

## Elastic scattering of electrons by hydrogen molecules using the eikonal approximation

P. K. Bhattacharyya

*Department of Physics, University College of Science, University of Calcutta, 92 Acharya P.C. Road, Calcutta-700009, India*

A. S. Ghosh

*Department of Theoretical Physics, Indian Association for the Cultivation of Science, Calcutta-700032, India*

(Received 5 November 1974)

The eikonal approximation has been used to investigate the elastic scattering of electrons by hydrogen molecules. In addition to the static potential, the effects of polarization and exchange have been included through potentials. The total and the differential cross sections have been calculated in the energy range 9.4–100.0 eV and compared with the experimental and other theoretical values. It is found that the eikonal approximation predicts reliable results for incident electron energies  $\geq 20.0$  eV.

### I. INTRODUCTION

In recent years the problem of elastic scattering of electrons by hydrogen molecules has received considerable attention by experimental<sup>1-3</sup> as well as theoretical workers.<sup>2,4-10</sup> Apart from some low-incident-energy calculations,<sup>4-6</sup> theoretical investigations are centered round the intermediate- and high-energy regions.<sup>7-10</sup> Khare and Moiseiwitsch<sup>7</sup> have employed the first Born and the first-order exchange approximation and neglected the polarization of the molecule. They have used a two-center wave function, and the results have been given in the separated-atom approximation. Rozsnyai<sup>8</sup> has also used the first Born approximation without taking into consideration the effect of polarization. Trajmar *et al.*<sup>2</sup> and Truhlar and Rice<sup>9</sup> have used the polarized Born and Born-Ochkur-Rudge approximations to investigate this problem. Khare and Shobha<sup>10</sup> have also applied the same approximation. The results of these calculations<sup>11</sup> are in good agreement with the experimental findings for the incident electron energies  $E \geq 100.0$  eV.

In this paper we have applied a modified form of the eikonal approximation<sup>12</sup> to investigate the elastic scattering of electrons by hydrogen molecules. In addition to the static potential which includes a semiempirical quadrupole term, we have considered the polarization potential and exchange effect through a model potential. The eikonal approximation, which has been used earlier in electron-atom collisions by different workers,<sup>13,14</sup> is applicable for intermediate and high energies. The main advantages of this method are that it obeys the important constraint of unitarity and is consistent with the requirement of time reversibility. The validity and the accuracy of the eikonal approximation have been discussed in detail by Glauber<sup>15</sup> and Newton.<sup>16</sup> Ghosh and his

co-workers<sup>12</sup> have applied the present method successfully to the problem of scattering of electrons (positrons) by hydrogen, helium, and lithium atoms. However, they have not considered the effect of exchange.

### II. THEORY

In the eikonal approximation the scattering amplitude is given by (throughout this paper atomic units are used)

$$F(\theta, \varphi, \theta_m, \varphi_m) = k_i (2\pi i)^{-1} \int e^{\vec{q} \cdot \vec{b}} (e^{-i\chi(\vec{b})} - 1) b db d\varphi, \quad (1)$$

where  $\vec{b}$  is the impact parameter measured from the center of mass of the hydrogen molecule;  $\vec{q} = \vec{k}_i - \vec{k}_f$ ,  $\vec{k}_i$  and  $\vec{k}_f$  being, respectively, the momenta of the incident and the scattered electrons;  $\theta, \varphi$  are the angles of scattering and  $\theta_m, \varphi_m$  denote the angles of orientation of the molecular axis. The phase-shift function  $\chi(\vec{b})$  is of the form

$$\chi(\vec{b}) = \frac{1}{v_i} \int_{-\infty}^{\infty} V_{\text{opt}}(\vec{r}_3) dz, \quad (2)$$

where  $\vec{v}_i$  is the velocity of the incident electron and  $\vec{r}_3$  denotes the position vector of the incoming electron relative to the center of mass,

$$\vec{r}_3 = \vec{b} + \hat{n}z, \quad (3)$$

$\hat{n}$  being the unit vector along the incident direction. The optical potential<sup>17</sup>  $V_{\text{opt}}$  is expressed as

$$V_{\text{opt}}(\vec{r}_3) = V_S(\vec{r}_3) + V_P(\vec{r}_3) + V_{\text{ex}}(\vec{r}_3). \quad (4)$$

