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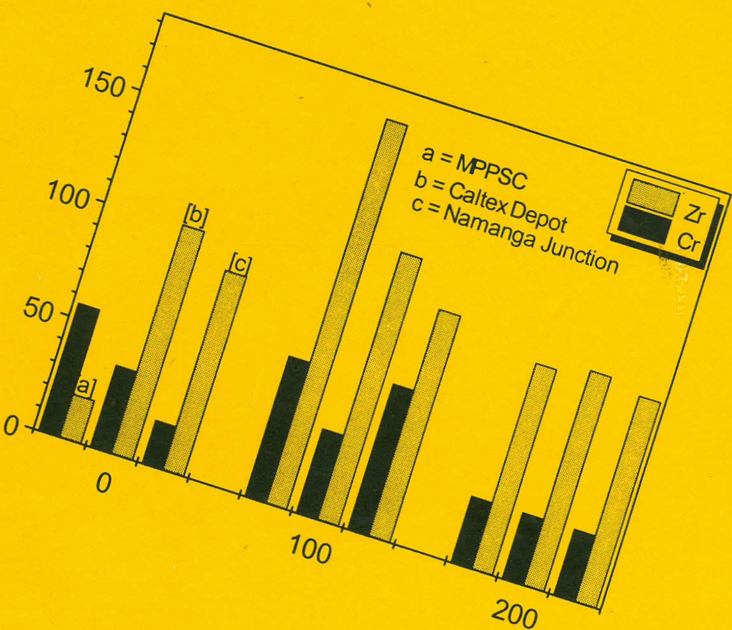
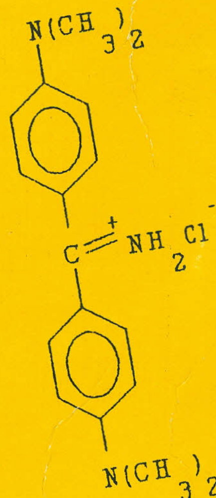
$$T = \left\langle \chi_f(\mathbf{k}_f, \mathbf{r}_2)\varphi_f(\mathbf{r}_1) \left| \frac{1}{r_{12}} \right| \Psi_i^+(\mathbf{r}_1, \mathbf{r}_2) \right\rangle$$

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# A generalized Coulomb-projected Born calculation using screened Coulomb potential

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The Coulomb-projected Born method proposed by Geltman has been generalized by using the screened Coulomb potential of the form $\frac{-Z}{r}e^{-r/a}$ in place of the nuclear potential $\frac{-Z}{r}$ experienced by the incident electron. The results obtained by using this generalized Coulomb-projected Born method for electron impact excitation of 2s state of hydrogen atom have been presented.

**Key Words** : electron impact excitation; coulomb-projected Born; screened coulomb potential; differential cross section.

## INTRODUCTION

The Coulomb-projected Born (CPB) methods suggested by Geltman (1971, 1976) and further generalized by Stauffer and Morgan (1975) improve upon the Born approximation by taking an explicit account of either the full (due to Geltman) or the partial (due to Stauffer and Morgan) interaction between the projectile electron and the target nucleus. In these methods the incident electron and the target nucleus interaction term is included either fully or partially in the unperturbed part of the hamiltonian and thus taking into account this interaction term in the form of the Coulomb-wave in the final channel. In the Born approximation this incident electron - nucleus interaction term, which is treated as a part of the perturbation, makes a vanishing contribution to the direct excitation amplitude because of the orthogonality of the atomic wavefunctions. The results obtained by using these CPB methods (Geltman 1971, 1976, Geltman & Hidalgo 1971, Stauffer & Morgan 1975) are in better agreement with the experimental results than the Born results.

