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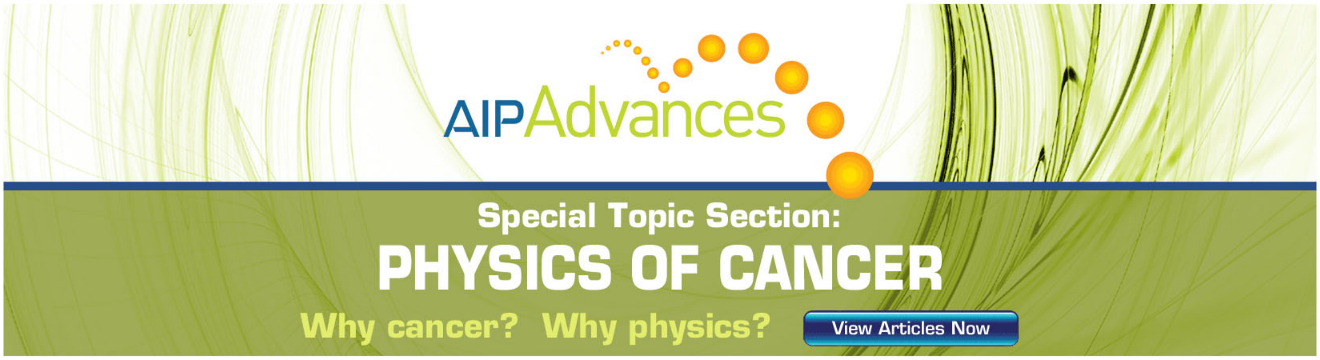

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Differential elastic electron scattering cross sections for CCl_4 by 1.5–100 eV energy electron impact

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We report absolute elastic differential, integral and momentum transfer cross sections for electron interactions with CCl_4. The incident electron energy range is 1.5–100 eV, and the scattered electron angular range for the differential measurements varies from 15°–130°. The absolute scale of the differential cross section was set using the relative flow technique with helium as the reference species. Comparison with previous total cross sections shows good agreement. Atomic-like behaviour in this scattering system is shown here for the first time, and is further investigated by comparing the CCl_4 elastic cross sections to recent results on the halomethanes and atomic chlorine at higher impact energies [H. Kato, T. Asahina, H. Masui, M. Hoshino, H. Tanaka, H. Cho, O. Ingólfsson, F. Blanco, G. Garcia, S. J. Buckman, and M. J. Brunger, J. Chem. Phys. **132**, 074309 (2010)]. © *2011 American Institute of Physics*. [doi:10.1063/1.3669429]

I. INTRODUCTION

Carbon tetrachloride (CCl_4) has been extensively used in many industrial applications such as in fire extinguishers, as a cleaning agent, a refrigerant precursor, and as a feed gas for plasma processing discharges. It was largely used to produce chlorofluorocarbons (CFCs), mainly CCl_3F and CCl_2F_2, and these refrigerants have been shown to play a major role in ozone depletion at stratospheric altitudes.[1–3] The primary motivation for measurements of electron scattering cross section data for CCl_4 is the need for a reliable database of information that can be used to model such interactions and applications of this molecule.

Previous experimental work on this molecule includes the grand total cross section (TCS) measurements by Szmytkowski *et al.*[4] covering an energy range of 0.5–200 eV. This TCS was also measured by Hamada and Sueoka[5] who covered the range of 0.7–400 eV, whereas the measurements of Jones[6] lie in 0.6–50 eV energy region, and Zecca *et al.*[7] in 75–4000 eV. Other relevant studies include the total (elastic and inelastic) cross sections of Jiang *et al.*[8] (and see references therein) over the energy range of 10–1000 eV, the elastic scattering calculations by Natalense and co-workers[9–11] using the Schwinger multichannel (SMC) method and the calculations of Curik *et al.*[12] who applied a close-coupling approach. CCl_4 is a non-polar molecule but has a dipole molecular polarizability (α) of considerable magnitude, 11.2 $\times 10^{-24}$ cm^3,[13] and this is expected to play a key role in determining the magnitude and the angular and energy dependent behaviour of the low to intermediate-energy electron-scattering cross sections. To our knowledge there is only one experimental elastic differential cross section (DCS) for the CCl_4 molecule by Dimon *et al.*[14] at impact energies of 70, 200, and 400 eV, however, there are no elastic DCS for the CCl_4 molecule in the wider energy range covered in the present work.

