ELECTRONIC AND ATOMIC COLLISIONS
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RESONANT EXCITATION OF HIGH VIBRATIONAL LEVELS BY SLOW ELECTRON COLLISIONS[1]

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A novel, highly sensitive trochoidal electron spectrometer is used to study the excitation of high vibrational levels *via* low-lying shape resonances in diatomic and polyatomic molecules. Recent theoretical prediction of an unexpected vibrational structure near threshold is confirmed in H_2. The results in H_2, N_2, and CO permit an evaluation of the ability of different theories to reproduce threshold effects. Study of large polyatomic molecules reveal two types of excitation, the "specific" excitation of low vibrational levels and the "unspecific" excitation of vibrational quasicontinua near threshold. Very complex near threshold excitation is found in the triatomic molecule CO_2.

1. INTRODUCTION

Its high sensitivity makes the trochoidal electron spectrometer suitable for the study of processes with low cross sections. The present contribution concentrates on the measurement of the excitation of high vibrational levels *via* low-lying shape resonances in three classes of molecules. The first class are the diatomic molecules, where the measurements in H_2, N_2, and CO are presented. The second class are the large polyatomic molecules, with *p*-benzoquinone serving as representative example. Finally the triatomic molecule CO_2 is studied since it represents an intermediate case between the diatomics with only one vibration and the polyatomics with many vibrations.

2. TROCHOIDAL ELECTRON SPECTROMETER

The instrument has been described previously (1, 2), and is shown schematically in Figure 1. It uses trochoidal analysers (3) both to prepare a beam of monoenergetic electrons and to analyse the energies of scattered electrons. The trochoidal analyser has often been used to prepare monoenergetic electron beams for transmission (4) and dissociative attachment studies (5), but the present instrument represents the first successful implementation of this device to analyse the energies of the scattered electrons. The crutial feature of the present instrument is the use of two analysers in series. This arrangement permits the attenuation of the intense unscattered electron beam which enters the analyser in the magnetically colimated instrument with its linear geometry, and has caused a large background of stray electrons in a first version of the instrument using only a single analyser stage.

Several advantages and drawbacks of the present instrument in comparison with an electrostatic apparatus may be recognized. Among the drawbacks is the inability to vary the scattering angle, the data obtained being a superposition

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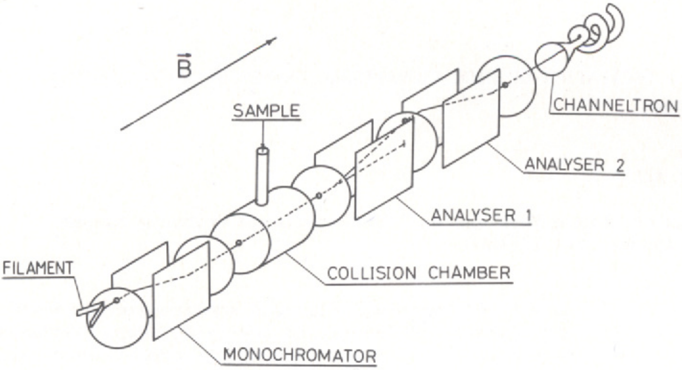

FIGURE 1
Schematic diagram of the apparatus.

of 0° and 180° differential cross sections. The resolution of the instrument, about 35 meV, suffices to resolve the vibrational structure in most cases, but is less than the best obtained with electrostatic instruments. These drawbacks are more than outweighted by several advantages for a number of applications. Most important is the high sensitivity, which appears to surpass that of the electrostatic instruments by several orders of magnitude. Important is the low energy capability; both the incident and the scattered electron energies may be varied down to 30 meV. The energy dependence spectra may be relatively easy corrected for the instrumental transmission function. In addition there are some practical advantages like low sample consumption and the capability of the instrument to record both the transmission and the energy-loss spectra.

