

Incoherent renormalised multicentre potential model for electron–linear-molecule scattering: elastic and vibrational transition cross sections for e^- -N₂ and e^- -CO

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Received 23 June 1982, in final form 1 September 1982

Abstract. The incoherent renormalised multicentre potential model has been applied to study the vibrationally elastic and inelastic scattering of electrons by N₂ and CO in the intermediate energy range. The comparison with the available experimental measured data shows fairly good agreement. The comparison with the other theoretical results is also discussed.

1. Introduction

Recently, we have proposed a theoretical model for electron–linear-molecule scattering: the incoherent renormalised multicentre potential model (IRMPM) (Lee and Freitas 1981a, b). The physical formulation of the IRMPM is similar to the two-potential approximation of Choi *et al* (1979), however, in the IRMPM, the static-exchange potential for the electron–molecule interaction is derived directly from the target molecular wavefunction. In this sense the IRMPM is physically more realistic.

The application of this theoretical model to treat the elastic scattering (Lee and Freitas 1981a, b) of electrons by H₂ in the energy range between 20 and 2000 eV, and also the 0→1 and 0→2 vibrational transitions in the ground electronic state of H₂ ($X^1\Sigma_g^+$) by electron impact in the 20–81.6 eV range show that the IRMPM is a very convenient theoretical approach for electron–linear-molecule interactions in the intermediate and high incident energy range.

In view of the simplicity of the IRMPM, it is clearly of interest to extend the applicability of this theoretical model to the interaction between electrons and more complicated linear molecules.

In this paper, we have applied the IRMPM to the vibrationally elastic and inelastic scattering of electrons by N₂ and CO in the intermediate energy range. These studies can provide a further test of this theoretical model. Moreover, the comparison of the cross sections for electron scattering by N₂ and CO is interesting since N₂ and CO are isoelectronic diatomic molecules. Previous studies (Bromberg 1969, 1970, Dubois and Rudd 1976, Tanaka *et al* 1978) have shown that the angular distribution of elastically scattered electrons from these two gases is very similar. However, some

differing behaviour in respect to the angular distribution of the vibrationally inelastic cross sections is to be expected since the CO molecule has a permanent dipole moment which changes with the molecular vibration.

In the recent years, absolute and normalised elastic differential cross sections for electron scattering by N₂ and CO in the intermediate energy range have been extensively measured (Arnot 1931, Bromberg 1969, 1970, Dubois and Rudd 1976, Jansen *et al* 1976, Srivastava *et al* 1976, Shyn and Carignan 1980, Truhlar *et al* 1977, Herrmann *et al* 1976). The cross sections for the vibrational transitions in N₂ and CO have also been measured by Truhlar *et al* (1977), Tanaka *et al* (1981) and Chutjian and Tanaka (1980). Previous theoretical studies for vibrationally elastic and inelastic e⁻-N₂ scattering have been reported by Sawada *et al* (1974), Rumble *et al* (1981) using the close-coupling approach, Choi *et al* (1979) in the two-potential method and Siegel *et al* (1980) in the multiple-scattering potential method. Finally, elastic e⁻-CO scattering has previously been reported by Truhlar *et al* (1972) in a polarised Born approximation and Khare and Raj (1979) in the independent atom model (IAM) approach. A theoretical study concerning the vibrational transitions of CO by the electron impact has been done by R T Poe (1979 unpublished), see Chutjian and Tanaka (1980).

Details of the theory have already been discussed in the previous studies (Lee and Freitas 1981a, b). In § 2 we outline briefly the relevant theory. The details of the calculation and the discussion of the results will be presented in § 3 and in § 4 we present our conclusions.

