CHAPTER IV

THE STUDY OF DIFFUSION CROSS SECTION

4.1 INTRODUCTION :-

In the previous chapter effect of phase shift on the scattering cross section was studied. It was also possible to determine the scattering cross section. In this chapter a comparative study of the scattering cross section is made.

One of the very interesting points in this particular problem was regarding the use of Born approximation. It was observed that Born approximation can be successfully applied for determining scattering amplitude. In 1955, Gerjouy and Stein pointed out that the rotational excitation cross sections for H_2 and N_2 in the Born approximation can explain quite satisfactorily the experimentally found behaviours of thermal electrons in these gases. In order to understand the situation more clearly K.Takayanagi (1964-65) made the partial wave analysis. The same study was repeated by Chang (1970). The

Born cross section was decomposed in to the partial cross section by expanding the incident and outgoing plane waves in terms of the partial waves. Each partial wave corresponds to a definite value of the orbital angular momentum. It has been found that success of Born approximation was first of all due to the long range nature of the relevant interaction and secondly due to the fact that the S wave, which is the only partial wave to be distored considerably in the low energy collision under consideration; does not contribute appreciably to the rotational transitions. In the Born approximation for the quadrupole interaction the change in the orbital quantum number ℓ for the scattered electron was either $\Delta\ell = 0$ ($0 \leftrightarrow 0$ forbidden) or $\Delta\ell = \pm 2$. More generally, in the scattering of electrons from a homonuclear diatomic molecule with $\Lambda = 0$ (Λ is the electronic angular momentum of the target molecule around the molecular axis). $\Delta\ell$ can not take an odd intiger. This selection rule was obtained by evaluating the angular part of the transition matrix element of the interaction potential which was written asymptotically in the form

$$V (r, \theta) = \sum_{\alpha \text{ even}} \mathcal{V}_\alpha (r) \; P_\alpha (\cos \theta) \qquad \ldots\ldots 4.1$$

where r is the position vector for the scattered electron relative to the centre of mass of the target; and θ the angle between $\vec{r}$ and the molecular axis. The short range part of V could not be written as in equation 4.1 because of the electron exchange interaction of nonlocal nature. But the selection rule remained valid. In the case of $\Lambda \neq 0$ this was not necessarily the case. It may be appropriate to mention in passing that for homonuclear diatomic molecule with $\Lambda = 0$. We had a similar selection rule for the rotational J for the molecule i.e. ΔJ = even In the case of $\Lambda \neq 0$, however, this rule did not apply, as was demonstrated by Temkin and Faisal (1971) in the frame work of so called adiabetic approximations. Their conclusion was consistent with the study by Itikawa (1972) of the rotational excitation of symmetric top molecules in the Born approximation. A symmetric top molecule rotating aroung its symmetric axis was equivalent in many ways to a liniar molecule with nonvanishing Λ . Similarly in the molecule with a non vanishing electron spin such as O_2 in the ground Σ state; ΔJ is not necessarily an even integer (Geltman and Takayanagi 1966).

In the electron scattering from H_2 or N_2, the dominant interaction was the quadrupole interaction. It was asymptotically written

$$- \frac{eQ}{r^3} P_2 (\cos \theta) \qquad \ldots\ldots \qquad 4.2$$

where - e is the electronic charge and Q the quadrupole moment of the molecule. If this interaction is used down to r = 0 and if Born approximation is applied it was found that the major contribution to the cross section in the low energy region came from the jump from the incident p wave to the outgoing p wave. The s wave was necessarily combined with the d wave since $\ell = 0 \rightarrow \ell = 0$ is forbidden by the above mentioned selection rule. The d wave function had a~~s~~n appreciable magnitude only at such a distant region where the interaction 4.2 was extremely small. This was the reason why the S wave does not contribute to the rotational transition in any important way, except in the very vicinity of the excitation thresold where only the S wave could go out of the interaction region. In the low energy region, the p wave passes the target at a fair distance where the interaction was still appreciable but not too large, so that the first order perturba--tion treatment was applicable. This was the reason why the Born approximation can be used in the present problem.

In case of the rotational excitation in the electron polar molecule scattering the Born approximation is valid in a wider energy region than in the electron non polar molecules scattering. The partial wave analysis for this type of interaction was made by K.Takayanagi (1966). The selection rule was $\Delta J = \pm 1$, $\Delta \ell = \pm 1$. He observed that contrarary to electron non polar molecule scattering, in the electron polar molecule scattering Born approximation was much more reliable even for the collision energy exceeds 1 e V. Born approximation to point dipole potential was applied by Altshuler (1957) and to Finite dipole potential by the author (1972). Altshuler had shown that Born approximation can be well applied to the point dipole potential. Though his calculations gave better agreement with experiment it could not give the perfect agreement. A variation method for point dipole potential was used considering wave function slightly different than Born approximation wave function. In the next section the variational approach to the problem is discussed.

4.2 VARIATIONAL APPROACH :-

Though Born approximation gave very satisfactory results for diffusion cross section, it did not give the perfact agreement with experiment. Moreover larger cross section of some of the molecules like H_2O can not be well explained by the Born approximation. A variational method has been applied to the problem. This method was established by Lyman Mower (1955) on the basis of variation method developed by J. Schwinger (1950). This method is described briefly.

Integral equation for the initial wave function $\varphi_i(r)$ could be written as

$$\varphi_i(r) = e^{iK.r} - \frac{2m}{\hbar^2}\int \frac{G(r, r')}{4\pi} V(r')\,\varphi_i(r')\,dr' \qquad \ldots.4.3$$

where $G(r, r') =$ Green's function

$$= \frac{e^{iK|\bar{r} - \bar{r}'|}}{|\bar{r} - \bar{r}'|} \qquad \ldots\ldots \quad \ldots \quad 4{\cdot}4$$

for $r >> r'$ equation 4·3 could be written as

$$\varphi_i(r) = e^{iK_i \cdot r} + f(n, n_i) \frac{e^{iKr}}{r} \qquad \ldots \quad 4{\cdot}5$$

$$\text{where } f(n, n_i) = - \frac{m}{2\pi\hbar^2} \int e^{iK \vec{n} \cdot \vec{r}'} V(r') \varphi_i(r') \, dr' \quad .. \quad 4{\cdot}6$$

By the help of equation 4·3 and 4·6 the expression for $f(\bar{n}_s, \bar{n}_i)$ may be obtained easily,

$$f(n_s, n_i) = - \frac{1}{4\pi} \Big\{ \int e^{-i\vec{K}_s \cdot \vec{r}'} U(r') \varphi_i(r') \, dr' +$$

$$\int e^{i\vec{K}_i \cdot \vec{r}} U(r) \varphi_{-s}(r) \, dr - \int \varphi_{-s}(r) U(r) \varphi_i(r) \, dr -$$

$$1/4\pi \int\int \varphi_{-s}(r) U(r) \; G(r, r') \; U(r') \varphi_i(r') \, dr \; dr' \Big\} \quad .. \quad 4{\cdot}7$$

where

$f(n_s, n_i)$ = Exact expression for scattering amplitude.

$U(r) = \frac{2m}{\hbar^2} V(r)$

$\vec{K}_i = K \vec{n}_i$; $\vec{n}_i$ = Unit vector in the direction of incidence.

φ_{-s} = wave function of integral equation 4.3 for a plane wave incidence in the direction of $(-n_s)$

A trial wave function satisfying very nearly (4.3) should be used to determine the approximate scattering wave function. This was taken as

$$\Phi(r) = \sum_{1}^{n} C_n \, X_m(r) \qquad \ldots \quad (4.8)$$

C_n are unknown constants and

X_n are known functions of r.

The necessary condition that $[f(\bar{n}_s, \bar{n}_i)]$ be stationary with respect to small variation of $\Phi_i(r)$ and $\Phi_{-s}(r)$ about $\varphi_i(r)$ and $\varphi_{-s}(r)$ was

$$\frac{\partial [f(n_s, n_i)]}{\partial C_n} = 0 \qquad \ldots\ldots \qquad (4.9)$$

Coefficiants C_n can be evaluated by the help of equation 4.9.

Application of variation method to point dipole.

The variation method discussed above is applied to point dipole potential, which was represented as

$$V(r) = -\frac{\vec{D}.\vec{r}}{r^3} e \qquad \ldots \qquad \ldots (4.10)$$

Where D = dipole moment of the molecule e = electronic charge and $\vec{r}$ = position vector.

A trial function selected was slightly different from Born approximation is given by

$$\Phi_i(r) = C_o e^{i \vec{K}_i \cdot \vec{r}}$$

$\Phi_s(r)$ was obtained from $\Phi_i(r)$ by replacing vector $\vec{K}_i$ by $(- \vec{K}_s)$. For simplicity the rotation f (θ) is used for $[f(\bar{n}_s, \bar{n}_i)]$. By substituting these values in equation 4.7 and performing elementary integration f (θ) was obtained as

$$f(\theta) = f_B(\theta) \left[2C_o - C_o^2 + C_o^2 \, T_o(\theta) \right] \qquad ..(4.11)$$

(see appendix I).

where $f_B(\theta)$ = Amplitude by using Born approximations

$$= \frac{2 i D e m \gamma'}{\hbar^2 K}$$

γ' = Direction Cosine of the dipole axis with K. K is a wave vector the magnitude of which is given by $K_o \left[2 (1 - \cos\theta) \right]^{\frac{1}{2}}$. θ = angle between initial and scattered direction.

$$T_o(\theta) = f_B(\theta) \frac{K^2}{2\pi^2} \int \frac{dn}{(n^2 - K^2)(n - K_s)(n - K_i)}$$

$$= \frac{i K}{2} f_B(\theta) \quad . \qquad ......(4.12)$$

This integration was derived by representing the Green's function in the double integral of equation 4.7 in the momentum space i.e.

$$G(r,r') = \frac{4\pi}{2\pi^3} \int \frac{e^{in.(r-r')}}{(n^2 - K^2)} \, d\vec{n} \qquad \ldots\ldots \quad (4.13)$$

By the help of equation 4.9 and 4.11 we obtained

$$C_o = \frac{1}{1 - T_o(\theta)} \qquad \ldots\ldots \quad (4.14)$$

which finally lead to an expression

$$f(\theta) = f_B(\theta) \left[1/1 - T_o(\theta) \right] \qquad \ldots\ldots \quad (4.15)$$

The term $\left[1 - T_o(\theta) \right]^{-1}$ was expanded binomially and with slow electrons the higher powers of K were neglected

$$f(\theta) \simeq f_B(\theta) \left[1 + T_o(\theta) \right] \qquad (4.16)$$

Now the differential scattering cross section averaging over the entire dipole orientation is represented as

$$\sigma_t = \sum \sum P_{l,m} \int \Theta^*(l,m) \; |f(\theta)|^2 \; \Theta(l,m) \, d\Omega \; (4.17)$$

where $\Theta(l, m)$ = Rotator eigen function.

$P(l, m)$ = Probability distribution function for non - degenerate energy states of the rotor; and under equilibrium condition is independent of m.

1, and m , are orbital and magnetic quantum number. 1 can have values 0 to infinity while m is the magnetic quantum number, which is the numerical value of orbital vector 1 of the field direction. m is an intiger, and have only any of the (2l + 1) values from - 1 to + 1 including zero.

Substituting the values of f (θ) from equation 4.16 in to equation 4.17 and performing integration, following equation was obtained.

$$
\begin{aligned}
&\int \Theta^{*}(1,m)\, \left| f(\theta,\phi) \right|^{2} \Theta(1,m)\; d\Omega = \\
&4\,(D\,e\,m/\hbar^{2})^{2}\ \frac{1}{K^{2}} \left\{ \left[\frac{(\ell+1)^{2}-m^{2}}{(2\ell+1)(2+3)} + \frac{(\ell-m^{2})}{(2\ell-1)(2\ell+1)} \right] + \right. \\
&\qquad (D\,e\,m/\hbar^{2})^{2} \left[\frac{(\ell-m)(\ell+m)}{(2\ell-1)(2\ell+1)} \left\{ \frac{(\ell-m)(\ell+m)}{(2\ell-1)(2\ell+1)} + \right. \right. \\
&\qquad\qquad \left. \frac{(\ell-1-m)(\ell-1+m)}{(2\ell-3)(2\ell-1)} \right\} + \frac{(\ell+1-m)(\ell+1+m)}{(2\ell+1)(2\ell+3)} \\
&\left. \left. \left\{ \frac{(\ell+2-m)(\ell+2+m)}{(2\ell+3)(2\ell+5)} + \frac{(\ell+1-m)(\ell+1+m)}{(2\ell+1)(2\ell+3)} \right\} \right] \right\} \qquad \ldots \quad (4.18)
\end{aligned}
$$

(For the method of simplification of this formula see appendix II).