3.DIATOMIC MOLECULES

3.1. Hydrogen

The shape of bands in the energy dependence of resonant vibrational excitation by electron impact is known to be a function of resonance lifetime. Resonances with lifetimes long compared to the vibrational period have sharp vibrational structure, a lifetime short relative to the vibrational period gives structureless bands, and intermediate lifetimes result in broad vibrational structure whose shape and spacing depend upon the channel of observation (5).

The $^2\Sigma_u$ resonance in H_2, responsible for the vibrational excitation in the low energy region, is one of the prototype cases of an extremely short lived resonance, with a lifetime comparable to the duration of the nonresonant scattering. One would thus expect no vibrational structure in the energy dependence curves. This expectation seemed confirmed by the available experimental data (Ehrhardt *et al.* (6), Trajmar *et al.* (7)).

Mündel, Berman, and Domcke (8) and Domcke, Mündel, and Cederbaum (9) recently reported a theoretical study of vibrational excitation and dissociative attachment in H_2 employing a sophisticated treatment of the nuclear dynamics. A striking result of this study, contradicting the intuitive expectation outlined above, is a prediction of a pronounced vibrational structure in the energy dependence of the excitation of the higher vibrational levels (υ>3). The present experiment is testing the unexpected theoretical

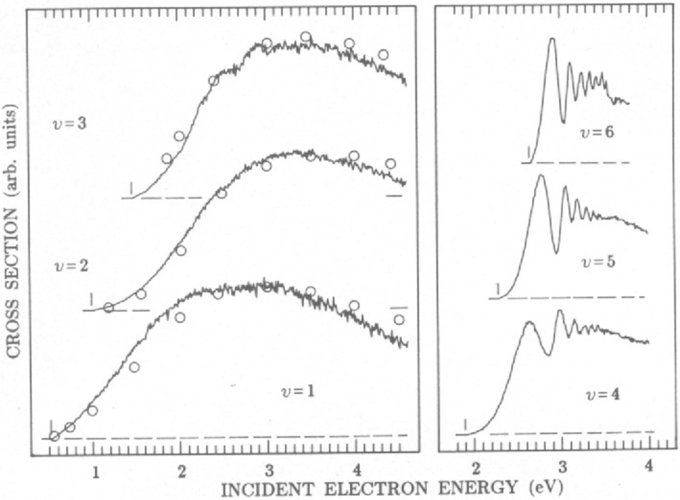

FIGURE 2
Vibrational excitation cross sections in H_2. The curves are not on the same vertical scale; the relative intensities at curve maxima were given in Ref. (10). The short vertical bars indicate threshold energies. The circles show the integral cross sections of Ehrhardt *et al.* (6), normalised to the present curves at the maximum of the υ=1 cross section.

prediction experimentally (10).

The experimental energy dependence curves are shown in Figure 2. The shapes of the first three curves are in a good agreement with the data of Ehrhardt *et al.*(6). Structures observed in the curves with υ=3 and higher confirm the theoretical predictions of Mündel *et al.*(8). In agreement with the prediction the structure is barely visible in the υ=3 curve and becomes progresively deeper with increasing υ. Revealing is the comparison of the experimental curves with the theoretical results, obtained with three different approximations, given by Mündel *et al.* The adiabatic nuclei approximation does not reproduce the vibrational structure. The local-complex-potential model gives structure in the cross section, its shape is, however, qualitatively incorrect and the cross section does not have the correct magnitude. The results thus emphasize the necessity of moving beyond the local approximation for proper treatment of nuclear dynamics in H_2.

3.2. Nitrogen

The efficient vibrational excitation of N_2 by electron impact in the 2.3 eV region has been the first observed manifestation of a resonance in electron molecule scattering (Haas (11)). Schulz (12) has found an unusual vibrational structure in the cross sections, whose explanation in terms of the "boomerang modell" by Birtwistle and Herzenberg (13) has been one of the most impressive successes of the theory of resonant electron-molecule scattering.

