cross section in this resonance region. The agreement with the data of Khakoo *et al* (2008b) is also very reasonable. We note in particular that our theoretical results lie between both set of experimental data at energies below 3 eV.

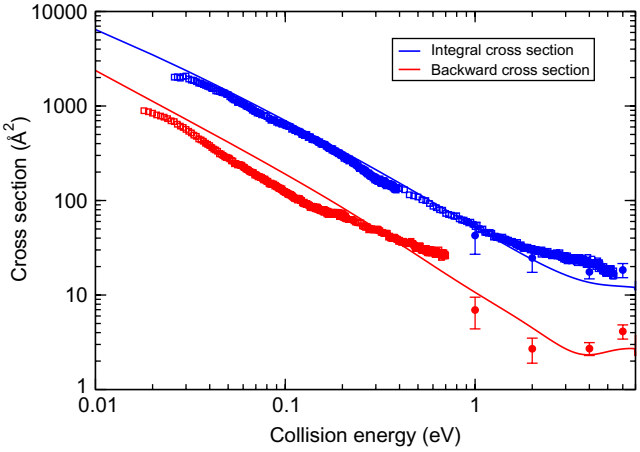

Figure 1. Elastic (rotationally summed) *effective* integral and backward cross sections as a function of the collision energy. Solid lines denote the present theoretical results. Open squares give the experimental data of Čurík *et al* (2006) while filled circles correspond to the differential data of Khakoo *et al* (2008b). See text for explanations.

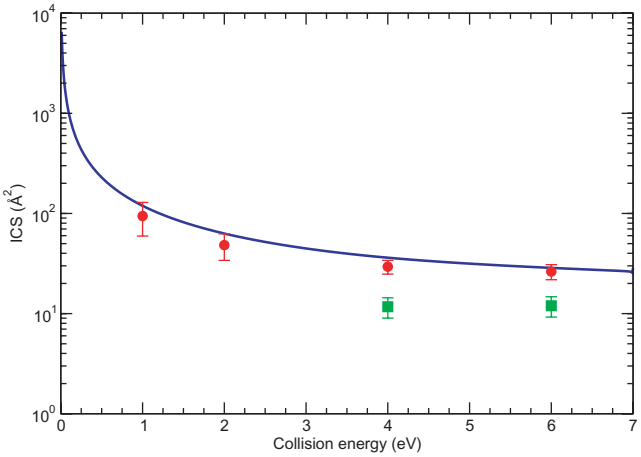

Figure 2. Elastic (rotationally summed) integral cross sections as a function of the collision energy. The solid line denotes the present theoretical results. Filled squares and circles give the experimental data of Cho *et al* (2004) and Khakoo *et al* (2008b), respectively.

The effective ICS in figure 1 correspond to the integration of the DCS over the experimental solid angle. As a result, these ICS are smaller than those published by Faure *et al* (2004b) by up to a factor of 2 at the highest energies (see also figure 2). This reflects the missed forward angles at which the DCS are heavily peaked. At the lowest energies (<20 meV), however, the peak is much less pronounced and the theoretical ICS in figure 1 agree to within a few percent with those plotted in figure 2.

It should be noted that while the effective ICS agrees well with the calculated ones above 40 meV, figure 1 suggests that the calculations overestimate somewhat the contribution due to backward scattering at energies below 200 meV. Backward scattering is not strongly influenced by the long-range dipole potential but is sensitive to short-range potential, suggesting that the effective short-range potential of the calculations is a little too hard. This observation is consistent with the results of recent studies (Gorfinkiel and Tennyson 2005, Tarana and Tennyson 2008) which show that it is only possible to get a converged description of the attractive polarization effects by using extended close-coupling expansions which also allow for effects of coupling to the continuum. The molecular *R*-matrix with pseudostates (RMPS) (Gorfinkiel and Tennyson 2004) allows for the inclusion of such effects but so far RMPS calculations have not been attempted for water. Finally, we note that the experimental, backward cross sections above 1 eV given in figure 1, which are derived from the differential measurements of Khakoo *et al* (2008b), are actually based only on measurements at three angles and none above 130°. The errors given in the figure are therefore likely to be underestimates.

