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Total electron scattering cross-sections for carbon monoxide at low electron energies

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Abstract. Absolute total electron scattering cross-sections for carbon monoxide have been measured at low electron energies using a photoelectron source. The measurements have been carried out at 22 electron energies varying from 0.73 to 9.14 eV with an accuracy of ±3%. The cross-sections obtained in the present experiment have been compared with other measurements and theoretical computations.

Keywords. Electron scattering; total cross-sections; carbon monoxide.

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1. Introduction

The scattering of low energy electrons by atoms and molecules plays an important role in a variety of collisional processes pertaining to weakly ionized plasmas, gaseous lasers, diffuse-discharge switching and gaseous dielectrics. Interest in both experimental and theoretical aspects of the subject has grown enormously over the last few years and as a result, investigations to study the collision cross-sections have been carried out using better experimental techniques and theoretical methods.

Total electron scattering cross-section for carbon monoxide at low electron energies have been obtained both experimentally as well as theoretically. The early measurements were carried out many years ago by Brüche [1] and Ramsauer and Kollath [2] up to electron energies smaller than 5.5 and 1.2 eV respectively. The later measurements have been made by Guskov *et al* [3], Szmytkowski and Zubek [4], Kwan *et al* [5], Sueoka and Mori [6] and Buckman and Lohmann [7]. Guskov *et al* [3] obtained total cross-section in the electron energy range 0.05–6.0 eV using a time-of-flight electron spectrometer whereas Szmytkowski and Zubek [4] carried out the measurements at energies 1.34–5.26 eV using a 127° electrostatic electron energy spectrometer in a transmission mode. The cross-section measurements in the energy range 1–500 eV have been carried out by Kwan *et al* [5] using beam-transmission technique whereas retarding-potential time-of-flight method was employed by Sueoka and Mori [6] at electron energies 1.2–403 eV. Similar measurements were reported by Buckman and Lohmann [7] in the electron energy range 0.5–5 eV using a linear time-of-flight electron-transmission spectrometer. In addition to the total cross-section measurements, momentum transfer cross-section for carbon monoxide were measured by Haddad and Milloy [8] whereas Gibson *et al* [9] reported the theoretically computed integral elastic cross-sections. A few *ab initio* calculations on *e*-CO collisions have been reported in literature in the past; the two prominent among these are from Chandra [10] and Jain and Norcross [11]. Chandra [10] used a static-model exchange plus polarization approach to obtain total electron-scattering cross-sections for carbon monoxide at 0–10 eV energies whereas exact-static-exchange plus polarization model in the fixed-nuclei approximation has been used for the cross-section calculations by Jain and Norcross [11]. A comparison of cross-section values reported by different researchers shows that there is a large variation in the cross-section values at the peak of the shape resonance $^2\Pi$ centered in the vicinity of 1.9 eV. The values differ from 27 to 69 Å^2, the extreme values being reported by Sueoka and Mori [6] and Chandra [10]. As a matter of fact, the cross-sections data available for the resonance peak can be categorized in three groups. One set of values vary from 60 to 69 Å^2 [10, 11], the second set from 43 to 45 Å^2 [5, 7] and the third set of values from 27 to 35 Å^2 [1, 3, 4, 6]. Thus there is obviously a discrepancy in the values of cross-section reported so far at the peak of the shape resonance. In view of this, we decided to measure the absolute total scattering cross-sections for carbon monoxide at low electron energies using a photoelectron source.

This paper is a part of the ongoing research programme taken up to measure the total electron scattering cross-sections for atoms and molecules in gas phase. Previously, absolute total cross-sections for helium, neon [12], argon, krypton, xenon [13], molecular hydrogen [14] molecular oxygen [15], carbon dioxide [16] and nitrous oxide [17] have been measured at electron energies from 0–10 eV. In this paper, we present measurements of scattering cross-sections for electrons scattered by carbon monoxide with projectile energy varying from 0.73–9.14 eV.