The vibrational excitation by the 2.3 eV resonance has been further studied by Ehrhardt and Willmann (14) and the measurements have been extended up to υ=10 by Boness and Schulz (15). Schulz (5,16) and Trajmar *et al.* (7) have extensively reviewed the existing experimental work.

The electron N_2 scattering in the 2.3 eV $^2\Pi_g$ resonance region has become a touchstone for the theories of the coupling of the electronic and nuclear

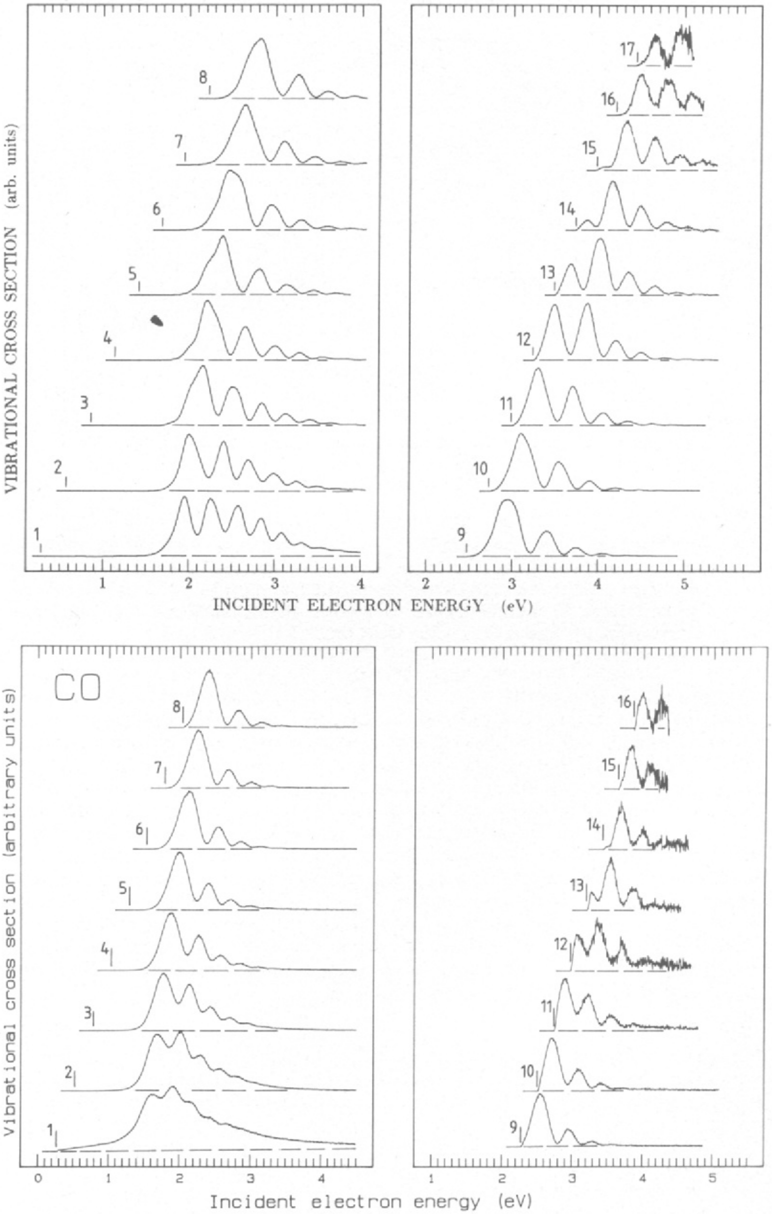

FIGURE 3
Vibrational cross sections in N_2 (top) and CO (bottom). Thresholds are indicated by vertical lines. The curves are not on the same vertical scale.

motions. This is well reflected in the numerous publications on this subject, reviewed for example by Śchulz (5,16), Lane (17), and Herzenberg (18). The recent studies (19-23) prove that the subject remains to be of current interest.

