LETTER TO THE EDITOR

Elastic scattering of intermediate and high energy electrons with N_2 and CO molecules

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Abstract. The elastic scattering of intermediate and high energy electrons with N_2 and CO molecules is investigated in a two-potential coherent approach in which the intramolecular scattering effects are also considered. The short-range static potentials centred at both the atoms are derived from target molecular wavefunctions. Results are compared with recent measurements and the corresponding calculations using Yukawa-type atomic scattering factors. The new results are in better accord with experiment.

The elastic scattering of electrons by molecules at intermediate and high energies has recently been studied theoretically in several approximations going beyond the trivial well known independent-atom model (IAM) (see for example, Jain 1982, Ganas and Green 1982, Jain *et al* 1983, Daimon *et al* 1983a, Lee and Freitas 1981a, b, 1983). The reason for this intense theoretical interest is the wealth of absolute experimental data that are now available in this energy range for several diatomic (H_2, N_2, CO, O_2, etc: Shyn and Carignan 1980, Shyn and Sharp 1982, Daimon *et al* 1982, Hoffman *et al* 1982), linear polyatomic (CO_2, HCN, C_2H_2, etc: Register *et al* 1980, Shyn *et al* 1978, Fink *et al* 1975, Srivastava *et al* 1978) and nonlinear polyatomic molecules (CH_4, NH_3, H_2O, SF_6, CCl_4, As_4, SO_2, C_2H_4, C_2H_6, etc: Srivastava *et al* 1976b, Fujita *et al* 1983, Okada *et al* 1980, Orient *et al* 1982, Daimon *et al* 1983a, b, Nagashima *et al* 1982, Lahmam Bennani *et al* 1979, Shibata *et al* 1980). The knowledge of e–molecule cross sections at intermediate energies is required in many applied sciences such as radiation physics, modelling of various laser systems, cometary and interstellar plasmas, etc.

An *ab initio* treatment of the e–molecule scattering problem is prohibitively difficult in the present energy range (however, some preliminary very sophisticated *ab initio* calculations have recently been reported by Noble *et al* (1983) for the e–N_2 system). The continuum multiple-scattering method (CMSM) along with various model exchange potentials has been used by Siegel *et al* (1980) for e–N_2 elastic scattering in a wide energy range 0–1000 eV (see also Dill and Dehmer 1974, 1977, Siegel *et al* 1976, 1978). A relatively simple but promising method, to be known as the two-potential

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coherent approach (TPCA) (Hayashi and Kuchitsu 1976a, Jain 1982), has recently been applied successfully to the investigation of elastic scattering of electrons with N_2, CO, O_2 (Hayashi and Kuchitsu 1976b, Daimon *et al* 1982, Jain 1982, 1983), CO_2 (Jain and Tayal 1982), HCN (Jain and Tayal 1984), CCl_4 (Daimon *et al* 1983b) and As_4 (Daimon *et al* 1983a) molecules.