2. Experimental set-up and method for analysis of data

The experimental set-up for the measurement of electron scattering cross-sections using a photoelectron source has been discussed in detail elsewhere [12, 13] along with the method for analysis of data and error analysis. A brief description is being given here for the sake of completeness. The experiment consists of measuring the intensities of the peaks in the photoelectron spectra of the source gas such as argon, krypton, xenon or carbon monoxide itself. The photoelectrons thus produced by the source gas are scattered by the target gas, the cross-section for which is to be determined. Each peak in the photoelectron spectrum of the source gas provides one point in the energy scale. Complete scanning of the electron energy is performed by varying the energy of the ionizing radiation as well as changing the source gas. Using different combinations of photons of three different wavelengths (HeI, 58.4 nm, NeI, 73.6 and 74.4 nm) and four different source gases and neglecting the energy points where the statistics for the photoelectron intensity were poor, it was possible to measure scattering cross-sections at 22 electron energies.

The microwave discharge light source for producing resonant emission lines of helium and neon, the beam splitter for monitoring any change in the intensity of the incident photon beam, the ionization and the scattering regions, the cylindrical mirror analyser, the electron detector (channeltron) and data acquisition systems have been described in detail previously [12, 13]. The pumping systems and additional fast pumps for different pumping of the various regions including the ionization region and some regions of the cylindrical mirror analyser and electron detector have also been discussed there. The details of absolute pressure measurement using an MKS capacitance manometer and the performance of the photoelectron spectrometer have been given in one of our previous publications [12].

The electron scattering cross-sections for carbon monoxide were measured using the method described previously. When source and target species are different, the electron scattering cross-sections, σ, can be evauated by using the following equation:

$$\ln\left(\frac{I_{e2}I_{\lambda 01}}{I_{e1}I_{\lambda 02}}\right) = \frac{P_1 - P_2}{760}[n_0\sigma x + k(al_1 + l_2)] \tag{1}$$

where I_{e1} and I_{e2} are the amplitudes of the photoelectron peaks at two different gas pressures P_1 and P_2, $I_{\lambda 01}$ and $I_{\lambda 02}$ are the incident photon intensities monitored by the beam splitter at the two pressures, l_1 is the distance from the center of the beam splitter to the circular aperture covering the ionization region, l_2 is the distance from the same aperture to the actual ionization region defined geometrically by the different slits in the accelerating region and cylindrical mirror analyser, x is the scattering path, a is the ratio of the pressures of the target gas outside and inside the ionizing region while k is the photoabsorption coefficient of the target gas at a particular photon wavelength. The total photoabsorption cross-sections at the three incident photon wavelengths have been taken from Samson and Yin [18]. The ratios $I_{\lambda 01}$ and $I_{\lambda 02}$ could be determined from the beam splitter.

When source and target gas species are the same, the electron scattering cross-sections could be evaluated by an equation given below:

$$\ln\left(\frac{I_{e2}I_{\lambda 01}P_1}{I_{e1}I_{\lambda 02}P_2}\right) = \frac{P_1 - P_2}{760}[n_0\sigma x + k(al_1 + l_2)]. \tag{2}$$

The electron scattering cross-sections for carbon monoxide were measured using equations (1) and (2) respectively in the two cases described above. In both these equations, all parameters I_{e1}, I_{e2}, $I_{\lambda 01}$, $I_{\lambda 02}$, P_1 and P_2 could be determined experimentally and cross-sections could be calculated.

All errors in the measurement of electron scattering cross-sections have been discussed in detail previously [12]. In the present experiment, the most probable error was estimated to be $\pm 3\%$. The problem of inadequate discrimination against forward scattered electrons has been attempted previously [16] to estimate the magnitude of this effect on the measured cross-sections in the experimental set-up used by us. A Monté Carlo method was developed and the electron trajectories originating from the ionization region and terminating at the detector were numerically studied using five random generators i.e. the finite length of the ionization region where photoelectrons are produced, random angle of projection within the allowed cone of ejection determined by the geometry, spread in energy of the photoelectrons determined by thermal broadening, place where a chosen fraction of the emitted photoelectrons are undergoing forward scattering and deflection in angle within a specified cone due to forward scattering. Assuming a differential scattering cross-section of 100 Å^2 per steradian, the error in total cross-section due to lack of discrimination of forward scattered electrons was found to be dependent on the overall cone

