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Differential cross sections for the ionization of the CO molecule by electron impact

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Abstract

Partial doubly differential cross sections (PDDCS) for the ionization of the CO molecule by electron impact have been calculated using a semiempirical approach. The incident electron energies used are 100, 500, and 1000 eV. The calculations are made as a function of energy loss suffered by the primary electron and the scattering angle. The present approach also leads to the calculations of partial singly differential cross sections (PSDCS). The results are compared with the only available experimental data at 500 eV electron energy [C.B. Opal, E.C. Beaty, W.K. Peterson, At. Data Tables 4 (1972) 209]. (Int J Mass Spectrom 184 (1999) 201–205) © 1999 Elsevier Science B.V.

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The present study deals with the ionization of the CO molecule by electron impact. The ever-increasing interest in the ionization processes of the CO molecule is due to its importance in the formation of ionosphere and interstellar clouds [1].

In this brief report, we have calculated the partial doubly differential cross sections (PDDCS) for the production of CO^+, O^+, C^+, CO^{+2}, C^{+2}, and CO^{+3} ions through direct, dissociative, and multiple ionization processes of the CO molecule by electron impact. For these calculations, the Khare et al. formula [2], which could provide good results for partial ionization cross sections [3], has been suitably modified to evaluate the partial doubly differential cross sections (PDDCS) and partial singly differential cross sections (PSDCS) [4,5]. The present calculations were undertaken at incident electron energies of 100, 500, and 1000 eV. These calculations have been done as a function of energy loss suffered by the incident electron at scattering angles of 30 °, 60 °, and 90 °. The energy loss W is defined as the sum of ejected electron(s) energy ε and the ionization threshold I_i. The PSDCS are calculated by integrating the PDDCS over the entire range of the scattering angles. For comparison with the experiment, only the data of Opal et al. [6] for total double and total single differential ionization cross sections at 500 eV was available. A reasonable agreement between the theoretically calculated and the experimental results has been noticed. To date, no experimental data for PDDCS and PSDCS values is available to compare

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with the present calculations. However, these calculations will prove to be of importance for future experiments.

The details of the modified Khare et al. formula used in the present calculations have been given in earlier publications [4,5]. It was shown that the formula yields reasonably good agreement with the experimental data available for the H_2 molecule. The PDDCS for the production of secondary electron(s) of energy ε through ith type of ionization mechanism from a molecule by an incident electron of energy E is given by

$$\begin{aligned} Q_i(E, W, \theta) = {} & (a_0^2 R^2/E)[(E - W)/(E - I_i) \\ & (1/W\, df_i(W, 0, \theta)\ \ln[1 + C_i(E - I_i)] \\ & + (E - I_i)/(E(\varepsilon_0^3 + \varepsilon^3))S_i\{\varepsilon - \varepsilon^2/(E - \varepsilon) \\ & + \varepsilon^3/(E - \varepsilon)^2\}]\sin\theta \end{aligned} \tag{1}$$

It is convenient to replace ε by $(W - I_i)$, where W is the energy loss suffered by the incident electron. We can then easily calculate the total double differential cross section, i.e. the sum of PDDCS over i. The integration of Eq. (1) over the entire range of scattering angles gives the PSDCS. In this treatment, no distinction has been made between the primary and the secondary electrons. However, ε stands for the energy of the secondary electron(s). Because PDDCS values are isotropic it is necessary to convert the differential generalized oscillator strengths into the cosine distribution form of linear oscillator strengths using the Lassettre theorem [7]. The asymmetric parameter for CO is taken to be the ionization probability of the electrons in the optical molecular orbit. The various symbols employed in Eq. (1) have their usual meaning [2]. The method of calculation and the input data used in the present calculations are the same as discussed earlier [3].

In the present investigation, we have designated i values from 1–6 corresponding to the CO^+, C^+, O^+, CO^{+2}, C2, and CO^{+3} ions, respectively. Figs. 1–4 present the results for PDDCS and PSDCS evaluations, where curves A, B, C, D, E, and F represent the cross sections corresponding to the production of CO^{+3}, C^{+2}, CO^{+2}, O^+, C^+, and CO^+ ions, respectively. Curve G represents the total partial differential cross sections. The latter can be compared with the available experimental data [6].

