

Elastic electron scattering by acetylene at low and intermediate energies

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Abstract. We report calculated differential and integral cross sections for e-C₂H₂ collisions in the 10–200 eV energy range. These cross sections were derived from fixed-nuclei scattering amplitudes in such a way that the low angular momentum components are obtained using the Schwinger iterative method and the large ones are treated by a Born closure. Using this combined theory, it can be shown that the elastic differential cross sections obtained at the static-exchange level are nearly exact, even at higher energies. The inclusion of a semi-empirical polarization potential is discussed as well.

1. Introduction

In the last few years, there have been several theoretical activities concerning the electron-molecule scattering at intermediate and high impact energies (Hayashi and Kuchitsu 1976a, b, Choi *et al* 1979, Bhattacharyya and Syamal 1985, Lee *et al* 1985, Jain *et al* 1983). As we know, with the increase of the kinetic energy, the penetration power of the incident electron into the molecule will also be increased. Therefore, the convergence of the partial-wave expansion for the continuum scattering wavefunction will become more difficult to be achieved. This fact, together with the difficulties in describing the non-spherical and non-local potentials for the electron-molecule interaction, makes the full *ab initio* calculations almost prohibitive. In particular, considering only the calculation at the static-exchange level, one should still deal with a set of coupled radial integro-differential equations which requires numerical solutions with formidable computational efforts. In this sense, several modified versions of the well known independent-atom model (IAM) have been proposed (Hayashi and Kuchitsu 1976a, b, Lee and Freitas 1981, Choi *et al* 1974). These theoretical models have been used to treat the elastic scattering of electrons by small molecules at the hundred eV region. The cross sections obtained with these models compare reasonably well with the experimental results. However, at lower incident energies, these methods, which are based on the impulse approximation (Bransden 1983) are expected to fail.

Although several alternative theoretical approaches have been proposed for studying electron-molecule scattering at intermediate energy range (Dill and Dehmer 1974,

Jain 1986, 1987, 1988), they generally deal with approximate interaction potentials: the non-spherical non-local potentials are replaced by spherically symmetric local potentials which are derived from the molecular charge densities. Physically, it is expected that the spherical potential approach should work reasonably well for the highly symmetric molecules or for the molecules in which the central atom is much heavier than the peripheral atoms. However, for linear polyatomic molecules with significant dipole or quadrupole moments, these theoretical models will not be able to describe realistically the dynamics of the collision.

In the present study we calculate the elastic differential cross sections for the e^- - C_2H_2 collision in the low and intermediate energy range, using a theory which combines the Schwinger variational iterative method (SVIM; Lucchese *et al* 1982) with the Born approximation. We will refer to this combined method as the Born closure Schwinger variational method (BCSVIM). The main purpose of the present work is to establish a theoretical formulation which is nearly exact at the static-exchange (SE) level of approximation and can be used to study the elastic electron-molecule scattering covering a wide energy range. The SVIM was introduced some time ago to study low-energy electron-linear-molecule scattering problems at the SE level. The essence of the BCSVM rests in the fact that the higher-order components of the partial-wave expansion of the transition T matrix, $T_{l'l'm}$, can be well described by a plane-wave type of approximation. Therefore, if one truncates the partial-wave expansion of the scattering wavefunction at a given angular momentum l_{\max} , the solution of the finite-size set of coupled integro-differential equations will be computationally feasible using the SVIM. The contribution of the higher partial waves can then be completed through the Born-type approximation (Thompson 1966, Nesbet 1980).

The idea itself is not new; it has already been applied to study e^- -polar-molecule scattering in the low-energy range (Padial *et al* 1983) and also to calculate the electron impact excitation processes involving optically allowed electronic transitions (Holley *et al* 1981). In both cases, the long-range dipole nature of interaction potentials leads to a slow convergence of the partial-wave expansion. However, to our knowledge, this is the first attempt to establish a theoretical formulation, at nearly exact SE level, with its applicability covering the intermediate incident energy region.

In this paper, we report calculated elastic differential and integral cross sections in the energy region from 10 to 200 eV. For e^- -acetylene scattering, experimental data covering the 100–1000 eV range are available in the literature (Fink *et al* 1975). The relative cross sections in the 4–800 eV range were also reported by Hughes and McMillen (1933) a long time ago. Thirumalai *et al* (1981) have reported calculated elastic and rotational excitation cross sections for 10 eV incident electrons. Jain *et al* (1983) have also calculated the elastic e^- - C_2H_2 cross sections in the 100–1000 eV range using a two-potential coherent approach.

In section 2 we present a review of the theory. The details of the calculation will be discussed in section 3. The comparison with previous theoretical and experimental results will be presented in section 4. In section 5 we summarize our conclusions.

2. Theory

In the Born–Oppenheimer approximation, the electronic part of the electron-molecule scattering wavefunction satisfies the fixed-nuclei Schrödinger equation

$$(-\frac{1}{2}\nabla^2 + V - \frac{1}{2}k^2)\Psi_k(\mathbf{R}; \mathbf{r}) = 0 \quad (1)$$

where the scattered electron momentum is denoted by k . The parametric dependence of the electronic wavefunction on the nuclear coordinate is expressed collectively as \mathbf{R} , and V is the electron-molecule interaction potential. For elastic scattering, the laboratory frame scattering wavefunction has the asymptotic form

$$\lim_{r \rightarrow \infty} \Psi_k \rightarrow e^{ik_0 \cdot r} + \frac{e^{ikr}}{r} f_k(\mathbf{R}', \hat{k}') \quad (2)$$