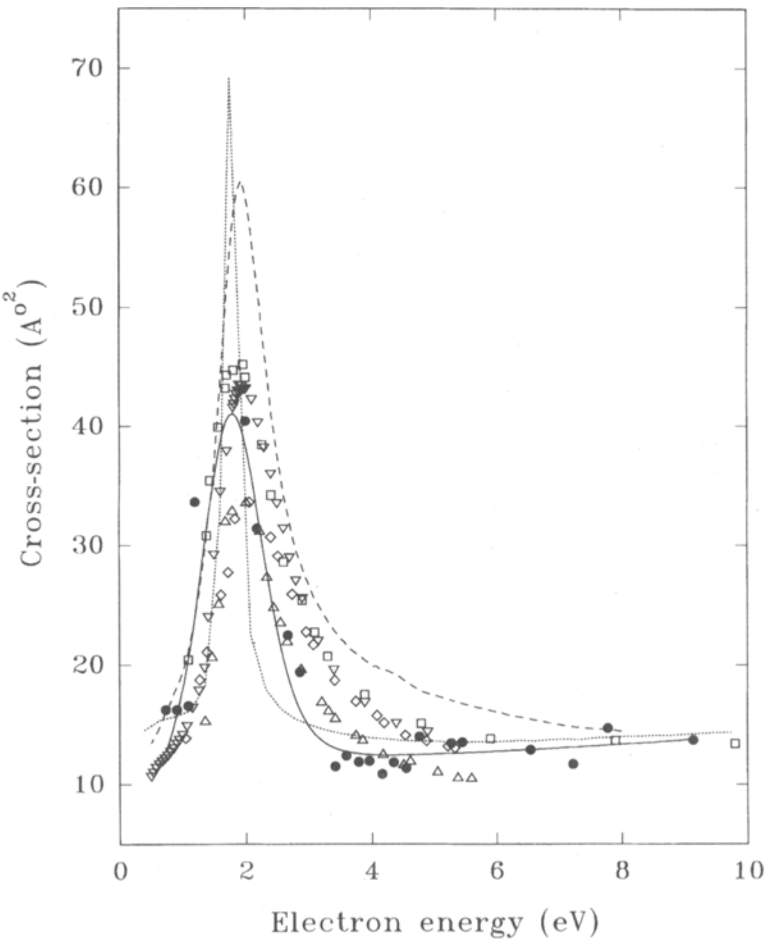

Figure 1. Total electron scattering cross-sections for carbon monoxide as a function of incident energy from 0.73 to 9.14 eV obtained by various researchers. The symbols denote: •, present result; ∇, Buckman and Lohmann; □, Kwan *et al*; ◇, Brüche *et al*; △, Symtkowski *et al*; – – – – – –, Jain and Narcoss; . . . . . . , Naresh Chandra; ———, present result curve fitted.

angle of emergence. For our experimental set-up where the overall cone angle of emergence has been estimated to be 6°, the maximum error has been found to be about 0.5%.

3. Results and discussion

The total electron scattering cross-sections for carbon monoxide as measured in the present experiment are shown in figure 1 for electron energies ranging from 0.73 to 9.14 eV. The lowest energy was 0.73 eV and it was not possible to go to energies below this value because of constraints on the photon beam wavelengths and the type of source gases available to us. Also shown in the figure are the measured cross-sections reported by Brüche [1], Szmytkowski and Zubek [4], Kwan *et al* [5] and Buckman and Lohmann [7]. The cross-section values given by Ramsauer and Kollath [2] have not been shown in the figure as there are only a few cross-section values available at energies less than 1.2 eV. Also not shown in the figure are the experimentally obtained cross-section values by Guskov *et al* [3] and Sueoka and Mori [6]. The cross-sections by these two groups have not been reported in tabular form and it has been quite difficult to obtain the values accurately after digitizing their cross-section curves even though repeated attempts were made. The cross-section curve after proper curve fitting to the results obtained in the present experiment has also been shown in figure 1. This has been carried out using an appropriate mathematical function in the library of large number of functions available in the Tablecurve-2D (Jandel Scientific) software. Kwan *et al* [5] reported a 5% estimated error in the total cross-section measurement and the energy width for electron beam used in the experiment was about 200 meV. An energy resolution of better than 50 meV for the electron beam was used by Szmytkowski and Zubek [4] to obtain total cross-sections with a standard deviation usually not exceeding 9% over the whole electron energy range 1.34 to 5.26 eV. An absolute uncertainty in the electron energy in the experiment reported by Buckman and Lohmann [7] was estimated to be about 54 meV at an energy of 1.5 eV and about 100 meV for energies above 1.5 eV. The theoretically computed electron scattering cross-sections for carbon monoxide reported by Chandra [10] and Jain and Norcross [11] have also been shown in figure 1.