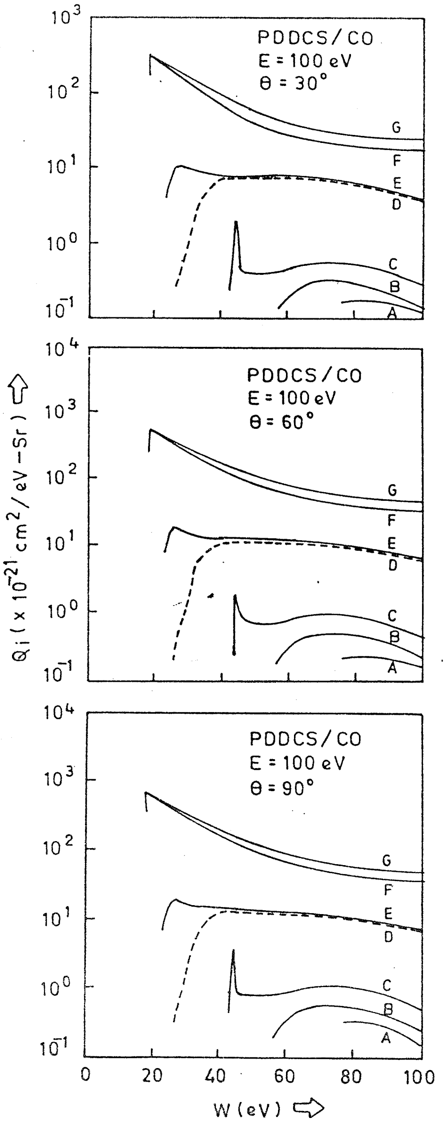

Fig. 1. The PDDCS for the CO molecule by the impact of 100 eV electrons. Curves A, B, C, D, E, and F correspond to the production of CO^{+3}, C^{+2}, CO^{+2}, C^+, O^+, and CO^+ ions, respectively. Curve G represents their sum, i.e. total PDDCS.

Figs. 1–3 show the PDDCS at incident electron energies 100, 500, and 1000 eV, respectively. At 100 and 1000 eV, neither partial nor total double differ-

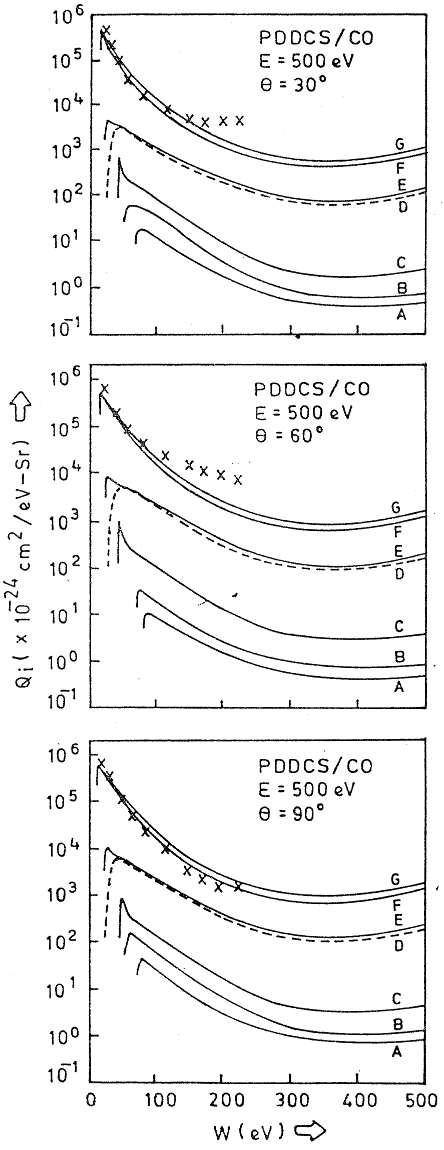

Fig. 2. As Fig. 1, but at $E = 500$ eV. Experimental data, X [6].

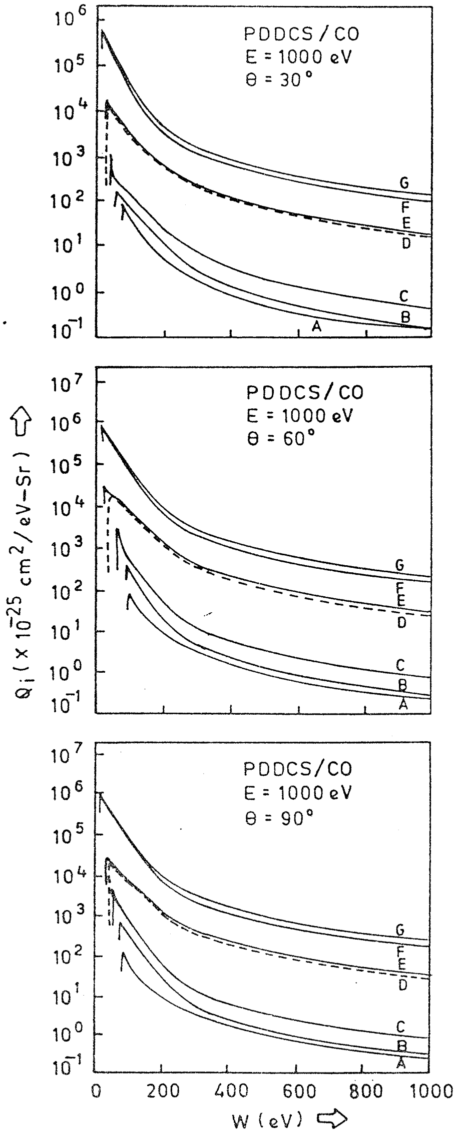

Fig. 3. As Fig. 1, but at $E = 1000$ eV.