where $f_k(\mathbf{R}', \hat{k}')$ is the laboratory frame fixed nuclei scattering amplitude and is related to the electronic portion of the $(N+1)$ -particle transition T matrix (Dill and Dehmer 1974) according to

$$f_k(\mathbf{R}', \hat{k}') = \frac{i\pi^{1/2}}{k} \sum_{l'l'} i^{l'-l'} (2l+1)^{1/2} T_{ll'mm'} D_{0m}^{l'*}(\hat{R}') Y_{l'm'}(\hat{k}') D_{m''m'}^{l'}(\hat{R}') \quad (3)$$

where $D_{mm'}^l(\hat{R})$ are usual rotation matrices (Edmonds 1974), and k is the magnitude of the incident electron momentum. It is convenient to work with the K matrix which satisfies the Lippmann-Schwinger equation

$$K = V + VG_0^P K \quad (4)$$

where G_0^P is the principal-value part of G_0^+ . The principal-value part of the wavefunction Ψ^P satisfies the same Schrödinger equation

$$(-\frac{1}{2}\nabla^2 + V - \frac{1}{2}k^2)\Psi_k^P = 0. \quad (5)$$

For closed-shell molecules the function Ψ_k^P can be single-centre expanded as:

$$\Psi_k^P(\mathbf{r}) = \sum_{lm} \Psi_{klm}^P(k, \mathbf{r}) Y_{lm}(\hat{k}) \quad (6)$$

and since $m = m'$ for linear molecules, $\Psi_{klm}^P(k, \mathbf{r})$ can be re-expanded as

$$\Psi_{klm}^P(k, \mathbf{r}) = \sum_l g_{ll'm}(k, \mathbf{r}) Y_{l'm}(\hat{r}). \quad (7a)$$

The asymptotic behaviour of the radial function $g_{ll'm}(r)$ is given by

$$\lim_{r \rightarrow \infty} g_{ll'm}(r) = j_l(kr) - K_{ll'm} y_l(kr) \quad (7b)$$

where $j_l(kr)$ and $y_l(kr)$ are respectively the regular and irregular spherical Bessel functions and $K_{ll'm}$ is the partial-wave K matrix element. The transition T matrix can be related to the K matrix through the expression

$$T = \frac{-2iK}{1-iK}. \quad (8)$$

The K matrix for the electron-molecule scattering is obtained through the resolution of equation (5) by the SVIM. In this case, it is convenient to transform the Schrödinger equation to an integral form

$$\Psi_{klm}^P = S_{klm}^P + G_0^P U \Psi_{klm}^P \quad (9a)$$

or

$$\Psi_{klm}^P = S_{klm}^P + G_0^P K S_{klm}^P \quad (9b)$$

where $U = 2V$, and S_{klm}^P is the appropriate partial element of the plane wavefunction. In the svim we first solve the Lippmann-Schwinger equation (9), by assuming an approximate separable form for the scattering potential U

$$U(r, r') \approx U^s(r, r') = \sum_{\alpha_i, \alpha_j} \langle r | U | \alpha_i \rangle (U^{-1})_{ij} \langle \alpha_j | U | r' \rangle \quad (10)$$

where $(U^{-1})_{ij}$ is the inverse of the matrix with elements $U_{ij} = \langle \alpha_i | U | \alpha_j \rangle$, and $\{\alpha_i\}$ is a set of square integrable basis functions, adequately chosen to represent the separable potential. With this approximation, the partial-wave K matrix element can be obtained as

$$K_{ll'm} = \sum_{i,j} \langle S_{klm} | U | \alpha_i \rangle [D^{-1}]_{ij} \langle \alpha_j | U | S_{kl'm} \rangle \quad (11)$$

where D_{ij} is a matrix element defined as

$$D_{ij} = \langle \alpha_i | U - UG^P U | \alpha_j \rangle. \quad (12)$$

The scattering wavefunction obtained using the approximate separable potential (equation (10)) can be improved through an iterative procedure. For this, a new basis set is formed by augmenting the old $\{\alpha_i\}$ by a set of new functions

$$S_0 = \{\Psi_{kl_1m}^{S_0}, \Psi_{kl_2m}^{S_0}, \dots, \Psi_{kl_{p_0}m}^{S_0}\} \quad (13)$$

which are the scattering solutions given by equation (9), and l_p is the maximum l included in the expansion. Using this augmented set of functions, a second set of scattering solutions

$$S_1 = \{\Psi_{kl_1m}^{S_1}, \Psi_{kl_2m}^{S_1}, \dots, \Psi_{kl_{p_1}m}^{S_1}\} \quad (14)$$

is obtained through equations (9) to (11). This iterative procedure is continued until convergence is achieved. It can be shown that when the wavefunctions do converge, they correspond to the solutions of the Lippmann-Schwinger equation for the exact potential U . The elastic differential cross section for the electron-molecule scattering is given in terms of the scattering amplitude $f^{(+)}$ by

$$\frac{d\sigma}{d\Omega} = \frac{1}{8\pi^2} \int d\hat{R} |f^{(+)}(\hat{R}, \hat{k}')|^2 \quad (15)$$

where \hat{k}' is measured relative to the incident electron direction \hat{k}_0 . However, it is convenient to represent the e^- -molecule scattering cross section in the so called j_t basis (Fano and Dill 1972). Within this representation, the differential cross section can be now expressed as an incoherent sum over j_t (Siegel et al 1978):

$$\frac{d\sigma}{d\Omega} = \frac{\pi}{k^2} \sum_{j_t=0}^{j_t^{\max}} \sum_{m_t, m_t'} (2j_t + 1)^{-1} |B_{m_t, m_t'}^{j_t}(\hat{k}')|^2 \quad (16)$$

with

$$B_{m_t, m_t'}^{j_t}(\hat{k}') = \sum_{l'l'm} (-1)^m (i)^{l-l'} (2l+1)^{1/2} T_{ll'm}(l-m, l'm | j_t m_t') (l_0, l'm_t | j_t m_t) Y_{l'm_t}(\hat{k}') \quad (17)$$

where j_t is the angular momentum transferred to the molecule during the collision. Here, $j_t = l' - l$ and m_t, m_t' are projections of j_t along the laboratory and molecule axes, respectively.