2. Theory

In the adiabatic-nuclei approximation (Chase 1956) the vibrationally elastic and inelastic differential cross sections for electron-linear-molecule collision can be written as:

$$\left(\frac{d\sigma}{d\Omega}\right)_{v \rightarrow v'} = \frac{k'}{k} \frac{1}{4\pi} \int d\hat{R} |F_{vv'}(\mathbf{q}; \mathbf{R})|^2 \quad (1)$$

where $\hat{R} = (\theta_R, \phi_R)$ represents the polar angle of the internuclear vector \mathbf{R} in the laboratory frame; k and k' are, respectively, the magnitudes of the wavevector of the incident and the scattered electron and $F_{vv'}(\mathbf{q}; \mathbf{R})$ can be written (Chase 1956, Lane 1980) as:

$$F_{vv'} = \langle v' | f^{S,L}(\mathbf{q}; \mathbf{R}) | v \rangle \quad (2)$$

where $|v\rangle$ and $|v'\rangle$ represent the initial and final vibrational state vectors in the ground electronic state, $f^{S,L}(\mathbf{q}; \mathbf{R})$ is the scattering amplitude due to the short-(S), or long-(L), range potentials which depend parametrically on the internuclear distance.

In the IRMPM, the short-range potentials are basically the spherical-averaged potentials centred on the nuclei and on the centre of mass of the system. These potentials, which include the exchange effect in a local potential formalism (Bransden *et al* 1976), are derived directly from the molecular wavefunction (Lee and Freitas 1981a, b). In this paper, the semiclassical exchange (SCE) formalism (Riley and Truhlar 1975) is used. The dominant term of the long-range potential is the polarisation potential of either a permanent or an induced nature, which is given by the general

expression:

$$V_L(\mathbf{r}; \mathbf{R}) \approx \left(\left| \frac{\alpha_0(R)}{2r^4} + \frac{\alpha_2(R)}{2r^4} P_2(\cos \theta) + \frac{D(R)}{r^2} P_1(\cos \theta) + \frac{Q(R)}{r^3} P_2(\cos \theta) \right| \right) \times |1 - \exp(-r/r_c)^5| \quad (3)$$

where $\cos \theta = \hat{\mathbf{r}} \cdot \hat{\mathbf{R}}$, α_0 and α_2 are, respectively, the symmetric and asymmetric parts of the induced polarisability of the molecule and $D(R)$ and $Q(R)$ are, respectively, the dipole and quadrupole moments of the molecule.

The cross sections for the total collision process are approximated by the incoherent sum of the contributions of the short- and long-range potentials. The interference effect of multicentre scattering is taken in account by the coherent sum of the scattering amplitudes from the short-range potentials, that is:

$$f^S(\mathbf{q}; \mathbf{R}) = \sum_{\alpha} f_{\alpha}(\mathbf{q}; \mathbf{R}) \exp(i\mathbf{q} \cdot \mathbf{R}_{\alpha}) \quad (4)$$

where \mathbf{R}_{α} is the coordinate of centre α , which can be one of the nuclei or the centre of mass of the molecule.

3. Calculation and discussion

In this study, the fixed-nuclei approximation is assumed for calculating the scattering amplitude $f_{\alpha}(\mathbf{q}; \mathbf{R}_e)$ defined in equation (4), where \mathbf{R}_e is the internuclear vector of the target molecules in the equilibrium position. Therefore, the only dependence of the internuclear distance in the scattering amplitudes $f^S(\mathbf{q}; \mathbf{R})$ comes implicitly from the coordinates of α . This approximation is expected to be reasonable since in the previous study (Lee and Freitas 1981b) we have shown that only at small angles is the adiabatic-nuclei scattering amplitude $f_{\alpha}(\mathbf{q}; \mathbf{R})$ sensitive to the variation of the internuclear distance. As the main contributions to the differential cross sections in this angular range come from the scattering by the long-range potentials, this implies that the error caused by the replacement of the adiabatic $f^S(\mathbf{q}; \mathbf{R})$ by the fixed-nuclei $f^S(\mathbf{q}; \mathbf{R}_e)$ in the vibrationally elastic and inelastic cross sections will be small (<5%) in the incident energies of this study.

The molecular wavefunctions of N_2 and CO at the equilibrium internuclear distances of 2.068 and 2.132 au are calculated, respectively, by Cade *et al* (1966) and by McLean and Yoshimine (1967).

