# Chapter 3
# Theoretical models

## 3.1 Introduction

In a typical collision experiment, a projectile with velocity ($v_p$) impinges on a target which is usually at rest in the laboratory frame. To interpret the experimental observations different theoretical models have been developed over decades. Accurate interpretation of the ionization cross sections in multielectronic target systems is a challenging task for theoretical models. The main difficulty is caused by the many-body feature of the collision, which involves the projectile (P) having charge state ($q_p$), the target nucleus (T) and the number of electron(s) in the target $N$. Each of the theoretical models uses some approximations that are required to solve the many-body problem associated with the ionization process. Majority of the earlier theoretical works were based on the Born approximation which is perturbative in nature. In this approach the projectile exerts very small perturbation to the target system and the projectile effectively goes almost undeflected from it's straight line trajectory. Such an assumption is valid only for fast moving projectiles, i.e., where the projectile velocity is sufficiently higher than the velocity of the orbital electron in the target. In such cases the projectile is represented as a plane wave both in the entrance as well as in the exit channel of the reaction. Here the interaction between the ejected electron and the projectile is not considered. Such an approach, although valid for high velocity projectiles, but fails for projectiles having intermediate collision energy or having high charge state.

For the different collision systems studied in the present thesis, in most of the cases, the projectile velocities were much higher than the orbital velocity of the electron in the target. For such cases we have used the perturbative treatment, the CB1 model, discussed in the following section. We next move on to the projectiles which are highly charged ions or having intermediate energy. For such cases, there exists a strong post collision interaction between the projectile and the ionized electron. In this regard, the continuum distorted wave-eikonal initial state (CDW-EIS) approximation is widely used, which takes into account the distortions by both the projectile and target centers. After discussing these quantum mechanical calculations, we have discussed about the CTMC model which deals with the collision partners from a classical point of view. All these models, obtained from different collaborators, are used to calculate the DDCS (hence SDCS and TCS) for electron emission. The calculations using the CB1 approximations were provided by Champion and co-workers, similarly those using the CDW-EIS model and the CTMC model were provided by Rivarola *et. al.* and Tokesi *et. al.*, respectively. The CSP-ic approximation which is a semi-empirical model has been used as a part of this work for evaluating the total ionization cross section (TCS) in case of electron impact ionization studies.

## 3.2 CB1 Model

In case of the first Born approximation (B1), the projectile is represented by a plane wave both in the incoming and outgoing channel, whereas the electron is described by bound and continuum wave functions of the target in the entrance and exit channel respectively [1]. In case of the CB1 model, the cross section have been calculated within the framework of B1 approximation with the initial and final wave functions satisfying the correct boundary conditions (hence named as CB1). Here, the ejected electron is described by a Coulomb wave (CW), taking care of the long range Coulomb interaction between the projectile and the ionized electron [59, 60, 61, 62].

In the present thesis, the CB1 model calculations were used extensively to compare the experimental results obtained for keV energy electron impact on $N_2$ molecules. Since in this case the energy of the electrons causing ionization are sufficiently high, one can resort to such perturbative models. In the present quantum mechanical calculation, an effective target charge ($Z_T^*$) has been introduced which is seen by the ejected electron. The effective charge is given by

$$Z_T^* = \sqrt{-2n^2\epsilon}. \tag{3.1}$$

Here $n$ is the principal quantum number of each atomic orbital component used in the target description and the active electron orbital energy $\epsilon$ is related to the ionization energies $B$ of each occupied molecular orbital by $\epsilon = -B$. Further, the well known frozen core approximation was used where the *passive* (not ionized) electrons are assumed to remain frozen in their molecular orbitals during the collision. This allows one to reduce the electron target interaction potential to a one-active electron problem. Using these conditions, the triple differential cross section, differential in the direction of the scattered electron $\Omega_s$, differential in the direction of the ejected electron $\Omega_e$ and differential in the ejected energy $E_e$ is denoted as :

$$\sigma^{(3)}(\Omega_s, \Omega_e, E_e) \equiv \frac{d^3\sigma}{d\Omega_s d\Omega_e dE_e} = \sum_{j=1}^{N} \frac{d^3\sigma_j}{d\Omega_s d\Omega_e dE_e}. \tag{3.2}$$

where $N$ is the number of molecular orbitals used in the description of the target and $\frac{d^3\sigma_j}{d\Omega_s d\Omega_e dE_e}$ is the triple differential cross section for the $j$-th orbital of the target. Each "molecular orbital" cross section is expressed as a weighted sum of the atomic triple differential cross sections corresponding to the different atomic components used in the description of the $N_2$