The vibrational cross sections obtained with the present instrument are shown in Figure 3 (24). The curves for υ=1 to υ=10 excitations agree well with previous experimental data. The qualitative trends observed with increasing channel up to υ=10 are (i) an increasing spacing between the peaks and (ii) an increasing dominance of the first peak in width and intensity. For υ=2 to υ=10 the first peak exhibits a "substructure" in form of shoulders. All the essential features were reproduced by the theoretical work of Domcke and Cederbaum (25), Dubé and Herzenberg (26), and Schneider *et al.* (27). For υ=11-17 the above mentioned trends are not continued. With the first peak approaching the threshold the peak spacing diminishes, the first peak becomes narrower, is no longer dominant in intensity and does not exhibit the "substructure". The discussion by Cederbaum and Domcke (28) of resonant scattering in the context of both the nonlocal and the local potentials has until very recently been the only theoretical study applicable to N_2 in this final channel range. These authors have calculated the vibrational cross sections up to υ=12 for an exactly solvable model whose parameters were chosen to simulate the $^2\Pi_g$ resonance in N_2. An important conclusion of this study has been that whereas for the low υ's the local-complex-potential model yielded satisfactory results, for the higher channels a dramatic qualitative difference has been found between the results of the local and the "exact" treatment, using using a non-local potential. Thus for the υ=12 curve the local approximation has predicted a dominant first peak, whereas the non-local treatment has predicted correctly, in qualitative agreement with the present experiment, its diminishing intensity relative to the second peak, thus confirming the importance of the non-local treatment for the higher channels.

Recently Morgan (29) has calculated the vibrational cross sections up to υ=19 using the R-matrix method and her results are in excellent qualitative agreement with the experiment.

3.3. Carbon monoxide

The vibrational cross sections in CO have been measured by Schulz (30), Boness and Schulz (15), Ehrhardt *et al.*(31), Jung *et al.*(32), Tronc and Azria (33) and by Chutjian and Tanaka (34). The present measurements aim at determining whether the shorter lifetime of the $^2\Pi$ resonance and the dipole moment of CO affect the excitation of high vibrational levels.

The cross sections obtained with the trochoidal electron spectrometer are shown in Figure 3. Only relatively minor differences between the CO cross sections and the N_2 cross sections may be observed. The cross section for the IR-active υ=1 transition is much larger in CO below the resonance region. The shorter lifetime of the resonance in CO causes the structure to be shallower in the υ=1 to υ=4 cross sections. Further, the "substructures", that is the weak shoulders observed in the υ=3 to υ=10 cross sections in N_2, are absent in CO, a fact possibly related to the shorter lifetime of the resonance in CO. Apart from these weak diferences the shapes of the cross sections are very similar in both molecules, in particular for the higher channels.

Relative differential cross sections at their maxima have been obtained by measuring the signal intensities at the maxima of the curves of Figure 3 at constant pressure and correcting them for the variation of the analyser sensitivity with residual energy. Under the assumption that the angular dependencies are the same for all υ's these relative differential cross sections are equal to the relative integral cross sections. The resulting values are compared with the results in N_2 in Figure 4. (The absolute values have been reviewed by Trajmar *et al.*(6).) The two curves are very similar except for small differences around υ=1 and υ=2, indicating that the small dipole moment of CO and the shorter lifetime of the resonance have little effect on the relative cross sections.

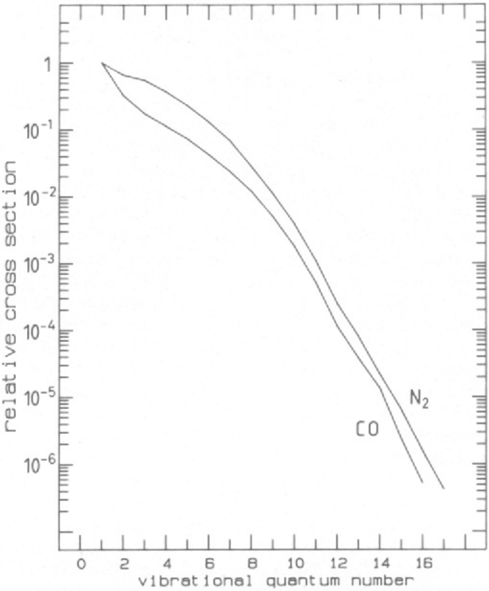

FIGURE 4
Relative vibrational cross-sections at their maxima.