The adiabatic-nuclei long-range interaction potential between the incident electron and the target molecule is generated according to equation (3) where the R-dependent α_0 and α_2 are taken from Onda and Truhlar (1979) for N_2 and from Bridge and Buckingham (1965) for CO. The permanent dipole (in CO) and quadrupole moments of the molecules are implicitly included in the molecule wavefunctions. However, we neglected the contribution of the quadrupole moment for both N_2 and CO since the calculation for the equilibrium distance reveals that the contribution of the quadrupole moment to the scattering is not important. The R-dependent dipole moment of CO used in this work is calculated by Huo (1965) in the Hartree-Fock (HF) approximation. It is well known that the HF method gives an inverted sign for the dipole moment of CO, however, this fact is not important in this study, since the cross section depends only on the square of the dipole moment of CO. Finally, the constant r_c which appears

in the cut-off function of equation (3) is defined as (Choi *et al* 1979):

$$r_c = \frac{1}{2}(R + 2)a_0. \quad (5)$$

The scattering amplitudes due to the spherical short-range potentials are obtained by the partial-wave method whereas the scattering amplitudes due to the long-range potentials are obtained within the first Born approximation (FBA). To obtain the vibrationally elastic and inelastic scattering factor defined in equation (2), the vibrational wavefunctions were approximated by harmonic oscillator functions (Flygare 1978) as only the first two vibrational levels were treated (Dehmer *et al* 1980).

In figure 1, we show our differential vibrationally elastic cross sections for electron scattered by N₂ in the 50–800 eV range, in comparison with the experimental measurements. In this case, only the results of Srivastava *et al* (1976) and Shyn and Carignan (1980) are vibrationally elastic cross sections. Although the measured cross sections

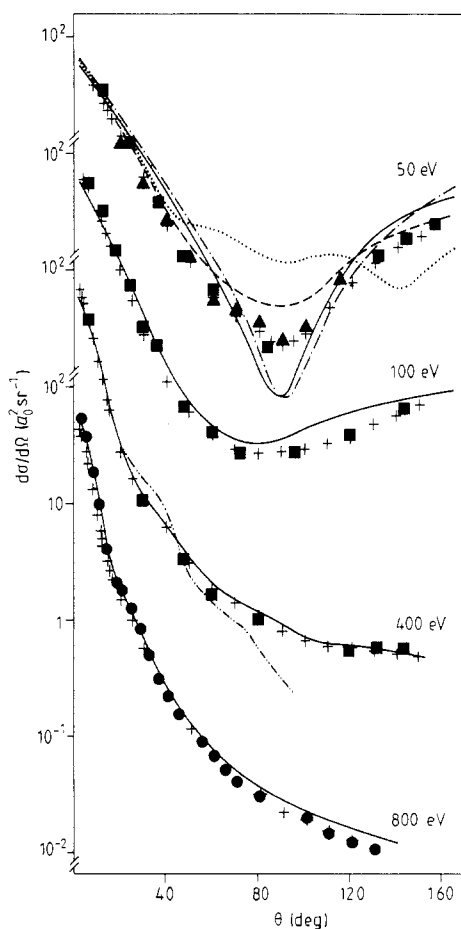


Figure 1. Elastic differential cross sections (DCS) for electron-N₂ scattering in the 50–800 eV range. Theoretical results of IRMPM (full curve), Brandt *et al* (1976) (dotted curve), Onda and Truhlar (1979) (broken curve), Choi *et al* (1979) (chain curve) and Sawada *et al* (1974) (double dotted chain curve). Experimental results are from DuBois and Rudd (1976) (+), Srivastava *et al* (1976) (▲), Shyn and Carignan (1980) (■) and Herrmann *et al* (1976) (●).

of Dubois and Rudd (1976) and Herrmann *et al* (1976) are vibrationally unresolved, comparison between these experimental data and our vibrationally elastic differential cross sections can be made directly, since the contribution of the vibrational excitation cross sections are much smaller in magnitude (Tanaka *et al* 1981) than vibrationally elastic cross sections.

One can see that the IRMPM reproduces the experimental data quite well both in shape and magnitude in the entire energy range. At 50 eV our results correctly predicted the position of the minimum of the experimental DCS except that our theoretical prediction is somewhat deeper at 50 eV. This deeper minimum from our theory can arise from the spherical averaging of the nuclei-centred short-range potentials (Choi *et al* 1979).