Which on substituting in equation 4.17 simplifying together with probability distribution factor gave very lengthy term, hence for simplicity it is represented as

$$\sigma_t = 4/3 \, (D e m / \hbar^2)^2 \, 1/K^2 \left[1 + 3 \, (D e m / \hbar^2)^2 \mathbf{\Delta}_{\ell,m} \right] \qquad \ldots\ldots(4.19)$$

as m takes values from $-\ell$ to $+\ell$ including zero $\mathbf{\Delta}_{\ell,m}$ was only ℓ dependent term and its value was given as

$$\mathbf{\Delta}_{\ell,m} = \sum\sum \left\{ \Delta_{\ell,m} \left(\Delta_{\ell,m} + \Delta_{\ell-1,m} \right) + \Delta_{\ell+1,m} \left(\Delta_{\ell+1,m} + \Delta_{\ell+2,m} \right) \right\} p_{\ell,m}$$

$$\Delta_{1,m} = \frac{(\ell - m) \quad (\ell + m)}{(2\ell - 1) \quad (2\ell + 1)} \qquad \ldots\ldots \quad (4.21)$$

Momentum transfer cross section or diffusion cross section was given as

$$Q_D = \int (1 - \cos\theta) \, \sigma_t \, d\Omega \qquad \ldots\ldots \quad (4.22)$$

substituting the values of σ_t from equation 4.19 and simplifying, following equation was obtained

$$Q_D = \frac{8\pi}{3} (D e m / \hbar^2 K_0)^2 \left[1 + 3 \, (D e m / \hbar^2)^2 \mathbf{\Delta}_\ell \right] \qquad \ldots \quad (4.23)$$

which is in C. G. S. units. In atomic units expression was derived as $$Q_D' = \frac{Q_D \, (\alpha)}{\pi a_o^2} \frac{E}{RY} = (2/3)\alpha^2 \left[1 + 3 \, (\alpha/2)^2 \mathbf{\Delta}_\ell \right] \qquad \ldots \quad (4.24)$$

where $\alpha = 2 D / e a_o$

The comparative statement for Born calculations, Mittleman and Vonhold calculations together with Q_D^8 calculated by equation 4·24 is exhibited in table I.

The term useful in the swarm experiment was the mean scattering cross section averaging over the Maxwellian distribution of velocity was defined as

$$\langle \sigma_m(v) \rangle = 4\pi \int_0^\infty \sigma_m(v)\, f_0(v)\, v^2\, dv \qquad \ldots\ldots \qquad \ldots \quad (4{\cdot}25)$$

where

$$f_0(v) = (m/2\pi kT)^{3/2} \exp\left[- \frac{m v^2}{2kT} \right] \ldots \qquad \ldots \quad (4{\cdot}26)$$

k is a Boltzman constant . Expression for $\langle \sigma_m(v) \rangle$ is calculated and is represented below

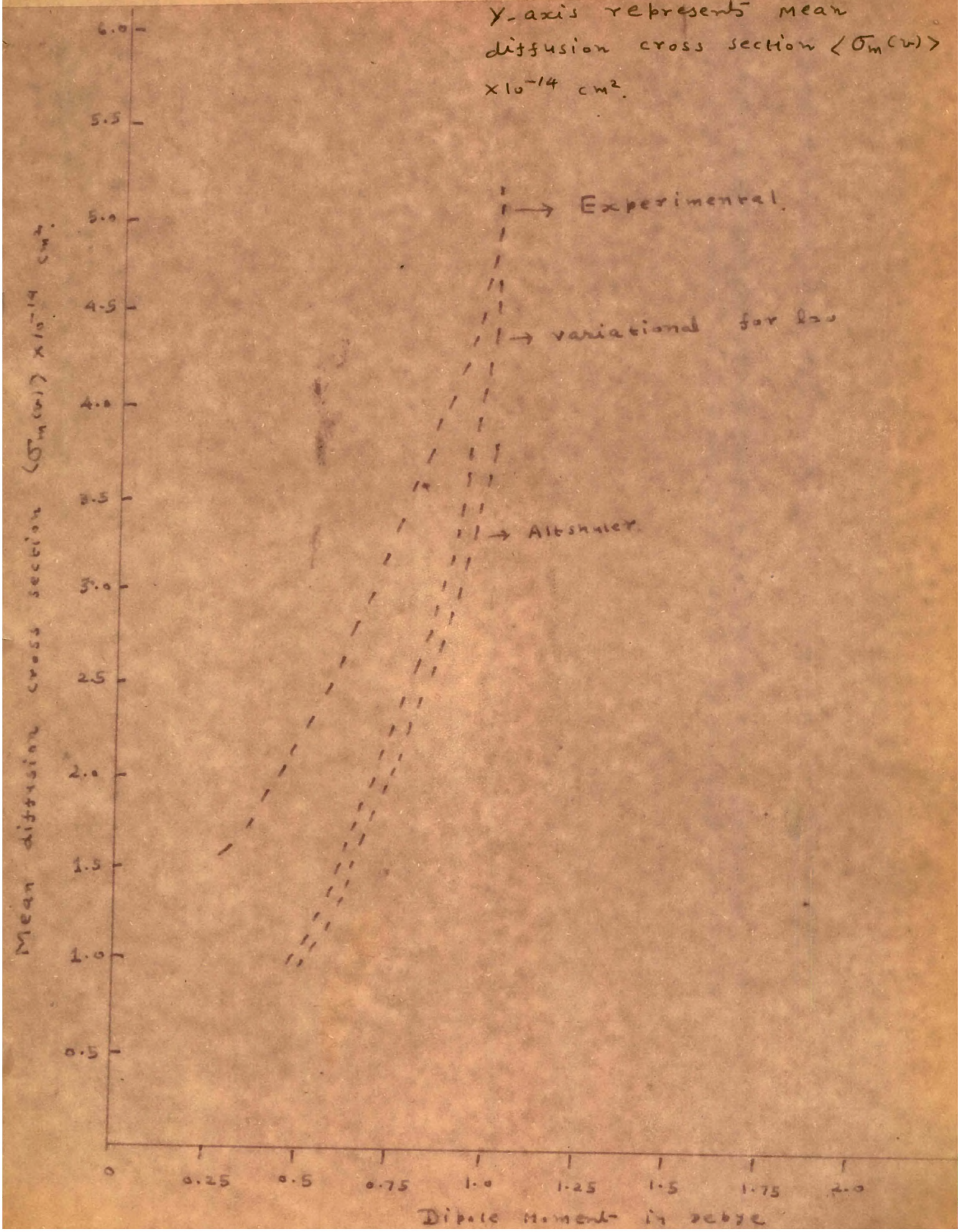
$$\langle \sigma_m(v) \rangle_{\text{variation}} = 3{\cdot}8083\, \mu^2 \left[1 + 1{\cdot}1736\, \mu\, \Delta_{l,m} \right] \times 10^{-14}\, \text{cm}^2 \qquad \ldots \quad (4{\cdot}27)$$

The first term in the bracket is due to Born approximation

$$\langle \sigma_m(v) \rangle_{\text{Born}} = 3{\cdot}8083\, \mu^2 \times 10^{-14}\, \text{cm}^2 \qquad \ldots \quad (4{\cdot}28)$$

The $\Delta_{l,m}$ in 4·27 is as defined in equation 4·21. The comparative statement for $\langle \sigma_m(v) \rangle$ calculated by Born approximation, variational method together with experimental values are exhibited in table II. Calculations for $\langle \sigma_m(v) \rangle$ were made for thermal electrons i.e. for which $T = 300^\circ$K.

Graph. 1.


Y-axis represents mean diffusion cross section $\langle \sigma_m(v) \rangle$ $\times 10^{-14}$ cm^2.
→ Experimental.
→ variational for l=0
→ Altshuler
Mean diffusion cross section $\langle \sigma_m(v) \rangle \times 10^{-14}$ cm^2.
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
0.25
0.5
0.75
1.0
1.25
1.5
1.75
2.0
Dipole moment in Debye

From the study of table II, it was observed that the cross section for $\ell = 1$ showed a maximum value. For $\ell = 2$ it decreased and for higher ℓ , cross section increased very slowly, hence a very slow divergence can be observed. As stated in chapter II divergency of total cross section in many cases was unavoidable fact of this problem (Garrett 1971). For $\ell = 0$ larger cross section than Born approximation was observed. The results for $\ell = 0$ are plotted in graph 1. It was observed from the graph that upto the dipole moment approximately equal to 2 Debye, variational method gave better agreement for cross section. The Born approximation on the other hand gave fairly well agreement with experimental values throughout the whole range of dipole moment.

Looking to the success of Born approximation, this approximation was applied to the problem. Altshuler had applied Born approximation to point dipole potential. Here it is applied to finite dipole potential. Takayanagi and Itikawa (1968) have studied the finite dipole potential by partial wave method. They have separated the waves in prolate spheroidal coordinates. It was observed (Desai and Maru 1972) that in the finite dipole expression,

$$V(r) = -2eq \sum_{K\,\mathrm{odd}} \frac{r_<^k}{r_>^{k+1}} P_K(\mathrm{Cos}\,\theta)$$

for K = 1 case Born approximation was applied satisfactorily. In the following section this case is described in detail.

4.3 FINITE DIPOLE CORRECTION :-

In this section an attempt is made to study the finite dipole potential, applying Born approximation. Consider a molecule as rigid rotor and the interaction potential between the molecule and electron is $V(r, \tau)$, Total Hamiltonian of the system can be represented as

$$H_o = \tau + H_{rot} + H_1 + H_2 \qquad \ldots\ldots \qquad (4.30)$$

where

τ = Kinetic energy operator of the electron.

H_{rot} = Hamiltonian for the rotational motion of molecule.

$H_1 + H_2$ = H' = Hemiltonian for vibrating and electronic part of the molecule.

Therefore total energy,

$$E = K_i^2 + W + \varepsilon_i \qquad \ldots\ldots \qquad \ldots \qquad (4.31)$$

where

K_i^2 = Kinetic energy of electron (Incident electron is free particle therefore it has no potential energy).

W_ℓ = Initial rotational eigen values of the molecule.

ε_i = Eigen values of vibrational and eletronic states of the molecule.

$$E - H_o = K_i^2 + W_\ell + \varepsilon_i - T - H_{rot} - H' \qquad \ldots\ldots \qquad (4.32)$$

Now W'_{ℓ} - H_{rot} represented the Hemiltonian and initial rotational eigen value of the molecule and as intially electron was moving very fast compare to the rotational motion of the molecule this part was neglected therefore,

$$E - H_o = K_o^2 + \varepsilon_i - T - H' \qquad \ldots\ldots \qquad (4.33)$$

when the electron collides with the molecule it will give some energy to molecule and then molecule will change the rotational state. The amplitude for this transition from the target state ℓ' to ℓ is then given by

$$f_{\ell\ell'}(\theta , \phi) = - \frac{1}{4\pi} \langle X_{\ell} V \varphi_{\ell}^{(+)} \rangle \qquad \ldots\ldots \qquad (4.34)$$

where $\varphi_{\ell}^{(+)}$= outgoing wave solution to the integral equation 4.35.

$$\varphi = X + \frac{1}{E-H_o} V \varphi \qquad \ldots\ldots \qquad (4.35)$$

with initial rotational state ℓ .

X_{ℓ} = Outgoing wave solution of the final state, when the scattered electron in plane wave state (Because at large distance the scattered electron will again behave as if it is free particle and will give plane wave)and the molecule in rotational state .