The first term on the right-hand side is the static potential and is obtained from the expression

$$V_S(\vec{r}_3) = -\left(\frac{1}{r_{3a}} + \frac{1}{r_{3b}}\right) + \int |\Phi_0(1,2)|^2 \left(\frac{1}{r_{13}} + \frac{1}{r_{23}}\right) d\vec{r}_1 d\vec{r}_2, \quad (5)$$

where  $r_{3a}$ ,  $r_{3b}$ , and  $r_{i3}$  are the distances of the incident electron from the nuclei  $a$ ,  $b$ , and the bound electrons, respectively. Using for the molecular wave function  $\Phi_0(1,2)$  the one used by Hara,<sup>4</sup> we get

$$V_S(\vec{r}_3) = V_S^0(\vec{r}_3) + [V_S^2(\vec{r}_3) + V_q(\vec{r}_3)] P_2(\cos\theta_3), \quad (6)$$

with<sup>18</sup>

$$V_S^0(\vec{r}_3) = -0.27734(1/r_3)(e^{tr_3} - e^{-tr_3}) + 0.13961(e^{tr_3} + e^{-tr_3}), \quad r_3 \leq 0.7$$

$$= -1.86577(1/r_3)e^{-tr_3} - 3.51477e^{-tr_3}, \quad r_3 \geq 0.7,$$

$$V_S^2(\vec{r}_3) = 5.01637(1/r_3^3)(e^{tr_3} - e^{-tr_3}) + 11.69816(1/r_3^2)(e^{tr_3} + e^{-tr_3}) - 10.27985(1/r_3)(e^{tr_3} - e^{-tr_3}) + 2.76688(e^{tr_3} + e^{-tr_3}), \quad r_3 \leq 0.7$$

$$= -0.96504(1/r_3^3)e^{-tr_3} - 2.25047(1/r_3^2)e^{-tr_3} - 2.81971(1/r_3)e^{-tr_3} - 2.49604e^{-tr_3}, \quad r_3 \geq 0.7,$$

$$V_q^2(\vec{r}_3) \rightarrow -Q/r_3^3, \quad \text{as } r_3 \rightarrow \infty,$$

where  $Q$  is the quadrupole moment of the hydrogen molecule and is equal<sup>4</sup> to  $0.464a_0^2e^2$ ,  $t = 2.332a_0^{-1}$ , and  $\theta_3$  is the angle made by  $\vec{r}_3$  with the molecular axis and is given by

$$\cos\theta_3 = \cos\theta \cos\theta_m + \sin\theta \sin\theta_m \cos(\varphi - \varphi_m). \quad (7)$$

The second term of the optical potential [Eq. (4)] is the polarization potential which in the adiabatic approximation takes the form

$$V_P(\vec{r}_3) = V_P^0(\vec{r}_3) + V_P^2(\vec{r}_3) P_2(\cos\theta_3), \quad (8)$$

with

$$V_P^0(\vec{r}_3) \rightarrow -\alpha_0/2r_3^4, \quad \text{as } r_3 \rightarrow \infty,$$

$$V_P^2(\vec{r}_3) \rightarrow -\alpha_2/2r_3^4, \quad \text{as } r_3 \rightarrow \infty,$$