In figure 2, the theoretical ICS corresponding to the integration of DCS over the full solid angle are compared to the experimental results of Cho *et al* (2004) and Khokoo *et al* (2008b). The agreement with the ICS of Khokoo *et al* (2008b) is very good while the results of Cho *et al* (2004) are lower by a factor of 2–3. Since the agreement between the three sets of DCS is much better (see figure 3), the differences in the ICS clearly reflect the extrapolation procedure used by Cho *et al* (2004). Indeed, in contrast to Khakoo *et al* (2008b), Cho *et al* (2004) did not apply Born-dipole results to their data, which is necessary to properly account for the strong forward scattering (see discussion in Khakoo *et al* (2008b)).

Finally, it is worth saying a few words about the DCS themselves. Faure *et al* (2004b) already noted that they got excellent agreement between their calculations and the measured DCSs of Johnstone and Newell (1991) and Cho *et al* (2004), even though the ICS did not give good agreement. Figure 3 gives a similar comparison with the more recent measurement of Khakoo *et al* (2008b). Again agreement is good although we note that the DCS of Khakoo *et al* (2008b) tend to be higher than other data at energies above 4 eV; they are also below the present theoretical results at lower energies for backward angles.

4. Positron–water collisions

Positron–water collisions have been less studied both theoretically and experimentally than their electron analogues and, in particular, there are no very low-energy measurements available. Furthermore collisions with positrons introduce a new channel, positronium (Ps) formation, at 6.8 eV below the ionization threshold. Given this complication we only consider energies up to 10 eV, as above this Ps formation becomes significant.

Theoretically, calculations of positron scattering cross sections are in general harder than the corresponding ones with electrons due to the very strong electron–positron correlation effects. The solution has often been to introduce semi-empirical factors into such calculations (Franz *et al* 2008). The dominance of the dipole interaction, however, means that positron collisions with strongly dipolar molecules are actually easier to model reliably and here we stick to purely *ab initio* procedures. In particular, we focus on the *R*-matrix calculations of Baluja *et al* (2007), which are the positron analogue of the electron calculations of Faure *et al* (2004b) discussed above; these positron–water calculations are in good agreement with the single-centre expansion study of Gianturco *et al* (2001), see figure 4.