target, namely, the $N_{1s}$, $N_{2s}$, and $N_{2p}$ orbitals, given by [62] :

$$\frac{d^3\sigma_j}{d\Omega_s d\Omega_e dE_e} = \sum_i \xi_{j,i}.\frac{d^3\sigma_{at,i}}{d\Omega_s d\Omega_e dE_e}. \tag{3.3}$$

where the effective number of electrons $\xi_{j,i}$ and the corresponding binding energy are calculated in the gas phase with the Gaussian 09 software.

Thus, in the laboratory framework, the atomic tripe differential cross sections are calculated as follows :

$$\frac{d^3\sigma_{at,i}}{d\Omega_s d\Omega_e dE_e} = (2\pi)^4 \frac{k_s k_e}{k_i} |[T_{a,b}]_i|^2. \tag{3.4}$$

where $k_i$, $k_s$ and $k_e$ denote the wave vectors of the incident, scattered and ejected electron respectively. $[T_{a,b}]_i$ denotes the atomic transition matrix element between an initial state $a$ and a final state $b$ given by :

$$[T_{a,b}]_i = \langle \phi_b^i(\mathbf{r}_0).\varphi_b^i(\mathbf{r}_1)|V(\mathbf{r}_0,\mathbf{r}_1)|\phi_a^i(\mathbf{r}_0).\varphi_a^i(\mathbf{r}_1)\rangle. \tag{3.5}$$

where $V(\mathbf{r}_0, \mathbf{r}_1)$ is the interaction potential between the incident electron and the target, $\mathbf{r}_0$ and $\mathbf{r}_1$ stands for the position vectors of the incident and the active target electron respectively. $\phi_a^i(\mathbf{r}_0)$ and $\phi_b^i(\mathbf{r}_0)$ are the incoming and outgoing projectile plane waves, respectively. $\varphi_b^i(\mathbf{r}_1)$ represents the ejected-electron Coulomb wave function whereas $\varphi_a^i(\mathbf{r}_1)$ represents the atomic wave function. Using the frozen core approximation, the multi-electron problem is reduced to a one active electron problem. Further, by using the well-known partial-wave expansion of the plane wave as well as that of the Coulomb wave, the DDCS are obtained for each molecular orbital by analytical integration of the triple differential cross section. Finally, the target ionization cross sections are obtained by summing up the contributions from all the subshells.

## 3.3 CDW-EIS Model

In the previous sections we have discussed about the perturbative models which are valid for projectiles with sufficiently high energy. However, for projectiles with collision energy in the intermediate energy regime or when the projectile is a highly charged ion, then the ionized electron experiences the long-range Coulomb field of both the residual target ion and the projectile. For example, in the present thesis we have performed studies on keV energy proton (intermediate energy regime) impact and MeV energy $C^{6+}$ (highly charged ion) ion impact on different molecular targets. In such cases, the collisional aspects are by far best explained in terms of the continuum distorted wave-eikonal initial state (CDW-EIS) approximation, taking care of the two center effect accurately. This model was initially introduced by D S F Crothers and J F McCann [63]. The CDW-EIS model is valid both in the intermediate and high velocity regime of the projectile. It takes into account the distortions both in the initial and final channels. Here the independent electron model is used, where the non-ionized (*passive*) electrons are assumed to remain frozen during the collision process with only one *active* electron, thus describing single ionization phenomena. The Coulombic behaviour due to the active electron-projectile interaction is included in the entrance channel by choosing a distorted initial wavefunction where the initial bound state is multiplied by an eikonal phase associated with that interaction [64]. In the final channel, it is assumed that the active electron feels the fields of the projectile and of the residual target simultaneously. So, the final wavefunction is proposed as a product of two continuum states of the active electron : one due to the presence of the projectile and the other due to the presence of the residual target.

In this model, the distorted wave function in the initial channel is given by :

$$\chi_i^+ = \varphi_i(\mathbf{x})\, \exp\left(-i\,\varepsilon_i\, t\right)\, \exp\left[-i\,\nu\, \ln\left(v\, s + \mathbf{v}\cdot\mathbf{s}\right)\right] \tag{3.6}$$

where $\varphi_i$ is the active-electron initial bound state with $\varepsilon_i$ its initial binding energy, $\nu$ is the perturbation strength i.e. $(q_p/v_p)$, with $q_p$ being the projectile charge and $v_p$ the collision velocity. The super-index (+) in Equation 3.6 indicates that it preserves correct outgoing boundary condition.