where  $\alpha_0$  and  $\alpha_2$  are linear combinations of the static parallel and perpendicular polarizabilities and their values<sup>10</sup> are taken to be  $5.18e^2a_0^3$  and  $1.20e^2a_0^3$ , respectively. For finite  $|\vec{r}_3|$  the asymptotic forms of  $V_q^2$ ,  $V_P^0$ , and  $V_P^2$  are replaced by  $-Qr_3^3(r_3^2 + R_0^2)^{-3}$ ,  $-(\alpha_0/2)(r_3^2 + R_0^2)^{-2}$ , and  $-(\alpha_2/2)r_3^2(r_3^2 + R_0^2)^{-3}$ , respectively, where the cutoff parameter  $R_0$  is taken equal<sup>4</sup> to  $1.6a_0$ . The third

term of the optical potential [Eq. (4)] accounts for the exchange of the incident electron with either of the two bound electrons and has been considered in the form given by Hara.<sup>4</sup> Using Eqs. (4), (6), and (8) in the expression for  $\chi(\vec{b})$  [Eq. (2)], we get

$$\chi(\vec{b}) = (1/v_i) \int_0^\infty [A' + B'P_2(\cos\theta_3)] dz, \quad (9)$$

with

$$A' = 2[V_S^0(\vec{r}_3) + V_P^0(\vec{r}_3) + V_{ex}(\vec{r}_3)],$$

$$B' = 2[V_S^2(\vec{r}_3) + V_P^2(\vec{r}_3) + V_q^2(\vec{r}_3)].$$

For averaging the molecular orientations ( $\theta_m, \varphi_m$ ) we have selected three orientations,<sup>19</sup>  $(0,0)$ ,  $(\pi/2,0)$ , and  $(\pi/2,\pi/2)$ . Remembering Eq. (7), Eq. (9) reduces to

$$\chi(\vec{b}) = A \pm B \cos 2\varphi, \quad (10)$$

with

$$A = (1/v_i) \int_0^\infty [A' + (\frac{3}{4} \sin^2\theta - \frac{1}{2})B'] dz,$$

$$B = (1/v_i) \int_0^\infty \frac{3}{4} B' \sin^2\theta dz,$$

where the plus and minus signs are for the orien-

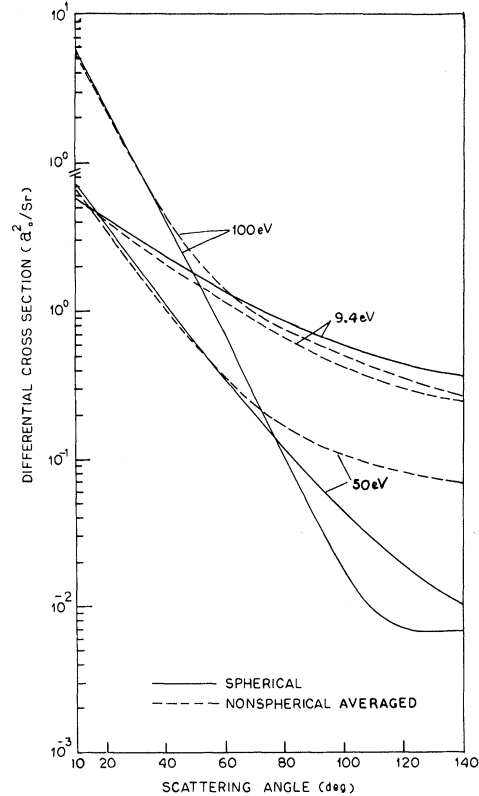


FIG. 1. Study of the effect of nonspherical parts of the effective potential on the differential cross section.