In brief, this two-potential approach adds in a coherent manner the contributions from the short- (located at each atomic centre of the molecule) and the long- (at the centre of mass (COM) of the molecule) range isotropic potentials. In addition, the intramolecular multiple scattering effects are also taken into account approximately. It has been found in all two-potential calculations to date (for references, see above) that the intramolecular multiple scattering effects are very important below 100 eV and improve the IAM results qualitatively. In the earlier application of the TPCA, the short-range potentials centred at each atom have been taken as either Yukawa-type (Jain 1982) (TPCAYTP) or semi-empirical ones of Green *et al* (1969) (see also Daimon *et al* 1983a, b). On the other hand, if the short-range potentials are derived directly from target molecular wavefunctions, a more realistic model can be constructed; Lee and Freitas (1981a, b, 1983) have derived such potentials for N_2 and CO. Very recently, Jain *et al* (1983) have used the short-range atomic potentials (derived from molecular wavefunctions) of Lee and Freitas for e-C_2H_2 elastic scattering in the TPCA; the results were in better accord with experiment compared with the results using Yukawa-type potentials. In other words, the TPCA along with the Lee and Freitas
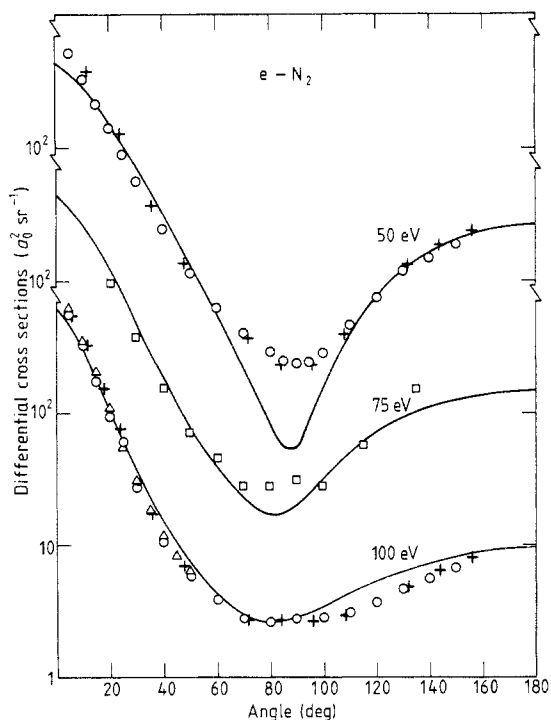

Figure 1. Elastic differential cross sections for e-N_2 scattering at 50, 75 and 100 eV. Present calculations are shown as full curves. Experimental data: $\bigcirc$, Dubois and Rudd (1976); $\triangle$, Jansen *et al* (1976); $+$, Shyn and Carignan (1980); $\square$, Srivastava *et al* (1976).

short-range potentials, is more suitable than theories where molecular effects (such as the binding effects) are ignored and the scattering amplitude is not a function of internuclear separation.

Therefore, the present letter is a follow up of our earlier work on C_2H_2 in this new approach. We report differential, integral and momentum transfer cross sections for N_2 and CO molecules in the regions 40–800 eV. In fact, Lee and Freitas (1983, for more details see Freitas 1981) have already determined scattering quantities for N_2 and CO using molecular wavefunctions to derive short-range interactions, but they did not account for the multiple scattering within the molecule (the other difference being in the choice of polarisation potential; they use a semi-empirical polarisation potential based on an adjustable parameter).

The theory and the formulae for various cross sections and the multiple scattering terms are exactly the same as described by Jain (1982). The method of generating the renormalised multicentre potentials has been discussed in detail by Lee and Freitas (1981a, b). For the long-range part of the potential, we use exactly the same potential V_L as employed by Jain (1982) (see § 2.2 of this article). We will not repeat that analysis here.

We first give numerical details of the new calculations. In order to generate the static potentials at each atomic location, we use near Hartree–Fock target wavefunctions of McLean and Yoshimine (1967) for CO and of Cade *et al* (1966) for N_2. The C_α coefficients (see equations (6)–(10) of Jain *et al* 1983) for all the three atoms C, O and N are calculated to be 1.211, 0.99 and 1.087, respectively.
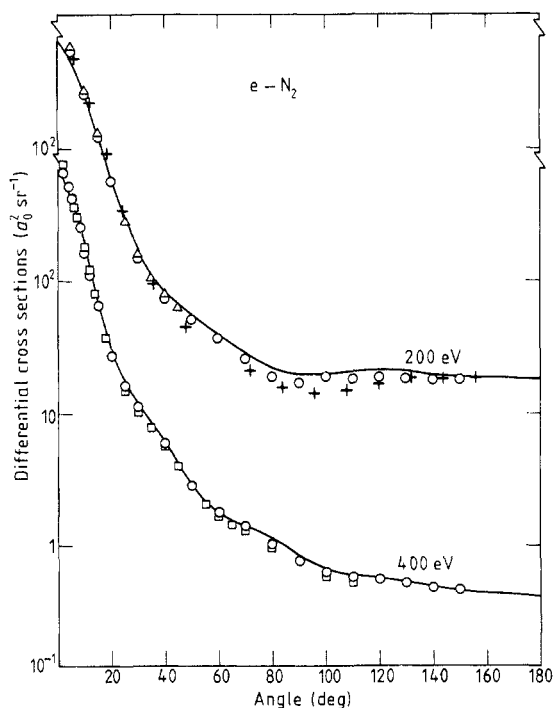