The approximation of neglecting the rotational kinetic energy in equation 4.35 allowed a factorization of $\varphi_{\ell}^{(+)}$as

$$\psi_l^{(+)} = \psi_{K_i}^{(+)} \Omega_{l'} \quad \ldots\ldots \quad (4.36)$$

$\Omega_{l'}$ = Rotational eigen function.

$\psi_{K_i}^{(+)}$ = Solution to the scattering problem with fixed molecular orientation.

Similarly final state can also be factorized as

$$X_1 = \lambda_{K_f} \Omega_l^*$$

equation 4.34 will becomes,

$$f_{ll'} = \int d\alpha\, \Omega_l^* \left\{ -\frac{1}{4\pi} \left\langle \lambda_{K_f} V\, \psi_{K_i}^{(+)} \right\rangle \right\} \Omega_{l'} \quad (4.37)$$

α = Rotational coordinates of molecule.

Inner bracket of 4.37 is the elastic amplitude of fixed molecular orientation $f\ (K_f, K_i, \alpha)$ or $f\ (\theta, \phi, \tau)$

$$f_{ll'}\ (K_f, K_i) = \int d\alpha\, \Omega_l^*\, f\ (K_f, K_i, \alpha)\, \Omega_{l'} \quad (4.38)$$

equation 4.38 is similar to the equation

$$f_{ni}\ (\theta, \phi) = \int d\tau\ \Phi_n^*\ (\tau)\ f\ (\theta, \phi, \tau)\ \Phi_i(\tau) \quad \ldots (4.39)$$

used by Altshuler (1957) and derived by Chase (1956).

The scattering amplitude for fixed molecular orientation $\left\{ f\ (\theta, \phi, \tau) \right\}$ may now be obtained from a solution of equation 4.35 which still contains the vibrational and electronic part of the molecular Hemiltonian. This may be eliminated in effect by representing 4.35 in the usual equivalent potential formalism which suppresses the vibrational and electronic degree of freedom by introducing a complicated potential operator in the equation of elastic scattering. Evaluation of this operator is prohibitively difficult except in the limit in which incident electron is well separated from the molecule. In that case the dominant interaction was the dipole one. Theoretically more correction should be made for quadrupole, octupole and short range terms, but in all cases the dipole term was found more suitable for polar molecule electron interaction.

Altshuler (1957) and Mittleman (1965) expected that at low enough energies longest range of part of the potential, the dipole part to dominate and so they replaced the entire interaction of an electron with point dipole.

The number of excited states of the target contributed significantly to the total wave function were limited and therefore the transversal time of the scattered particle through the interaction region was small compared to the period of the target motion excitable in the collision. The exact expression for the excitation amplitude was given by

$$f_{ni} = -\frac{m}{2\pi\hbar^2}\iint e^{iK_n\cdot r}\,\phi_n^*(\tau)\,V(R,\tau)\,\Psi(R,\tau)\,d^3r\,d\tau$$

$$= \frac{m}{2\pi\hbar^2} \iint e^{i\bar{K}_n . \bar{R}} \sum_{\alpha} F_{\alpha}(\bar{R}) \langle n \mid V \mid \alpha \rangle \qquad (4.40)$$

where $\psi(\bar{R}, T)$ = Total wave function.

It was found that in case of dipole, the energy states which were immediately above or below in

$$\psi(\bar{R}, T) = \sum F_{\alpha}(\bar{R}) \, \phi_{\alpha}(T)$$

contributed in f_{ni} i.e. $n = \alpha \pm 1$. Consequently if α's involved in ψ were limited than so were the excited states. Therefore equation 4.39 can be applied formally for all n without violating the time of passage criterian as a result of this consideration, the total differential cross section may be written as

$$\sigma_i(\theta, \phi) = \sum_n |f_{ni}|^2$$

$$= \sum \iint d\tau \, d\tau_0 \, \phi_n^*(\tau) \, \phi_n(\tau_0) \, f(\theta, \phi, \tau) \, f^*(\theta, \phi, \tau) \, \phi_i^*(\tau_0) \, \phi_i(\tau) \quad \ldots\ldots \; 4.41$$

and for the property

$$\sum_n \phi_n^*(\tau) \, \phi_n(\tau_0) = \delta(\tau - \tau_0)$$

it was shown that

$$\sigma_i(\theta, \phi) = \int d\tau \, |f(\theta, \phi, \tau)|^2 \, \phi_i(\tau) \quad \ldots\ldots \; 4.42$$

which gave the expectation value for the differential cross section when calculated with the target coordinates held fixed. If P_i is the probability for finding target in the ith states then

$$\sigma_i(\theta, \phi) = \sum_i P_i \, \sigma_i(\theta, \phi) \qquad (4.43)$$

The quantity measured by Townsend swarm method was diffusion or momentum transfer cross section and was defined as

$$Q_D = \int (1 - \cos\theta)\, \sigma_i(\theta, \phi) \, d\Omega \qquad (4.44)$$

Q_D in the probability form ca be introduced as

$$Q_D = \int (1 - \cos\theta) \sum_i P_i \, \sigma_i(\theta, \phi)\, d\Omega \qquad (4.45)$$

For the numerical calculation of momentum transfer cross section it was necessary to evaluate $f(\theta, \phi, T)$ for scattering in the field of a fixed finite dipole, in which two charges $+q$ and, $-q$ were separated from each other by a distance 2a is

$$V(r, T) = -2eq \sum_{K=\text{odd}} \frac{r_<^K}{r_>^{K+1}} P_k(\cos\quad) \quad \ldots\ldots \qquad (4.46)$$

where $r_<$ and 2 $r_>$ are smaller and greater of r and a, $P_k(\cos\theta)$ = Legendre polynomials. Consider the case for K = 1, that is we seek a solution to the problem

$$\left\{ - \frac{\hbar^2}{2m} \nabla^2 + V(R, T) \right\} \Psi(R) = \Psi(R) \qquad \ldots \quad (4.47)$$

for fixed T. Subject to the outgoing boundary condition,

$$\Psi(R) = e^{i\vec{K}_o \cdot \vec{R}} + f(\theta, \phi, T) \frac{e^{iK_o R}}{R} \qquad \ldots \quad (4.48)$$

The exact expression for $f(\theta, \phi, T)$ was given by

$$f(\theta, \phi, T) = \frac{m}{2\pi\hbar^2} \int d\bar{R} \; e^{i\bar{K}\cdot\bar{R}} V(R, T) \; \Psi(R) \quad (4.49)$$

The expression for amplitude in Born approximation was written in the form (for fixed T)

$$f(\theta, \phi) = - \frac{m}{2\pi\hbar^2} \int e^{i\bar{K}\cdot\bar{r}} V(r) \; d^3r \quad (4.50)$$

substituting the values of $V(r)$

$$f(\theta, \phi) = \frac{m}{2\pi\hbar^2} \int e^{iK\cdot r} \, 2eq \sum_{K=odd} \frac{r_{<}^{K}}{r_{>}^{K+1}} P_K(\cos\theta) \; d^3r$$

For K = 1, this expression reduces to

$$f(\theta, \phi) = \frac{m}{2\pi\hbar^2} \left[\int_0^{\pi}\int_0^{2\pi}\int_0^{a} \frac{r}{a^2} e^{iK\cdot r} P_1(\cos\theta) \, d^3r + \int_0^{\pi}\int_0^{2\pi}\int_a^{\infty} \frac{a}{r^2} e^{iK\cdot r} P_1(\cos\theta) \; d^3r \right] \quad (4.51)$$

on performing the elementary integration and substituting $D = 2\,q\,a$ final result is obtained as

$$f(\theta,\phi) = \frac{2i\,D\,e\,m\,\gamma'}{\hbar^2 K}\left[3\left(\frac{\operatorname{Sin} K a}{K^3 a^3} - \frac{\operatorname{Cos} K a}{K^2 a^2}\right)\right] \qquad (4{\cdot}52)$$

where γ' = Direction cosine of dipole axis with respect to direction of $\vec{K}$

$\vec{K}$ = wave vector, the magnitude of which is given by $K_o\left[2\,(1 - \operatorname{Cos}\theta)\right]^{\frac{1}{2}}$. It is noted that as $a \to o$

$$f(\theta,\phi) = \frac{2\,i\,D\,e\,m\,\gamma'}{K} \qquad \ldots\ (4{\cdot}53)$$

which is the expression for amplitude for a point dipole. Now the coordinate of target is measured relative to the fixed direction of K, hence differential scattering cross section equation 4.43 can be expressed as

$$\sigma_T = 4\,(D\,e\,m/\hbar^2 K)^2 .\ 9\left[\frac{\operatorname{Sin} K a}{K^3 a^3} - \frac{\operatorname{Cos} K a}{K^2 a^2}\right]^2 \sum_{l=0}^{\infty}\sum_{m=-l}^{+l}\int\left|\Theta(l,m)\right|^2 \gamma'^2\, d\Omega \qquad (4{\cdot}54)$$

where $P_{l,m}$ = Probability distribution for non degenerate enery state of the rotor and under equivilibrium condition is independent of m. Θ (l, m) = Rotator eigen function. Now performing elementary integration by streight forward way it was shown that

$$\sum_{l=0}^{\infty} \sum_{m=-l}^{+l} P_1 \int \left| \Theta (1, m) \right|^2 \mathrm{Cos}^2 \gamma \; d\Omega = 1/3 \qquad (4.55)$$

(For details of this simplification see appendix II),

putting this value in 4.54 the expression for σ_T will be

$$\sigma_T = 12 \; (D e m / \hbar^2 K)^2 \left\{ \frac{\mathrm{Sin} K a}{K^3 a^3} - \frac{\mathrm{Cos} K a}{K^2 a^2} \right\}^2 \qquad (4.56)$$

Now momentum transfer cross section as defined in the last section was evaluated as follows

$$Q_D = 2\pi \int_0^{\pi} (1 - \mathrm{Cos}\, \theta) \; \sigma_T \; \mathrm{Sin}\, \theta \; d\theta$$

putting the value of σ_T from equation 4.56

$$Q_D = 24 \pi \, (D e m / \hbar^2)^2 \int_0^{\pi} \frac{1 - \mathrm{Cos}\, \theta}{K^2} \left(\frac{\mathrm{Sin} K a}{K^3 a^3} - \frac{\mathrm{Cos} K a}{K^2 a^2} \right)^2 \mathrm{Sin}\, \theta \; d\theta \; \ldots . (4.57)$$

Now expanding Sin K a, Cos K a in terms of Ka and performing integration

$$Q_D = \frac{8\pi}{3} (D e m / \hbar^2 K_o)^2 \left\{ 1 - 0.4 \, K_o^2 \, a^2 + 0.053 \, K_o^4 \, a^4 \right\} \qquad (4.58)$$

which also for small values of Ka → point dipole results.

In equation 4.58 Q_D is in C.G.S. units, which is in πa_o^2 units takes up the form

$$Q_D' = \frac{Q_D}{\pi a_o^2} = \left[5{\cdot}6 \; \frac{D'^2}{E'} - 0{\cdot}006579 \; D'^4 \right] \qquad (4{\cdot}59)$$

where $D' = D/10^{-18}$, $E' = \frac{E}{e} \frac{X}{X} \frac{c}{10^8} = \sqrt{\text{volt}}$.

(Details of the conversions of units are given in appendix III).

In equation 4·59 the cross section was derived in πa_o^2 units and moreover it was converted in such a manner that Q_D' was dependent on energy E'. E' is in $\sqrt{\text{volt}}$ units. Comparision of results were made with Altshuler's calculations and Townsend's experiment. The comparative statement for this quantity is made in table III. Q_D' was calculated for energy range 0·6 $\sqrt{\text{volt}}$ to 1·0 $\sqrt{\text{volt}}$. It was observed from the table that the value of cross section considering finite dipole potential gave very small correction. Takayanagi and Itikawa also observed the same effect in their calculations.

For the comparision of finite dipole results with the present experimental studies it was necessary to find out the mean cross section $\langle \sigma_m(v) \rangle$ averaging over the Maxwellian distribution of velocities. The expression for $\langle \sigma_m(v) \rangle$ was given by

$$\langle \sigma_m(v) \rangle = 4\pi \int_0^\infty \sigma_m(v) \, f_o(v) \, v^2 \, dv$$

$$f_o(v) = (m/2\pi KT)^{3/2} e^{-mv^2/2KT}$$

= Maxwellian distribution factor.