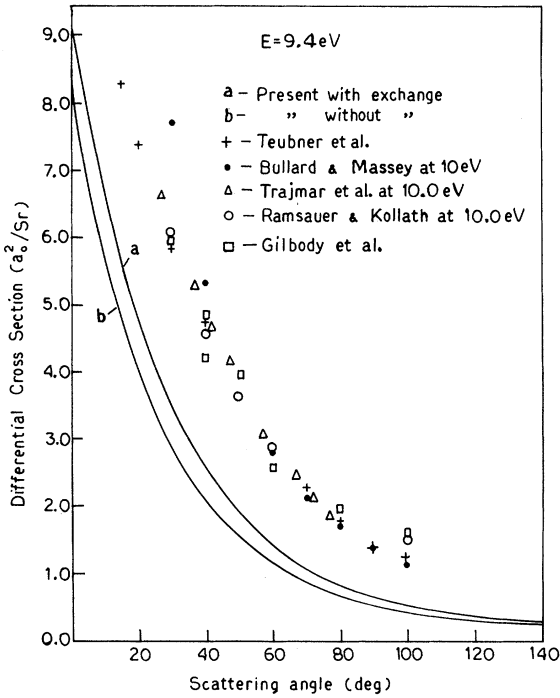


FIG. 2. Comparison of theoretical and experimental differential cross sections for  $e\text{-H}_2$  scattering, at  $E = 9.4$  eV.

tations  $(\pi/2, 0)$  and  $(\pi/2, \pi/2)$ , respectively. Equation (10) becomes independent of  $\varphi$  for the orientation  $(0, 0)$  and the integration is straightforward. Using Eqs. (10) and (1), we obtain

$$F(\theta, \varphi, \theta_m, \varphi_m) = (k_i/2\pi i) \int e^{i(qb \cos\varphi \mp B \cos^2\varphi - A)} b db d\varphi + ik_i \int J_0(qb) b db. \quad (11)$$

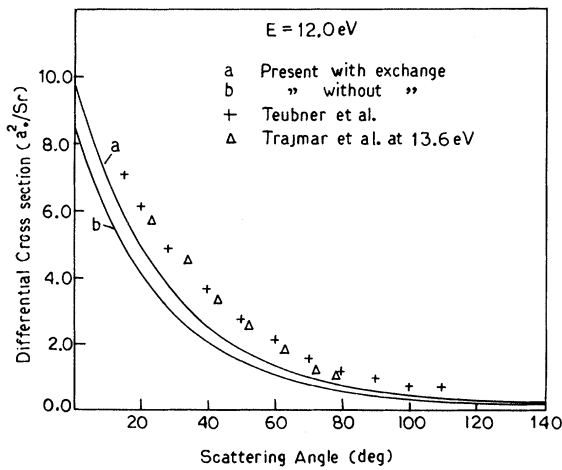


FIG. 3. Theoretical and experimental differential cross sections for  $e\text{-H}_2$  scattering, at  $E = 12.0$  eV.

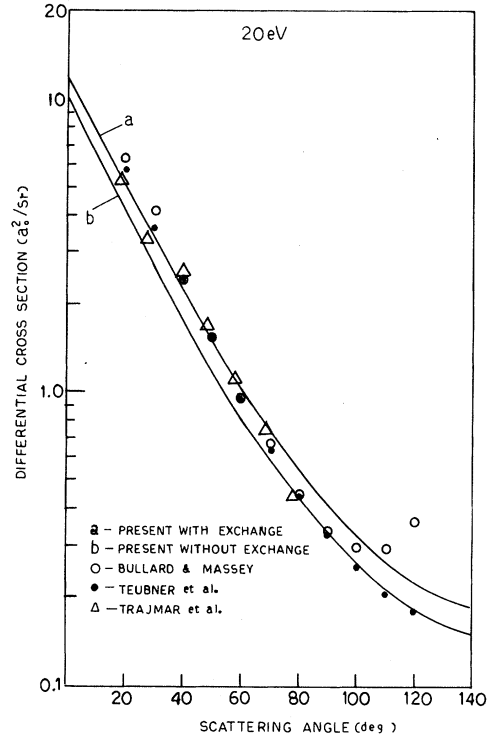


FIG. 4. Comparison of theoretical and experimental differential cross sections for  $e\text{-H}_2$  scattering,  $E = 20.0$  eV.