Figure 2. Elastic differential cross sections for e–N_2 scattering at 200 and 400 eV. Symbols are the same as in figure 1 except that here, $\square$, are the experimental points of Bromberg (1970).

The phaseshifts for the short-range forces in both the Yukawa-type and the RMPM atomic potentials are calculated up to an accuracy of 10^{-4}. However, for V_L, we included phaseshifts up to an accuracy of 10^{-3} only. There is a considerable difference between f_i^{YTP} and f_i^{RMPM} (f_i stands for the scattering amplitude in the Yukawa-type potential (YTP) and the RMPM potential). See Freitas (1981) for details of this comparison.

In figure 1 we have displayed the present differential cross sections (DCS) for e–N_2 elastic scattering at 50, 75 and 100 eV. For clarity, we have not plotted the calculations of Jain (1982) or Lee and Freitas (1983). (However, we shall compare their calculations for the integral (σ_I) and the momentum transfer (σ_m) cross sections later.) The present results (full curve) are compared with the experimental data of Dubois and Rudd (1976), Jansen *et al* (1976), Bromberg (1970), Shyn and Carignan (1980) and Srivastava *et al* (1976a). The agreement is very good at all energies except at 50 and 75 eV at middle angles, where the theoretical dip is much deeper than the experimental one. The same discrepancy occurred in Jain (1982) (using YTP but multiple scattering included), and Lee and Freitas (1983) (using RMPM but multiple scattering effects neglected) calculations. It means that the earlier conclusion of Jain (1982) that the discrepancy at middle angles may be partly due to the neglect of the anisotropic part of both the short and the long range potentials and partly due to the neglect of exchange seems to be correct. For example, including quadrupole terms in the interaction means to allow for the $J = 0$ to $J' = 2$ (J and J' being the initial and the final rotational quantum numbers) rotational excitation contribution to the cross section. A semi-classical calculation (Gianturco *et al* 1977) indicated that the quadrupole transition
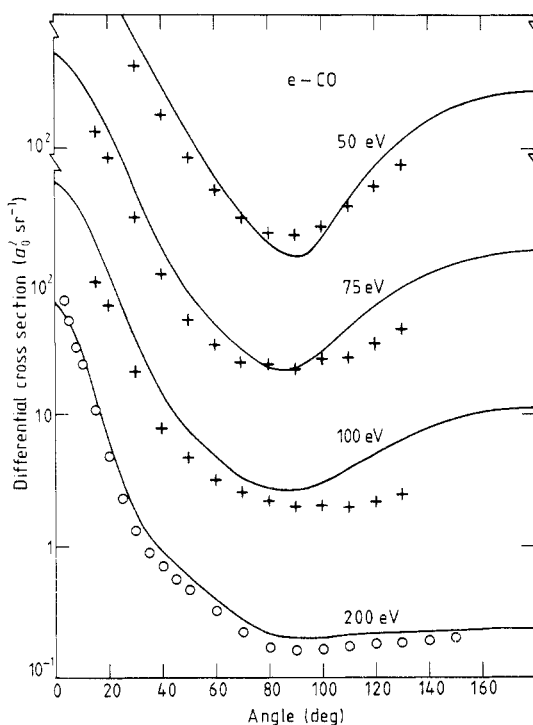

Figure 3. Elastic DCS for e–CO collisions. Present theory, full curve. Experimental points are: +, Tanaka *et al* (1978); O, Dubois and Rudd (1976).

cross sections for N_2 (also CO, CO_2, O_2) are nearly isotropic at middle angles. This, however, remains a point for future investigation. At 200 and 400 eV (figure 2), the agreement is very good and at further higher energies (not shown) we obtain excellent agreement with experiment (of course, at these higher energies, the earlier calculations of Jain (1982) and Lee and Freitas (1983) give equally excellent results too).

