Low energy elastic electron scattering from polyatomic targets.

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Abstract: New differential cross-section measurements for elastic electron scattering from ethylene (C₂H₄), three primary alcohols, methanol (CH₃OH), ethanol (C₂H₅OH) and propanol (C₃H₇OH) are reported. The measurements are obtained using the relative flow method with a thin aperture as the collimating target gas source. The relative flow method is applied without the molecular diameters restriction imposed by the relative flow pressure condition on helium (the calibrating gas) and the unknown gases (the primary alcohols). The experimental data were taken at incident electron energies of 1eV, 2eV, 5eV, 10eV, 15eV, 20eV, 30eV, 50eV and 100eV, but only a brief survey of these results will be made here. The experimental results are compared to theoretical differential cross-sections are obtained by using the variational multi-channel Schwinger method. Initial comparisons between theory and experiment show that present theory is well-able to model low electron scattering from these polyatomic targets.

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1. Introduction.

Accurate differential elastic scattering cross-sections for low energy electrons from atomic and molecular gases have provided very useful tests of electron scattering theory, and has resulted in measurement/modeling of other differential scattering processes such as excitation, ionization and electron attachment [1]. These processes play important roles in a range of processes in plasmas [2, 3], astrophysics [4] and in DNA break-up [5]. Elastic electron scattering, a dominant process in the transport of low energy electrons through gaseous media and condensed matter, is important in our understanding of the transport of electrons in various media such as organic tissue made of biomolecules [6], planetary atmospheres [4] and interstellar media, lasers and fusion plasmas [7].

Recently, we developed a novel version of the relative flow method using an aperture gas collimating source, to replace our conventional tube collimating source [8]. The aim was to be able to apply the relative flow method without the restriction imposed by the requirement that the pressures behind the source be in the ratio of the gas kinetic molecular diameter squared. This is because the aperture source’s gas profile is not dependent on the source pressure over a large pressure range up to when the mean-free path of the gas behind the source becomes comparable to the thickness of the aperture. This innovation is therefore useful for large molecules where the values of these diameters are not available or not
accurately known. A series of recent measurements in Tetrahydrofuran [9,10,11] have used a molecular diameter from a very old source [12]. Whereas these measurements show good qualitative agreements (shapes), there exist some quantitative disagreements (magnitudes) and the situation could be improved, if the molecular diameter requirements in these experiments were eliminated. A recent important synopsis of these measurements which includes further work using an aperture-like source by Allen [13], shows that there exists a significant dependence on the pressure ratios used which affect the cross-section ratios.

Presently, there are no measurements of elastic electron scattering (differential) cross-sections from most polyatomics molecules since the gas kinetic molecular diameters of these polyatomics are unavailable or unreliable. In particular, for the alcohols, or molecules with permanent dipole moments, one expects the gas kinetic molecular diameter to deviate significantly from that of a hard-sphere type of molecule, and make these sticky targets more difficult to work with in the conventional relative flow type of experiment.

In this paper report the extension of our recent implementation of the relative flow method, using an aperture source [8], to alcohols. The proposed method is a simple modification of the conventional relative flow method in which a collimating tube source is replaced by an aperture source. The results are supported by new large theoretical calculations using the variational multi-channel Schwinger method with polarization effects included [14].

2. Method

The most successful method that has been used for measuring differential elastic electron scattering from relatively light atomic and molecular targets has been the relative flow method, which was first formulated by Srivastava et al. [15] and has been applied extensively in the last 30 years to determine elastic electron scattering DCSs for many (mostly light) targets. The reader is referred to the extensive review of Brunger and Buckman [1] for the most recent summary of this work. The experimental apparatus (spectrometer, vacuum chamber, control equipment) has been detailed in previous papers, e.g. Khakoo et al. [8]. The target aperture of 0.3mm diameter was located on a thin disc of 0.025mm thick brass shim stock located flush at the end of a 6.35mm o.d. and 4.3mm i.d. brass tube [8]. The tube was incorporated into a moveable source [16] arrangement.

We followed the recipe given in [17] to calibrate our relative flow rate (RFR) vs. the pressure behind the source \( P_s \). A second-order polynomial in the input gas pressure behind the source \( P_s \) served adequately to express relative flow rate as a function of \( P_s \) in the form \( \text{RFR} = aP_s(1+\varepsilon P_s) \). The coefficients \( a \) and \( \varepsilon \) are related to the mass and the molecular diameters of the gases [18,19]. These coefficients are given in table 1 for all gases used in our aperture gas system to date. As can be seen the gas kinetic molecular diameters determined from \( a \) and \( \varepsilon \) values from our flow measurements for the alcohols are large, typifying the long-range dipole forces these molecules must exert on each other as compared to hard-sphere molecules. However, the ‘\( a \)’ term for these molecules deviates markedly by a factor of \( \approx \sqrt{2} \) from its molecular mass dependence (last column in table 1: Mass Factor). The reason for this is not certain, but it could be speculated that these molecules form dimers during their flow through the gas system from the liquid phase into the gas phase. This is under discussion at the present time.
We operated our experiment at low pressures, typically <2 Torr for He, <0.2 Torr for CH$_3$OH, <0.12 for C$_2$H$_5$OH and <0.1Torr for C$_3$H$_7$OH (n-propanol), which are well below the critical mean-free path (when this equals the aperture thickness of 0.025mm) conditions for our system. The experimental chamber typically remained in the pressure range of 0.7 to 2 x 10$^{-6}$ Torr for the range of pressure used in this work and the incident electron current remained stable during operation within 10% at maximum.