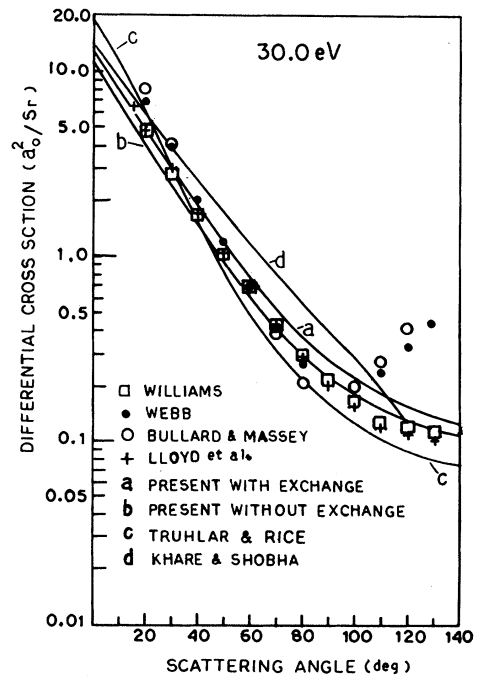


FIG. 5. Comparison of theoretical and experimental differential cross sections for  $e\text{-H}_2$  scattering,  $E = 30.0$  eV.

Expanding  $e^{iqb \cos \varphi \mp iB \cos 2\varphi}$  in terms of Bessel functions and carrying out the integration over  $\varphi$ , we get

$$F(\theta, \theta_m, \varphi_m) = -ik_i \int \left[ \left( J_0(qb) J_0(B) + 2 \sum_{m=1}^{\infty} (\pm)^m J_{2m}(qb) J_m(B) \right) e^{-iA} - J_0(qb) \right] b db, \quad (12)$$

where  $J_n$ 's are the Bessel functions of order  $n$ .

Finally, differential cross sections  $\langle I(\theta) \rangle$  and total cross sections  $\langle \sigma \rangle$ , averaged over molecular orientations, are computed from the following expressions:

$$\langle I(\theta) \rangle = \frac{1}{3} [ |F(\theta, 0, 0)|^2 + |F(\theta, \pi/2, 0)|^2 + |F(\theta, \pi/2, \pi/2)|^2 ], \quad (13)$$

$$\langle \sigma \rangle = \frac{1}{3} [ \sigma(0, 0) + \sigma(\pi/2, 0) + \sigma(\pi/2, \pi/2) ]. \quad (14)$$

### III. RESULTS AND DISCUSSIONS

We have evaluated the expressions  $A$  and  $B$  [Eq. (10)] numerically. The reduced one-dimensional integration [Eq. (12)] over the impact pa-

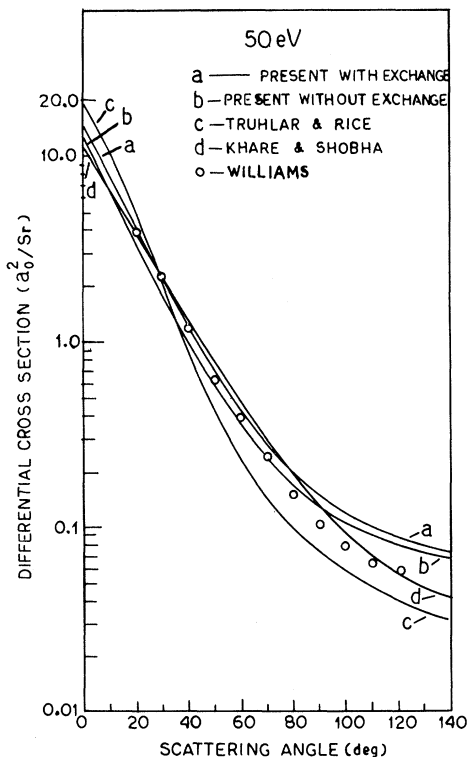


FIG. 6. Comparison of theoretical and experimental differential cross sections for  $e$ - $H_2$  scattering,  $E=50.0$  eV.

rameter  $b$  has also been performed numerically. The Gaussian quadrature method has been used in both the cases taking special care of the presence of Bessel functions in the integrand for the scattering amplitude. It may be mentioned that the series which occurs in the integrand is rapidly convergent and the maximum number of terms required for a well-converged amplitude at 100.0 eV is only three.