Our results for e–CO scattering are illustrated in figure 3 at 50, 75, 100 and 200 eV. Experimental data of Tanaka *et al* (1978) and Bromberg (1970) are plotted along with the theoretical curves. The discrepancy at 50 eV in the middle angular region seems to be improved by using the RMPM method in the case of CO. It means that molecular effects are more pronounced in the CO case (for example, the value of C_α coefficients is maximum for the carbon atom, see above). Further discrepancy may be attributed to the same reasons as mentioned earlier for the nitrogen molecule. Results at 500 and 800 eV (not shown) are in excellent agreement with measurement.

Let us now look at the new results for σ_l and σ_m for both the molecules. Here we also compare the present results with earlier calculations of Jain (1982) (TPCAYTP), and Lee and Freitas (1983) (IRMPM). In table 1, we have given all the three theoretical calculations for σ_l along with recent experimental values. The new results improve upon the old calculations with respect to the absolute experimental data of Dubois and Rudd (1976), Srivastava *et al* (1976a), and Finn and Doering (1975). A similar situation occurs for CO results. In table 2, the same data for σ_m are tabulated. Here not many experimental sets of data are available. Therefore, a definite conclusion cannot be drawn. Certainly, the new results compare better with respect to Shyn and

Table 1. Integral (σ_l) cross sections (in units of a_0^2) for e–N_2 and e–CO elastic scattering.

Energy (eV)	Theory			Experiment			
	Present	TPCAYTP	IRMPM	a	b	c	d
N_2							
50	26.14	27.62	35.90	25.8	20.4	28.6	30.35
75	20.85	22.60	25.12	—	16.7	20.7	—
100	19.14	20.94	20.20	17.7	13.6	—	19.99
200	12.66	14.31	12.90	12.6	—	—	13.2
400	8.15	9.35	7.94	7.54	—	—	8.18
500	6.97	8.04	—	—	—	—	—
800	4.87	5.67	4.33	3.8	—	—	—
CO							
50	28.08	30.26	35.1	19.6[e]			
75	23.02	24.70	26.2	14.2[e]			
100	20.29	21.79	21.1	10.7[e]			
200	13.62	14.84	13.7	11.3[f]			
500	7.54	8.29	6.59	6.15[f]			
800	5.30	5.85	4.94	3.74[f]			

[a] Dubois and Rudd (1976).
[b] Finn and Doering (1975).
[c] Srivastava *et al* (1976a).
[d] Shyn and Carignan (1980).
[e] Tanaka *et al* (1978).
[f] Obtained through the numerical integration of the published data of Dubois and Rudd (1976).

Table 2. Momentum transfer (σ_m) cross sections (in units of a_0^2) for e–N_2 and e–CO elastic scattering.

Energy (eV)	Theory		Experiment	
	Present	TPCAYTP	a	b
N_2				
50	12.73	13.53	14.64	21.1
75	9.66	10.34	—	13.2
100	7.46	8.05	6.28	—
200	3.29	3.53	2.68	—
400	1.28	1.36	1.25	—
500	0.92	0.98	—	—
800	0.45	0.48	—	—
CO				
50	13.23	13.58	11.46[c]	
75	10.17	10.37	5.71[c]	
100	7.92	8.05	3.94[c]	
200	3.44	3.52	—	
400	0.96	0.98	—	
500	0.47	0.48	—	
800	0.33	0.33	—	

[a] Shyn and Carignan (1980).
[b] Srivastava *et al* (1976a).
[c] Tanaka *et al* (1978).

Carignan (1980) numbers. For CO, the new results are certainly better than the TPCAYTP calculations of Jain (1982).

The present model can straightforwardly be applied to the vibrational excitation of these molecules. We plan to work on such a calculation.

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