In a recent pioneering work on elastic electron scattering from the halomethane molecules CH_3X (X = F, Cl, Br, and I),[15] atomic-like behaviour in these scattering systems was also considered by comparing these halomethane elastic cross sections to results from other previous works for the corresponding noble gases Ne, Ar, Kr, and Xe, respectively. Moreover, by making use of optical potential calculations and assuming an independent atom configuration including screening corrections for larger molecules (IAM-SCAR),[16] Kato *et al.*[15] have shown for the first time a qualitative correspondence in the DCSs, at each energy and for each species of an atomic-like effect in the scattering process. Therefore, they have concluded that the charge distribution of the electrons in the target molecule plays an important role in the energy range that was considered, i.e., 50–200 eV.

The present study represents a new and original experimental contribution for the measurement of elastic DCS

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data for CCl_4. This study, in combination with other previous measurements of excitation and ionisation also enables a meaningful comparison to be made against the TCS measurements.[4–8]

In Sec. II, we provide details on the experimental apparatus and the measurement techniques that have been used. In Sec. III, we present a brief discussion on the fitting and integration methods used and in Sec. IV the experimental results are presented together with a discussion and comparison with other results, where that is possible. Finally some conclusions that can be drawn from this study are given in Sec. V.

II. APPARATUS AND OPERATING PROCEDURES

The electron spectrometer used in the present work has been described in detail elsewhere,[17] so only a brief discussion will be presented here. A monochromatic electron beam is generated with a hemispherical electron monochromator and crossed at right angles with an effusive molecular beam that enters the interaction region through a 5 mm long capillary with a 0.3 mm inner diameter. After the electron interaction with the target gas, the scattered electrons are energy analysed with a hemispherical electron analyser, which can rotate about the gas jet, and detected by an electron multiplier. Both the electron monochromator and the energy analyser are enclosed in separate, differentially pumped housings. This greatly reduces the effect of background gases and improves the stability of the spectrometer, particularly when reactive gases are being studied. The typical base pressure in the main chamber was 2.0×10^{-5} Pa and, upon gas admission (CCl_4), this increased to a pressure of 2.0×10^{-4} Pa. In addition, the spectrometer and molecular beam source are heated to a temperature of about 60 °C, in order to reduce any possible contamination during the measurements. The gas sample was supplied from Wako Pure Chemical Industries Ltd. (Osaka, Japan) and used as delivered. The stated purity was 99.5%.

In the current experiments, the energy resolution of the incident electron beam was 40 meV [full width at half maximum (FWHM)], with incident electron currents of a few nanoamperes (depending on the initial electron energy). Such a value means that, in principle, there could be contributions to the elastic signal from some of the lower lying vibrational modes of CCl_4. However, in the energy range above 10 eV, these possible vibrational contributions are expected to be very small compared to the elastic intensity, and thus are not expected to make any significant contribution to the measured elastic cross sections, whereas below 10 eV, those have been extracted by deconvoluting the energy loss spectra with the Gaussian profiles and separated from the elastic DCSs. The incident electron energy was calibrated with respect to 19.365 eV, ^2S resonance in He (Ref. 18) and with respect to the $^2\Pi_g$ resonance in N_2 for the vibrational excitations around 2.4 eV.[19] The hemispherical electron analyser is placed on a turntable stage and can be rotated from –10° to +130°, with respect to the incident electron beam, with an angular resolution of about ± 1.5° (FWHM).

The absolute scale of the present DCSs was set using the relative flow technique,[20] in which the ratio of the elastic scattering intensity for the CCl_4 molecules to that of helium under the same experimental conditions was determined. Then employing the known helium elastic DCSs, as reported in Boesten and Tanaka,[21] we can derive the CCl_4 DCSs of interest. The values of the hard sphere diameters for He and CCl_4 were taken as 2.18 and 6.53 Å, respectively. Note that the value for CCl_4 was obtained from the atomic radii of C and Cl and the bond length. We estimate that the experimental uncertainties on the resulting CCl_4 DCS lie in the range of 15%–20%, with the actual value depending on the specific incident electron energy (E_0) and scattered electron angle (θ) under consideration. This overall error is largely comprised of an uncertainty in the reference helium DCSs, an uncertainty in keeping the correct flow conditions for the relative flow technique and, to a much lesser extent, an error associated with the statistical accuracy of the data and the stability of the incident electron beam (<1%).