Now the final distorted wave function at the exit channel is given by :

$$\begin{aligned}\chi_f^- =& \varphi_f(\mathbf{x})\, \exp\left(-i\,\varepsilon_f\, t\right)\\ &\times\, N^*(\lambda)\, {}_1F_1[-i\,\lambda; 1; -i(k\, x - \mathbf{k}\cdot\mathbf{x})]\\ &\times\, N^*(\xi)\, {}_1F_1[-i\,\xi; 1; -i(p\, s - \mathbf{p}\cdot\mathbf{s})]\end{aligned} \tag{3.7}$$

Here $\varphi_f$ is a free-electron plane wave with momentum $\mathbf{k}$, $\varepsilon_f = \frac{1}{2}k^2$, $\xi = Z_P/p$, being $\mathbf{p} = \mathbf{k} - \mathbf{v}$, $\lambda = \tilde{Z}_T/k$ with $\tilde{Z}_T$ and effective target nuclear charge describing the interaction of the active electron with an effective residual-target Coulomb potential. In both Equation 3.6 and Equation 3.7 $\mathbf{x}$ and $\mathbf{s}$ are the active-electron coordinate in a target-fixed and projectile-fixed reference frame respectively. Also ${}_1F_1$ is the hypergeometric function and $N(a) = \exp\left(\pi\, a/2\right)\Gamma(1 - i\, a)$ its normalization factor (with $\Gamma$ the Euler Gamma function).

This model has a prior and post version. When the perturbative potentials are applied to the initial channel distorted wave function it gives rise to the prior version of the transition matrix element and similarly when applied to the exit channel, the post version of transition matrix elements are generated. In the present thesis, the prior version of this model has been applied extensively to check with the experimentally observed DDCS in case of ion impact ionization of small molecules and large biomolecules.

## 3.4 CTMC Model

The classical trajectory Monte Carlo (CTMC) method was introduced by Abrines and Percival to study ion-atom collisions [65, 66]. This model provides a classical treatment to the collision involving three particles i.e., the projectile, the active target electron and the remaining target ion, comprising of the target nucleus and the remaining target electrons. The three particles are characterized by their masses and charges. Here the many-body interactions are exactly taken into account during the collisions on a classical level [67]. Newton's classical non-relativistic equations of motions for a three-body system are solved numerically for a statistically large number of trajectories for given initial conditions. Using this method one can calculate the time evolution of a classical distribution $f(\mathbf{x}, \mathbf{p}, t)$ in phase space. In case of multi-electronic target system, the independent electron approximation is employed which considers only the active electron whereas the passive electrons along with the target nucleus formed the target ion.

Considering a collision system consisting of the projectile of mass $M_P$, target core of mass $M_T$ and one active electron initially bound to the target. The Hamiltonian of the system is written as :

$$H = \frac{p^2}{2\mu_T} + V_T(\mathbf{x}) + V_P(\mathbf{s}) \tag{3.8}$$

where $\mu_T = M_T/(M_T + 1)$ and $V_T$ and $V_P$ are the electron-target core and electron-projectile interaction potentials respectively. $\mathbf{x}$ and $\mathbf{s}$ are the position of the active electron with respect to the target and projectile respectively. Here the projectile-target core interactions are neglected assuming that the projectile and the target core move rectilinearly. Now for a given set of initial conditions in the phase space, the dynamics of the system is determined from the classical Hamilton's equations :

$$\frac{dx_j}{dt} = \frac{\partial H}{\partial p_j} \tag{3.9}$$

$$\frac{dp_j}{dt} = -\frac{\partial H}{\partial x_j} \tag{3.10}$$

where $(x_j, p_j)$ are phase space coordinates and $j = 1, 2, 3$. The equations of motion were integrated using the Runge-Kutta method. A microcanonical ensemble characterizes the initial state of the target. The CTMC method can be visualized as a computer experiment. The interaction between the active target electron and the projectile is Coulombic is nature. The interaction between the electrons and the target nucleus is described by a central model potential which is based on the Hartree-Fock calculations [68]. In the present thesis, this model has been used to compare the experimental DDCS investigations for keV energy electron impact on $N_2$

molecules. The total and double differential cross-sections for a particular process are obtained as follows :

$$\sigma = \frac{2\pi b_{max}}{T_N} \sum_j b_j^{(i)}, \tag{3.11}$$

$$\frac{d^2\sigma}{dEd\Omega} = \frac{2\pi b_{max}}{T_N \Delta E \Delta\Omega} \sum_j b_j^{(i)}. \tag{3.12}$$