In this paper we have further generalized the CPB method by using a screened Coulomb potential (nuclear potential experienced by the incident electron) in which the screening is position dependant. In the Stauffer and Morgan's generalization this screening had a fixed value. We have applied our method to electron impact excitation of 2s state of hydrogen atom and compared the results with other theoretical and experimental results. Though there are several more sophisticated accurate calculations available, *e.g.* multichannel pseudopotential close coupling calculations of Wyngaarden and Walters (1986), intermediate energy R-matrix calculation of Scholz *et al.* (1991), exact second order distorted wave results due to Madison *et al.* (1991), convergent close coupling results due to Bray and Stelbovics (1992), convergent J-matrix calculation of Konovalov and McCarthy (1994) and Pseudopotential close coupling calculation due to Wang *et al.* (1994), we are doing this calculation to see how the inclusion of screened Coulomb potential as the new screening parameter affects the original simple Coulomb-projected Born calculation.

## THEORY

Coulomb-projected Born approximation was formulated by Geltman, using the fact that the total Hamiltonian $H$ of a system can be split arbitrarily into an unperturbed part $H_0$ and a perturbation $V$. The most common choice is to assume that the unperturbed part consists of a noninteracting incident electron and the target atom (we consider e-H scattering (Singh 1989)):

$$H_0 = -\frac{1}{2}\nabla_1{}^2 - \frac{1}{2}\nabla_2{}^2 - \frac{1}{r_1}\,, \quad \text{-------------} \quad (1)$$

$$V = -\frac{1}{r_2} + \frac{1}{r_{12}}\,. \quad \text{---------------------------} \quad (2)$$

$\mathbf{r}_1$ and $\mathbf{r}_2$ represent the position coordinates of the target electron and projectile electron respectively. Then the transition matrix element T for a transition in which the target atom goes from an initial state i to a final state f can be written as

$$T = \left\langle e^{i\mathbf{k}_f \cdot \mathbf{r}_2}\varphi_f(\mathbf{r}_1) \right| -\frac{1}{r_2} + \frac{1}{r_{12}} \left| \Psi_i^+(\mathbf{r}_1,\mathbf{r}_2) \right\rangle . \quad \text{---} \quad (3)$$

$\varphi_f$ is the final state of the atom, $\mathbf{k}_f$ is the final wave vector of the projectile electron, and $\Psi_i^+$ is the total exact initial scattering wave function.

In his variation Geltman included the $-{}^1\!/_{r_2}$ term (projectile electron and target nucleus interaction term) in the unperturbed part of the Hamiltonian and thus

$$H_0 = -\frac{1}{2}\nabla_1{}^2 - \frac{1}{r_1} - \frac{1}{2}\nabla_2{}^2 - \frac{1}{r_2} \quad \text{----------} \quad (4)$$

$$V = \frac{1}{r_{12}} \quad (5)$$

The T matrix then takes the form

$$T = \left\langle \chi_f(\mathbf{k}_f,\mathbf{r}_2)\varphi_f(\mathbf{r}_1) \right| \frac{1}{r_{12}} \left| \Psi_i^+(\mathbf{r}_1,\mathbf{r}_2) \right\rangle, \quad \text{---} \quad (6)$$

where the final state plane wave of the projectile electron in (3) is replaced by the Coulomb wave $\chi_f$ in the field of the target nucleus. It is due to this reason that (6) is referred to as the Coulomb-projected form of the T matrix.

The usual Born approximation and the Coulomb-projected Born approximation can be obtained by replacing the exact scattering wave function $\Psi_i^+$ by $e^{i\mathbf{k}_i \cdot \mathbf{r}_2}\varphi_i(\mathbf{r}_1)$ in (3) and (6), respectively. $\varphi_i$ is the wave function of the target atom in the initial state. In the Coulomb-projected Born formulation (6) the effect of the projectile electron-nucleus interaction is included in the T matrix in the form of the Coulomb wave $\chi_f$, whereas in the Born approximation the incident electron-nucleus interaction term $-{}^1\!/_{r_2}$ makes a vanishing contribution to the direct excitation amplitude because of the orthogonality of the atomic wave functions.