In an actual calculation, the partial-wave expansion of the scattering function has to be truncated in some maximum values l_p and m_p . At high impact energies, large values of l_p and m_p are needed, increasing formidably the computational efforts.

On the other hand, it is well known that because of the centrifugal barrier, the incident electron with relatively high angular momentum has very small penetration power into the molecule. These electrons are kept away from the molecule and interact only with the relatively weak long-range potentials. Under these conditions, the Born approximation is able to provide very accurate K -matrix elements for e^- -molecule scattering. Therefore, one can truncate the partial-wave expansion of equation (6) at some reasonable values of l_p and m_p , and the contribution of higher angular momenta to the cross sections can be accounted for through the Born approximation. Then $B_{m_i m_i}^{j_i}$ can be written as

$$B_{m_i m_i}^{j_i}(\hat{k}') = B_{m_i m_i}^{\text{Born } j_i}(\hat{k}') + \sum_{l'l'm}^{l_p, m_p} (-1)^m (i)^{l-l'} (2l+1)^{1/2} (T_{l'l'm} - T_{l'l'm}^{\text{Born}}) (l-m, l'm | j_i m_i) \times (l0, l'm | j_i m_i) Y_{l'm_i}(\hat{k}'). \quad (18)$$

In equation (18), $T_{l'l'm}^{\text{Born}}$ is the Born partial T matrix element given by

$$T_{l'l'm}^{\text{Born}} = \langle S_{klm} | U | S_{k'l'm} \rangle \quad (19)$$

and $B_{m_i m_i}^{\text{Born } j_i}$ is the j_i -basis expansion coefficient of the Born scattering amplitude, namely

$$B_{m_i m_i}^{\text{Born } j_i}(\hat{k}') = \left(\frac{2j_i+1}{8\pi^2} \right) \frac{k}{i\pi^{1/2}} \int d\hat{R}' f_k^{\text{Born}}(\hat{R}'; \hat{k}') D_{m_i m_i}^{j_i*}(\hat{R}'). \quad (20)$$

If the molecular wavefunction is expressed in a Cartesian Gaussian basis function, the Born scattering amplitude can be obtained analytically as shown in previous works (see, for example, Fliflet and McKoy 1980). By combining equations (18), (19), (20) and (16) we obtain the differential cross sections for electron-molecule scattering.

3. Calculations

The ground-state electronic configuration of acetylene is $1\sigma_g^2 1\sigma_u^2 2\sigma_g^2 2\sigma_u^2 3\sigma_g^2 1\pi_u^4$. In its equilibrium geometry, the molecule belongs to the $D_{\infty h}$ group with C—C and C—H bond lengths of 2.2734 and 2.003 au, respectively. The SCF wavefunction for the C_2H_2 neutral molecule was constructed from a (3s2p/2s) Cartesian Gaussian basis set (Lynch *et al* 1984) contracted from a primitive (9s5p/4s) basis, augmented by a set of d and p polarization functions on the C and H centres, respectively. With this basis and geometry, the SCF energy is -76.831406 au.

The scattering wavefunction and the K matrices are obtained through the solution of equations (9) and (11). We have limited the SVM calculation to only six symmetries: σ_g , σ_u , π_g , π_u , δ_g and δ_u . In these calculations, all matrix elements were computed by a single-centre expansion technique with radial integrals evaluated using a Simpson's rule quadrature. The various partial-wave expansion parameters were chosen as follows.

(1) Maximum partial wave included in the expansion of the scattering solution $l_p = 10(\sigma_g, \pi_g, \delta_g)$ and $9(\sigma_u, \pi_u, \delta_u)$.

(2) All other partial wave expansions were truncated at $l = 20$.

For the radial integrations, the grid contained 1000 points and extended to 79 au with the smallest step size being 0.01 au and the largest step size 0.16 au.

Table 1 lists the initial basis sets used in equation (6) for each symmetry. An iterative procedure has been applied in order to obtain the converged K -matrix elements. It has been verified that two iterations are needed for the σ_g channel and only one iteration for other symmetries.

Table 1. Basis set used in equation (10).

Continuum symmetry	Centre	Type of Cartesian Gaussian function ^a	Exponents (α)
σ_g	C	s	4.0, 1.0, 0.3
		z	1.0, 0.3
		x^2	0.5
		z^2	0.5
	H	s	1.0, 0.3
		z	1.0, 0.3
σ_u	C	s	4.0, 1.0, 0.3
		z	1.0, 0.3
		x^2	0.5
		z^2	0.5
	H	s	1.0, 0.3
		z	1.0, 0.3
π_g	C	x	4.0, 1.0, 0.3
		xz	1.0, 0.3
	H	x	1.0, 0.3
π_u	C	x	4.0, 1.0, 0.3
		xz	1.0, 0.3
	H	x	1.0, 0.3
δ_g	C	xy	4.0, 1.0, 0.3, 0.1
	H	xy	1.0, 0.3, 0.1
δ_u	C	xy	4.0, 1.0, 0.3, 0.1
	H	xy	1.0, 0.3, 0.1

^a Defined as $\phi^{\alpha,l,m,n,A}(\mathbf{r}) = N(x - A_x)^l(y - A_y)^m(z - A_z)^n \exp(-\alpha|\mathbf{r} - \mathbf{A}|^2)$.