At higher impact energies, the agreement between our theoretical results and the experimental measured data is quite good both in absolute magnitude and in shape. Comparisons with other theoretical calculations have also been shown in figure 1. The vibrational-rotational close-coupling calculation of Brandt *et al* (1976) shows a general shape of the differential cross section, in particular, the position of the minimum, which is quite different. Another theoretical formulation for elastic scattering is by Sawada *et al* (1974) who employed a phenomenological potential. Their theory predicts the differential cross section reasonably well in shape for incident energies below 50 eV. At higher energies, their theory predicts values of the differential cross sections two orders of magnitude lower than the experimental one. The results for the DCS at 50 eV from the close-coupling calculation of Onda and Truhlar (1979) agree quite well in shape with our results, nevertheless, their theory overestimates the DCS in the region of the minimum.

The agreement between our results and those of the two-potential theory of Choi *et al* is quite good. Another recent theoretical formulation for elastic scattering was by Siegel *et al* (1980) who employed the continuum multiple-scattering method. Their results for the DCS at 300, 400 and 500 eV show good agreement with the experimental data of Bromberg (1969). However, their calculations show a bump around 90° at 300 eV and around 60° at 500 eV which are not seen in the experimental data.

In figure 2, we show our inelastic DCS for the vibrational transition $0 \rightarrow 1$ in N_2 for incident energies in the 50 to 500 eV range. A comparison with the experimental data of Truhlar *et al* (1977) at 50 and 75 eV shows fairly good agreement. At 50 eV, our theory predicts quite well the position of the minimum. Again our theoretical curve shows that the minimum around 90° is somewhat deeper than the experimental data. The theoretical results of Choi *et al* (1979) are quite similar in shape with our results, however their theory predicts vibrationally inelastic DCS values lower than ours at all points. The qualitative angular dependence of the theoretical results of Brandt *et al* (1976) is also similar to our results, except an additional minimum around 140° is observed in their results which is not clearly seen in the experimental data. Moreover, the magnitude of the results of Brandt *et al* (1979) is in general larger than our results. At 75 eV, the agreement between our results and the experimental data is considerably better than at 50 eV both in magnitude and in shape. The results of Choi *et al* are lower than our results in the entire angular range, whereas the results of Brandt *et al* are quite different both in magnitude and in shape. At higher incident energies there are no experimental measurements for comparison. A comparison has been made with the theoretical results of the two-potential formulation (Choi *et al* 1979). One can see that the shapes of these two theoretical curves are similar, nevertheless, the results of Choi *et al* (1979) show systematically lower magnitudes.

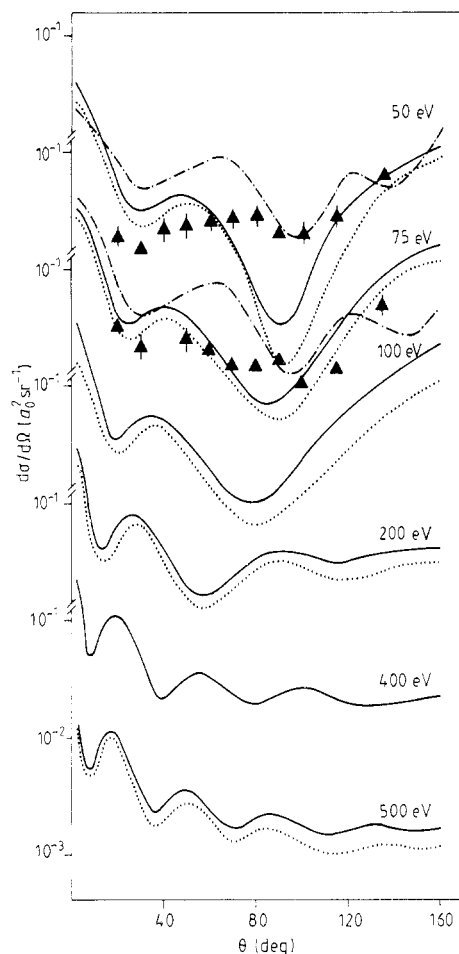


Figure 2. DCS for vibrational excitation of $v = 0$ to $v' = 1$ in N_2 in the 50–500 eV range. Theoretical results of IRMPM (full curve), Truhlar *et al* (1977) (chain curve), Choi *et al* (1979) (dotted curve). The experimental measurements are from Truhlar *et al* (1977) (\blacktriangle).