Later, Stauffer and Morgan (1975) generalized the CPB approximation due to Geltman. They argued that the incident electron never 'sees' the bare nucleus because part of the nucleus is screened by atomic electron(s). So it 'sees' a partially screened nucleus. Thus in this case

$$H_0 = -\frac{1}{2}\nabla_1{}^2 - \frac{1}{r_1} - \frac{1}{2}\nabla_2{}^2 - \frac{\xi}{r_2}, \quad \text{---------} \quad (7)$$

$$V = -\frac{1-\xi}{r_2} + \frac{1}{r_{12}}\,. \quad \text{------------------------} \quad (8)$$

The corresponding T matrix takes the form

$$T = \left\langle \chi_f(\xi,\mathbf{r}_2)\varphi_f(\mathbf{r}_1) \right| -\frac{1-\xi}{r_2} + \frac{1}{r_{12}} \left| \Psi_i^+(\mathbf{r}_1,\mathbf{r}_2) \right\rangle . \quad \text{----------} \quad (9)$$

Here $\chi_f$ is a Coulomb wave describing the projectile electron in the field of a charge $\xi$ situated at the position of the nucleus. Stauffer and Morgan made calculations for different values of the screening parameter $\xi$ varying from 0 to Z. When $\xi = 0$, the Generalized Coulomb-projected Born method of Stauffer and Morgan converges to simple Born approximation and when $\xi = Z$ it reduces to CPB method of Geltman. Between these two values it is a generalized form of CPB method.

Since the incident electron 'sees' the screened nucleus and this screening depends on the position of the incident electron, we thought that instead of taking any fixed value of $\xi$ between 0 and Z, it is worthwhile to include the screened potential of the form $-\frac{Z}{r}e^{-r/a}$ in the unperturbed part of the hamiltonian. So the unperturbed part of the Hamilton $H_0$, interaction $V$ and the T matrix have the same form as in case of generalized CPB method of Stauffer and Morgan but the screening parameter $\xi$ is now position dependent and it is given as $\xi = Ze^{-r/a}$. The above form of the screened Coulomb potential behaves like the nuclear Coulomb potential for atomic number Z for small $r$ and falls of rapidly when $r$ is large in comparison with $a$ assumed to be the 'radius' of the atomic electron cloud that screens the nucleus. Thus this potential gives a picture which is much closer to the actual physical picture of the electron – atom collision.

## RESULTS AND DISCUSSION

We performed the calculation for e-H scattering by making use of the above variation in the CPB method. In the screened Coulomb potential $-\frac{Z}{r}e^{-r/a}$ we substituted $a = a_0$ = first Bohr radius and Z = 1 for hydrogen. In the calculation we used a computer program as used by Singh (1989) with necessary modifications.

The differential cross section results of our calculation for 1s – 2s excitation of hydrogen atom by electron impact at impact energies 54.4 eV and 100 eV are shown in figures 1 and 2 respectively. The present results are compared with the CPB results. The multichannel pseudopotential close coupling results of Wyngaarden and Walters (1986) are also plotted. At 54.4 eV we have plotted the experimental results of Williams (1981) also. We see from the two figures that at higher angles the present results are closer to the experimental as well as to the more reliable theoretical multichannel pseudopotential close coupling results compared to the CPB results. Though the change, as we go from CPB results to the present results, is not too much, but it is obvious that the present results are in better agreement with the experimental and more accurate theoretical close coupling results than the CPB results. This indicates that the CPB method used with screened Coulomb potential as the potential for distortion of the projectile electron wave is better than the simple CPB method where the total nuclear potential is used as the potential for distortion.