From equation 4.58 neglecting the third term of the bracket the velocity dependent $\sigma_m(v)$ was derived by substituting

$K_o = m\,v/\hbar$

$$\sigma_m(v) = \frac{8\pi}{3} (D\,e\,m/\hbar^2)^2 \left\{ \frac{\hbar^2}{m^2\,v^2} - 0.4\,a^2 \right\} \quad (4.60)$$

substituting this value of $\sigma_m(v)$ in the expression for $\langle\sigma_m(v)\rangle$ was

$$\langle\sigma_m(v)\rangle = \langle\sigma_m(v)\rangle_A - \frac{3.2}{3} (D\,e\,ma/\hbar^2)^2 \quad (4.61)$$

Here the temperature of gas taken was 300°K. The calculations could made for different values of T also, but generally the experiments are performed for thermal electrons for which D = 300°K . Moreover for polar molecules the experimental values of $\langle\sigma_m(v)\rangle$ at various temperature were not available.

The comparision of the results for $\langle\sigma_m(v)\rangle$ for finite dipole together with Born approximation and experimental values are made in table IV. It was observed that here also correction terms were very small.

The study of Q_D^* and $\langle\sigma_m(v)\rangle$ by finite dipole confirmed that Born approximation to this potential can be well applied. Born approximation to point dipole potential gave better values hence the point dipole potential was found more useful in this problem. The advatage of finite dipole potential was to have the potential resonance effect in the expression of Q'_D.

The expression 4.58 for Q'_D takes up the form in atomic units as

$$Q'_D = \frac{8}{3}\,\frac{(D)^2_{a.u.}}{(K_o)^2_{a.u.}}\left[1 - 0.1\,(K_o D)^2_{a.u.}\right] \qquad (4.62)$$

$$Q'_D = \frac{8}{3}\,\frac{\mu^2}{K'^2_o}\left[1 - 0.1\;K'^2\mu^2\right] \qquad (4.63)$$

where μ = Dipole moment in ea_o units. $K'_o = K_o$ in atomic units.

It was observed that equation 4.63 represents the resonance effect; of course the value of minimum dipole moment comes out to be large. In case of $K'^2_o = 0.1$, $(\mu)_{min} = 7\ ea_o$ This was expected due to our original approximation of K = 1 in the expression for finite dipole potential. It was observed that at $\mu = 10$ and for $K_o^2 = 0.1$, $Q'_D = 0$. This result was due to the fact that we had dropped IIIrd term of equation 4.58. The

Graph. 2.


Y-axis represents Momentum transfer cross section in πa_0^2 units.
800
600
400
200
0
2
4
6
8
10
Dipole Moment in Debye.

results for K_o^{2} = 0.1 is represented in graph 2.

The finite dipole expression though reduced the momentum transfer cross section by a very small amount, it gives the possibility of bound states in the dipole field. Point dipole potential had no such possibility. A point dipole together with the consideration of some short range force could give the bound state.

Though the point dipole had disadvantage of not having bound states, its success for the satisfactory agreement of diffusion or momentum transfer cross section is unavoidable fact. In the next section short range force of coulomb one centred potential field is super imposed on the point dipole field. Short range force varies from molecule to molecule. An attempt was made to see the effect of attractive and repulsive short range force.

4.4 SHORT RANGE FORCE :-

For the numerical calculations of diffusion cross section, it was necessary to evaluate f (θ, ϕ, T) in the field of a fixed point dipole with short range screened coulomb potential. This is given as

$$V(r) = -e\,\frac{\bar{D}\cdot\bar{r}}{r^3} \pm \frac{B\,e^{-\alpha r}}{r} \qquad (4.64)$$

where + sign to second term indicates that short range term is repulsive while negative sign indicates that it is attractive α is screening constant, is equal to $1/r_s$, r_s is screening length. B is a parameter which is different for different molecules.

Schrodinger equation can be written in the form

$$\varphi(R) = \left\{ -\frac{\hbar^2}{2m}\nabla^2 + V(R, T) \right\} \varphi(R) \qquad (4.65)$$

for fixed T. The expression for scattering amplitude in Born approximation was

$$f(\theta, \phi) = -\frac{m}{2\pi\hbar^2} \int e^{i\bar{K}\cdot\bar{r}} V(r)\, d^3 r$$

substituting the value of V (r) we get in case of attractive potential

$$f(\theta, \phi) = \frac{m}{2\pi\hbar^2} \int e^{iK\cdot r} \left[e \frac{D\cdot r}{r^3} - \frac{B e^{-\alpha r}}{r} \right] d^3 r$$

$$f(\theta, \phi) = \frac{m}{2\pi\hbar^2} \left[\int_0^\infty \int_0^\pi \int_0^{2\pi} e^{iK\cdot r}\, e \frac{D\cdot r}{r^3}\, r^2\, dr\, \sin\theta\, d\theta\, d\phi \right.$$

$$+ \int_0^\infty \int_0^\pi \int_0^{2\pi} e^{iK\cdot r} \frac{B}{r} e^{-\alpha r}\, r^2\, dr\, \sin\theta\, d\theta\, d\phi$$

performing elementary integration we get

$$f(\theta, \phi) = \frac{2\, i\, D\, e\, m\, \gamma'}{\hbar^2 K} + \frac{2\, m\, B}{\hbar^2 \alpha} \left(\frac{1}{K^2 + \alpha^2} \right) \qquad (4.66)$$

Differential scattering cross section averaging over the entire dipole range is

$$\sigma_T = 4/3 \; (D e\, m/ \hbar^2 K)^2 + 4 \; (m B/\hbar^2 \alpha)^2 \; (1/K^2+\alpha^2)^2 \qquad (4{\cdot}67)$$

The diffusion or momentum transfer cross section turn out to be

$$\sigma_m (v) = \frac{8\pi}{3} \; (D e m / \hbar^2 K_0)^2 - 2 \left(\frac{m B}{\hbar^2 + K_0^2} \right) \left[\log \; (4K_0^2 + \alpha^2 / \alpha^2) - 4K_0^2 / 4K_0^2 + \alpha^2 \right] \qquad (4{\cdot}68)$$

It is seen from the above equation that increase of attractive short range potential has the same effect as the increase of dipole moment. As the value of B increases the cross section moves towards smaller values of D. Finally the expression for the mean scattering cross section obtain as

$$\langle \sigma_m (v) \rangle = \langle \sigma_m (v) \rangle_{Alt} - 2 \pi G P^2 \sqrt{\pi} \left(\frac{1}{q} - \sqrt{\frac{P}{4}} \right) \qquad \ldots\ldots \; (4{\cdot}69)$$

$$\langle \sigma_m (v) \rangle_{Alt} = \frac{8\pi}{3} \; (D e / \hbar)^2 \; \frac{m}{K_T} =$$

$$3{\cdot}8083 \; D^2 \times 10^{-14} \; cm^2$$

$$G = \frac{m B}{2 K T}, \quad q = \sqrt{\frac{m}{2 K T}}, \quad P = \frac{2 m}{\hbar \alpha}$$

For a repulsive screening short range potential the value of

$\langle \sigma_m (v) \rangle$ becomes

$$\langle \sigma_m (v) \rangle = \langle \sigma_m (v) \rangle_{Alt} + 2 \pi G P^2 \sqrt{\pi} \left(\frac{1}{q} - \frac{\sqrt{P}}{4} \right) \tag{4.70}$$

Comparative statements for these potentials are given in table V and table VI. Attempt was made to calculate $\langle \sigma_m (v) \rangle$ for thermal electrons. The calculations could be made for different values of temperature also but as the experimental evident for different temperatures does not available the calculations for this case is avoided. It can be observed from table V and VI that the consideration of attractice short range potential reduces the Altshuler's cross section while repulsive potential increases the Altshuler's cross section.

The correction term due to short range attractive potential is

$$- 2 \pi G P^2 \sqrt{\pi} \left(\frac{1}{q} - \frac{\sqrt{P}}{4} \right)$$

while due to repulsive short range potential it is

$$+ 2 \pi G P^2 \sqrt{\pi} \left(\frac{1}{q} - \frac{\sqrt{P}}{4} \right)$$

here $P = \frac{2m}{\hbar\alpha}$, which means that second term decreases with the increase of α , Moreover $G = \frac{mB}{2\pi KT}$, $q = \sqrt{\frac{m}{2KT}}$ also suggests that with the increase of T second term decreases and reduces the repulsive cross section while increases the attractive cross section.

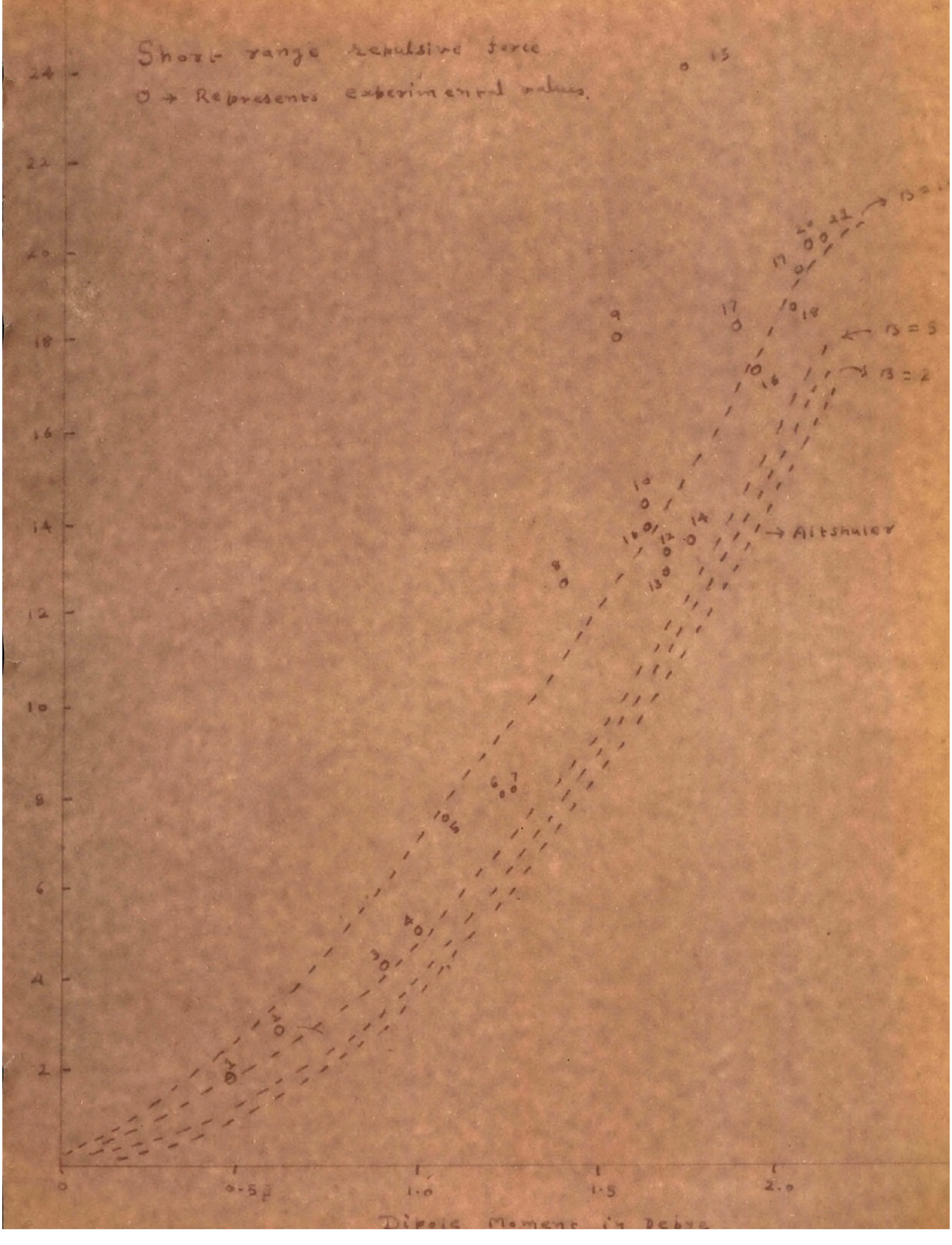
The potential $\frac{B e^{-\alpha r}}{r}$ represents the screened one centre coulomb potential. In order to see the qualititive feature of the effect of short range potential the mean momentum transfer cross section was calculated, for some typical values of B and α . When an electron is isolated from molecule, and is far from the rest of the system the wave function decays in a radial direction, approximately as e^{-Zr} where Z is the effective charge and r is the distance from the centre of the molecule. In this case the screening factor in the potential was roughly proportional to e^{-2Zr} which means that $\alpha = 2Z$. If Z is taken as unit charge $\alpha = 2$. The reasonable value of B was expected to vary from molecule to molecule. Firstly B was taken as 1 that is B = 1 a.u. and α = 2 a.u. Then as exhibited in table 5 and 6 for fixed α , various values of B was considered and the effect of short range attractive and repulsive force was accounted.