In figure 3, we compare the IRMPM elastic DCS for electron scattering by CO in the energy range of 50–800 eV with the experimental measurements of Bromberg (1970), DuBois and Rudd (1976) and Tanaka *et al* (1978). One can see that the agreement between our results and the experimental data is quite good for all the incident energies. For elastic scattering of electrons by CO, limited theoretical calculations have been reported in the literature in this energy range. Truhlar *et al* (1972) have calculated the elastic DCS by using the polarised Born approximation. Their theory predicts an elastic DCS in the 50–80 eV range quite different from the experimental data. Another recent theoretical approximation was formulated by Khare and Raj (1979) who employed the independent-atom model (IAM). Their results seem to reproduce the experimental data of Bromberg at 400 eV quite well.

Comparisons of the IRMPM elastic DCS for electrons scattered by N_2 and CO at 75 and 200 eV, together with the corresponding experimental data, are shown in figure 4. As expected, both the shape and magnitude of the two sets of theoretical

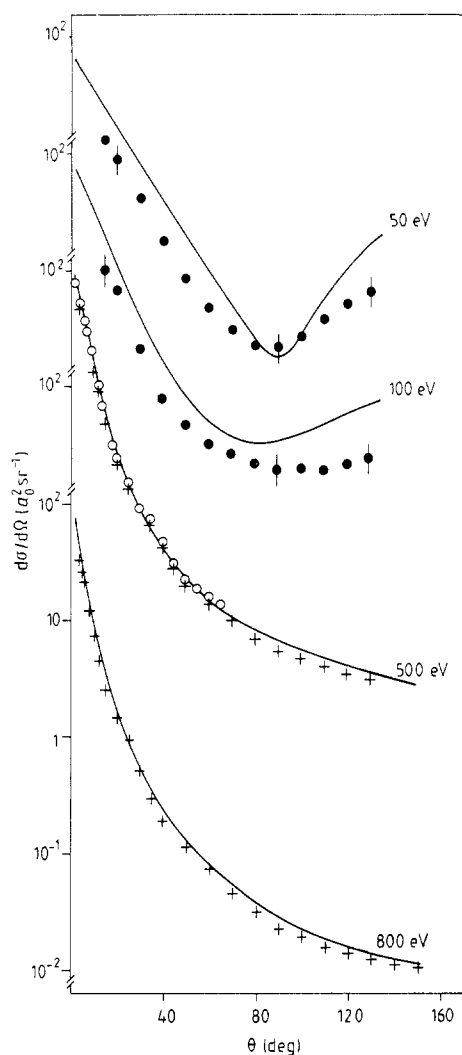


Figure 3. Elastic DCS for electron-CO scattering in the 50–800 eV range. Theoretical results of IRMPM (full curve); experimental measurements of DuBois and Rudd (1976) (+), Tanaka *et al* (1978) (●) and Bromberg (1970) (○).

data are very similar, in agreement with the previous studies (Bromberg 1969, 1970, DuBois and Rudd 1976, Tanaka *et al* 1978). Nevertheless, as the CO molecule has a permanent dipole moment which varies with the molecular vibration, one expects that the vibrationally inelastic DCS for electron scattering by N_2 and CO would be different. Comparisons of the IRMPM inelastic DCS for the vibrational transition $0 \rightarrow 1$ in N_2 and CO by electron impact at 50, 75 and 100 eV together with the available experimental data are shown in figure 5. In the first place, one can observe that, for the vibrationally inelastic DCS for e^- -CO collisions, our IRMPM theory reproduces the shape of the experimental data quite well. The agreement in magnitude is also quite good for scattering angles less than 100° , for the larger scattering angles our theory overestimates the DCS. However, our results and the experimental data are getting closer, as