For each symmetry, using only the static part of the interaction potential, a partial-wave representation of the Born T matrix is also calculated up to l_p . Then, the full Born scattering amplitude is calculated analytically and the differential elastic cross sections are obtained via equations (16) and (18).

4. Results and discussions

First we will show the results obtained at the static-exchange level. The comparison between the Born closure results and those obtained separately from the Born approximation and from the truncated svim at 10 and 100 eV are shown in figures 1 and 2, respectively. In figure 2, we also show the available experimental data of Fink *et al* (1975). At 10 eV the good agreement between the Born closure data and those from truncated svim shows clearly that at this energy the chosen parameters for truncation of the partial-wave expansion provide a good description of the scattering wavefunction. The contribution originated from the angular momenta higher than l_p does not exceed 20% in the entire angular range. As expected, the differential cross sections (DCS) obtained from the Born approximation disagree significantly with those obtained from the two other theoretical methods. On the other hand, at 100 eV the DCS obtained from the truncated svim lie above the experimental data by about a factor of three. Even qualitatively, the truncated svim curve presents some oscillations which seem to be unphysical, since they are not seen in the experimental data. The disagreement with the experimental data together with the unphysical oscillations in the svim curve reveals

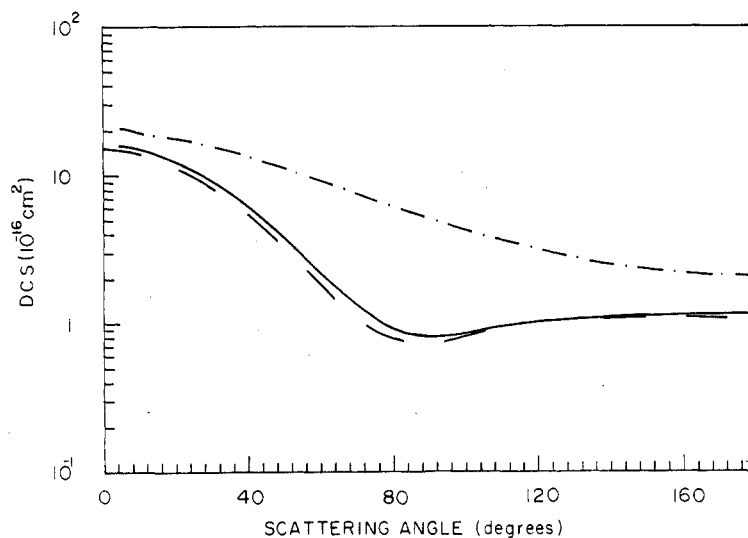


Figure 1. DCS for elastic e^- - C_2H_2 scattering at 10 eV: full curve, calculated results using the Born closure method; broken curve, truncated SVIM results; chain curve, first Born approximation (FBA) results.

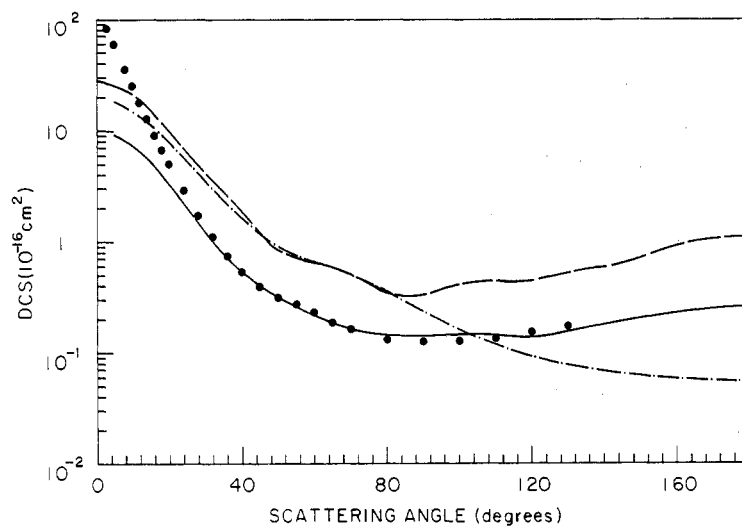


Figure 2. DCS for elastic e^- - C_2H_2 scattering at 100 eV: dots, experimental results (Fink *et al* 1975); other symbols are the same as figure 1.

clearly that with the chosen parameters for truncation, the convergence of the partial-wave expansion is still not achieved. The contribution of the higher angular momenta is important and cannot be neglected, as it can be seen in figure 2, where one notes a very good agreement between the Born closure results and the experimental data for scattering angles larger than 30° . At small angles, however, our formulation underestimates the DCS. The difference between the theoretical results and experimental data can be explained by the neglect of polarization effects in the calculated cross sections,

as we will see below. The DCS obtained via both the Born approximation and the SVIM lie above the Born closure data at angles below 100° . It is important to emphasize that although the SVIM data themselves lie well above the experimental data, the contributions of higher l s via Born approximation reduce substantially the cross sections.

In order to improve the calculated results in the small scattering angular range, we include the polarization effects in our calculation via an effective semiempirical polarization potential which can be written as

$$V_{\text{pol}} = - \left(\frac{\alpha_0}{2r^4} + \frac{\alpha_2}{2r^4} P_2(\cos(\theta)) \right) \{1 - \exp[-(r/r_c)^n]\} \quad (21)$$

where α_0 and α_2 are the symmetric and asymmetric part of the dipole polarizability, respectively, and r_c is a cut-off parameter. This semiempirical form of the polarization potential presents a correct asymptotic behaviour. For C_2H_2 , $\alpha_0 = 22.449$ au and $\alpha_2 = 12.102$ au (Hirschfelder *et al* 1964). The values of r_c and n are taken to be 2.073 au and 4.0, respectively. These values are the same as those used by Jain *et al* (1983) in their previous study and we did not attempt to find a better value for r_c . However, some studies concerning the influence of the r_c on the DCS have been made and will be discussed below.