In Equation 3.11 and Equation 3.12 $T_N$ is the total number of trajectories calculated for impact parameters less than $b_{max}$, $T_N^{(i)}$ is the number of trajectories that satisfy the criteria for ionization and $b_j^{(i)}$ is the actual impact parameter for the trajectory corresponding to the ionization process under consideration in the energy interval $\Delta E$ and the emission angle interval $\Delta\Omega$ of the electron.

## 3.5 CSP-ic Model

In addition to the models for DDCS, the total ionization cross section (TCS) for electron impact on $N_2$ were computed with the CSP-ic model [69]. The complex scattering potential-ionization contribution (CSP-ic) model, a semi-empirical model is used to calculate the TCS for electron impact on any target atoms/molecules. In this case the projectile electron energies can vary from threshold to few keV. Initially the total inelastic cross sections are calculated based on a spherical complex optical potential, $V_{opt}$. When the incident electron approaches the target, it experiences both short and long range potentials. On the other hand, the target electron cloud also feels an electric field due to the incoming electron. The potentials experienced by both the incident electron and the target due to the presence of each other is added up together to form the $V_{opt}$ potential. This potential comprises of the real term and an imaginary term and is defined as follows :

$$V_{opt}(E_i, r) = V_R + iV_{Im} \tag{3.13}$$

$$V_{opt}(E_i, r) = V_{st}(r) + V_{ex}(E_i, r) + V_{pol}(E_i, r) + iV_{abs}(E_i, r) \tag{3.14}$$

The real part ($V_R$) of the interaction potential takes into account the static ($V_{st}$), exchange ($V_{ex}$) and polarization ($V_{pol}$) potentials whereas the imaginary part ($V_{Im}$) comprises of the absorption potential ($V_{abs}$). The interaction between the projectile electron and the target is determined by these potentials. These potentials are constructed using the target molecular charge density ($\rho(r)$) which is formulated by a linear combination of atomic charge densities and $E_i$ is the incident electron energy.

### 3.5.1 Static Potential

The static potential ($V_{st}$) represents the Coulomb potential that is experienced by the incoming projectile electron while approaching the field of an undisturbed target charge cloud. The static potential at a distance $r$ is given by

$$V_{st}(r) = -\frac{Z}{r} + 4\pi\Big[\frac{1}{r}\int_0^r \rho(r')r'^2dr' + \int_r^\infty \rho(r')r'dr'\Big]. \tag{3.15}$$

Here $Z$ is the atomic number and $\rho(r')$ is the charge density of the target atom. For a multielectronic target atom/molecule, it is difficult to obtain an exact expression of the static potential and target charge density. Following the prescription of Cox and Bonham [70], the static potential of target can be represented by an analytical expression comprising of a sum of the Yukawa terms starting with Hartree-Fock and the relativistic wave functions for all the neutral atoms. The analytic expression of the static potential is given by :

$$V_{st}(r) = -\frac{Z}{4\pi r}\sum_{i=1}^{n}\gamma_i exp(-\lambda_i r). \tag{3.16}$$

where $\lambda_i$ and $\gamma_i$ are the potential field parameters.

The Dirac-Hartree-Fock - Slater (DHFS) method is an improved version of the Roothan-Hartree-Fock (RHF) method which takes into account the relativistic effects [71]. This approximation depends on the parameters for the atomic screening function, which are determined by DHFS self-consistent data. The analytical expression for the static potential is,

$$V_{st}(r) = -\frac{Z}{r}\sum_{i=1}^{n}A_i exp(-\alpha_i r). \tag{3.17}$$

Here $A_i$ and $\alpha_i$ are the atomic screening parameters. This potential is real and acts only at short ranges.