The value of B require for exact agreement with experiment was also calculated, which is exhibited in table 7.

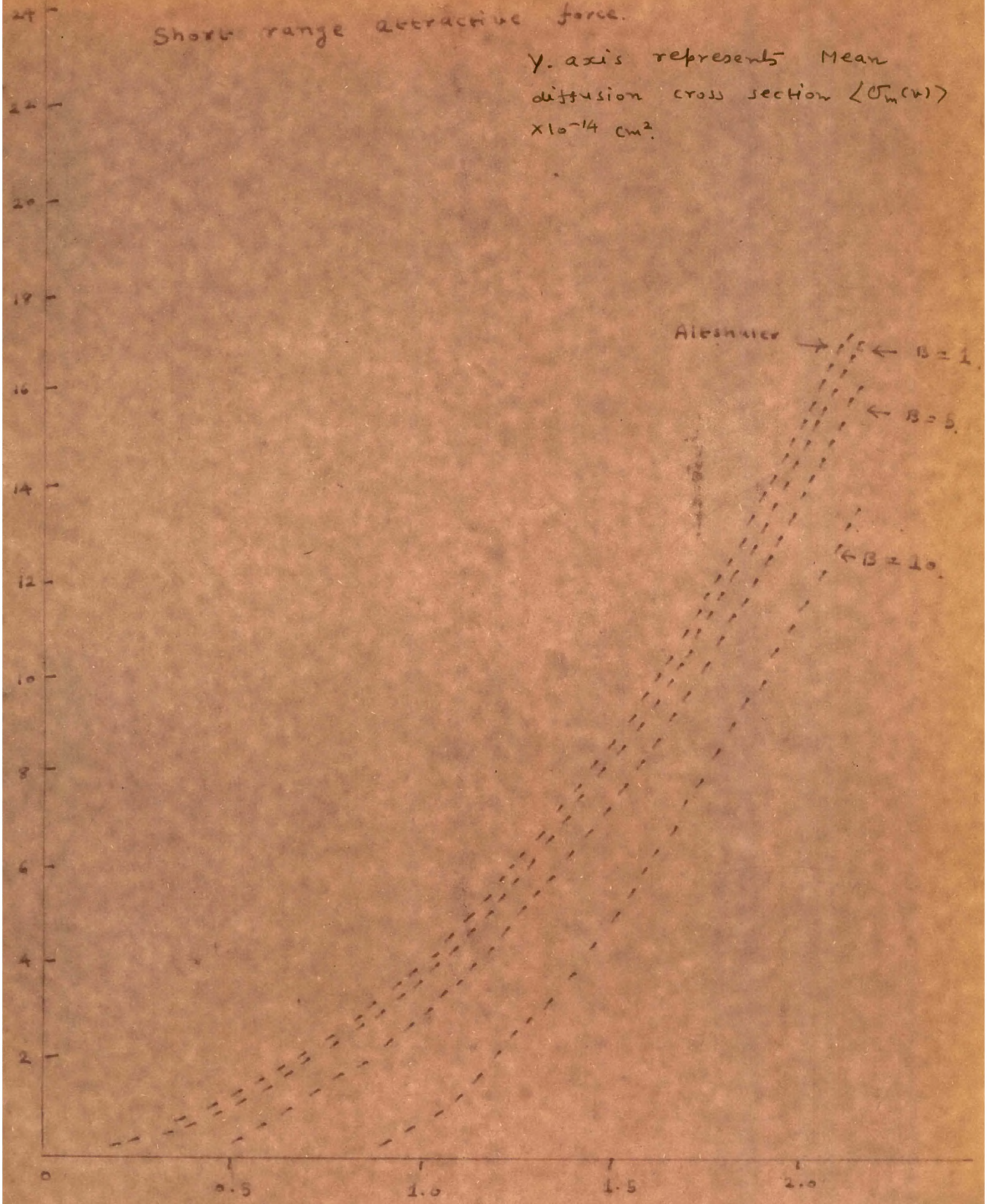
Further it was observed that for some of the groups of molecules, for better agreement with experiment an attractive short range force was required while for some group the repulsive force was required. For Ledogen derivetive of Methone, Estor, Alkyl Halide, Amine, Alcohol group repulsive force gave the better agreement. For Cynogen, Aldihide and Ketone group the attractive force gave better agreement. This may due to certain similarity in the molecular structure and the charge distribution in the molecule. In general for organic and inorganic polar molecules, the molecules having dipole moment less than (≤ 2.74) repulsive force was found suitable while for the molecules having dipole moment (≥ 2.74) the attractive short range force was the better fit for agreements with experiments. It was further observed that for some of the organic group of molecules the value of " B " approximately remains same for the whole group while for some of the group the major variation for B from molecule to molecule was observed. The graphical representation of this effect is exhibited in graph 3, 4, 5.

A very few attempt of short range force for polar molecules are made. Bordman and Smmpnathe (1969) used

Graph. 3.


Short range repulsive force
O → Represents experimental values.
24
22
20
18
16
14
12
10
8
6
4
2
0
0.5
1.0
1.5
2.0
Dipole Moment in Debye
B = 1
B = 5
B = 2
Altshuler
1
2
3
4
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22

Graph. 4.



Short range attractive force.

Y. axis represents Mean diffusion cross section $\langle \sigma_m(v) \rangle$ $\times 10^{-14}$ cm^2.

the screening potential in place of pure dipole potential in the form

$$V(r) = e\,\frac{\vec{D}\cdot\vec{r}}{r^3}\,\exp(-r/r_s) \qquad (4.71)$$

they thought that screening effect was due to the pressure of the gas. As expected they found the value of cross section lower than unscreened case. Takayanagi and Itikawa had also tried the coulomb two centred short range force to finite dipole potential. They have accounted total cross section for dipole field. A very systemetic application of short range force for CN, HCl, CO molecule was made by Itikawa (1969). For CO molecule considering inter atomic distance Itikawa found that short range force takes up the form

$$V_{S.R'} = -\frac{6.09}{r}\exp(-1.59r) - \frac{8.71}{r}\operatorname{Exp}(-2.11r) \qquad \ldots\ldots (4.72)$$

Considering close coupling method the cross section for rotational transitions was calculated. For making the comparision with Coulomb one centred short range potential the attempt was made to calculate $\langle \sigma_n(v) \rangle$. It was observed that though, our short range potential was crude, it gave better value over the Itikawa potential.

In summing up the discussion a very general remark can be made that the point dipole potential super imposed by the short range force $\frac{B\,e^{-\alpha r}}{r}$ with proper choice of B, is the best fit potential for accounting the cross sections for slow electron polar molecule collision.

T A B L E I

Comparision of the quantity $Q'_D = \frac{Q_D(\alpha)}{\pi a_o^2}$ E/Ry.

α	Q'_D(Born)	Q'_D ditt. (For differente values of l)						Q'_D (Variational) For different values of l					
		0	1	2	3	4	5	0	1	2	3	4	5
0.2 [a]	2.666 [b] (-2)	4.639 (-4)	5.004 (-4)	4.900 (-4)	4.382 (-4)	4.376 (-4)	4.373 (-4)	2.632 (-1)	2.712 (-2)	2.652 (-2)	2.672 (-2)	2.663 (-2)	2.670 (-2)
0.4	1.066 (-1)	7.575 (-3)	3.150 (-3)	7.936 (-3)	7.953 (-3)	7.943 (-3)	7.943 (-3)	1.092 (1)	1.374 (-1)	1.045 (-1)	1.057 (-1)	1.070 (-1)	1.030 (-1)
0.6	2.4 (-1)	3.923 (-2)	4.266 (-2)	4.135 (-2)	4.172 (-2)	4.167 (-2)	4.164 (-2)	2.530 (-1)	2.732 (-1)	2.296 (-1)	2.296 (-1)	2.422 (-1)	2.430 (-1)
0.73	3.552 (-1)	-	-	-	-	-	-	3.336 (-1)	4.343 (-1)	3.324 (-1)	3.544 (-1)	3.593 (-1)	3.622 (-1)
0.8	4.266 (-1)	1.392 (-1)	1.427 (-1)	1.403 (-1)	1.399 (-1)	1.397 (-1)	1.397 (-1)	4.773 (-1)	5.416 (-1)	3.934 (-1)	4.153 (-1)	4.330 (-1)	4.364 (-1)
1.0	6.666 (-1)	3.659 (-1)	3.354 (-1)	3.793 (-1)	3.739 (-1)	3.736 (-1)	3.734 (-1)	7.666 (-1)	9.463 (-1)	5.190 (-1)	6.636 (-1)	6.323 (-1)	6.912 (-1)
1.2	9.6 (-1)	9.633 (-1)	1.005	9.944 (-1)	9.927 (-1)	9.920 (-1)	9.917 (-1)	1.670	1.540	7.922 (-1)	9.536 (-1)	9.934 (-1)	1.0103
1.25	1.0642	1.360	1.349	1.347	1.346	1.346	1.346	1.283	1.723	3.430 (-1)	1.033	1.073	1.100

N.B. a. α is in the units of $ea_o/2$

b. The notation (-n) means a factor of 10^{-n}

TABLE 2.

COMPARATIVE STATEMENT OF $\langle\sigma_m(v)\rangle$

For $\langle\sigma_m(v)\rangle_{\text{variational}}$ the trial function

$\psi_i(r) = C_o\, e^{i\vec{K}_i\cdot\vec{r}}$ is used

No.	Molecule	Dipole moment in Debye		$\langle\sigma_m(v)\rangle_{var.}$ $\times 10^{-14}$ cm^2	$\langle\sigma_m(v)\rangle_{Alt.}$ $\times 10^{-14}$ cm^2	$\langle\sigma_m(v)\rangle_{exp.}$ $\times 10^{-14}$ cm^2
1	2	3	4	5	6	7
1	$CClF_3$	0.48	0	0.9759	0.877	1.79
			1	1.154		
			2	0.7971		
			3	0.8487		
			4	0.8928		
			5	0.9016		
			6	0.9086		
			7	0.9095		
			8	0.9120		
			9	0.9137		
			10	0.9200		
2	$(CH_3)_3N$	0.62	0	1.677	1.464	2.80
			1	2.061		
			2	1.292		
			3	1.457		
			4	1.499		
			5	1.517		
			6	1.531		
			7	1.534		
			8	1.540		
			9	1.545		
			10	1.548		

1	2	3	4	5	6	7
3	$(C_2H_5)_2NH$	0.91	0	3.829	3.154	4.32
			1	5.041		
			2	2.606		
			3	3.134		
			4	3.264		
			5	3.321		
			6	3.365		
			7	3.378		
			8	3.394		
			9	3.406		
			10	3.416		
4	$(CH_3)_2NH$	1.0	0	4.701	3.808	5.16
			1	6.704		
			2	3.084		
			3	3.781		
			4	3.951		
			5	4.028		
			6	4.090		
			7	4.105		
			8	4.128		
			9	4.143		
			10	4.158		
5	$C_2H_5NH_2$	1.07	0	5.453	4.360	7.58
			1	7.727		
			2	3.473		
			3	4.328		
			4	4.538		
			5	4.630		
			6	4.704		
			7	4.718		
			8	4.752		
			9	4.775		
			10	4.788		