In Fig. 1 differential cross sections (DCS) for the spherically symmetric part of the potential and those for the total potential, both the spherical and the nonspherical, averaged over the molecular axis, have been compared at three incident electron energies (9.4, 50.0, and 100.0 eV). At the lowest energy the DCS's for the two cases differ slightly in magnitude maintaining, however, identical shape with respect to the scattering angles. It implies that at low energies only the spherical potential is sufficient to reproduce the DCS correctly, which has also been noticed by Hara.<sup>4</sup> At higher energies this is no longer true. Near the forward directions the effect of the nonspherical potential is still very little. At larger scattering angle, however, the influence of the nonspherical potential becomes dominant so that the averaged DCS's differ considerably from those obtained by using the spherical potential only. Trajmar *et al.*<sup>2</sup> have also noticed this feature at the incident energy 60.0 eV. The difference increases with increasing energy. This behavior is quite apparent owing to the fact that large-angle

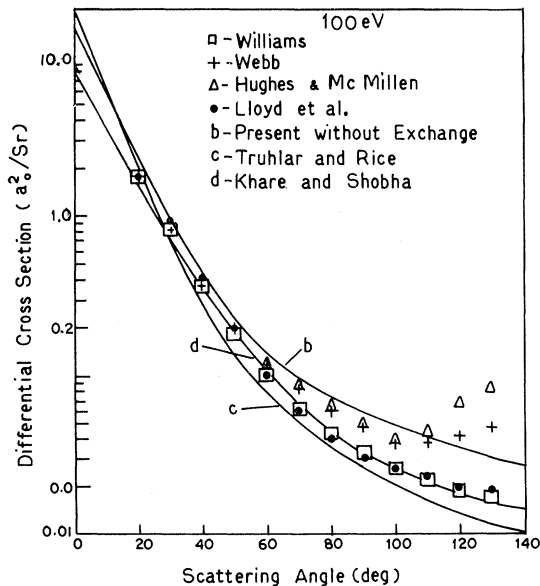


FIG. 7. Comparison of theoretical and experimental differential cross sections for  $e$ - $H_2$  scattering,  $E=100.0$  eV.

TABLE I. Calculated total elastic cross sections (in  $\pi a_0^2$ ).

Energy (eV)	Model C <sup>a</sup>	Model F <sup>a</sup>	Model B/P <sup>b</sup>	Present work	
				With exchange	Without exchange
9.4				4.67	3.83
12.0				4.43	3.63
20.0			5.33	3.90	3.17
30.0	4.77	4.87	3.67	3.30	2.70
50.0	2.28	2.33	2.26	2.42	2.03
100.0	0.95	0.98	1.16		1.22

<sup>a</sup>Reference 10: model C was quoted as their best potential model, and model F is based on the Lane-Henry polarization potential<sup>5</sup> (Table 3 of Ref. 10).

<sup>b</sup>References 2 and 9: calculated with an analytic polarization potential fitted to Lane-Henry polarization potential<sup>5</sup> (Tables III and IV in Ref. 2 and Table IX, Column 5 in Ref. 9).

scattering is governed by the small- $r$  interaction region, where the nonspherical part of the potential is expected to play a significant role.