### 3.5.2 Exchange Potential

This potential takes care of the exchange of the incident electron with one of the target electrons. According to the free electron gas exchange model by Hara [72], the electron gas is considered as a Fermi gas of non-interacting electrons when the total wave function is antisymmetrized in accordance with Pauli's exclusion principle. The exchange energy is calculated by summing all momentum states up to Fermi level $E_f$. The Hartree exchange potential energy is given by,

$$V_{ex}(E_i, r) = -\frac{2}{\pi}k_F\Big[\frac{1}{2} + \frac{1+\eta^2}{4\eta}ln\Big|\frac{1+\eta}{1-\eta}\Big|\Big]. \tag{3.18}$$

Here $k_F$ is the Fermi wave vector given by

$$k_F = \sqrt[3]{3\pi^2\rho(r)}. \tag{3.19}$$

and

$$\eta = \frac{\sqrt{k^2 + k_F^2 + 2I}}{k_F}. \tag{3.20}$$

This approximation is referred as the 'Hara Free Electron Gas Exchange'(HFEGE) model. The target electron being bound has a negative energy and hence the minimum energy required to make it zero is the ionization energy, which is denoted as $I$ (in Hartree). Here the approximation of the numerator in Equation 3.20 implies that the electron kinetic energy is given by $E + I$ in the asymptotic region. However, for large $r$ this is corrected by removing the ionization energy which further gives rise to the 'Asymptotically Adjusted' approximation [73, 74, 75] where $\eta$ is given as

$$\eta = \frac{\sqrt{k^2 + k_F^2}}{k_F}. \tag{3.21}$$

### 3.5.3 Polarization Potential

This potential takes care of the distortion of the target charge density cloud due to the incoming projectile. This potential is of particular importance while treating the elastic scattering of electrons by atoms/molecules. The transient distortion of the target by the approaching electron is due to the induced multipole moments and is attractive in nature, giving rise to the polarization potential. The adiabatic expression for asymptotic polarization potential is given by

$$V_{pol}(E_i, r) = -\frac{\alpha_d}{2r^4} - \frac{\alpha_q}{2r^6}. \tag{3.22}$$

Here $\alpha_d$ and $\alpha_q$ are the dipole and quadrupole static polarizabilities of the target atom where the higher order multipolar terms have been neglected. The potential is attractive and long range in nature and varies asymptotically as $r^{-4}$ at $r \to \infty$. At $r = 0$, there is a singularity and this is avoided by introducing a cut off parameter ($r_c$) in Equation 3.22 as follows :

$$V_{pol}(E_i, r) = -\frac{\alpha_d}{2(r^2 + r_c^2)^2}. \tag{3.23}$$

This is the well known Buckingham polarization potential [76]. Here the system is considered to be adiabatic, however at high incident energies the response of the target charge cloud should also depend on the speed of electrons. So for high projectile energies, an energy dependent form of the polarization potential is required which was proposed by Khare et. al. [77] as

$$V_{pol}(E_i, r) = -\frac{1}{2}\left[\frac{\alpha_d r^2}{(r^2 + r_c^2)^3} + \frac{\alpha_q r^4}{(r^2 + r_c^2)^5}\right]. \tag{3.24}$$

$r_c$ being the energy dependent cut-off parameter. Using the Born approximation [78, 79], it is found

$$r_c = \frac{3k}{8\Gamma}. \tag{3.25}$$

Here $\Gamma$ is the average excitation energy of the atom. This potential is long range in nature and so the simple $r^{-4}$ behaviour does not hold for short distances. Therefore one has to account for the electron correlation effects at short distances [79].

An approximated local density functional form of the correlation for short range (SR) and the long range polarization potential is given by

$$V_{pol}(r) = \begin{cases} V_{SR}^{corr}, & \text{at } r \leq r_0 \\ -\frac{\alpha_d}{2r^4}, & \text{at } r > r_0 \end{cases} \tag{3.26}$$

where $r_0$ is the point of intersection of the short range correlation potential $V_{SR}^{corr}$ and the long range potential $\frac{-\alpha_d}{2r^4}$ and $r_0$ is roughly taken as the radius of the atomic short range potentials. The short range part of the potential in Equation 3.26 is known as Perdew-Zunger (PZ) form of the potential, named after the authors [80]. The PZ form is given by :

$$V_{SR}^{corr}(r) = \begin{cases} 0.0311 ln r_s - 0.058 + 0.00133 r_s ln r_s - 0.0084 r_s, & \text{at } r_s \leq 1 \\ \frac{\gamma(1+\frac{7}{6}\beta_1\sqrt{r_s}+\frac{4}{3}\beta_2 r_s}{(1+\beta_1\sqrt{r_s}-\beta_2 r_s)^{-2}}, & \text{at } r_s \geq 1 \end{cases} \tag{3.27}$$

The constants in Equation 3.27 are as follows : $\gamma$=-0.1423, $\beta_1$=1.0529, $\beta_2$=0.3334 in a.u. and $r_s = \sqrt[3]{\frac{3}{4\pi\rho(r)}}$ is related to the electronic charge density of the target. Thus for high incident energies (above 100 eV) the polarization potential defined in Equation 3.24 is used whereas at intermediate electron energies (typically below 100 eV) the correlation potential given in Equation 3.26 for $r \leq r_0$ is considered in the calculations.