Elastic integral cross sections (ICSs) and momentum transfer cross sections (MTCSs) are subsequently obtained by integration of the CCl_4 DCSs, at each E_0, by making use of the well-known formula.[22] The DCSs for $\theta < 15°$ and $\theta > 130°$ are obtained by an extrapolation based on a modified partial-wave expansion including polarisation and the Born approximation for higher phaseshifts.[23] Due to the uncertainty involved in the extrapolation process, we estimate an error of ~30% in the present elastic ICSs and MTCSs.

III. FITTING AND INTEGRATION METHODS

The measured elastic DCSs were extrapolated with the help of two fitting methods and then integrated numerically. Briefly, we have made use the Simpsons' rule and the quadrature by parts in very small steps. Both methods showed very good agreement within 1% error, which was included within the experimental error. In the first step, the fitting formulas were used by a single expression as

$$\frac{d\sigma(\theta)}{d\Omega} = |f(\theta)|^2 ,$$

and

$$2ikf(\theta) = N(k)\left\{\sum_{\ell=0}^{L}[S_\ell(k)-1](2\ell+1)P_\ell(\cos\theta)+C_L(\theta)\right\}$$

with

$$C_L(\theta) = 2i\pi\alpha k^2\left\{\frac{1}{3}-\frac{1}{2}\sin\left(\frac{\theta}{2}\right)-\sum_{\ell=1}^{L}\frac{P_\ell(\cos\theta)}{(2\ell+3)(2\ell-1)}\right\},$$

where C_L is the Born approximation of the higher phases in the Thompson form,[24] k is the wave number of the free electron, α (11.2×10^{-24} cm^3) the atomic/molecular polarisability, P_ℓ are the Legendre polynomials, and $f(\theta)$ is the scattering amplitude. In simple phase shift fitting,[25] $N(k) = 1$, and the scattering function becomes $S_\ell(k) = \exp(2i\delta_\ell)$ where δ_ℓ are the usual phase shifts. The parameter L is set to be as small as possible (generally <5) but still compatible with a given (noisy) dataset. In the second step, the DCSs for $\theta < 15°$ and $\theta > 130°$ were used as the guide for an extrapolation based on the theoretical results by the Schwinger

TABLE I. Differential (10^{-16} cm^2/sr), integral (10^{-16} cm^2), and momentum transfer (10^{-16} cm^2) cross sections for elastic scattering from CCl_4. Error on the DCS are typically 15%–20%, on the ICS ∼30% and on the MTCS ∼30%.

Angle	Impact energy (eV)									
(deg)	1.5	2.0	3.0	5.0	8.0	10	20	30	60	100
15	4.884	3.384	3.662	13.979	32.685	47.351	48.620	36.206	17.545	7.267
20	5.784	4.682	4.693	12.682	28.908	36.983	24.923	15.373	4.739	3.316
30	6.237	5.633	6.214	9.649	13.303	13.489	4.237	2.510	2.945	2.057
40	5.772	6.116	7.138	7.043	3.670	2.765	3.821	3.905	1.133	0.614
50	5.018	5.121	6.008	5.674	1.481	1.701	5.628	2.814	0.355	0.424
60	3.784	3.797	4.778	3.766	1.956	2.892	2.909	0.741	0.258	0.305
70	3.458	2.742	3.574	2.449	2.832	3.828	0.932	0.602	0.254	0.230
80	3.123	2.233	2.514	3.010	3.526	3.806	0.967	0.716	0.343	0.338
90	3.065	2.096	2.550	4.031	3.964	3.242	1.381	0.973	0.437	0.333
100	3.031	1.967	2.502	4.064	3.574	2.527	1.573	1.562	0.565	0.247
110	2.623	2.104	2.299	3.256	2.485	2.016	1.741	1.373	0.507	0.138
120	2.310	2.229	2.001	1.936	1.793	1.926	1.660	0.899	0.326	0.070
130	2.336	2.373	1.585	1.321	2.526	2.503	1.165	0.483	0.210	0.124
ICS	46.623	42.419	41.483	49.824	68.496	67.540	43.887	31.606	20.378	12.448
MTCS	38.422	34.781	30.639	34.454	54.961	39.358	25.862	13.605	8.776	5.432