4. POLYATOMIC MOLECULES.

The decay of the shape resonances in H_2, N_2, and CO described above resulted in strong excitation of low vibrational levels, with the cross section decreasing rapidly with increasing exit channel. Similar observation is made in polyatomic molecules and in addition the excitation is often characterized by a pronounced selectivity: only few of the many available vibrational modes are in general observed. Thus predominant excitation of the N-O stretch vibration *via* the 2.3 eV resonance in N_2O has been observed by Azria *et al.*(35) and Andric and Hall (36) and interpreted by Herzenberg and Dubé (37) within the impulse approximation in terms of different slopes of the negative ion potential surface along the different normal coordinates. Later it has been shown that even in large polyatomic molecules with many vibrations, like benzene (38) and ethylene (39) only very few vibrations are excited by resonant electron scattering, the change of the geometry in the negative ion and symmetry selection rules (38-40) being the determining factors.

On the other hand trapped electron (41) and ion scavenger (42) studies have shown intense (in comparison to electronic excitation) threshold electron peaks at energies of low-lying shape resonances for many polyatomic molecules. These early results have indicated that the polyatomic molecules are also excited to very high vibrational levels, leaving the scattered electron with nearly zero kinetic energy.

This work employs the trochoidal electron spectrometer to study the excitation of high vibrational levels in several polyatomic molecules.

Qualitatively similar results have been obtained with a number of organic molecules, and are illustrated here on the example of *p*-benzoquinone (43).

The transmission (44, 45) and vibrational excitation (43) spectra in *p*-benzoquinone have revealed three low-lying resonances, *a*, *b*, *c*, at 0.8 eV, 1.4 eV, and 2.1 eV (probably the ^2A_u, $^2B_{3u}$, $^2B_{3u}$ states (43-46)), which all appear to have some π^* shape resonance character because of configuration interaction (47), and a broad σ^* shape resonance *d* with a maximum around 5 eV. The vibrational excitation caused by these resonances is illustrated in Figure 5. With all four resonances distinct peaks are observed on the left side of the Figure, where the energy-loss is relatively small and the energy of the departing electron relatively large. These distinct peaks point to high selectivity of the excitation process because the density of the vibrational states is very large even for relatively small vibrational energies for a molecule of this size. The selectivity is associated with the changes of the molecular geometry in the negative ion. The π^* orbitals are antibonding along the C=C and C=O bonds and their occupation causes lengthening of these bonds and excitaion the υ_2 (and perhaps also υ_3) vibration, which contains the C=C and C=O stretch motions. The 5 eV resonance with occupation of a σ^* orbital, antibonding along the C-H bonds, excites strongly the C-H stretch vibration.

Signal is observed even for very high energy losses up to the value of the incident energy for the three π^* resonances, however. In contrast to the low energy losses no distinct vibrational levels may be discerned at high energy

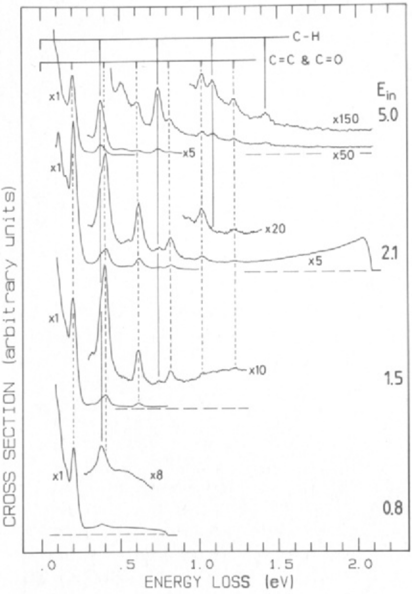

FIGURE 5
Energy-loss spectra in *p*-benzoquinone (not on the same vertical scale), recorded at constant incident energies corresponding to the π^* resonances *a*, *b*, *c*, and the σ^* resonance *d*.