### 3.5.4 Absorption Potential

The imaginary part of the optical potential ($V_{opt}$) in Equation 3.14 consists of the absorption potential ($V_{abs}$) which corresponds to the absorption or loss of the scattered flux into the inelastic channels of electronic excitation and ionization. The modified absorption potential [81, 82, 83] which has been used in the present calculations is given by :

$$V_{abs} = -\frac{1}{2}\rho(r) v_{loc} \sigma_{ee}. \tag{3.28}$$

where $v_{loc}$ is the velocity of the projectile electrons and $\sigma_{ee}$ is the average total cross section of the binary impact collision of the incident electron with a target electron.

The partial wave approach under the spherical approximation is used leading to complex phase shifts $\delta_l(k)$ which carry the signature of the interaction between the incident electrons and target molecule.

### 3.5.5 Deriving total ionization cross section

Using the above mentioned $V_{opt}$ potential and then by using the partial wave approach one can get information about the total elastic and inelastic cross sections for electron impact on any target atom or molecule. Now to extract the contribution of ionization cross section ($Q_{ion}$) from the inelastic cross section, the complex scattering potential- ionization contribution (CSP-ic) method is employed which is a semi-empirical model. This method uses the fact that the total inelastic cross section contains the total cross sections for all allowed ionization processes and all the excitation cross sections for all accessible electronic transitions summed together which is given as follows :

$$Q_{inel}(E_i) = \sum Q_{exc}(E_i) + Q_{ion}(E_i). \tag{3.29}$$

The sum total of electronic excitation cross section is contributed mostly from the low lying dipole allowed transitions for which the cross section decreases rapidly at higher energies [84].

The CSP-ic approximation originates from the inequality

$$Q_{inel}(E_i) \geq Q_{ion}(E_i). \tag{3.30}$$

Now to extract the total ionization contribution from the total inelastic cross section, we define a dynamic ratio given by :

$$R(E_i) = \frac{Q_{ion}(E_i)}{Q_{inel}(E_i)}. \tag{3.31}$$

such that $0 \leq R \leq 1$. When $E_i \leq I$, then $R = 0$, i.e., when ionization has not begun. Experimentally it is observed that the ratio *R* rises steadily as the incident projectile energy increases above the threshold, such that

$$R(E_i) \begin{cases} = 0, & \text{for } E_i \leq I \\ = R_P, & \text{at } E_i = E_P \\ \cong 1, & \text{for } E_i \gg E_P \end{cases} \tag{3.32}$$

Here $E_P$ stands for the incident projectile energy at which the calculated $Q_{inel}$ attains its maximum value or peak value. The peak of $Q_{inel}$ occurs at an energy where the electronic excitation cross sections have started receding and $Q_{ion}$ is rising. $R_P$ stands for the value of $R$ at $E_i = E_P$ (see Equation 3.32). The value of $R_P$ is chosen to be ≈ 0.7 to 0.8. Such a choice is made based on the general observation that at energies close to the peak of the ionization cross section the contribution of the target $Q_{ion}$ is about 70 - 80% of the total inelastic cross sections ($Q_{inel}$). The present value of $R_p$ stems from the fact that as the incident energy increases gradually above threshold, the transition to the continuum starts dominating giving rise to an infinite number of open scattering channels. An iterative method is followed for calculating the value of $R$. For calculating $Q_{ion}$ from $Q_{inel}$, $R$ should be a continuous function of energy (for $E_i \geq I$) and hence we represent the ratio $R$ in the following manner :

$$R(E_i) = 1 - C_1\Big[\frac{C_2}{U + a} + \frac{lnU}{U}\Big]. \tag{3.33}$$

where $U = \frac{E_i}{I}$, $E_i$ is the impact energy and $I$ is the ionization potential of the target. The three constants $C_1, C_2$ and $a$ in Equation 3.33 are evaluated by applying the conditions in Equation 3.32 and finally $R(E_i)$ is obtained which finally provides information about the total ionization cross section for the collision system under investigation.