The cross-section curve (figure 1) in the entire electron energy range from 0.73 and 9.14 eV can be divided into two regions. The low energy region below 3.5 eV is dominated by excitation of the $^2\Pi$ shape resonance centered at around 1.9 eV whereas the second energy region covers the range from 3.5 to 9.14 eV. In the first region, the cross-section values show a sharp increase up to the maximum of the shape resonance followed by a sharp decrease. In figure 1, it is clear that there is a large discrepancy in the cross-section value at the maximum of the resonance peak and a similar trend could also be seen at the wings on both sides of the peak. To have a clear comparison, the cross-section curves reported by Brüche [1], Szmytkowski and Zubek [4], Kwan *et al* [5], Buckman and Lohmann [7], Chandra [10] and Jain and Norcross [11] alongwith the curve obtained in the present experiment have been made to undergo proper curve fitting procedure. This has been done with the help of Tablecurve-2D (Jandel Scientific) software. The energy and cross section values thus obtained at the peak of the shape resonance are given in table 1 alongwith the full width at half maximum (FWHM) of the resonance peak. Also given in the table are the values of energy resolution of electron beam used in different experiments. These characteristic parameters for the shape resonance by Guskov *et al* [3] have also been given in the table. However, the cross-section curve by Guskov *et al* [3] has not been shown in figure 1 for reasons described above. The electron energy value at the peak of the shape resonance as reported by different researchers has been found to vary from 1.75 eV [10] to 2.1 eV [1] with an overall average value of 1.9 eV. The variations from 1.9 eV is not much and in case of measured data, it is almost within the reported experimental errors. But the cross-section values obtained by different research groups appear to differ by a large amount. A close look at these cross-section values calls for putting them in different groups. The values of 69.2 Å^2 and 60.3 Å^2 by Chandra [10] and Jain and Norcross [11] respectively could constitute one group whereas the second group could include the cross-section values of 33.8 Å^2 [1], 35.0 Å^2 [3] and 34.8 Å^2 [4].

Table 1. Some characteristic parameters of the shape resonance as obtained after proper curve fitting to the results reported by different experimental groups. Also given in table is the energy resolution used in different experiments.

	Energy resolution in meV	Peak value		FWHM (eV)
		Electron energy (eV)	Cross-section (Å^2)	
Chandra [10]	—	1.75	69.2	0.35
Jain and Norcross [11]	—	1.94	60.3	1.35
Brüche [1]	Not available	2.1	33.8	2.5
Guskov *et al* [3]	<50	1.8	35.0	~2.3
Szmytkowski and Zubek [4]	50	1.9	34.8	1.7
Kwan *et al* [5]	200	1.9	45.6	1.9
Buckman and Lohmann [7]	100	2.0	44.1	1.8
Present results	45	1.8	41.1	1.5

The rest of the measurements by Kwan *et al* [5], Buckman and Lohmann [7] and authors of the present work with cross-section values at 45.6, 44.1 and 41.1 Å^2 respectively form the third group. The general agreement in cross-section values reported by researchers in each group is reasonably good but the difference in cross-sections are appreciably larger when compared with values reported in different groups.

A detailed discussion is in order to find out which cross-section values are more reliable. Let us first discuss the results obtained theoretically by Chandra [10] and Jain and Norcross [11]. The theoretical cross-section reported by Chandra [10] exhibits a much narrower resonance peak than that obtained in any of the experiments (table 1). Lane [19] has commented that the theoretical curve obtained by Chandra [10] for $^2\Pi$ shape resonance would be broadened and reduced in magnitude at the peak if the vibrational motion of the nuclei had been included in the calculation. Chandra used a static-model exchange plus polarization approach in his calculations and his model was modified by Jain and Norcross [11] in their calculation using exact-static-exchange plus polarization method in the fixed-nuclei approximation. However, the nuclear vibrational motion was neglected in their study also as in the case of Chandra. They suggest that the higher value of cross-section at the peak of the shape resonance could be reduced if proper vibrational close-coupling calculations are carried out.