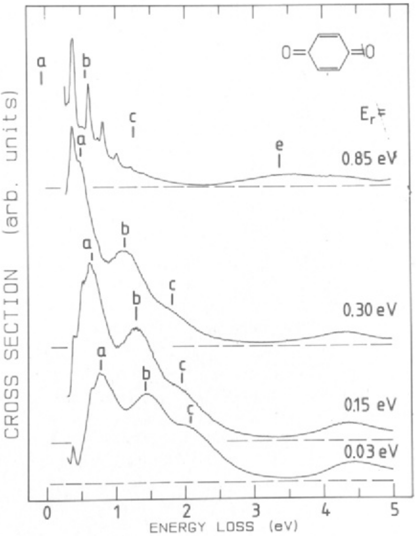

FIGURE 6
Energy-loss spectra in *p*-benzoquinone (on the same vertical scale), recorded at constant energies above threshold. Incident energies corresponding to the resonances are indicated.

losses with the available resolution, indicating that the excitation is unselective, with many (or all) of the vibrational states present being excited with comparable intensities. In the following the selective excitation mechanism will be called the "specific" vibrational excitation and the unselective mechanism the "unspecific" excitation.

The intensity of the unspecific excitation as a function of increasing energy-loss (decreasing scattered electron energy) is different for the three resonances. It decreases for the lowest resonance at 0.8 eV, remains approximately constant for the 1.5 eV resonance, and increases for the 2.1 eV resonance, resulting in a peak of zero-energy electrons.

The role of the resonances in the unspecific excitation may be seen in the constant E_r spectra of Figure 6. At low residual energies unspecific excitation results in strong peaks at the energies of the π^* resonances (a, b, and c). These peaks shift to the left on the energy-loss scale with increasing residual energy, indicating that they are fixed on the incident energy scale. No structure due to individual vibrational levels appears on these peaks, confirming the unselectivity of the unspecific vibrational excitation. The weak structure on the peak a in the spectra with E_r=0.03 and 0.15 eV is probably the boomerang structure of the negative ion, which is also seen in the transmission spectrum (44, 45). The specific vibrational excitation of long progressions in the ν_2 vibration is observed in the spectrum recorded with E_r=0.85 eV, that is higher above threshold, and in the low energy-loss region on the left side of the Figure 6. The spectra in Figure 6 thus prove that the same resonances a, b, and c are involved in both the specific and the unspecific excitation.

The specific and unspecific wibrational excitation have been observed in many polyatomic molecules with low-lying shape resonances, for example acetaldehyde, benzene, naphtalene, and octatetraene and appear to be characteristic for all larger polyatomic molecules with low-lying shape resonances.

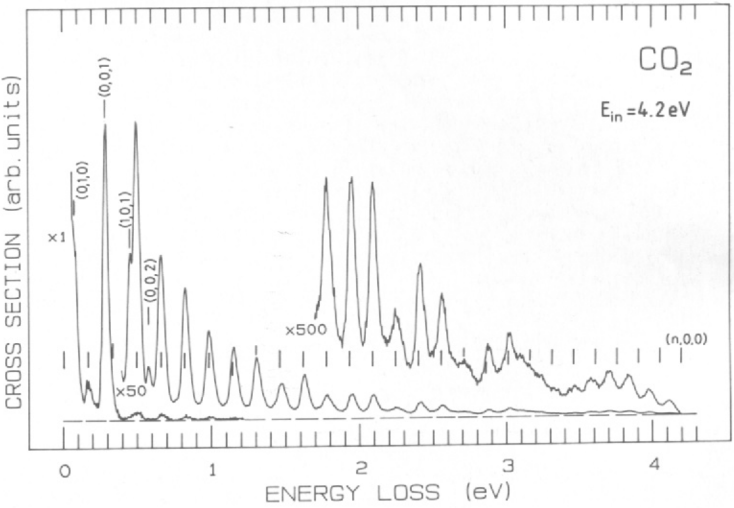

FIGURE 7
Energy-loss spectrum in CO_2, recorded at a constant incident energy.

