

## ELECTRON IMPACT VIBRATIONAL EXCITATION OF CO IN THE RANGE 1–4 eV

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The cross sections for resonant vibrational excitation of the CO molecule by electron impact in the range 1–4 eV have been calculated. The calculations have been done on the basis of resonance scattering theory for the vibrational transitions from the ground level as well as from the excited levels.

The scattering of electrons with energies of 1–4 eV by CO molecules is affected by the formation of a negative-ion resonance state  $\text{CO}^-$ . This process plays a significant role in the electron impact vibrational excitation of the CO molecule since it considerably increases the cross sections for vibrational excitation. In addition the oscillatory resonance structure appears in the cross sections.

The differential cross sections for the vibrational excitation from the ground state were studied by Schulz [1]. The angular distributions of the elastic scattering and vibrational excitation were studied later more precisely by Ehrhardt et al. [2]. The cross sections for vibrational states up to  $\nu = 8, 9, 10$  were recently analyzed by Boness and Schulz [3].

The results of these works suggest that the vibrational excitation of the CO molecule is dominated by the formation of the  $\text{CO}^-$  shape resonance state of  $^2\Pi$  symmetry. The angular distributions for inelastic processes for the  $\nu = 1$  to  $\nu = 6$  levels are almost constant in the investigated energy range, which suggests that one could neglect the contribution of potential scattering. The analysis of the experimental data [3] suggests the predominance of the partial p-wave over the d-wave in the resonant electron scattering although the theoretical results [4] showed that the contribution of the d-wave may be substantial.

In the vibrational cross sections one can observe an oscillatory resonance structure. The characteristic feature of that structure for the successive vibrational levels is that the positions of the peaks are not constant

but seem to shift toward higher energies with increasing final state quantum number. Similar features are shown by the oscillatory structure observed for  $\text{N}_2$  [5] and  $\text{CO}_2$  [6].

The purpose of this work was to study, using the "boomerang" model [7], the vibrational excitation of the CO molecule from the ground state. To give a complete view of the vibrational processes taking place in the CO molecule, as well as to satisfy the recently felt need to investigate the cross sections for vibrational de-excitation and excitation from excited vibrational states, these cross sections were calculated.

We made use of a procedure similar to the one proposed by Birtwistle and Herzenberg [7] and that used in the preliminary calculations [8]. All functions in the complex potential  $W(R) = E^-(R) - \frac{1}{2}i\Gamma(R)$  used in our calculations were written down for electrons with angular momentum  $l = 1$ .  $E^-(R)$  was taken as Morse's potential. The calculated cross sections were fitted to the experimental results, which permitted establishing the molecular parameters of the resonance state.

The total cross sections for the excitation from the vibrational ground state are shown in fig. 1. The calculations were done for final levels  $\nu = 1$  to  $\nu = 6$  and quite good agreement with experiment [2] was obtained. The normalization between the theoretical and experimental curves was done for the  $\nu = 0 \rightarrow 2$  curve at the second maximum. In the calculations the following molecular parameters of the  $\text{CO}^-$  state in the complex potential  $W(R)$ , obtained from fitting to the experiment were used:  $E^-(R_0^-) - E(R_0) = 1.50$  eV,  $\hbar\omega^- = 0.23$  eV,

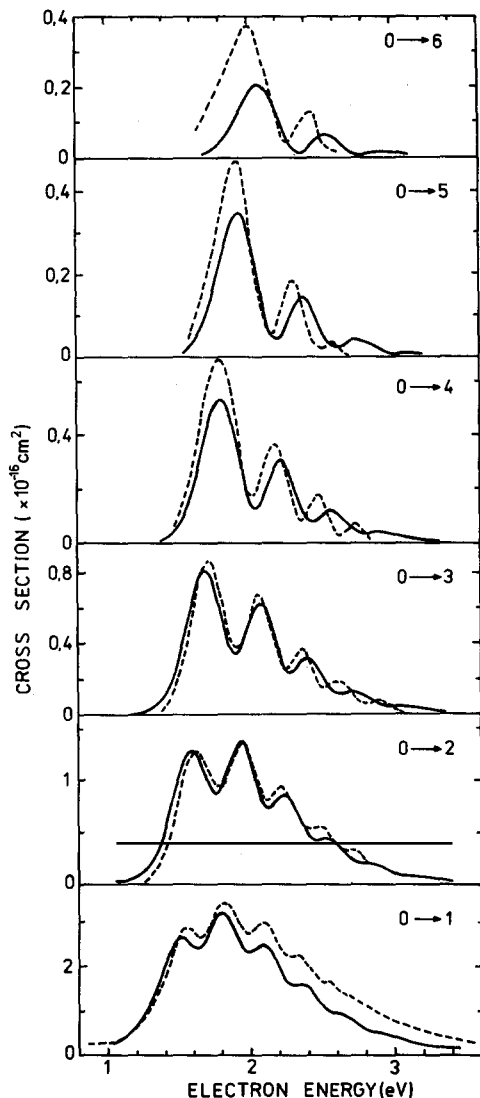


Fig. 1. Energy dependence of the total cross sections for the vibrational excitation of CO from the ground level  $v = 0$ : full curves, present calculations; broken curves, experiment [2] (as listed by Kieffer [14]). Vibrational transitions are indicated on the right.