ential cross sections are available for comparison of the presently calculated results. A similar situation has been noticed in case of PSDCS depicted in Fig. 4. However, our calculations do show the qualitative trend expected for PDDCS and PSDCS with the secondary electron energy.

Figs. 2 and 4 show that the calculated PDDCS and PSDCS values, respectively, at 500 eV incident electron energy, can be folded to compare with the experimental data [6] available for total PDDCS and total PSDCS utilizing curve G. At scattering angle 30 °, the calculated results for double differential cross sections below electron energy loss of 100 eV are in satisfactory agreement with the experimental data. However, above the energy loss of 100 eV, the deviations increase significantly. A similar trend has

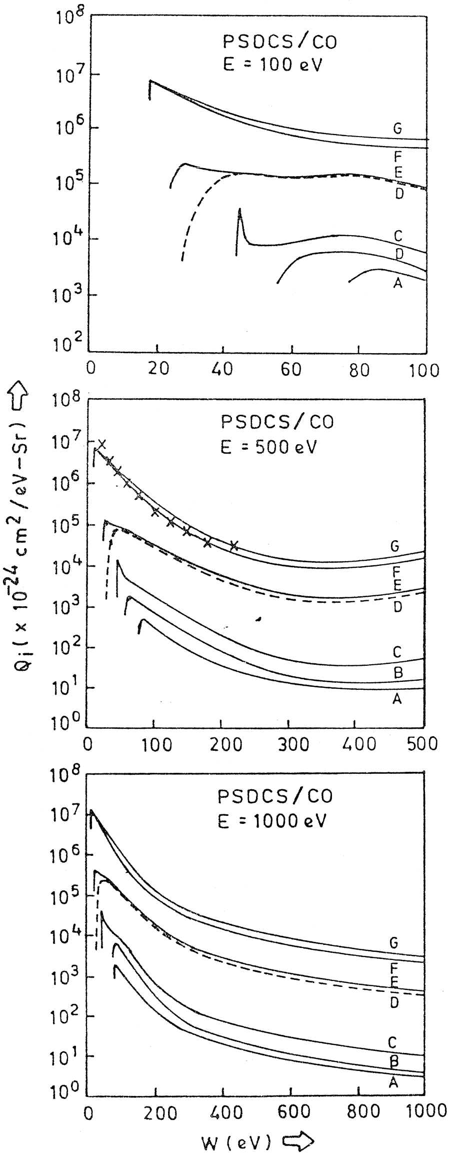

Fig. 4. As Fig. 1, but for PSDCS at 100, 500, and 1000 eV. Experimental data, *X* [6].

been noticed at scattering angle of 60 °. The situation is rather different at the scattering angle of 90 ° where the experimental data is underestimated by about 40% in the entire secondary electron energy covered by the experiment. The theoretical calculations for total PSDCS shown in Fig. 4 are in satisfactory agreement with the experimental data in the energy loss range from ionization threshold to 65 eV. As the energy loss increases from 65 eV to 150 eV the deviation increases up to 30%. Above 150 eV, the present calculations (curve G) are again in satisfactory agreement with the experimental data. However, below an energy loss of 50 eV, the present calculations show a good perspective of the threshold behavior. It is interesting to note that we predict differential cross sections to be asymmetric about the energy loss value $W/2$. It may however, be noted that the cross sections are symmetric about $W/2$ for the case of symmetric molecules [4,5,8].

In this article, for the first time, we have calculated the PDDCS and PSDCS for the CO molecule at various incident electron energies. The accuracy of the present calculations are directly linked to the accuracy of oscillator strengths that were used as inputs. These calculations take into account the contribution of exchange effects through the second term in Eq. (1). Such effects are not easily identifiable in the experiments. In all the ionization processes, the calculations predict the threshold behavior of the ionization cross sections as a function of energy loss clearly. The present investigations justify the extension of the semiempirical formula [2,5] for the evaluation of partial differential cross sections for molecules in the complete energy spectrum of the ejected electrons, i.e. 0 to $(E - I_i)$. However, it will be helpful if experimental investigations are conducted in order to check the calculations more specifically.

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