multichannel method[10] at impact energies of 5, 8, 10, 20, and 30 eV, respectively. Note that the use of this formula assumes that the highly symmetrical configuration in the T_d symmetry of CCl_4 allows the adaptation of a central field theory. In the case of the theoretical results not being available, this approach has been employed to estimate the integral cross sections for many molecules, such as CH_4, CF_4, Si_2H_6, and GeH_4. The χ^2–fitting followed the well-known Boyden-Fletcher-Goldfarb-Fannon algorithm.[26,27] Due to the uncertainty involved in the extrapolation process, we estimate an error of ∼30% of the present elastic ICSs and MTCSs.

IV. RESULTS AND DISCUSSION

Table I gives the measured DCS, ICSs, and MTCSs for the elastic electron scattering from CCl_4. Figure 1 illustrates the angular distribution with the quality of the fits obtained and Figure 2 shows for comparison, the corresponding theoretical results from the application of the IAM-SCAR model for the Cl atom and the previous experimental DCS for CH_3Cl (Ref. 15) at impact energies of 60 and 100 eV. The ICS is plotted in Fig. 3(a) in comparison with the total cross section[4–8] and the SMC theoretical calculation. The momentum transfer cross section is shown in Fig. 3(b), again in comparison with the SMC calculation. A typical energy-loss spectrum is also shown in Figure 4, as an example of the decomposition at an impact energy of 1.5 eV and the scattering angle of 20° into the elastic and the vibrational excitations. In Figure 4, ν_1 and ν_3 represent the symmetric stretch and degenerate stretch, whereas ν_2 and ν_4 represent the degenerate deformation, respectively.

A. Elastic DCS

The overall total cross section in CCl_4[4–6] reveals the well-known Ramsauer-Townsend minimum at around 0.5 eV and two broad peaks, the first at ∼1.2 eV and the second at ∼6.8 eV with a shoulder at 10 eV. The Ramsauer-Townsend minimum in the $^2A_1$ state is outside of the present energy range from 1.5 to 100 eV, but we are interested in the effect that the resonances of the $^2T_2$ state (see below) have on