$R_0 - R_0^- = 0.092 \text{ \AA}$ ,  $D^- = 14 \text{ eV}$  and  $\Gamma(R_0) = 0.75 \text{ eV}$ . The average autoemission width for the energy 1.75 eV is equal to  $\langle \Gamma \rangle = 0.6 \text{ eV}$ .

The partial lack of agreement seen in fig. 1 can be caused by adopting in the model a function for the autoemission width which can only be a rough approximation. Testing calculations done in this work for  $\Gamma$  other

than the ones anticipated by the expressions given by Blatt and Weisskopf [9] show that the positions of the peaks in the cross sections on the higher energy side depend on the shape of the function  $\Gamma(R)$ .

Another reason for the discrepancies between the calculations and experiment for high vibrational levels may be the partial breakdown of the approximations of the local potential theory, because for these levels the energy of the detaching electrons becomes com-

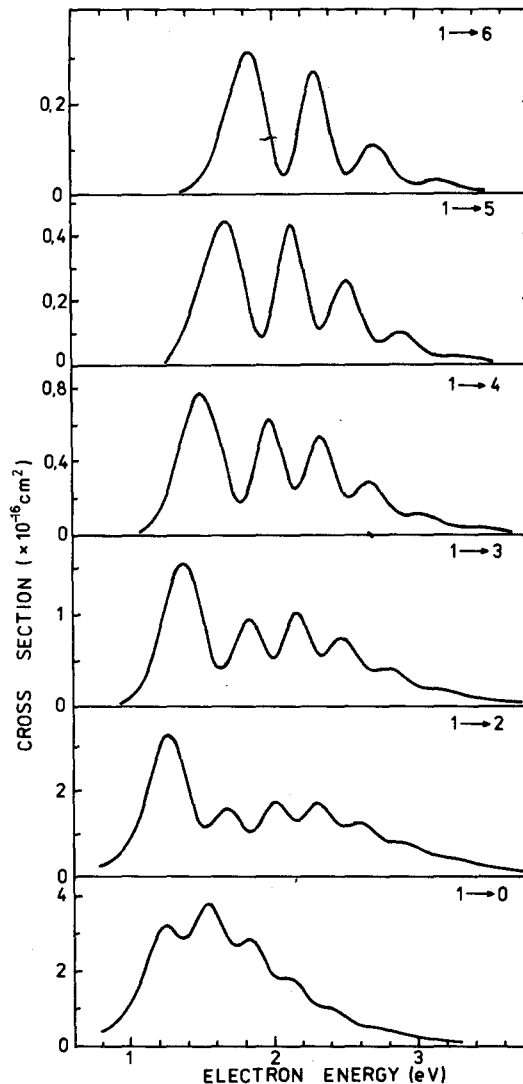


Fig. 2. Energy dependence of the total cross sections for the vibrational transitions (indicated on the right) of CO from the vibrationally excited level  $v = 1$ .

parable to the vibrational spacing of the molecule [10]. The same behaviour for high vibrational levels was observed for  $N_2$  [11].

It seems also that inclusion of two partial waves  $l = 1$  and  $l = 2$  [4] should improve the agreement between calculations and experiment.

Making use of the complex potential parameters obtained in the fitting, calculations were made for vibrational transitions from vibrationally excited states of the CO molecule. It was assumed that the function  $\Gamma(R)$  is independent of the initial vibrational level and the same form was adopted as that for the  $\nu = 0$  level. Fig. 2 shows the cross sections for de-excitation and excitation from the  $\nu = 1$  level.

In these cross sections one can observe a resonance structure. These structures occur in a greater energy interval than in the case of transitions from  $\nu = 0$ . It is caused by the increase of the Franck-Condon region with the change of the initial level to the excited levels. Some of the curves (e.g.  $\nu = 1 \rightarrow 2$ ) have a slightly different shape, compared to the ones shown in fig. 1. In these curves, a strong peak is followed by a bump with an oscillatory structure. On the other hand, it seems, that the shape of these first peaks is similar to those of the first peaks in the curves for  $\nu = 0$  (e.g.  $\nu = 0 \rightarrow 4$ ). A new feature of the studied excitation processes is that the positions of the peaks in the successive cross sections for superelastic processes almost do not change, as is shown in fig. 3 for transitions from the  $\nu = 4$  level.

An experimental investigation of the cross section of the type described in this section was recently started by Wong et al. [12] for  $N_2$ . The measurements for CO are in progress but the preliminary comparison of the results of our work with the experimental results for the  $\nu = 1 \rightarrow 2$  transition indicate that the main feature in the energy dependence can be well accounted for by the calculations [13].

All cross sections calculated in this work obey well the principle of detailed balance.

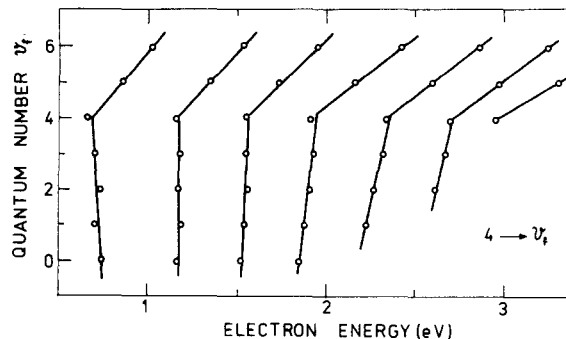


Fig. 3. Energy positions of the peaks in the cross sections for transitions from the vibrationally excited level  $\nu = 4$  to the final levels  $\nu_f = 0, 1, \dots, 6$ .

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