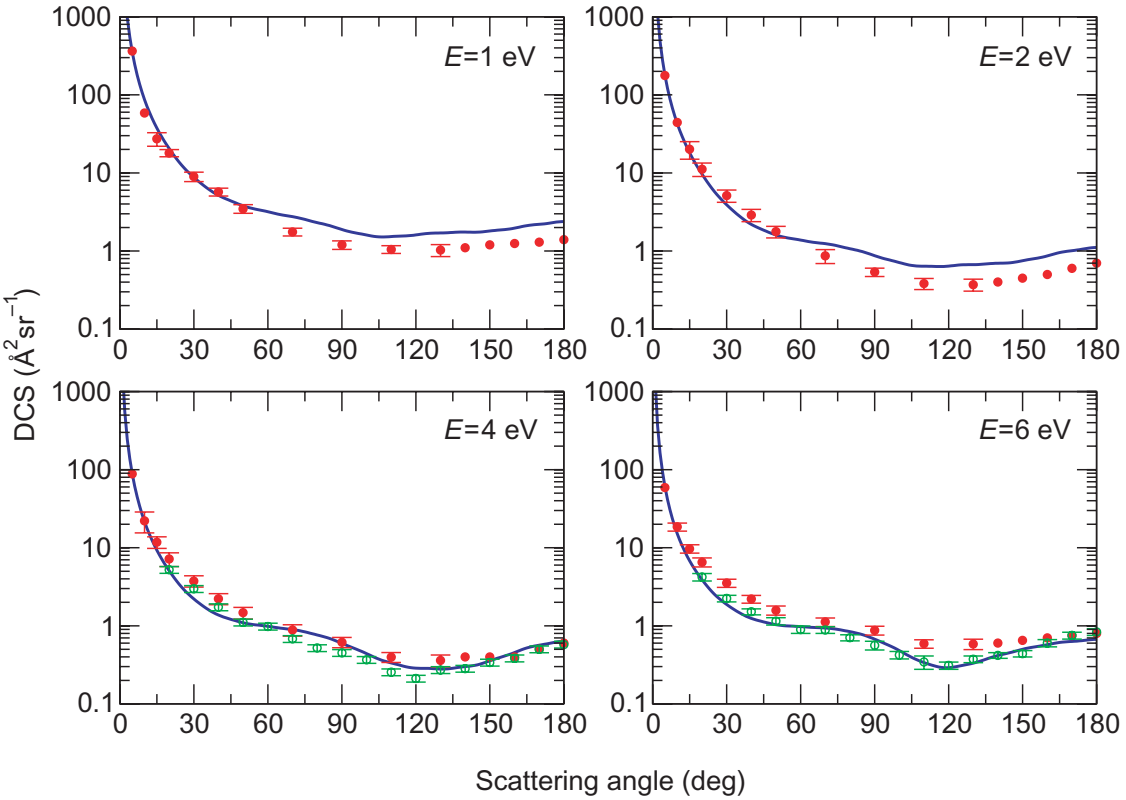

Figure 3. Elastic (rotationally summed) differential cross sections at collisional energies of 1, 2, 4 and 6 eV. The solid line denotes the present theoretical results. Filled squares and circles give the experimental data of Cho *et al* (2004) and Khakoo *et al* (2008b), respectively.

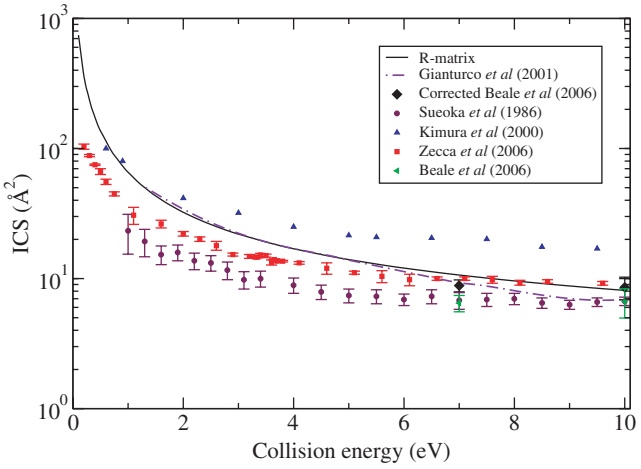

Figure 4. A comparison of theory (Gianturco *et al* 2001, Baluja *et al* 2007) with uncorrected experiment (Sueoka *et al* 1986, Kimura *et al* 2000, Zecca *et al* 2006, Beale *et al* 2006) and corrected one for integral cross sections for positron–water collisions as a function of the collision energy.

As noted above the measurements of elastic positron–molecule collision cross sections give less good agreement with each other at least in part due to the fact that most of them are uncorrected for problems associated with detecting collisions which are strongly forward scattered. However, we note that the most recent study, due to Beale *et al* (2006), actually characterizes the acceptance angle for the apparatus used. Here, we therefore give a theoretical correction to Beale *et al*'s measured cross section based on theoretical estimates of the collisions into the low angle region to which their measurements were not sensitive. In this fashion we aim for the best estimate of the cross section in this region.

Our procedure was as follows. We developed a functional form which reproduced our DCS at low angles. This function was then integrated to give the correction to the total cross section. Beale *et al*'s acceptance angle is energy dependent and corresponds approximately to angles above 12° for collisions at 7 eV and above 11° for 10 eV collisions.