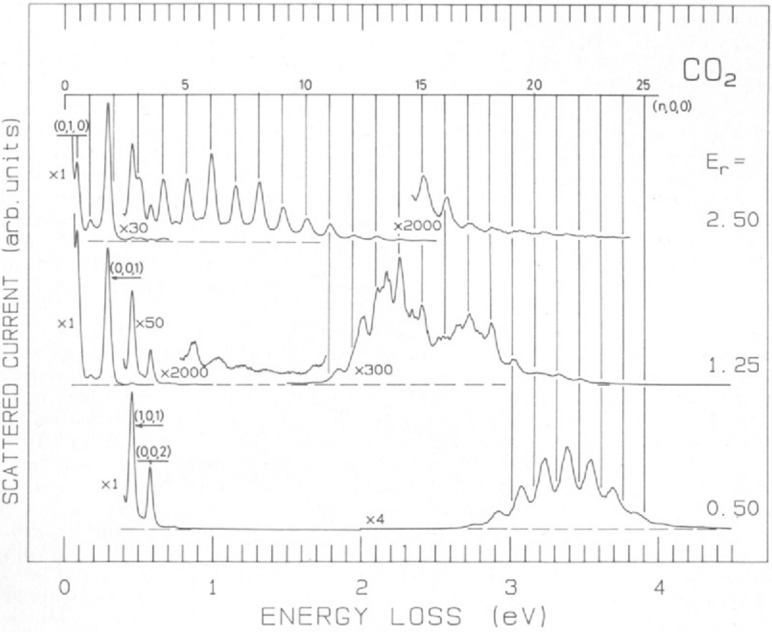

FIGURE 8
Constant-residual-energy spectra in CO_2. The three spectrea are not on the same vertical scale.

5. CARBON DIOXIDE

After the recognition of the presence of the two types of vibrational excitation in many large polyatomic molecules it appeared interesting to examine the excitation of high vibrational levels in a small polyatomic molecule like CO_2 to determine whether the excitation is selective near threshold and what kind of selectivity is encountered (48).

Vibrational excitation via the first shape resonance $^2\Pi_u$ at 3.6 eV has been studied over a large range of energy-losses by Boness and Schulz (49) and Cadez *et al.*(50). Both groups observed a strong selectivity expected for the specific vibrational excitation; the occupation of the π^* orbital causes the CO_2^- state to have longer C=O distances and to be bent and consequently a long progression in the ν_1 symmetric stretch and weaker excitation of the bending vibration ν_2 have been observed. On the other hand the excitation of high vibrational levels in threshold spectra has also been reported (51).

Figure 7 shows the vibrational excitation spectrum obtained with the trochoidal electron spectrometer at an incident electron energy within the $^2\Pi_u$ resonance. For energy-losses up to about 3 eV the spectrum agrees well with the previously published spectra, in particular with the E_{in} =4.2 eV, θ=20° spectrum of Ref.(50). For very high energy-losses the spectra are not incompatible, but the improved signal/noise ratio of the present spectrum permits a closer examination of the energy-loss region above 3 eV. Up to an energy-loss of about

3 eV the specific excitation is observed. The spectrum is dominated by a long progression in the υ_1 symm. stretch vibration, the bending vibration υ_2 being weaker at low scattering angles. The intensity of the peaks does not drop quite monotonically because of the pronounced boomerang structure observed in the vibrational cross sections (49).