With the theoretically computed data out of the discussion, one needs to concentrate on the cross-section values obtained experimentally by researchers in second and third groups as given in table 1. It may be worthwhile to discuss about the error in all these measurements associated with incomplete discrimination against projectiles at small angles in the forward direction. In all the three experiments by Brüche [1], Guskov *et al* [3] and Szmytkowski and Zubek [4], no discussion about this potential source of error associated with their instruments has been taken up. It appears that in all the above experiments, the error in cross-section values due to lack of discrimination against small angle scattering is extremely large. Also, in case of measurement by Szmytkowski and Zubek [4], only relative cross-sections for carbon monoxide with respect to argon were obtained and the relative total cross-sections were then made absolute by normalizing to the results in argon by Golden and Bandel [20] in the 2–20 eV energy range. In view of

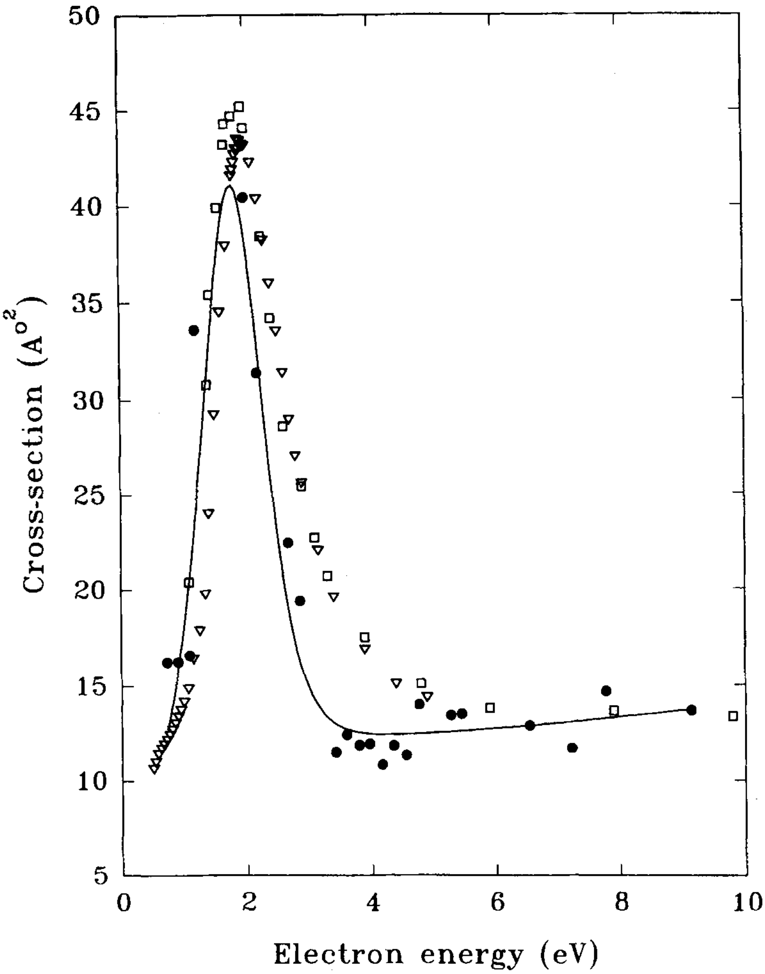

Figure 2. Total electron scattering cross-sections for carbon monoxide as a function of incident energy from 0.73 to 9.14 eV obtained by various researchers. The symbols denote: •, present result; ∇, Buckman and Lohmann; □, Kwan *et al*; ——, present result curve fitted.

this it is clear that the above three experiments could lead to large errors in cross-section values at the peak of the shape resonance.