The DCS at low energy is very sharply peaked at 0° so finding a satisfactory function with which to perform the fit was not straightforward. After some trial and error we used a function of the form

$$F(\theta) = C_0 + \sum_{i=1}^{3} C_i \theta^{-i} \tag{2}$$

to fit the low angle DCS. This fit was tested for both positron and electron DCSs and using it we were able to get residuals of less than 1% at angles below 10°. Coefficients for the fits are given in table 1.

We then integrated the fit function equation (2) analytically over the whole range 0–180°:

$$\sigma^{\mathrm{corr}} = \int x(\theta) F(\theta) \sin\theta \, \mathrm{d}\theta, \tag{3}$$

where $x(\theta) = \mathrm{e}^{-\lambda\theta^2}$ is the acceptance profile given by Beale *et al* (2006), and for θ in degrees $\lambda = 0.0206$ at 7 eV, 0.0266 at 10 eV. In practice, $x = 0$ for θ greater than 14°. For positrons, this procedure gives $\sigma^{\mathrm{corr}} = 2.346$ Å^2 at 7 eV. This value is very close to the value obtained by fitting the electron DCS data of Faure *et al* (2004b) which gives 2.340 Å^2. At 10 eV,

Table 1. Coefficients for fit function given by equation (2) used to represent the angular behaviour of the positron (and electron) DCS in the forward region. Angles are given in degrees for a DCS in $Å^2/^\circ$. A separate fit is given for each collision energy, E.

	Electron	Positron	Positron
E	7 eV	7 eV	10 eV
C_0	0.918729	−0.292103	−0.578577
C_1	0.0717311	0.033907	0.129589
C_2	0.383493	0.386788	0.265902
C_3	−0.0000129725	−0.0000131518	0.0000463739

the correction for positrons is 1.904 $Å^2$. We note that at lower collision energies the proportion of particles scattered into the forward 10° is much higher.

Our best estimate, σ^{final}, for the elastic cross section is then obtained using

$$\sigma^{\text{final}} = \sigma^{\text{obs}} + \sigma^{\text{corr}}, \tag{4}$$

where σ^{obs} are the measured cross sections reported by Beale *et al* (2006).

Figure 4 compares the calculated total positron water cross sections of Gianturco *et al* (2001) and Baluja *et al* (2007) with the published measurements (Sueoka *et al* 1986, Kimura *et al* 2000, Zecca *et al* 2006, Beale *et al* 2006) and the corrected experimental results. We can see that the corrected data give agrees better than the uncorrected results. In particular, we note that the error bars for corrected experimental results are the same as original experimental results (Beale *et al* 2006) and therefore must be an underestimate of the error associated with σ^{final}.

Kimura *et al* (2000) used electron DCS measurements to characterize the correction required to their earlier (Sueoka *et al* 1987) positron collision measurements. Our results do indeed confirm that the forward cross sections for the electron case are very close to those for the positron one if we assume that the acceptance profiles $x(\theta)$ for electrons and positrons are the same. The discrepancy with the corrected measurements of Kimura *et al* (2000), which appear to overestimate the total cross section at energies below 10 eV, must therefore arise from another source.

5. Conclusions

We have considered electron and positron collisions with the polar water molecule for collision energies below 10 eV. Provided that an appropriate treatment of the long range dipole interactions involved in these collisions is used, it would appear that various different theoretical methods yield very similar results for both the electron and the positron cases. This situation is not so clear cut experimentally where issues with the acceptance angle of the experiment for strongly forward scattered collisions leads to serious difficulties in determining total collision cross sections. However, as demonstrated above, the most recent experiments, while not always agreeing with earlier measures, do give results consistent with the available theoretical treatments. We therefore suggest that the present theory provides the best method of obtaining reliable elastic, and rotationally inelastic, cross sections for low-energy collisions for both electron and positron collisions with strongly dipolar molecules.

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