| Gas | T (C) | P$^*$ | P | a | $\delta$ (cm) | M | a$^*$/$M$ | s/$\delta^*$ | Mass Factor |
|-----|------|------|--|---|--------------|--|----------|-----------|------------|
| H$_2$ | 22 | 0.2290 | 0.2181 | 0.2181 | 1.9501 | 2.74E-08 | 2.016 | 0.310 | 1.40E+15 | 1 |
| He | 22 | 0.1146 | 0.1551 | 0.1551 | 0.7391 | 2.18E-08 | 4.002 | 0.310 | 1.56E+15 | 1 |
| He | 47 | 0.1028 | 0.1611 | 0.1611 | 0.6380 | 2.18E-08 | 4.002 | 0.322 | 1.34E+15 | 1 |
| He | 74 | 0.1064 | 0.1615 | 0.1615 | 0.6587 | 2.18E-08 | 4.002 | 0.323 | 1.39E+15 | 1 |
| N$_2$ | 22 | 0.1261 | 0.0596 | 0.0596 | 2.1145 | 3.75E-08 | 28.02 | 0.316 | 1.50E+15 | 1 |
| C$_2$H$_4$ | 22 | 0.2305 | 0.0566 | 0.0566 | 4.0705 | 4.95E-08 | 28.03 | 0.300 | 1.66E+15 | 1 |
| CH$_3$OH | 47 | 0.2214 | 0.0387 | 0.0387 | 5.7222 | 6.20E-08 | 32.04 | 0.310 | 1.49E+15 | 2 |
| C$_2$H$_5$OH | 47 | 0.2582 | 0.0352 | 0.0352 | 7.3462 | 7.02E-08 | 46.07 | 0.337 | 1.49E+15 | 2 |
| C$_3$H$_7$OH | 74 | 0.2328 | 0.0288 | 0.0288 | 8.0953 | 7.35E-08 | 60.11 | 0.315 | 1.50E+15 | 2 |

Table 1. Gas flow parameters for the aperture source for various gases. See text for discussion.

We took measurements of elastic scattering from CH$_3$OH and C$_2$H$_5$OH and C$_3$H$_7$OH at $E_0$ values of 1eV, 2eV, 5eV, 10eV, 15eV, 20eV, 30eV, 50eV and 100eV at scattering angles of 5° to 130°, over a coarser interval (20°) at large scattering angles than at small scattering angles (10°). The data were normalized via the relative flow method to the established He DCS values from [20] and [21].

3. Results:

A brief review of our DCS measurements is reported here. More complete reports on this are currently in progress. The methanol DCSs are compared to theory in figures 1 and for ethanol in figures 2. The Schwinger multi-channel theory both includes (Born dipole-polarization) and excludes (static) dipole-polarization effects and was developed and computed by theoretical groups in Brazil and the USA [14]. Agreement of our experiment theory is qualitatively excellent at all $E_0$ values for CH$_3$OH and C$_2$H$_5$OH. It is especially good at lower $E_0$ values where both the dipole-polarization calculations from Brazil and from USA show agreement. Clearly, getting the dipole-polarization correct becomes very important for theory at low $E_0$ values, e.g. at 5eV or below when compared to only the static potential calculations. At $E_0$=10eV, 15eV, 20eV and 30eV agreement between theory and experiment is very good.
The experiment remains lower than theories for large angles at $E_0=100\text{eV}$ and has a steeper rise at small $\theta$ values. Even at low energy (e.g. 5eV), polarization in the scattering (steep forward-peaking) is strong, and is also evident to a similar extent for $\text{C}_2\text{H}_5\text{OH}$. However at higher $E_0$ values, the differences between theory and experiment are larger for $\text{C}_2\text{H}_5\text{OH}$ than for $\text{CH}_3\text{OH}$. The shapes of the DCSs for these 3 alcohols are almost identical as can be observed in figure 3 at $E_0=30\text{eV}$. We note that the small angle DCSs show similarly strong polarization dependence, which is expected as these alcohols have almost
equal dipole moments (\(\approx 1.6\) Debyes). However, at lower energies, we observe significant differences in large angle behavior.

![Figure](image.png)

**Figures 3.** Sample of present DCSs (connected by dashed lines) with error bars for elastic electron scattering from methanol at (a) \(E_0=30\text{eV}\) and (b) \(5\text{eV}\). Legend: ▲ Propanol, ● Ethanol and ■ Methanol

### 4. Conclusions.

In conclusion, the present work shows that theory and experiment have made significant progress towards the determination of DCSs for elastic scattering from large polyatomics, a fact that was not considered possible until recently. Presently we are considering the extension of our measurements to butanol, \(C_4H_9OH\).

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