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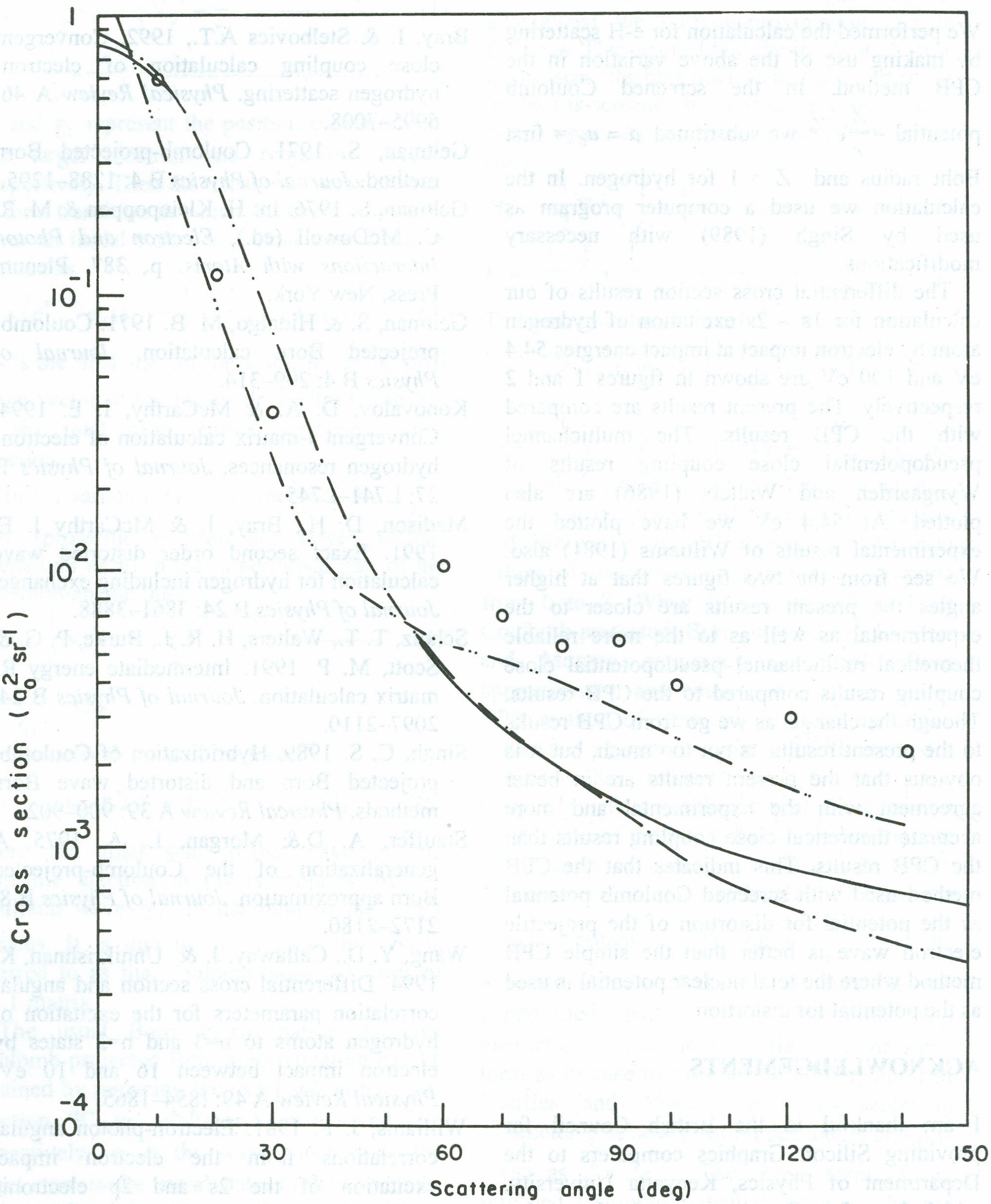


**Figure 1.** Differential cross section for 1s – 2s excitation of hydrogen atom by electron impact at 54.4 eV electron impact energy.