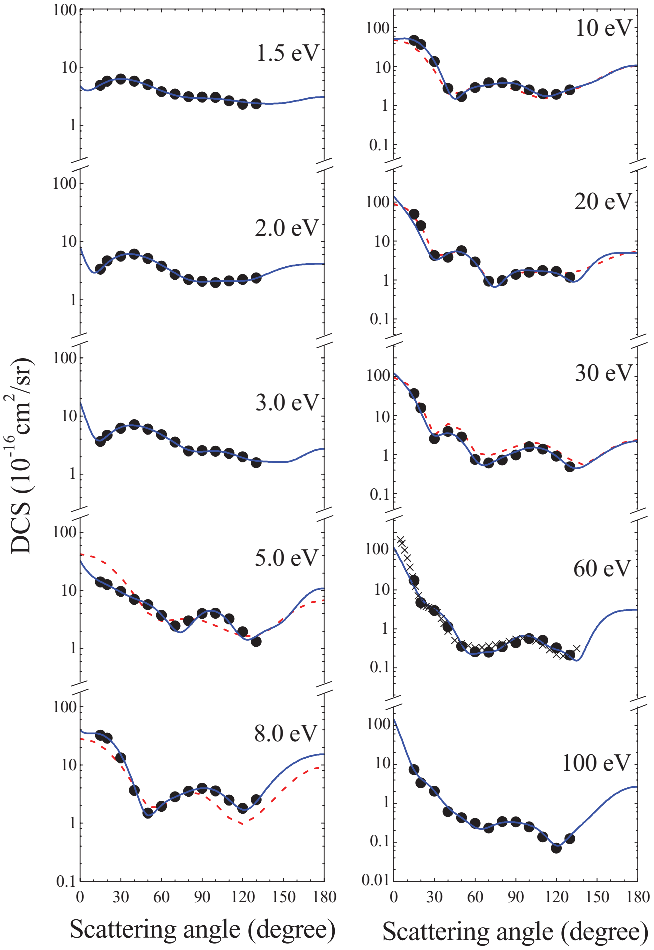

FIG. 1. Present DCS (10^{-16} cm^2/sr) for elastic electron scattering from CCl_4 in the incident electron energy region 1.5–100 eV; (●) present elastic DCS; (×) Dimon *et al.*[14] at 70 eV rescaled by a factor of 0.5. Solid curve: our fitting results; dashed curve: SMC calculation.[11]

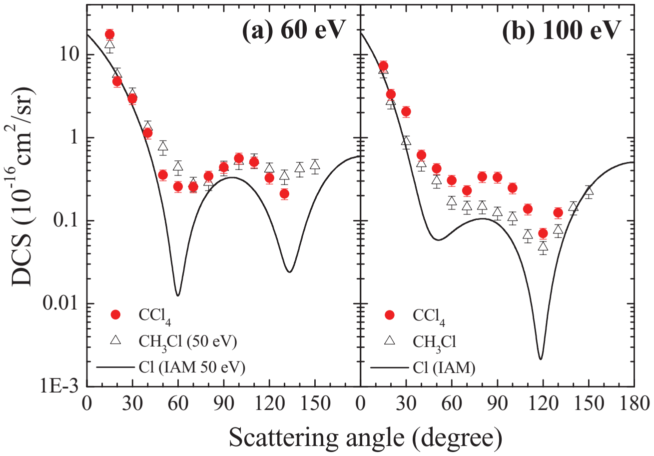

FIG. 2. A comparison between the elastic DCS of CCl4 and CH3Cl.[15] Also included are the results from the IAM-SCAR calculations for Cl atom.[15]

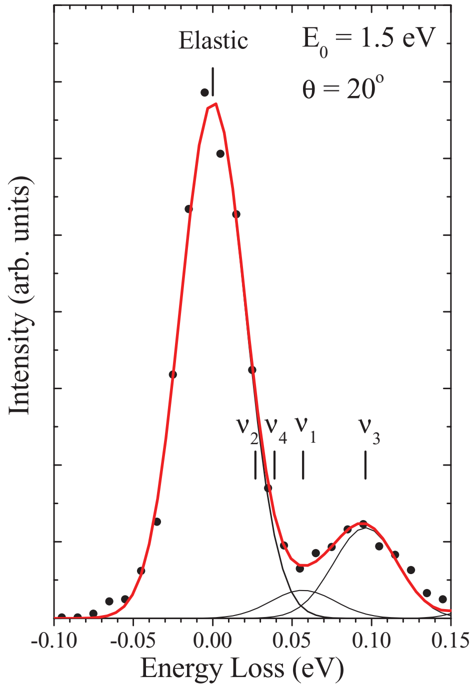

FIG. 4. Typical energy loss spectrum at 1.5 eV recorded at the energy resolution of ~40 meV (FWHM). The contributions of ν_2 and ν_4 are hidden in the elastic peak whereas ν_1 and ν_3 have been assigned by adjusting a Gaussian fit.

the DCS, and the overall DCS behaviour up to 100 eV. From Figure 1 we can see that, generally speaking above about 5 eV incident electron energy, the measured DCSs are peaked at the more forward scattering angles, which is consistent with the significant magnitude (~70 a.u.) of the dipole polarisability of CCl$_4$. Although tetrachloromethane (CCl$_4$) has no permanent dipole moment, the result in the measured DCS at 100 eV shows the strongest enhancement. These observations suggest that at higher energies the most dominant interaction mechanism is direct scattering from the longer range polarisation potential.

The theoretical calculations of Curik *et al.*[12] reported that at the lowest collision energy they studied (1 eV), the angular distribution changes completely and the presence of a minimum region in the ICS is reflected in a rather oscillatory dependence on the scattering angle of the corresponding DCS. In general, the trends that they observe in the shape of the DCS at energies below about 15 eV are also largely reflected in the present experimental results. The strong forward scattering that occurs at higher energies gives way to a relatively isotropic DCS at 3 eV and below with the forward angle cross section decreasing with angle at these energies. This is reminiscent of the behaviour noted previously[15] in a number of molecules at energies near or above the position of low energy shape resonances.