We have plotted our results for the DCS with and without exchange (denoted by  $a$  and  $b$ , respectively) against the scattering angles at the incident electron energies 9.4, 12.0, 20.0, 30.0, 50.0, and 100.0 eV in the Figs. 2–7. The corresponding experimental DCS's measured by different workers<sup>1–3,20</sup> are given for comparison. We have not normalized any of the observed DCS's with our results. The data of the Australian group<sup>3</sup> is absolute, the details of the normalization of their data are given in their papers. Except for the absolute DCS of Ramsauer and Kollath<sup>20</sup> at 10.0 eV and the relative DCS of Williams<sup>1</sup> at 50.0 eV all other relative experimental angular distributions have been normalized at the results of the Australian group for the best visual fit. At 30.0, 50.0, and 100.0 eV we have presented the available theoretical DCS of Truhlar and Rice<sup>11</sup> (curve  $c$ ) and Khare and Shobha<sup>11</sup> (curve  $d$ ). The results of Williams at 50.0 eV have been normalized at the theoretical results of the above workers at 30° scattering angle.

Figures 2–6 show that our curves with exchange,  $a$ , lie above our curves without exchange,  $b$ , the slopes of the two curves remaining the same at all energies. The difference between the two curves decreases as the energy increases and becomes negligible at 100.0 eV. From 20.0 to 50.0 eV our results are in very good agreement with the experimental findings. On the other hand, the theoretical curves  $c$  and  $d$  fail to reproduce the proper shape of the DCS at energies 30.0 to 100.0 eV. At 100.0 eV the curve  $d$  underestimates the experimental values in the forward directions whereas the curve  $c$  is somewhat steeper than our curve  $b$ . The apparent discrepancy of our results

with those of Lloyd *et al.*<sup>3</sup> may be attributed to the fact that the Australian group has normalized their data at 60° scattering angle with those of Khare and Moiseiwitsch.<sup>7</sup> Our large-angle DCS differ from those measured experimentally at intermediate energies. But at those energies the experimental data of different workers also deviate considerably amongst themselves.

The lower values of DCS at 9.4 and 12.0 eV obtained in the present work cannot be attributed to a different choice of one-center or two-center wave functions in calculating the short-range static potential. It has been noted by Baille *et al.*<sup>21</sup> that a rather crude wave function may give a reasonably good static potential in the energy range considered here. However, the effective exchange potential used by us is not expected to account completely for the exchange, particularly at low energies where the exchange effect plays a dominant role. A better way of accommodating the effect of exchange may improve the results to a great extent. As noted earlier, the large-angle behavior of the DCS is not very clear from the observed values. In this context we point out that the present approximation is valid at angles larger than that originally anticipated.<sup>13,16</sup> However, the major shortcoming of the theoretical study of the large-angle scattering is that the small- $r$  behavior of the potential, a dominating factor in the large-angle region, is not known accurately. We believe that more accurate theoretical calculations as well as experimental studies are required to settle the large-angle behavior of the DCS. Nevertheless, Figs. 2–7 show that the eikonal approximation, unlike other approximations, gives the best fit (covering a wider range of scattering angle) to the experimental data available until now. This is particularly true for intermediate energies (20.0 to 100.0 eV). Since the present approximation is

more theoretically sound than any other high-energy approximation,<sup>13</sup> it is expected to give better results in the high-energy region also. But we have not calculated the DCS at higher energies.

Finally, in Table I the total cross sections of the present work along with those of Khare and Shobha,<sup>10</sup> based on their two potential models C and F, and Trajmar *et al.*<sup>2</sup> and Truhlar and Rice<sup>9</sup> have been presented. Judging from the DCS behavior our results seem to be reliable in the energy region 20.0–100.0 eV.

## ACKNOWLEDGMENTS

The authors are thankful to Professor N. C. Sil, Department of Theoretical Physics, Indian Association for the Cultivation of Science, for valuable suggestions. They are also thankful to Professor P. C. Bhattacharya, Department of Physics, University of Calcutta, for his keen interest in the problem. One of us (P.K.B.) is grateful to the Computer Center, University of Calcutta, for providing computing facilities.

<sup>1</sup>K. Williams, in *Proceedings of the Sixth International Conference on the Physics of Electronic and Atomic Collisions, Cambridge, Massachusetts, 1969* (MIT Press, Cambridge, Mass., 1969), pp. 735–737.