It follows that there are two ways to include polarization effects into our calculations. In the first one, to be referred to as method A, we incorporate polarization effects simply via the Born approximation in a two-potential formalism (Hayashi and Kuchitsu 1976a, b). In this case, the partial-wave expansion T -matrix elements $T_{ll'm}$ and $T_{ll'm}^{\text{Born}}$ used in equation (18) are computed as before: at the static-exchange and static levels, respectively. Nevertheless, the full Born scattering amplitude is now formed by two parts, namely:

$$f_k^{\text{Born}} = f_k^{\text{Born st}} + f_k^{\text{Born pol}} \quad (22)$$

where $f_k^{\text{Born st}}$ is the static part of the Born scattering amplitude and is computed analytically, using the target molecular wavefunction. The $f_k^{\text{Born pol}}$ is the polarization part of the Born scattering amplitude and, in the body frame, is calculated as follows:

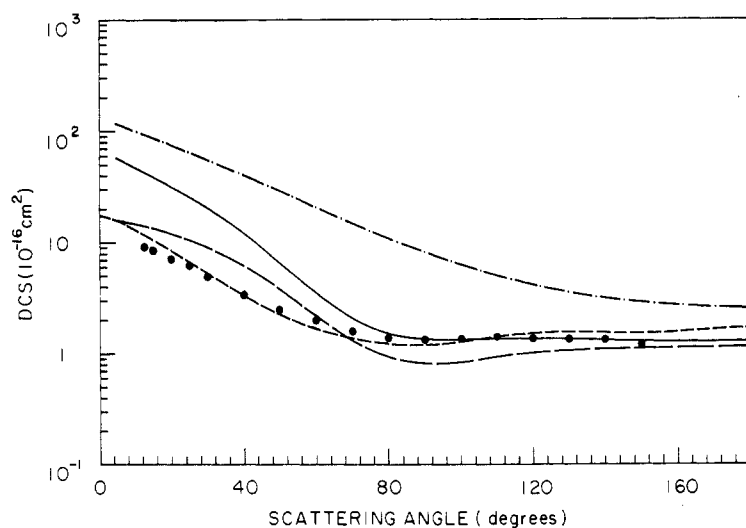
$$f_k^{\text{Born pol}} = -\frac{2}{q^2} \int e^{i\mathbf{q}\cdot\mathbf{r}} V_{\text{pol}}(\mathbf{r}) d\mathbf{r} \quad (23)$$

where \mathbf{q} is the elastic momentum transfer vector. Using the potential of equation (21), equation (23) can be reduced to two radial integrals and then evaluated using a Simpson's quadrature rule. The inclusion of polarization effects via the Born approximation is expected to provide reliable results whenever V_{pol} is relatively weak, which generally stands for high incident energies.

In table 2 we present the calculated differential and integral cross sections via method A for incident energies of 10, 50, 100 and 200 eV. The DCS are also shown in figures 3–6. In these figures, comparisons are made with the available experimental data and also with the static-exchange Born closure results. At 100 and 200 eV we compare our results also with those calculated by Jain *et al* (1983) using the coherent two-potential method. The Born results including polarization effects are shown as well. At 100 and 200 eV, the Born closure results with polarization are in excellent agreement with experimental data. Particularly at 200 eV our calculation reproduces well some oscillations due to the electron diffraction by the nuclei. The results of Jain *et al* (1983) lie on average 30% below our results.

Table 2. Elastic DCS (in 10^{-16} cm^2) for electron scattering by acetylene using svim + Born closure method A.

Angle	Incident energy (eV)			
	10	50	100	200
0.0	58.33	54.58	52.48	46.05
10.0	47.73	38.23	29.19	19.19
20.0	32.25	13.71	6.800	2.422
30.0	20.43	4.256	1.450	0.613
40.0	12.02	1.304	0.607	0.403
50.0	6.621	0.529	0.361	0.272
60.0	3.564	0.311	0.218	0.158
70.0	2.073	0.243	0.161	0.094
80.0	1.483	0.208	0.142	0.070
90.0	1.326	0.186	0.139	0.066
100.0	1.326	0.188	0.144	0.070
110.0	1.354	0.228	0.139	0.072
120.0	1.358	0.315	0.135	0.068
130.0	1.336	0.422	0.151	0.058
140.0	1.303	0.519	0.173	0.048
150.0	1.278	0.572	0.195	0.040
160.0	1.261	0.614	0.221	0.034
170.0	1.270	0.645	0.245	0.037
180.0	1.272	0.658	0.255	0.044
ICS	63.65	20.00	12.42	7.123

**Figure 3.** DCS for elastic e^- - C_2H_2 scattering at 10 eV: full curve, Born closure results which include the polarization through method A (see text); broken curve, Born closure results without polarization effects; chain curve, FBA results with polarization effects; short-dashed broken curve, calculated results of Thirumalai *et al* (1981); dots, experimental data (Hughes and McMillian 1933).