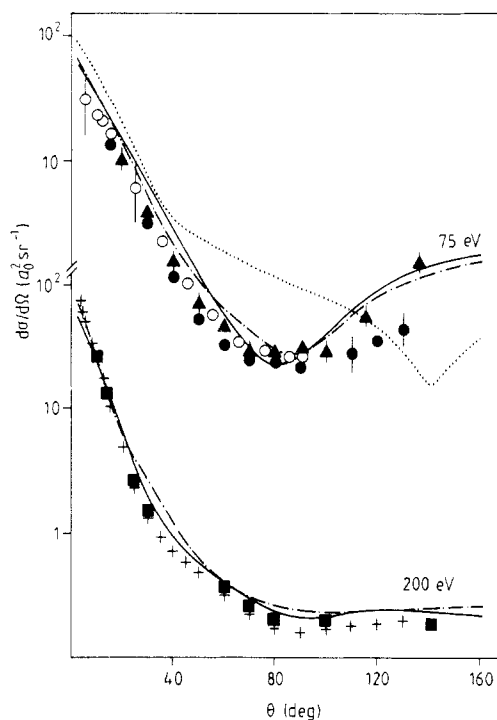


Figure 4. Comparison of the elastic DCS for electron- N_2 and electron-CO scattering in 75 and 200 eV. Theoretical results for e^- - N_2 from IRMPM (full curve), Brandt *et al* (1976) (dotted curve); IRMPM results for e^- -CO (chain curve); experimental measurements for e^- - N_2 of Finn and Doering (1975) (\circ), Srivastava *et al* (1976) (\blacktriangle) and DuBois and Rudd (1976) (\blacksquare); experimental measurements for e^- -CO of Tanaka *et al* 1978 (\bullet) and DuBois and Rudd (1976) (+).

expected, with increasing impact energy. One can also see that the agreement between our results and those of the two-potential theory of Poe (see Chutjian and Tanaka 1980) is good.

Next, we observe that the IRMPM DCS for the vibrational transition $0 \rightarrow 1$ for electron scattering by N_2 and CO are very similar both in shape and magnitude in the entire angular range except for very small scattering angles where the DCS for the e^- -CO interaction is larger. This fact might indicate that the contribution of the permanent dipole to the vibrational transition of CO is very small in the energy range considered in this work. The similar conclusion was obtained also by Chutjian and Tanaka (1980). However, it is interesting to observe that the experimental inelastic DCS for N_2 is larger than that for CO at larger scattering angles.

The integral cross sections for vibrationally elastic as well as inelastic ($0 \rightarrow 1$) e^- - N_2 and e^- -CO collisions are shown in tables 1 and 2. For elastic e^- - N_2 scattering, our results agree well with the experimental measurements of Shyn and Carignan (1980) in the 50–200 eV range. The agreement with other experimental data (Finn and Doering 1975, DuBois and Rudd 1976, Srivastava *et al* 1976) is also fairly good. Comparisons with other theoretical results show that our integral elastic cross sections agree quite well with those of Choi *et al* (1979) in the entire energy range. However,

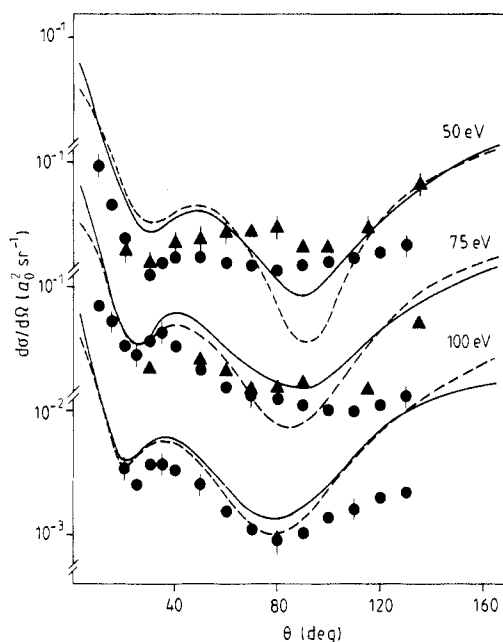


Figure 5. Comparison of the DCS for vibrational excitation of $v=0$ to $v'=1$ N_2 and CO by electron impact. IRMPM results for e^- -CO (full curve) and e^- - N_2 (broken curve); experimental measurement for e^- - N_2 , Truhlar *et al* (1977) (\blacktriangle) and for e^- -CO, Chutjian and Tanaka 1980 (\bullet).

the calculated cross section of Brandt *et al* (1979) is 20% larger than ours at 75 eV, although the agreement is good at 50 eV.