<sup>2</sup>S. Trajmar, D. G. Truhlar, and J. K. Rice, *J. Chem. Phys.* **52**, 4502 (1970).

<sup>3</sup>P. J. O. Teubner, C. R. Lloyd, and E. Weigold, *Phys. Rev. A* **9**, 2552 (1974); C. R. Lloyd, P. J. O. Teubner, E. Weigold, and B. R. Lewis, *Phys. Rev. A* **10**, 175 (1974).

<sup>4</sup>S. Hara, *J. Phys. Soc. Jpn.* **22**, 710 (1967).

<sup>5</sup>N. F. Lane and R. J. W. Henry, *Phys. Rev.* **173**, 183 (1968).

<sup>6</sup>S. Hara, *J. Phys. Soc. Jpn.* **27**, 1009 (1969).

<sup>7</sup>S. P. Khare and B. L. Moiseiwitsch, *Proc. Phys. Soc. Lond.* **85**, 821 (1965).

<sup>8</sup>B. F. Rozsnyai, *J. Chem. Phys.* **47**, 4102 (1967).

<sup>9</sup>D. G. Truhlar and J. K. Rice, *J. Chem. Phys.* **52**, 4480 (1970).

<sup>10</sup>S. P. Khare and P. Shobha, *J. Phys. B* **5**, 1938 (1972).

<sup>11</sup>D. G. Truhlar and J. K. Rice, *Phys. Lett.* **47A**, 372 (1974).

<sup>12</sup>B. C. Saha, Kalpana Sarkar, and A. S. Ghosh, *J. Phys. B* **6**, 2303 (1973); Kalpana Sarkar, B. C. Saha, and A. S. Ghosh, *Phys. Rev. A* **8**, 236 (1973); B. C. Saha, Kalpana Sarkar, and A. S. Ghosh, *Proc. Indian Natl. Sci. Acad. A* **39**, 382 (1973).

<sup>13</sup>E. Gerjuoy, in *Invited Papers and Progress Reports of the Seventh International Conference on the Physics*

*of Electronic and Atomic Collisions, Amsterdam, The Netherlands, 1971* (North-Holland, Amsterdam, 1971), p. 247.

<sup>14</sup>See, e.g., F. W. Byron, Jr. and C. J. Joachain, *Phys. Lett.* **38A**, 185 (1972); A. Tenney and A. C. Yates, *Chem. Phys. Lett.* **17**, 324 (1972); M. H. Mittleman, *Phys. Rev. A* **2**, 1846 (1970).

<sup>15</sup>R. G. Glauber, in *Lectures in Theoretical Physics, Summer Institute for Theoretical Physics, University of Colorado, Boulder, 1958*, edited by W. E. Brittin and L. G. Dunham (Interscience, New York, 1959), Vol. 1, p. 315.

<sup>16</sup>R. G. Newton, *Scattering Theory of Waves and Particles* (McGraw-Hill, New York, 1966), p. 582.

<sup>17</sup>M. L. Goldberger and K. M. Watson, *Collision Theory* (Wiley, New York, 1964), p. 788.

<sup>18</sup>The coefficients of the potentials given in Ref. 4 are not correct (private communication).

<sup>19</sup>D. P. Sural and N. C. Sil, *J. Chem. Phys.* **42**, 729 (1965).

<sup>20</sup>C. Ramsauer and R. Kollath, *Proc. R. Soc. A* **113**, 637 (1932); E. C. Bullard and H. S. W. Massey, *Proc. R. Soc. A* **130**, 637 (1931); A. L. Hughes and J. H. McMillen, *Phys. Rev.* **41**, 154 (1932); G. M. Webb, *Phys. Rev.* **47**, 379 (1935); N. B. Gilbody, R. F. Stebbings, and W. L. Fite, *Phys. Rev.* **121**, 794 (1961).

<sup>21</sup>P. Baille, J. W. Darewych, and J. G. Lodge, *Can. J. Phys.* **52**, 667 (1974), and references therein.