1	2	3	4	5	6	7
6	$C_3H_7NH_2$	1·25	0	7·693	5·950	8·15
			1	11·31		
			2	4·537		
			3	5·899		
			4	6·234		
			5	6·386		
			6	6·503		
			7	6·540		
			8	6·573		
			9	6·610		
			10	6·633		
7	$(CH_3)_2O$	1·30	0	8·397	6·436	8·15
			1	12·47		
			2	4·848		
			3	6·378		
			4	6·750		
			5	6·920		
			6	7·062		
			7	7·086		
			8	7·136		
			9	7·174		
			10	7·199		
8	$CHClF_2$	1·41	0	10·08	7·571	12·67
			1	15·27		
			2	5·544		
			3	7·499		
			4	7·982		
			5	8·193		
			6	8·366		
			7	8·405		
			8	8·464		
			9	8·523		
			10	8·752		

1	2	3	4	5	6	7
9	CH_2Cl_2	1.59	0	13.22	9.628	18.1
			1	20.67		
			2	6.722		
			3	9.523		
			4	10.21		
			5	10.52		
			6	10.76		
			7	10.82		
			8	10.91		
			9	10.98		
			10	11.04		
10	C_4H_9OH	1.63	0	14.00	10.118	14.45
			1	22.02		
			2	6.984		
			3	10.01		
			4	10.74		
			5	11.09		
			6	11.34		
			7	11.04		
			8	11.50		
			9	11.57		
			10	11.63		
11	C_3H_7OH	1.66	0	14.57	10.494	13.86
			1	23.05		
			2	7.348		
			3	10.37		
			4	11.15		
			5	11.50		
			6	11.78		
			7	11.34		
			8	11.95		
			9	12.03		
			10	12.09		

1	2	3	4	5	6	7
12	C_2H_5OH	1.70	0	15.40	11.006	13.43
			1	24.50		
			2	7.456		
			3	10.88		
			4	11.73		
			5	12.11		
			6	12.40		
			7	12.47		
			8	12.58		
			9	12.66		
			10	12.73		
13	CH_3OH	1.70	Same as Molecule No.12		11.006	13.00
14	$C_2H_4O_2$	1.77	0	16.89	11.931	13.73
			1	27.02		
			2	7.918		
			3	11.79		
			4	12.70		
			5	13.15		
			6	13.52		
			7	13.57		
			8	13.70		
			9	13.79		
			10	13.87		
15	H_2O	1.35	0	18.66	13.034	23.67
			1	30.28		
			2	8.45		
			3	12.86		
			4	13.94		
			5	14.42		
			6	14.83		
			7	14.90		
			8	15.05		
			9	15.17		
			10	15.24		

1	2	3	4	5	6	7
16	$(CH_2NH_2)_2$	1·94	0	20·84	14·333	17·46
			1	34·21		
			2	9·048		
			3	14·19		
			4	15·39		
			5	15·94		
			6	16·39		
			7	16·49		
			8	16·66		
			9	16·80		
			10	16·89		
17	CH_3Cl	1·88	0	19·39	13·46	18·38
			1	31·54		
			2	8·65		
			3	13·28		
			4	14·42		
			5	14·92		
			6	15·34		
			7	15·44		
			8	15·59		
			9	15·70		
			10	15·79		
18	C_2H_5Cl	2·03	0	23·33	15·694	18·93
			1	38·72		
			2	9·645		
			3	15·47		
			4	16·90		
			5	17·54		
			6	18·06		
			7	18·17		
			8	18·35		
			9	18·51		
			10	18·58		

1	2	3	4	5	6	7
19	C_3H_7Cl	2·05	0	23·71	16·006	19·6
			1	39·75		
			2	9·774		
			3	15·79		
			4	17·26		
			5	17·89		
			6	18·45		
			7	18·58		
			8	18·77		
			9	18·91		
			10	19·02		
20	C_4H_9Cl	2·08	0	24·52	16·476	20·22
			1	42·41		
			2	9·965		
			3	16·25		
			4	17·78		
			5	18·47		
			6	19·03		
			7	19·15		
			8	19·36		
			9	19·51		
			10	19·63		
21	C_4H_9Br	2·12	0	25·65	17·116	20·33
			1	43·34		
			2	10·23		
			3	16·39		
			4·	18·50		
			5	19·23		
			6	19·33		
			7	19·95		
			8	20·17		
			9	20·32		
			10	20·46		

1	2	3	4	5	6	7
22	C_2H_5CHO	2·74	0	46·97	28·591	26·49
			1	85·21		
			2	13·71		
			3	28·05		
			4	31·56		
			5	33·12		
			6	34·39		
			7	34·70		
			8	35·17		
			9	35·50		
			10	35·75		
23	C_3H_7CHO	2·73	0	46·57	28·383	25·62
			1	84·37		
			2	13·67		
			3	27·85		
			4	31·32		
			5	32·86		
			6	34·14		
			7	34·40		
			8	34·87		
			9	35·23		
			10	35·50		
24	C_2H_8O	2·77	0	48·25	29·221	28·99
			1	87·78		
			2	13·84		
			3	28·67		
			4	32·28		
			5	32·96		
			6	35·24		
			7	35·53		
			8	36·02		
			9	36·38		
			10	36·64		

1	2	3	4	5	6	7
25	C_3H_6O	2·87	0	52·52	31·369	30·35
			1	99·29		
			2	14·28		
			3	30·75		
			4	32·40		
			5	34·08		
			6	35·44		
			7	35·77		
			8	36·28		
			9	36·64		
			10	36·91		
26	$C_5H_8O_2$	3·03	0	59·81	34·964	29·59
			1	110·9		
			2	14·85		
			3	34·24		
			4	38·97		
			5	41·12		
			6	42·83		
			7	43·29		
			8	43·84		
			9	44·34		
			10	44·69		
27	C_2H_3CN	3·89	0	110·3	57·628	42·71
			1	219·7		
			2	15·05		
			3	56·67		
			4	66·15		
			5	70·65		
			6	74·29		
			7	75·08		
			8	76·40		
			9	77·45		
			10	78·20		

1	2	3	4	5	6	7
28	CH_3CN	3·96	0	115·3	59·721	43·59
			1	230·7		
			2	14·08		
			3	58·11		
			4	68·74		
			5	73·45		
			6	77·29		
			7	78·09		
			8	79·54		
			9	80·61		
			10	81·45		
29	C_2H_5CN	4·03	0	120·9	61·851	43·69
			1	242·10		
			2	14·51		
			3	60·16		
			4	71·32		
			5	76·33		
			6	80·41		
			7	81·23		
			8	82·17		
			9	83·89		
			10	88·74		
30	C_3H_7CN	4·06	0	122·60	62·775	43·84
			1	247·0		
			2	14·36		
			3	61·03		
			4	72·44		
			5	77·52		
			6	81·74		
			7	82·64		
			8	84·18		
			9	85·31		
			10	86·20		

1	2	3	4	5	6	7
31	C_5H_8O	3.3	0	73.60	41.473	31.02
			1	140.40		
			2	15.84		
			3	40.53		
			4	46.65		
			5	49.39		
			6	51.62		
			7	52.20		
			8	52.95		
			9	53.58		
			10	54.03		
32	$C\ O$	0.13	0	0.06598	0.064	0.26
			1	0.07003		
			2	0.06241		
			3	0.06395		
			4	0.06431		
			5	0.06449		
			6	0.06465		
			7	0.06465		
			8	0.06471		
			9	0.06476		
			10	0.06476		
33	N_2O	0.164	0	0.1059	0.102	0.81
			1	0.1140		
			2	0.09883		
			3	0.1019		
			4	0.1026		
			5	0.1030		
			6	0.1032		
			7	0.1033		
			8	0.1034		
			9	0.1035		
			10	0.1035		

1	2	3	4	5	6	7
34	CO_2	0.18	0	0.1281	0.123	3.04
			1	0.1389		
			2	0.1188		
			3	0.1228		
			4	0.1238		
			5	0.1243		
			6	0.1246		
			7	0.1248		
			8	0.1248		
			9	0.1249		
			10	0.1250		
35	NH_3	1.46	0	10.90	8.118	12.89
			1	16.68		
			2	5.865		
			3	8.035		
			4	8.572		
			5	8.808		
			6	8.999		
			7	9.040		
			8	9.114		
			9	9.173		
			10	9.204		

TABLE 3

Comparative statment of diffusion cross section calculated by Altshuler and by finite dipole approximation :-

No.	Dipole moment in Debye.	Enery of electron $\sqrt{\text{Volt}}$.	$(Q'_D)_{Alt}$ πa_0^2 Units.	$(Q'_D)_{\text{Finite Dipole}}$ πa_0^2 Units.	Correction factor.
1	2	3	4	5	6
1	0.48	0.6	3.583	3.58265	0.00035
		0.7	2.633	2.63265	
		0.8	2.016	2.01565	
		0.9	1.593	1.59265	
		1.0	1.290	1.28965	
2	0.62	0.6	5.978	5.97703	0.0009723
		0.7	4.393	4.39203	
		0.8	3.363	3.36203	
		0.9	2.659	2.65803	
		1.0	2.153	2.15203	
3	0.91	0.6	12.87	12.8655	0.004510
		0.7	9.462	9.6575	
		0.8	7.244	7,2395	
		0.9	5.275	5.7205	
		1.0	4.636	4.6315	
4	1.00	0.6	15.55	15.5434	0.006579
		0.7	11.43	11.4234	
		0.8	8.750	8.7434	
		0.9	6.915	6.9084	
		1.0	5.601	5.5944	

1	2	3	4	5	6
5	1.07	0.6	17.80	17.7918	0.008219
		0.7	13.08	13.0718	
		0.8	10.02	10.0118	
		0.9	7.918	7.9098	
		1.0	6.412	6.4038	
6	1.225	0.6	24.30	24.284	0.01606
		0.7	17.85	17.834	
		0.8	13.68	13.664	
		0.9	10.80	10.791	
		1.0	8.75	8.734	
7	1.30	0.6	26.28	26.261	0.01878
		0.7	19.32	19.301	
		0.8	14.79	14.771	
		0.9	11.69	11.671	
		1.0	9.462	9.443	
8	1.41	0.6	30.91	30.884	0.02600
		0.7	22.72	22.694	
		0.8	17.40	17.374	
		0.9	13.75	13.724	
		1.0	11.14	11.114	
9	1.59	0.6	39.31	39.268	0.04206
		0.7	28.89	28.848	
		0.8	22.12	22.078	
		0.9	17.48	17.438	
		1.0	14.16	14.118	

1	2	3	4	5	6
10	1.63	0.6	41.32	41.273	0.04645
		0.7	30.37	30.323	
		0.8	23.25	23.203	
		0.9	18.38	18.333	
		1.0	14.38	14.333	
11	1.66	0.6	42.35	42.301	0.04898
		0.7	31.49	31.441	
		0.8	24.11	24.061	
		0.9	19.05	19.001	
		1.0	15.43	15.381	
12	1.70	0.6	44.93	44.875	0.05493
		0.7	33.02	32.965	
		0.8	25.24	25.185	
		0.9	19.98	19.925	
		1.0	16.18	16.125	
13	Same as Molecule No.12				
14	1.77	0.6	48.73	48.665	0.06460
		0.7	35.81	35.745	
		0.8	27.42	27.355	
		0.9	21.67	21.605	
		1.0	17.55	17.485	
15	1.85	0.6	53.23	53.153	0.07709
		0.7	39.12	39.043	
		0.8	29.95	29.873	
		0.9	23.67	23.593	
		1.0	19.15	19.073	

1	2	3	4	5	6
16	1.94	0.6	58.53	58.437	0.09319
		0.7	43.01	42.917	
		0.8	32.94	32.897	
		0.9	26.02	25.927	
		1.0	21.08	20.987	
17	1.88	0.6	54.98	54.896	0.08914
		0.7	40.40	40.316	
		0.8	30.93	30.846	
		0.9	24.44	24.356	
		1.0	19.80	19.716	
18	2.03	0.6	64.09	63.973	0.1118
		0.7	47.10	46.988	
		0.8	36.06	35.948	
		0.9	28.49	28.378	
		1.0	23.08	22.968	
19	2.05	0.6	65.37	65.254	0.1162
		0.7	48.04	47.924	
		0.8	36.78	36.664	
		0.9	29.07	28.954	
		1.0	23.54	23.424	
20	2.08	0.6	67.30	67.177	0.1232
		0.7	49.45	49.327	
		0.8	37.86	37.737	
		0.9	29.92	29.797	
		1.0	24.26	24.137	