——— Present results

—·— CPB results

—··— Multichannel pseudopotential close-coupling results (Wyngaarden & Walters 1986)

O Experimental results of Williams (1981)

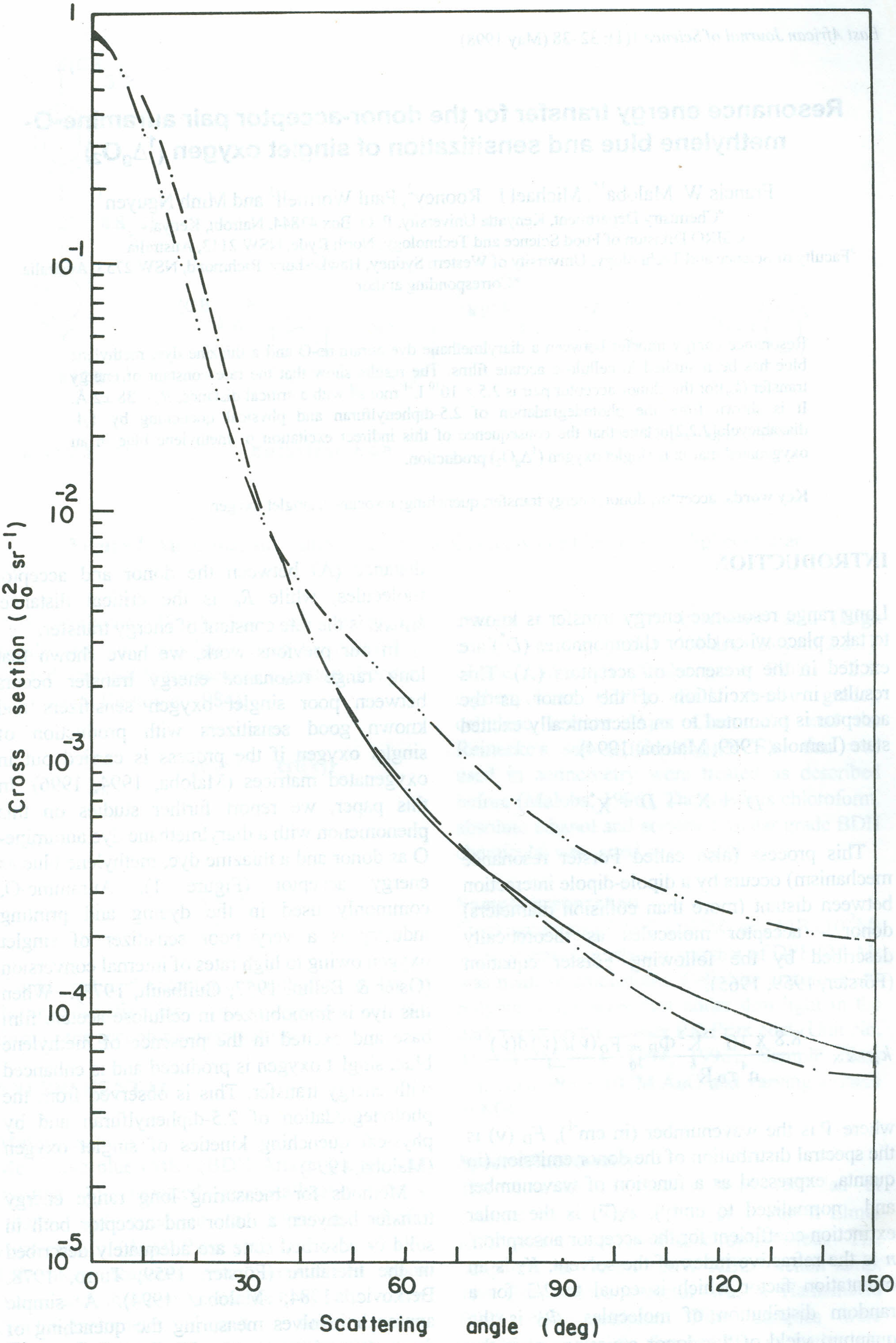


**Figure 2.** Same as Fig. 1 but at 100 eV electron impact energy.