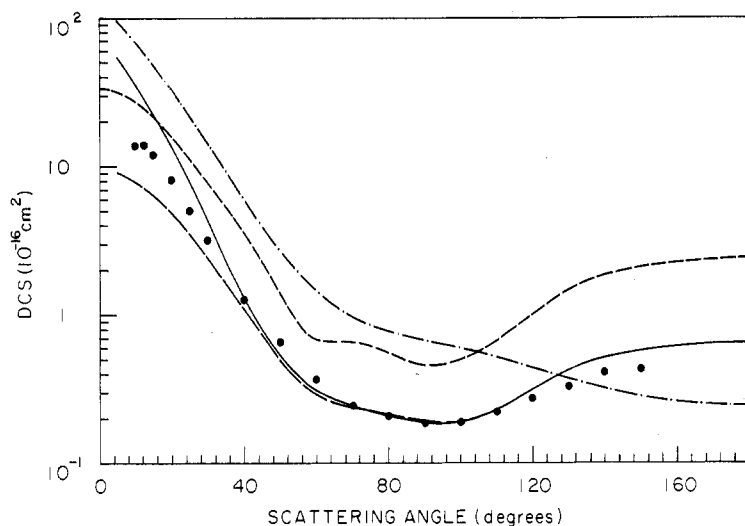


Figure 4. DCS for elastic e^- - C_2H_2 scattering at 50 eV; short-dashed broken curve, truncated SVIM results; other symbols are the same as figure 3.

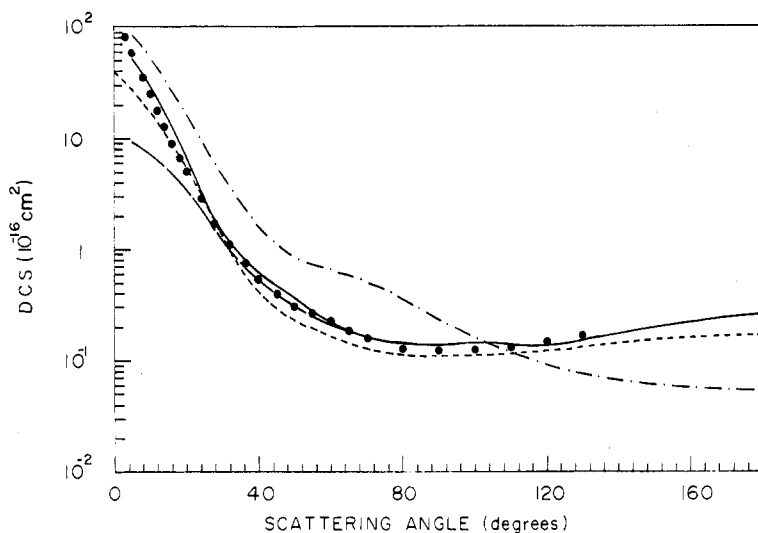


Figure 5. DCS for elastic e^- - C_2H_2 scattering at 100 eV; short-dashed broken curve, two-potential results of Jain *et al* (1983); dots, experimental data (Fink *et al* 1975); other symbols are the same as figure 3.

Comparison with the SE Born-closure data reveals that the polarization potential contributes mainly to the small-angle scattering. At lower energies, as shown in figures 3 and 4, one can see that the influence of the polarization potential is more significant. At 10 eV the discrepancy between the Born closure data with and without polarization extends to angles beyond 100°. At 10 and 50 eV, comparison is made through the normalization with the relative experimental data of Hughes and McMillen (1933) normalized to our calculated results. The normalization was carried out at 90° for both energies. At 50 eV, Born closure results both with and without polarization reproduce

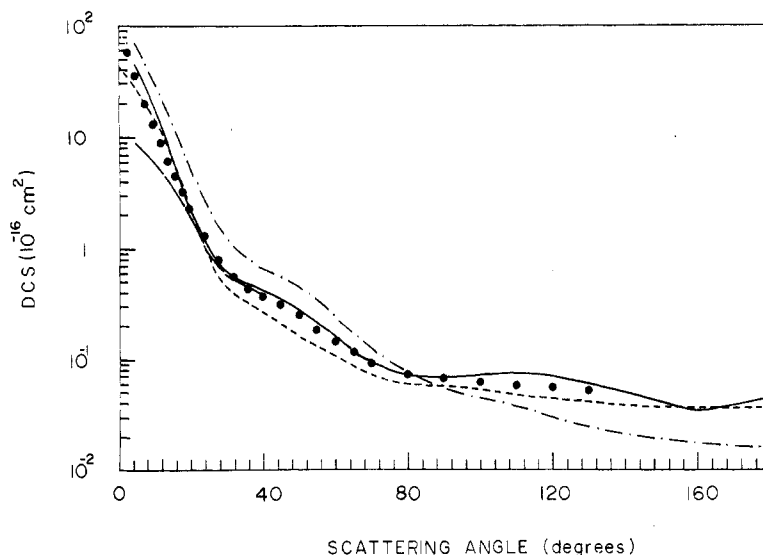


Figure 6. DCS for elastic e^- - C_2H_2 scattering at 200 eV: symbols are the same as figure 5.

well the shape of the experimental data. The agreement in magnitude is good as well, for scattering angles larger than 30° . Nevertheless, at small angles the Born closure results with polarization are more forward peaked than the experimental data. At 10 eV, the results obtained through the method A agree with the experimental data for angles above 80° . At small angles, however, our formulation overestimates the DCS. The discrepancy between theory and experiment (which is by nearly a factor of four at 15°) can possibly be attributed to the inadequacy of the cut-off parameter in the polarization potential in equation (21). Indeed, the DCS for electron-molecule scattering at the low-energy range is very sensitive to this cut-off parameter as we will show below. At 10 eV, we also show the theoretical elastic DCS, calculated by Thirumalai *et al* (1981). In comparison with our results obtained by method A, one can see that the agreement is fair at large scattering angles. However at small scattering angles the results of Thirumalai *et al* (1981) lie below our results and agree better with the experimental data. Besides the different types of polarization potentials used in the calculations, another fundamental difference between these two theoretical studies concerns the treatment of the exchange effect. In their work, Thirumalai *et al* (1981) employed a semiclassical local exchange potential, whereas the exchange effect is treated exactly in our calculation.