At the energy-loss range 3.0-3.4 eV no distinct vibrational peaks are observed. At energy-losses above 3.4 eV vibrational structure reappears, but the peaks lie in-between the extrapolated positions for the $n\upsilon_1$ progression and must correspond to excitation of vibrations other than the $n\upsilon_1$ progression. Spectra recorded at other incident energies within the first shape resonance indicate that the "structureless" region occurs approximately at a constant energy above threshold. Insight into the behavior of the three regions may thus be gained by considering the spectra recorded at constant residual energies shown in Figure 8. A long progression in the υ_1 vibration is observed at E_r=2.5 eV, that is in the specific excitation region. The observed peak positions agree with the predicted positions (52) up to about $18\upsilon_1$. At E_r=1.25 eV, approximately in the "structureless" region, the $n\upsilon_1$ progression is still observed, but together with a large number of other, partially resolved peaks, whose energies or intensities do not exhibit any apparent regularity and which could not be assigned. At E_r=0.5 eV, in the near-threshold region, a series of equidistant peaks whose energies fall in-between the extrapolated $n\upsilon_1$ positions are observed. At closer inspection these peaks are found to be significantly broader than the instrumental resolution and to exhibit a number of weak shoulders, that is to consist of groups of closely-spaced levels.

The vibrational excitation near threshold in CO_2 thus have some resemblance to the unspecific excitation in larger molecules in the sence that it does not follow the selectivity of the specific excitation and that many more vibrational levels are excited than in the specific, farther above threshold excitation. It differs from the larger molecules in the sence that although many vibrations are excited near threshold, they can still be partially resolved, and that certain selectivity remains preserved even near threshold, the many vibrations being not excited with equal intensity, but with intensity modulated with a period close to the symm. stretch vibration.

6. CONCLUSIONS

The local-complex-potential model (Boomerang model) is adequate for resonance with moderate lifetimes, and for cross sections not including thresholds, like the excitation of low vibrational levels in N_2. It has the advantage of giving a transparent physical picture of the excitation process.

Recent advances in theory and experiment indicate, however, that it becomes inadequate for very short-lived resonances and near excitation threshold. In this situations the non-local potential treatment proves to be successful. The R-matrix method could also well reproduce the N_2 cross sections.

It appears that for any larger polyatomic molecule two types of vibrational excitation via low-lying shape resonances occur.

One is the specific vibrational excitation, which occurs higher than about 0.5-1 eV above threshold, is highly selective with respect to the vibrational modes excited, and has been studied in several molecules. The dominant factor determining the selectivity are the changes in molecular geometry upon the transition from the neutral molecule to the negative ion. In symmetrical molecules symmetry selection rules apply and in some cases vibronic interactions between two resonances may cause the excitation of particular vibrations (53). The cross section of the specific vibrational excitation decreases in general very rapidly with increasing vibrational quantum excited.

The present report concentrates on the second type, the unspecific excitation, which results in slow scattered electrons ($E_r \lesssim 0.5$ eV) and excites a quasi-continuum of vibrational states without any apparent selectivity. Depending on the compound and resonance involved the cross section may decrease (but slowlier than the specific cross section), may remain approximately constant, or may even increase with increasing energy-loss, resulting in a peak of threshold electrons. Thus, there is a tendency for the scattered electron to lose a large fraction or all of its energy to the vibrational degrees of freedom of the target molecule. Many low-lying shape resonances in many "large" molecules studied so far result in both the specific and the unspecific vibrational excitation.

A theoretical study which may point towards the interpretation of the unspecific vibrational excitation is presented at this conference by Gauyacq (54). He studies a model system with two vibrations, one large, representing the specific excitation, and the second very small, representing the vibrational quasi-continuum. When the two vibrations are treated together, this model was able to reproduce the essential qualitative features of the unspecific excitation, that is a strong excitation of the quasi-continuum and the tendency of the electron to loose almost all its energy.

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