Where comparable cross section determinations exist from theory, our DCSs are in very good general agreement in overall shape with previous publications (see Figure 7 in Ref. 12 and Figure 3 in Ref. 11 at 10 eV). We may expect that several of the resonance features that are apparent in the various total scattering measurements and theoretical calculations will also play a role in the nature of the DCS at energies below 10 eV.

Several features dominate in our experimental DCSs: (a) the resonance in the vicinity of 1.2 eV[28] (0.94 eV from Ref. 28) has been attributed to triply degenerate $^2T_2$ state[29] (electron captured into a $\sigma^*_{\text{C–Cl}}$ MO) whereas at ~7.5 eV (Refs. 28 and 29) it may also be partly attributed to a resonant electron capture[4,28] which has been assigned to a broad

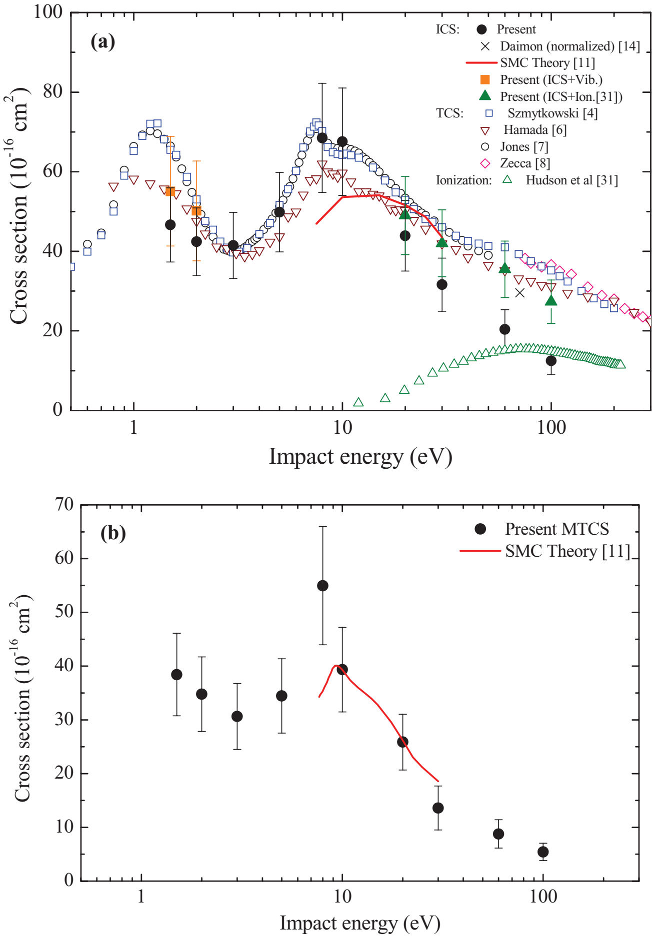

FIG. 3. Present experimental (a) ICSs (10^{-16} cm^2) and (b) MTCSs (10^{-16} cm^2) in comparison with other previous work. See text for details.

resonance of *E* symmetry around 9 eV (Ref. 12); (b) the general shapes of the DCSs may be divided into two categories, those above the resonances at 1.2 eV and below 7.5 eV. In particular, the DCSs show a minimum that shifts towards lower angles with increasing energies and a maximum at ∼30° that becomes noticeable at 3 eV and vanishes at higher energies. Such a maximum disappearance may be connected with the opening of another channel related to the threshold of formation of the second resonance peaking at 7.5 eV; (c) the general shapes show different features, again, above 8 eV. The experimental data show a second minimum at ∼120° at both 8 and 10 eV, which vanish at higher energy before becoming noticeable again at 100 eV; (d) above 10 eV, the minimum at ∼45° shifts to lower angles with increasing energy.