The second way to account for polarization effects, method B, can be described as follows. The scattering amplitude is written as

$$-2\pi f_k = \sum_{l'm'}^{l_p m_p} (T_{ll'm}^{\text{SVIM pol}} - T_{ll'm}^{\text{Born pol}}) + T_k^{\text{Born pol}}. \quad (24)$$

Here the $T_{ll'm}^{\text{SVIM pol}}$ and $T_{ll'm}^{\text{Born pol}}$ are the partial-wave transition T matrix elements, including polarization and calculated by the svim and Born approximation, respectively. In this case, the polarization potential is added to the static potential and the exchange is treated exactly in the computation of $T_{ll'm}^{\text{SVIM pol}}$, but neglected in computing the $T_{ll'm}^{\text{Born pol}}$. The $T_k^{\text{Born pol}}$ in equation (24) is the Born T matrix and can be related to

the polarized Born scattering amplitude, defined in equation (22) as:

$$T_k^{\text{Born}} = -2\pi f_k^{\text{Born}}. \quad (25)$$

The formulation of method B leads to the following physical conception: polarization effects are taken into account through svim for the low- l partial waves and via the Born approximation for high l partial waves. The calculated DCS using method B for incident electrons of 10 and 100 eV are shown in figures 7 and 8, respectively, in comparison with the Born closure results of method A and with the experimental data (Hughes and McMillen 1933). For both energies the agreement with the experimental data becomes worse in the entire angular range. At 100 eV the DCS obtained by method B show unphysical oscillations beyond 80°. Since the large-angle behaviour is determined fundamentally by the low- l partial waves, one can deduce that these low- l partial waves have been affected significantly by adding polarization effects into the scattering interaction potential. Although the polarization potential given by equation (21) has the correct asymptotic behaviour, one expects that there will be some distortions in the radial region around r_c . Because of the centrifugal barrier, the high- l partial waves would not be affected sensitively, nevertheless the low- l partial waves would be influenced by the distortions which lead to erroneous DCS. From equation (21) one can verify that the increase of r_c means physically that it limits the action of the polarization potential in a region away from the target. In this case the low- l partial waves will be less affected.

In order to examine the influence of the different cut-off parameters in the calculated DCS through method A, we show in figures 9 and 10 the results at 10 and 100 eV respectively, obtained using three values of r_c : 1.673, 2.073 and 2.473 au. At 100 eV,

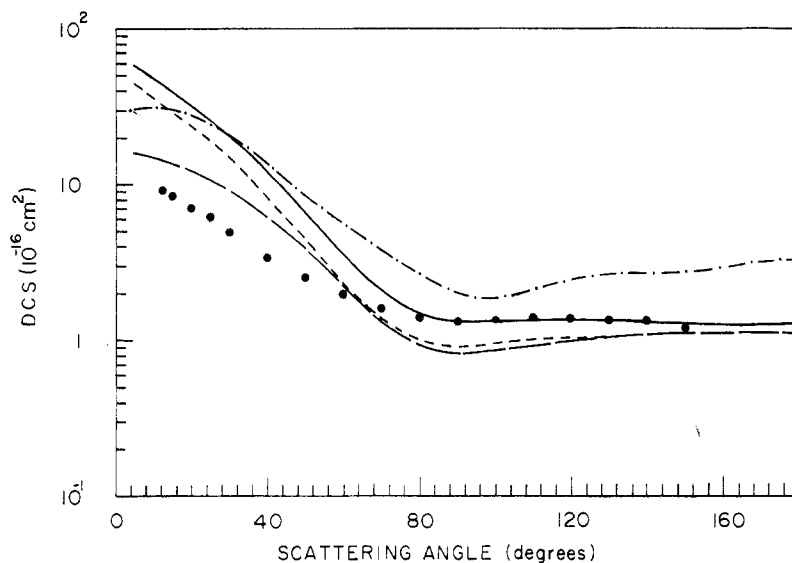


Figure 7. DCS for elastic e^- - C_2H_2 scattering at 10 eV: full curve, Born closure results including polarization through method A (see text); broken curve, Born closure results without polarization; chain curve, Born closure results with polarization via method B using cut-off parameter $r_c = 2.073$; short-dashed broken curve, Born closure results with polarization via method B using $r_c = 5.0$ au (see text); dots, experimental data (Hughes and McMillan 1933).

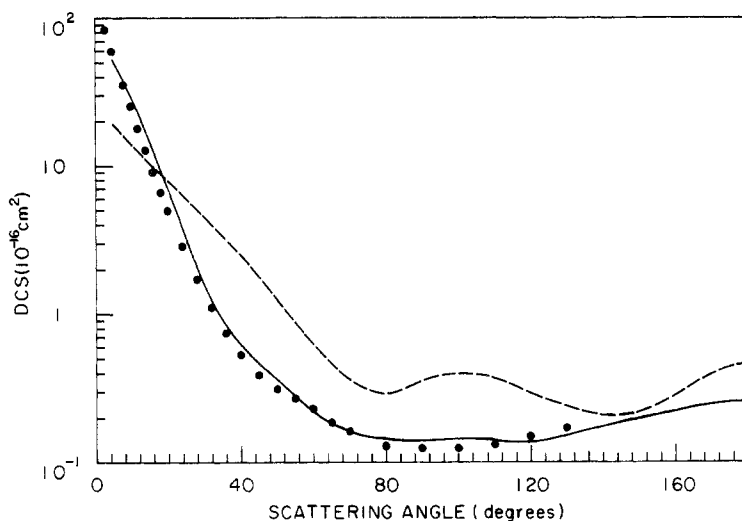


Figure 8. DCS for elastic e^- - C_2H_2 scattering at 100 eV: full curve, Born closure results including polarization through method A; short-dashed broken curve, Born closure results with polarization via method B; dots, experimental data (Fink *et al* 1975).