For the vibrationally ($0 \rightarrow 1$) excitation of e^- - N_2 , our integral cross section at 50 eV agrees well with the experimental data of Truhlar *et al* (1977). However at 75 eV, our theoretical model overestimates the cross sections by 66%, although the agreement between the theoretical and experimental differential cross sections at 75 eV seems to be better. Our results are also larger than those of Choi *et al* by approximately 20% in the entire energy range.

In our calculation, both vibrationally elastic and excitation cross sections for e^- - N_2 and e^- -CO collisions are similar in the entire energy range. Nevertheless, it is interesting to observe that in the impact energies up to 100 eV, the experimental integral inelastic cross sections for e^- -CO scattering (Tanaka *et al* 1978) are approximately half the magnitude of those for e^- - N_2 scattering. The same observation is also valid for the vibrational excitation cross sections. We cannot offer a particular reason for this discrepancy. For higher energies, our integral elastic cross sections for e^- -CO scattering agree well with the experimental results.

4. Conclusions

We have applied the IRMPM to calculate the vibrationally elastic and inelastic cross sections for electrons scattered by N_2 and CO in a wide range of incident energies. The good agreement between our calculated cross sections and the experimental

Table 1. Integral cross sections for vibrationally elastic and inelastic ($0 \rightarrow 1$) scattering for $e^- - N_2$ in units of a_0^2 .

$E(\text{eV})$	Integral cross sections			
	$0 \rightarrow 0$		$0 \rightarrow 1$	
	Theory	Experiment	Theory ($\times 10^{-2}$)	Experiment ($\times 10^{-2}$)
50	35.9	35.7 ^d	4.98	4.6 ^d
	37.4 ^a	20.4 ^e	4.01 ^a	
	36.7 ^b	25.8 ^f	8.4 ^b	
	27.3 ^c	28.6 ^g	2.07 ^c	
75	25.12	16.7 ^e	5.85	3.4 ^h
	27.4 ^a	20.7 ^g	5.02 ^a	
	32.7 ^b		5.7 ^b	
100	20.2	19.9 ^d	7.68	
	22.5 ^a	13.6 ^e	5.39 ^a	
		17.7 ^f		
200	12.9	13.2 ^d	4.57	
	14.8 ^a	12.6 ^f	3.75 ^a	
400	7.94	8.18 ^d	3.42	
		7.54 ^f		
500			3.01	
			2.44 ^a	
800	4.33	3.8 ^f		

^a Choi *et al* (1979).^b Brandt *et al* (1976).^c Onda and Truhlar (1979) (potential a).^d Shyn and Carignan (1980).^e Finn and Doering (1975).^f DuBois and Rudd (1976).^g Srivastava *et al* (1976).^h Truhlar *et al* (1977).**Table 2.** Integral cross sections for vibrationally elastic and inelastic ($0 \rightarrow 1$) scattering for $e^- - CO$ in units of a_0^2 .

$E(\text{eV})$	Integral cross sections			
	$0 \rightarrow 0$		$0 \rightarrow 1$	
	Theory	Experiment	Theory ($\times 10^{-2}$)	Experiment ($\times 10^{-2}$)
50	35.1	19.6 ^a	4.91	2.70 ^c
75	26.2	14.2 ^a	6.02	1.92 ^c
100	21.1	10.7 ^a	7.23	2.51 ^c
200	13.7	11.3 ^b		
500	6.59	6.15 ^b		
800	4.94	3.74 ^b		

^a Tanaka *et al* (1978).^b Obtained through the numerical integration of the published data of DuBois and Rudd (1976).^c Chutjian and Tanaka (1980).

measurements suggests that the IRMPM is a very useful theoretical model to treat e^- -molecule interactions in the intermediate- and high-energy ranges. In view of the simplicity of this model, it is clearly of interest to extend the applicability of IRMPM to more complicated polyatomic molecules. Efforts in this direction are now in progress.

Acknowledgments

The authors would like to thank Dr José Carlos Nogueira and Dr Ione Iga for many fruitful discussions. We also thank Miss Elisabeth A de Oliveira for typing this manuscript. Calculations were done on a B-6700 computer at the Centro de Computação da Universidade de São Paulo. This work is supported by Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq) and one of us (LCGF) acknowledges the CNPq for the award of a scholarship.

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