1	2	3	4	5	6
21	2.12	0.6	69.88	69.747	0.1328
		0.7	51.36	51.227	
		0.8	39.30	39.267	
		0.9	31.08	30.947	
		1.0	25.17	25.037	
22	2.74	0.6	116.8	116.429	0.3710
		0.7	85.82	85.449	
		0.8	65.70	65.329	
		0.9	51.93	51.559	
		1.0	42.06	41.689	
23	2.73	0.6	116.0	115.634	0.3656
		0.7	85.19	84.824	
		0.8	65.22	64.854	
		0.9	51.54	51.174	
		1.0	41.75	41.384	
24	2.77	0.6	119.3	118.912	0.3875
		0.7	87.70	87.312	
		0.8	67.14	66.752	
		0.9	53.07	52.682	
		1.0	42.97	42.582	
25	2.87	0.6	128.1	127.653	0.4465
		0.7	92.0	91.553	
		0.8	72.07	71.623	
		0.9	56.97	56.523	
		1.0	46.13	45.683	

1	2	3	4	5	6
26	3.03	0.6	142.8	142.246	0.554
		0.7	104.9	104.346	
		0.8	80.32	79,766	
		0.9	63.48	62.926	
		1.0	51.40	50.846	
27	3.89	0.6	235.3	233.792	1.508
		0.7	172.9	171.392	
		0.8	132.3	130.792	
		0.9	104.6	103.092	
		1.0	84.72	83.212	
28	3.96	0.6	243.9	242.282	1.613
		0.7	179.3	177.682	
		0.8	137.2	135.582	
		0.9	108,4	106,782	
		1.0	87.82	86.202	
29	4.03	0.6	252.5	250.764	1.736
		0.7	179.3	177.682	
		0.8	137.2	135.582	
		0.9	108.4	106.782	
		1.0	87.82	86.202	
30	4.06	0.6	254.6	254.613	1.787
		0.7	188.4	186,613	
		0.8	144.2	142.513	
		0.9	114.0	112.213	
		1.0	92.3	90.513	

1	2	3	4	5	6
31	3.3	0.6	169.3	168.52	0.7802
		0.7	124.5	123.72	
		0.8	95.28	94.50	
		0.9	75.30	74.52	
		1.0	60.98	60.20	
32	0.13	0.6	0.2626		1.878×10^{-6}
		0.7	0.1932		
		0.8	0.1479		
		0.9	0.1169		
		1.0	0.09462		
33	0.164	0.6	0.4182		$4.757 \ X10^{-6}$
		0.7	0.3073		
		0.8	0.2353		
		0.9	0.1860		
		1.0	0.1506		
34	0.18	0.6	0.5040		$6.908 \ X \ 10^{-6}$
		0.7	0.3073		
		0.8	0.2835		
		0.9	0.2241		
		1.0	0.1841		
35	1.46	0-6	33.16	33.13	0.0299
		0.7	24.36	24.33	
		0.8	18.69	18.66	
		0.9	14.74	14.71	
		1.0	11.94	11.91	

TABLE IV

Comparative statement of mean scattering cross section.

No.	Dipole moment in Debye	$\langle \sigma_w(v) \rangle_{Exp}$ X 10^{-14} cm^2	$\langle \sigma_w(v) \rangle_{Alt}$ X 10^{-14} cm^2	$\langle \sigma_w(v) \rangle_{F.D}$ X 10^{-14} cm^2	Correction factor X
1	2	3	4	5	6
1	0.48	1.79	0.877	-	0.00000-7466
2	0.62	2.80	1.464	-	0.0000-2079
3	0.91	4.32	3,154	-	0.0000-9645
4	1.00	5.16	3.808	3.807859	0.0001407
5	1.07	7.58	4.360	4.3598	0.0001845
6	1.25	8.15	5.950	5.9496	0.0003435
7	1.30	8.15	6.436	6.4356	0.0004017
8	1.41	12.67	7.571	7,5704	0.0005560
9	1.59	18.1	9.628	9.6271	0.0008993
10	1.63	14.45	10.118	10.117	0.0009933
11	1.66	13.86	10.494	10.4929	0.001069
12	1.70	13.43	11.006	11.0048	0.001174
13	1.70	13.00	11.006	11.0048	0.001174
14	1.77	13.73	11.931	11.9296	0.001381

1	2	3	4	5	6
15	1.85	23.67	13.034	13.0323	0.001648
16	1.94	17.46	14.333	14.331	0.001993
17	1.88	18.38	13.460	13.458	0.001758
18	2.03	18.93	15.694	15.692	0.002390
19	2.05	19.6	16.006	16.004	0.002486
20	2.08	20.22	16.476	16.473	0.002634
21	2.12	20.33	17.116	17.113	0.002840
22	2.74	26.49	28.591	28.583	0.007934
23	2.73	25.62	28.383	28.375	0.007818
24	2.77	28.99	29.221	29.221	0.008343
25	2.87	30.35	31.369	31.369	0.009548
26	3.03	29.59	34.964	34.964	0.01185
27	3.89	42.71	57.628	57,628	0.03221
28	3.96	43.59	59.721	59.721	0.03460
29	4.03	43.69	61.851	61.814	0.03711
30	4.06	43.84	62.775	62.737	0.03822
31	3.3	31.02	41.473	41.456	0.01668

1	2	3	4	5	6
32	0.13	0.26	0.064	-	4.017×10^{-8}
33	0.164	0.81	0.102	-	9.989×10^{-8}
34	0.18	3.04	0.123	-	1.478×10^{-7}
35	1.46	12.89	8.118	8.1174	0.0006396

TABLE V

Comparision of $\langle \sigma_m(v) \rangle$ for short range (attractive) force

$\alpha = 2A^{0}U^{-1}$

$T = 300^{0}K$

No.	Dipole moment in Debye	$\langle \sigma_m(v) \rangle_{expt}$ $\times 10^{-14}$ cm^2	$\langle \sigma_m(v) \rangle_{Alt}$ $\times 10^{-14}$ cm^2	$\langle \sigma_m(v) \rangle$ short range X 10^{-14} cm^2 for different values of B					
				B = 1	B = 2	B = 3	B = 4	B = 5	B = 6
1	2	3	4	5	6	7	8	9	10
1	0.48	1.79	0.877	0.3436	0.7434	0.5764	0.3426	0.0220	--
2	0.62	2.80	1.469	1.4356	1.3354	1.1684	0.9346	0.614	0.2670
3	0.91	4.32	3.154	3.1206	3.0204	2.8534	2.6196	2.299	1.952
4	1.00	5.16	3.808	3.7746	3.6744	3.5074	3.2736	2.953	2.606
5	1.07	7.58	4.360	4.3266	4.2264	3.3594	3.3256	3.505	3.158
6	1.25	8.15	5.950	5.9166	5.8164	5.6494	5.4156	5.095	4.748
7	1.30	8.15	6.436	6.4026	6.3024	6.1354	5.9016	5.581	5.134
8	1.41	12.67	7.571	7.5376	7.4374	7.2704	7.0366	6.716	6.369
9	1.59	18.1	9.623	9.4946	9.4344	9.3174	9.0936	8.773	8.426

1	2	3	4	5	6	7	8	9	10
10	1.63	14.45	10.118	10.0846	9.9894	9.8174	9.5836	9.263	8.916
11	1.66	13.86	10.494	10.4606	10.3604	10.1934	9.9596	9.639	9.292
12	1.70	13.43	11.006	10.9726	10.8724	10.7054	10.4716	10.151	9.804
13	1.70	13.00	11.006	10.9726	10.8724	10.7054	10.4716	10.151	9.804
14	1.77	13.73	11.931	11.8976	11.7974	11.6304	11.3966	11.076	10.729
15	1.85	23.67	13.034	13.0006	12.9004	12.7334	12.4996	12.179	11.832
16	1.94	17.46	14.333	14.2996	14.1994	14.0224	13.7986	13.578	13.131
17	1.88	18.38	13.460	13.4266	13.3264	13.1594	12.9256	12.605	12.258
18	2.03	18.93	15.694	15.6606	15.5604	15.3934	15.0596	14.739	14.492
19	2.05	19.6	16.006	15.9726	15.8724	15.7054	15.4716	15.151	14.804
20	2.08	20.22	16.476	16.4426	16.3424	16.1754	15.9416	15.621	15.274
21	2.12	20.33	17.116	17.0826	16.9824	16.8154	16.5816	16.261	15.914
22	2.74	26.49	28.591	28.5576	28.4574	28.2904	28.0566	27.736	27.389
23	2.73	25.62	28.383	28.3496	28.2494	28.0824	27.8486	27.528	27.181

1	2	3	4	5	6	7	8	9	10
24	2.77	28.99	29.221	29.1876	29.0874	28.9204	28.6866	28.366	28.019
25	2.87	30.35	31.369	31.3356	31.2354	31.0684	30.8346	30.514	30.167
26	3.03	29.59	34.964	34.9306	34.8304	34.6634	34.4296	34.109	33.762
27	3.89	42.71	57.628	57.5946	57.4944	57.3274	57.0936	56.773	56.426
28	3.96	43.59	59.721	59.6876	59.5674	59.4209	59.1366	58.866	58.519
29	4.03	43.69	61.851	61.8176	61.6974	61.5509	61.3166	60.796	60.649
30	4.06	43.84	62.775	62.7416	62.6214	62.4749	62.2406	61.620	61.573
31	3.3	31.02	41.473	41.4399	41.3394	41.1724	40.9336	40.618	40.271
32	0.13	0.26	0. 064	0.0306	-	--	--	--	--
33	0.164	0.81	0.102	0.0686	--	--	--	--	--
34	0.18	3.04	0.123	0.0896	- -	--	--	--	--
35	1.46	12.89	8.113	8.0846	7.9844	7.8174	7.5736	7.263	6.916

TABLE VI

Comparision of $\langle \sigma_m(v) \rangle$ for short range (repulsive) force

1	2	3	4	5	6	7	8	9	10
1	0.48	1.79	0.877	0.9104	1.0106	1.1776	1.4114	1.732	--
2	0.62	2.80	1.469	1.4974	1.5976	1.7646	1.9934	2.3190	2.666
3	0.91	4.32	3.154	3.1874	3.2876	3.4596	3.6334	4.009	4.356
4	1.00	5.16	3.808	3.3414	3.9416	4.1036	4.3424	4.663	5.010
5	1.07	7.58	4.360	4.3934	4.4936	4.6606	4.8944	5.215	5.562
6	1.25	8.15	5.950	5.9834	6.0836	6.2506	6.24344	6.845	7.152
7	1.30	8.15	6.436	6.4694	6.5696	6.7366	6.9704	7.291	7.638
8	1.41	12.67	7.571	7.6044	7.7046	7.8716	8.1054	8.4260	8.773
9	1.59	18.1	9.628	9.6614	9.7616	9.9286	10.1624	10.483	10.83
10	1.63	14.45	10.118	10.1514	10.2516	10.4186	10.6524	10.973	11.32
11	1.66	13.86	10.494	10.5274	10.6276	10.7946	11.0284	11.349	11.696
12	1.70	13.43	11.006	11.0394	11.1396	11.3066	11.5404	11.8610	12.208