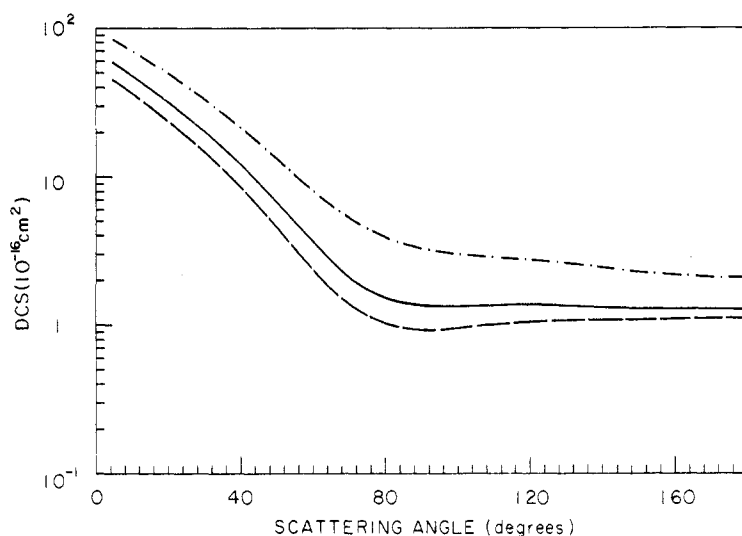


Figure 9. Influence of the cut-off parameter r_c on the DCS at 10 eV: full curve, $r_c = 2.073a_0$; broken curve, $r_c = 2.473a_0$; chain curve, $r_c = 1.673a_0$.

the DCS obtained with the last two cut-off parameters agree very well with each other in the entire angular range and both agree with the experimental data as well. The discrepancy is more significant when $r_c = 1.673$ au is used. However, even in this case the agreement with the experimental data is fair. Nevertheless, at 10 eV, the difference among these three theoretical curves is more significant, which confirms the expectation that the distortion of the polarization potential affects more sensitively the low-energy electrons.

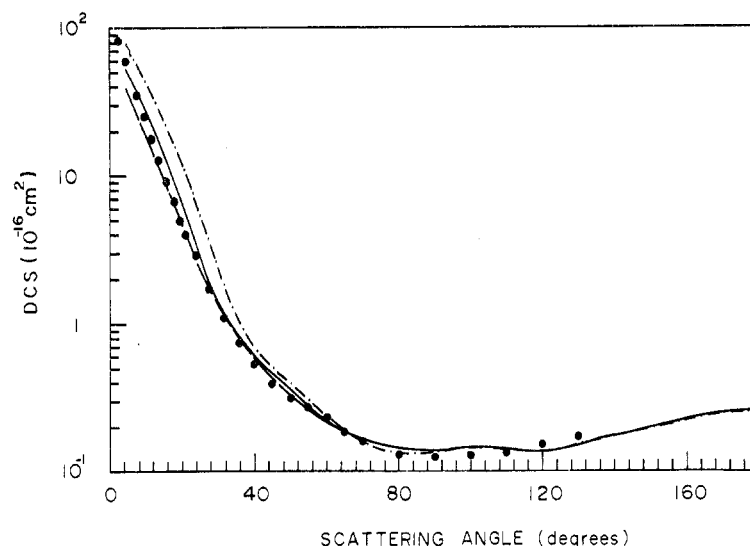


Figure 10. Influence of the cut-off parameter r_c on the DCS at 100 eV: dots, experimental data (Fink *et al* 1975); other symbols are the same as figure 9.

Through the above analysis, one can conclude that, although the distortion of the polarization potential caused by an inadequate cut-off parameter will affect both calculations via method A and method B, it seems that method A is less affected by this distortion. Nevertheless, we believe that reliable DCS can be calculated via method B if a realistic polarization potential can be obtained either through some *ab initio* method or by adjusting the best value for the cut-off parameter. In this work, no attempt in this direction has been made.

5. Conclusion

We have shown that the *ab initio* svim, designed for low-energy electron-molecule scattering, can be extended to the intermediate-energy range via the incorporation of the Born approximation to correct the contribution of the high- l partial waves. It has been shown that even at 200 eV, only few symmetries with relatively few partial-wave terms should be treated by the svim, which makes this approach computationally feasible.

On the other hand, two formulations have been tested to include polarization effects into the scattering process. The first one, that we have named method A, includes the polarization effects through the Born approximation only, whereas the second method, B, treats the contribution of polarization effects to the low- l partial waves via svim and the high- l partial waves through the Born approximation. It has been shown that the method B is more affected by the distortion of the polarization potential. In addition, in both methods A and B, the low-energy electrons are more affected by these distortions as we showed in the last section. Finally we conclude that reliable cross sections for electron-molecule scattering can be calculated with this formulation. Particularly, at the higher energies, the scattering is less affected by the distortion of the potential and our method A would be very useful in such studies.

Calculations of elastic electron scattering by other linear and non-linear molecules are underway.

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