That leaves us with the third group which includes three different measurements of cross-section for carbon monoxide resonance peak. Kwan *et al* [5] have not estimated the error in cross-section values due to lack of discrimination against small angle scattering but using the same experimental set-up, Hoffman *et al* [21] have pointed out that in case of carbon dioxide, their measurements may be 1% too low at 4 eV and less than 1% too low at 10 eV because of inadequate discrimination against forward scattered electrons. It can safely be assumed that the error in cross-section in case of carbon monoxide is almost similar to that estimated for carbon dioxide. An estimate of such error in the cross-section values reported by Buckman and Lohmann [7] indicates that the effect on the

Table 2. Total electron scattering cross-sections for carbon monoxide at various electron energies. Also given are the photon wavelength, the source gas and the photoion state for the corresponding electron energy.

Wavelength λ (Å)	Source gas	Photoion state	Electron energy (eV)	Cross-section (Å^2)
744	Ar	$^2P_{1/2}$	0.73	16.20
744	Ar	$^2P_{3/2}$	0.91	16.22
736	Ar	$^2P_{3/2}$	1.09	16.55
584	CO	$B^2\Sigma^+(\nu=0)$	1.20	33.62
744	Kr	$^2P_{1/2}$	2.00	40.43
736	Kr	$^2P_{1/2}$	2.18	31.39
744	CO	$\tilde{X}^2\Sigma^+(\nu=0)$	2.67	22.45
736	CO	$\tilde{X}^2\Sigma^+(\nu=0)$	2.86	19.38
584	CO	$\tilde{A}^2\Pi^+(\nu=6)$	3.42	11.49
584	CO	$\tilde{A}^2\Pi^+(\nu=5)$	3.60	12.39
584	CO	$\tilde{A}^2\Pi^+(\nu=4)$	3.80	11.85
584	CO	$\tilde{A}^2\Pi^+(\nu=3)$	3.97	11.93
584	CO	$\tilde{A}^2\Pi^+(\nu=2)$	4.17	10.85
584	CO	$\tilde{A}^2\Pi^+\nu=1)$	4.36	11.82
584	CO	$\tilde{A}^2\Pi^+(\nu=0)$	4.56	11.33
736	Xe	$^2P_{3/2}$	4.77	13.99
584	Ar	$^2P_{1/2}$	5.28	13.42
584	Ar	$^2P_{3/2}$	5.46	13.49
584	Kr	$^2P_{1/2}$	6.55	12.87
584	CO	$\tilde{X}^2\Sigma^+(\nu=0)$	7.23	11.67
584	Xe	$^2P_{1/2}$	7.78	14.67
584	Xe	$^2P_{3/2}$	9.14	13.66

cross-section at the resonance peak is less than 0.1%. In the present experiment, it has been shown by Rawat *et al* [16] that error in scattering cross-section at low angles due to lack of discrimination is about 0.5%. The above discussion leads to a conclusion that all those three measurements are highly reliable. The cross-section curves reported in these three experiments only are shown in figure 2 in order to have a better comparison of data in the three cases. Our cross-section value at the peak of the shape resonance in 11% and 7% lower than those reported by Kwan *et al* [5] and Buckman and Lohmann [7]. It is very difficult to say which of the three values is more reliable. In the present work, there are less number of energy points available at the peak. But there may be two other factors viz. narrower electron energy width and better discrimination against small angle scattering in different experiments. The combined effect of these two factors may go in favour of our results but the argument is, by no means, conclusive.

In the second energy region from 3.5–9.14 eV, the cross-section values reported in the three experiments (figure 2) need to be compared. At electron energies between 3.5 to 5.0 eV, the cross-sections obtained in the present experiment are found to be smaller as compared to those reported by Kwan *et al* [5] and Buckman and Lohmann [7]. This part of the energy spectrum is the tail end of the right wing of the shape resonance. The discrepancy in the result is the direct result of difference in the FWHM value of the shape resonance obtained in the three experiments. In the electron energy region from 5.0 to 9.14 eV, our cross-section values are in good agreement with those reported by Kwan *et al*

[5]. No measurements have been carried out by Buckman and Lohmann [7] in this energy region.

The values of scattering cross-sections for carbon monoxide as measured in the present experiment are given in table 2 alongwith the photon wavelength, source gas and photoion state for the corresponding electron energy.

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