Finally, for the comparison, we displayed the elastic DCS for CCl_4 at 70 eV by Dimon *et al.*[14] in Figure 1 together with our DCS at 60 eV. It is noted that since their data were about twice larger than our DCS, we rescaled them by a factor of 0.5. The angular distributions of our DCS at 60 eV are good agreement with the rescaled data.

B. Comparison with the atomic Cl-DCS

The 50 and 100 eV DCS, show a structure that was also observed in CH_3Cl and reproduced in the IAM-SCAR theory.[15] At these energies we enter a region where simple independent atom model calculations represent the data in the observed angular region rather well, and contain at least some of the structure. It may be due to "interference between single scattering centres" in multiple scattering within a single molecule. At the highest energy studied (100 eV) another deep minimum is seen at around 120°. In Figure 2 we compare in detail the present experimental data with the previous experimental DCSs for CH_3Cl and theoretical ones for the Cl atom at 50 and 100 eV. The magnitude of the present cross sections has been normalised in order to be comparable with the CH_3Cl and Cl atom (IAM) calculations. From a qualitative point of view, there is good agreement in both cases (but particularly at 50 eV) between our measurements and calculations, with the rich angular structure in these cross sections being observed. Given that the IAM-SCAR theoretical approach is built upon scattering from atomic centres, the level of agreement seen in Figure 2 is strong evidence in support of the assertion that atomic-like effects may remain prevalent in what are fundamentally molecular systems. Kato *et al.*[15] have concluded that in many cases the structure observed in the CH_3X halomethanes was also partly found in the corresponding noble gas species, suggesting therefore that a bonded halogen atom, F, Cl, Br, and I, behaves somewhat such as a Ne, Ar, Kr, and Xe atom, respectively. Though the bonded halogens are acting like their corresponding noble gas counterparts, so the atomic-like behaviour manifests itself in the measured cross sections. In Figure 2 we include for comparison the DCSs for Cl at the IAM-SCAR level of theory. As far as CCl_4 is concerned, at 50 and 100 eV incident electron energies, the structures observed in the calculated DCSs are reminiscent of those observed in the corresponding measured CH_3Cl DCSs.[15] This constitutes further evidence for atomic-like behaviour in the scattering dynamics in addition to the electron scattering collisional data on CH_3X molecules.[15] A close inspection at Figure 2 shows that there are differences with respect to the magnitude of the depths of the critical minima, suggesting perhaps that "molecular-like" effects are still playing a role here. This seems a reasonable assumption, and the reason why the molecular DCS is relatively smoother is most likely the random molecular orientations in the gas, which was proposed by da Paixao *et al.*[30] We also note that in Figure 1 as we go to lower energies, at least until ∼8.0 eV, the data suggest that molecular-like behaviour becomes increasingly important.

C. Comparison of integral and total cross sections

Finally, in Figure 3 we compare the present experimental ICSs with the available total cross sections in the literature. Generally, we find a very good level of agreement between the present data and the total scattering data,[4–8] although below 20 eV the calculated (SMC) elastic ICS are smaller than the TCS of Hamada and Sueoka[5] and our elastic ICS, which agree with the TCS of Szmytkowski *et al.*[4] and Jones.[6] On the other hand, below 3 eV and above about 30 eV our data are lower. This is most likely due to the contribution of the vibrational and electronic excitation and ionisation channels. In order to compare our estimated ICS with the TCS, information is needed for the inelastic integral cross sections, but only the ionisation cross section is available. As shown in the figure, by summing the elastic and ionisation contributions, our data agree with the TCS. Note that we show the ionisation cross sections of Hudson *et al.*[31] At lower energies in the region of the first resonance at 1.2 eV, the addition of the vibrational cross sections integrated intensities to our estimated elastic integral cross shows a reasonable agreement with the TCS.

V. CONCLUSIONS

We report experimental elastic differential, integral and momentum transfer cross sections for electron scattering from carbon tetrachloride molecules, CCl_4. Corresponding comparison with recent theoretical differential cross sections from IAM-SCAR model for CH_3Cl and Cl atom have also been discussed. Agreement between these sets of data is generally very good, at 60 and 100 eV incident electron energy, in terms of the shapes and angular distributions of the cross sections. The level of agreement reported here suggests that atomic-like behaviour in the scattering process may be of considerable relevance, at least in the energy range above 7 eV.

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