1	2	3	4	5	6	7	8	9	10
13	1.70	13.00	11.006	11.0394	11.1396	11.3066	11.5404	11.8610	12.208
14	1.77	13.73	11.931	11.9644	12.0646	12.2316	12.4654	12.7860	13.133
15	1.85	23.67	13.034	13.0674	13.1676	13.3346	13.5684	13.889	14.236
16	1.94	17.46	14.333	14.3634	14.4666	14.5336	14.8674	15.1880	15.535
17	1.88	18.38	13.460	13.4934	13.5936	13.7606	13.9944	14.315	14,662
18	2.03	18.93	15.694	15.7274	15,8276	15.9946	16.2284	16.549	16.896
19	2.05	19.6	16.006	16.0394	16.1396	16.3066	16.5404	16.861	17.208
20	2.08	20.22	16.476	16.5094	16.6096	16.7766	17.0104	17.331	17.678
21	2.12	20.33	17.116	17.1494	17.2496	17.4166	17.6504	17.971	18.318
22	2.74	26.49	28.591	28.6244	28.7246	28.8916	29.1254	29.4406	29.793
23	2.73	25.62	28.383	28.4164	28.5166	28.6836	28.9174	29.238	29.585
24	2.77	28.99	29.221	29.2544	29.3546	29.5216	29.7554	30.076	30.423

1	2	3	4	5	6	7	8	9	10
25	2.87	30.35	31.369	31.4024	31.5028	31.6696	31.9034	32.224	32.571
26	3.03	29.59	34.964	34.9974	35.0976	35.2946	35.9934	35.319	36.166
27	3.89	42.71	57.623	57.6614	57.7616	57.9236	58.1629	58.433	58.83
28	3.96	43.59	59.721	59.7544	59.8546	60.0216	60.2554	60.576	60.923
29	4.03	43.69	61.851	61.8344	61.9846	62.1516	62.3854	62.606	63.053
30	4.06	43.84	62.775	62.8084	62.9086	63.0756	63.3094	63.53	63.977
31	3.3	37.02	41.473	41.5064	41.6066	41.7736	42.0074	42.328	42.675
32	0.13	0.26	0.064	0.0974	0.1976	0.3646	--	--	--
33	0.164	0.31	0.102	0.136	0.2356	0.4026	0.6364	0.9570	--
34	0.18	3.04	0.123	0.1564	0.2566	0.4236	0.6574	0.9780	1.3250
35	1.46	12.89	8.113	8.1514	8.2516	8.4136	8.6524	8.973	9.32

TABLE VII

Exact value of " B " for perfact agreement with experiment.

No.	Dipole moment in Debye.	| B |	No.	Dipole moment in Debye	| B |
1	0.48	5.2	19	2.05	10.37
2	0. 62	6.07	20	2.08	10.59
3	0.91	5.909	21	2.12	9.656
4	1.00	6.362	22	2.74	7.932
5	1.07	9.819	23	2.73	9. 076
6	1.25	8.007	24	2.77	2.629
7	1.30	7.164	25	2.87	5.522
8	1.41	12.36	26	3.03	12.69
9	1.59	15.92	27	3.89	21.13
10	1.63	11.39	28	3.96	21.98
11	1.66	10.03	29	4.03	23.32
12	1.70	3.517	30	4.06	23.81
13	1.70	7.727	31	3.3	17.69
14	1.77	7.343	32	0.13	2.159
15	1.85	17.84	33	0.164	4.603
16	1.94	9.677	34	0.18	9.346
17	1.88	12.27	35	1.46	11.95
18	2.03	9.842			

N.B. For molecules No.1 to 21 and 2 to 35 for the agreement with the experiment Repulsive short range force should be considered while for molecules No.22 to 31 attractive short range force should be considered.

APPENDIX I

Detailed calculations of equation 4.11

Our aim is to solve the equation 4.7 for a point dipole potential. Equation 4.7 is given by

$$\left[f(n_s, n_i) \right] = -1/4\pi \left\{ \int e^{-i\vec{K}_s \cdot \vec{r}'} \, U(\vec{r}') \, \psi_i(r') \, dr' + \int e^{i\vec{K}_i \cdot \vec{r}} \, U(r) \, \psi_{-s}(r) \, dr - \int \psi_{-s}(r) \, U(r) \, \psi_i(r) \, dr - 1/4\pi \iint \psi_{-s}(r) \, U(r) \, G(r, r') \, U(r') \, \psi_i(r') \, dr \, dr' \right\}$$

Here $\psi_{-s}(r)$ is the wave function represents a solution of integral equation 4.3 for a plane wave incident in the direction $(-n_s)$. As a trial wave function we have taken

$$\Phi_i(r) = C_0 e^{i\vec{K}_i \cdot \vec{r}}, \quad V(r) = -\frac{e \, D \cos\theta}{r^2}, \quad U(r) = \frac{2m}{\hbar^2} V(r),$$

$$\Phi_{-s}(r) = C_0 e^{-i\vec{K}_s \cdot \vec{r}}$$

(A) First erm of equation 4.7 turn out to be

$$I_1 = -1/4\pi \int e^{-i\vec{K}_s \cdot \vec{r}'} \, U(r') \, \psi_i(r') \, dr'$$

substituting the values and performing elementary integrations we get $I_1 = C_0 f_B(\theta)$, $f_B(\theta)$ = Amplitude using Born approximation $= \frac{2i \, D \, e \, m \, \gamma'}{\hbar^2 K}$

(B) $$I_2 = -1/4\pi \int e^{i\vec{K}_i \cdot \vec{r}}\, U(r)\, \Psi_{-s}(r)\, dr = C_o\, f_B(\theta)$$

(C) $$I_3 = 1/4\pi \int \Psi_{-s}(r)\, U(r)\, \Psi_i(r)\, dr = -C_o^2\, f_B(\theta)$$

(D) $$I_4 = 1/16\pi^2 \iint \Psi_{-s}(r)\, U(r)\, G(r,r')\, U(r')\, \Psi_i(r')\, dr\, dr'$$

For the integration of this term

$$G(r,r') = \int \frac{4\pi}{(2\pi)^3} \frac{dn\, e^{i\vec{n}\cdot(\bar{r}-\bar{r}')}}{(n^2-k^2)}$$

substituting this we get final integration as

$$C_o^2 \left\{ f_B(\theta) \right\}^2 \frac{K^2}{2\pi^2} \int \frac{dn}{n^2-k^2} \int \frac{\cos\alpha}{r^2} e^{i(\vec{n}-\vec{K}_s)\cdot r}\, dr \int e^{-i(n-K_i)\cdot r'} \frac{\cos\alpha'}{r'^2}\, dr'$$

$$I_4 = \frac{C_o^2 \left\{ f_B(\theta) \right\}^2 K^2}{2\pi^2} \int \frac{dn}{(n^2-K^2)(n-K_i)(n-K_s)}$$

This integration is determine applying Cauchy's theorem according to which

$$\oint f(Z)\, dZ = 2\pi i \sum \text{Residule of } f(Z)$$

the integrand has poles at n = K and n = -K but since we integrate from 0 to ∞ we take only n = K we get $I_4 = C_o^2\, f_B(\theta)\, T_o(\theta)$

$$T_o(\theta) = f_B(\theta) \frac{K^2}{2\pi^2} \int \frac{dn}{(n^2-k^2)(n-k_i)(n-k_s)} = \frac{f_B(\theta) K_i\, i}{2}$$

APPENDIX II

Simplification of equation 4.55

We wish to simplify equation

$$\sum_{\ell=0}^{\sigma} \sum_{m=-\ell}^{+\ell} P_1 \int \left| \Theta(\ell,m) \right|^2 \cos^2\gamma \, d\Omega$$

$$\Theta(1,m) = \sqrt{\left\{ \frac{(2\ell+1)\ (\ell-m)}{2(\ell+|m|)} \right\}} \quad P_1^m \ (\cos\theta)\ e^{im\phi}$$

Where $P_1^m\ (\cos\theta)$ = Associated Legendre function

Now $\cos\gamma\,\Theta(\ell,m) = \Theta(\ell+1,m)\,C_1 + \Theta(\ell-1,m)\,C_2$

where $C_1 = \sqrt{\left\{ \frac{(\ell+1-m)\ (\ell+1+m)}{(2\ell+1)\ (2\ell+3)} \right\}}$

$C_2 = \sqrt{\left\{ \frac{(\ell-m)\ (\ell+m)}{(2\ell-1)\ (2\ell+1)} \right\}}$

$$\cos^2\gamma \left| \Theta(\ell,m) \right|^2 = \Theta^2(\ell+1,m)\,C_1^2 + 2C_1C_2\,\Theta(\ell+1,m)\,\Theta(\ell-1,m) + C_2^2\,\Theta^2(\ell-1,m)$$

$$\int \cos^2\gamma \left| \Theta(\ell,m) \right|^2 d\Omega = C_1^2 \int \Theta^2(\ell+1,m)\,d\Omega \ +$$

$$2C_1C_2 \int \Theta(\ell+1,m)\ \Theta(\ell-1,m)\,d\Omega + C_2^2 \int \Theta^2(\ell-1\ m)\ d\Omega$$

on integrating by straight forward way we get

$$C_1^2 \int \Theta^2(l+1,\, m)\; d\Omega \;=\; C_1^2 \;=\; \frac{(l+1)^2 - m^2}{(2l+1)(2l+3)}$$

$$2C_1\, C_2 \int \Theta\,(l+1,m)\;\Theta\,(l-1,m)\; d\Omega \;=\; \text{Zero}$$

$$C_2^2 \int \Theta^2(l-1,\, m)\; d\Omega \;=\; C_2^2 \;=\; \frac{l^2 - m^2}{(2l+1)(2l-1)}$$

$$\int \left|\Theta\,(l,\, m)\right|^2 d\Omega \times \operatorname{Cos}^2\gamma \;=\; \frac{(l+1)^2 - m^2}{(2l+1)(2l+3)} + \frac{(l^2 - m^2)}{(2l-1)(2l+1)}$$

$$\sum_{l=0}^{\infty}\ \sum_{m=-l}^{l} P_1 \int \left|\Theta\,(l,m)\right|^2 \operatorname{Cos}^2\gamma\; d\Omega$$

$$= \sum_{l=0}^{\infty} P_1 \sum_{m=-l}^{l} \frac{(l+1)^2 - m^2}{(2l+1)(2l+3)} + \frac{l^2 - m^2}{(2l-1)(2l+1)}$$

$$= \sum_{l=0}^{\infty} P_1\; \frac{2l+1}{3}$$

Now putting the value of $P_1 = 1/2l+1$ we get

$$\int \left|\Theta\,(l,\, m)\right|^2 \operatorname{Cos}^2\gamma\; d\Omega \;=\; 1/3$$

APPENDIX III

We wish to convert momentum transfer cross section Q_D in πa_o^2 units. Q_D is given in C.G.S. units as

$$Q_D = \frac{8\pi}{3} \left(D e m / \hbar^2 K_o \right)^2 \left\{ 1 - 0.4 K_o^2 a^2 + 0.53 K_o^4 a^4 \right\}$$

considering first term $\frac{8\pi}{3} \left(D e m / \hbar^2 K_o \right)^2$

$$= \frac{8\pi}{3} \frac{D^2 e^2 m^2}{\hbar^4} \quad \frac{\hbar^2}{2mE} \quad \text{where} \quad K_o^2 = 2m E/\hbar^2$$

putting $m e^2/\hbar^2 = 1/a_o$ where a_o = Bohr radius, E may be converted in $\sqrt{\text{volt}}$ units

$$\frac{8\pi}{3} \frac{D^2}{2E} \frac{1}{a_o} = \frac{8\pi}{6} \left(\frac{D}{10^{-18}} \right)^2 X \; 10^{-36} \quad \frac{1}{a_o \left(\frac{E \times C}{e \times 10^8} \right) \frac{e}{C} X \, 10^8}$$

$$= \frac{8}{6} \left(\frac{D'}{E'} \right)^2 \quad \frac{10^{-36} X \, C}{e \, X \, 10^8 \, a_o^3} \quad (\pi a_o^2)$$

putting the values of C (Velocity of light) and e and on simplifying we get the first term $= 5.6 \, (D')^2 / E' \, \pi \, a_o^2$

Similarly second term will be $= 0.006579 \, D^4 \, \pi \, a_o^2$ and third term $= 0.253 \, X \, 10^{-5} (D')^6 \, \pi \, a_o^2$

$$Q_D' = \frac{Q_D}{\pi a_o^2} = \left[5.6 \frac{(D')^2}{E'} - 0.006579 \, (D')^4 + 0.253 \times 10^{-5} (D')^6 E' \right]$$