A Brief Study on Dissociative Ionization Cross Section of Atom and Molecule

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Abstract:

Investigations, both theoretical and experimental, into the microscopic structure of matter rely heavily on studies of the collision phenomena. As a result, accurate estimates of atomic and molecular collisional cross sections are increasingly important for the advancement of many scientific and technological disciplines, including astrophysics, astronomy, gas lasers, plasma physics, controlled thermonuclear fusion, transport phenomena, chemical reactions, biophysics, gaseous electronics, auroral airglow, etc.

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Introduction

High in the atmosphere, energetic particles and electromagnetic radiations are continually pounding the area. Extremely high levels of X-rays, ultraviolet light, cosmic rays, ions, and electrons are emitted from the sun during solar flares. Additional photoelectrons and secondary electrons are created by these radiations, cosmic rays, ions, and electrons. These electrons eventually get thermalized after losing energy through elastic and inelastic processes. This means that the electron energy spectrum is a crucial factor in determining the state of the atmosphere. The chemical composition, density, and temperature of the atmosphere's component elements may be inferred from the energy spectrum caused by collision events [1–5]. Solar radiations ionise the neutral component of the atmosphere, creating energetic free electrons and ions, which in turn create the ionic layers in the ionosphere of breath. Due to the particle's subsequent excitation by these high-energy electrons, fluorescence is produced when its excited states decay back to less-excited ones. That's a crucial part of what makes day glow possible. Auroras are atmospheric emissions caused by these ionised and excited species. Therefore, a thorough familiarity with atomic and molecular collisional processes is required for an appropriate comprehension of the many phenomena taking place in the upper atmosphere[6].

There is significant theoretical and practical interest in electron transport in gases. It reveals the fundamentals of scattering potential and molecular structure. Studies of electron transport, especially in the low energy region involving sub-ionized and sub-excited electrons, are of particular interest in a variety of fields, including radiation dosimetry, stopping power calculations, plasma and upper atmospheric physics, and the broad field of gaseous electronics[7-8]. These electrons' energy is less than the initial electronic excitation potential of the material they're passing through. These electrons dissipate energy via elastic collisions and inelastic collisions through vibrational and rotational excitations. An important topic in radiation physics is the determination of the cross sections for the aforementioned processes for different molecules as a function of electron energy. Electron-molecule collisional cross sections are useful in molecular chemistry for assessing a wide range of factors relevant to the study of molecular structure. These cross sections find use in high-energy molecular gas lasers[9-12].

Overexposure to powerful radiation is a common complication of radiation treatment. When radiations strike damaged cells, they release secondary charged particles that ionise nearby atoms.

Additionally, harm is done to living tissues as a result of this prolonged exposure. The dosage and duration of radiation exposure may be managed to reduce the resulting harm to live tissues. Knowing the ionisation cross sections is necessary for calculating the different parameters needed for this, such as stopping power and energy expanded per ion pair[13-15].

Fusion is one of the most promising processes for producing energy in the present period of energy challenges. However, the fusion plasma is cooled by a variety of collosional mechanisms. Accordingly, familiarity with collosional cross sections for the many processes occuring in the fusion process is essential.

Literature Review

In principle, ionization cross section may be calculated quantum mechanically but because of the complicated nature of the process , the quantum mechanical calculation are quite involved. Most of the theoretical calculations are limited to the first born approximation and in almost all the cases the agreement between the theory and the experiment is not encouraging. Since 1920's scientists have recognized the similarity between high energy photo produced. Much of this understanding was formulated by bethe (1930)[20]. Even today bethe's work remains the basis of all the energy deposition studies.Fano (1953)[21] and platzman (1955)[22]set down to the basic relation upon which great part of the work carried out today is based.

In the first Born approximation the differential cross section for the inelastic scattering of an electron , of intial energy E,in which the atom makes a transition from the intial ground state | 0 > to the excited state | n > is given by

$$dQ_n(E,K^2a_0^2) = \frac{4\pi a_0^2 R^2}{E} \frac{f_n(Ka_0)}{W_n} d[\ln(K^2a_0^2)] \tag{1}$$

Where W_n ,a_0 and R are excitation energy , first Bohr radius and Rydberg constant , respectively ħK is the change in momentum vector of the incident electron due to scattering. $f_n(K a_0)$ is the generalized oscillator strength defined by

$$f_n(K a_0) = \frac{W_n}{R} \frac{1}{K^2a^2} |< n | \sum_{i=1}^{Z} e^{ik.ri} | 0 >|^2 \tag{2}$$

wherer_i represents the position of the i^{th} atomic electron and |< n| A | 0 > is matrix element for the operator A taken between the states | n > and | 0 >. Integrationof (2) over ka_0 yields total excitation cross section $Q_n(E)$.

$$Q_n(E) = \int_{(K^2a_0^2)\min}^{(K^2a_0^2)\max} dQ_n(E,K^2a_0^2) \tag{3}$$

For ionization the excitation energy W_n is replaced by the variable W which changes in continuous manner and the generalized oscillator strength reduces generalized oscillator strength per unit energy range.Thus the cross section per unit energy range for the production of a secondary electron of energy *E* due to electron impact ionization of a target is given by

$$Q(E\ ,\mathcal{E}) = \frac{4\pi a_0^2 R^2}{E} \int_{(K^2a_0^2)\min}^{(K^2a_0^2)\max} \frac{1}{W} \frac{df(W,\mathrm{K}^2a_0^2)}{dW}\, d[\ln(\mathrm{K}^2 a_0^2)\,] \tag{4}$$

On the assumption that the producing ion is in its ground state.W is equal to (*E+)*I where I is the ionization potential of the target.The generalized oscillator strength is represented comprehensively by a three dimensional plot of

$$\frac{df(W,\mathrm{K}^2a_0^2)}{dW}$$

As a function of $\ln(\mathrm{K}^2\ a_0^2)$ and W/R. Such a plot gives Bethe surface which is marked by two distinct domains. The first domain, where the energy loss W/R and $(\mathrm{K}^2\ a_0^2)$ are both small, represents soft collision domain and (4) at large value of E reduced to

$$Q_B(E,\mathcal{E}) = \frac{4\pi a_\circ^2 R^2}{E}\frac{1}{W}\frac{df(W,O)}{dw}\ln[C(W)E] \tag{5}$$

Where df(W,O)/dW is the optical oscillator strength per unit energy range for the ionization of the target by a photon of energy W is proportional to the photo ionization cross section $Q_P(W)$.

The relationship is given by

$$\frac{df(W,O)}{dW} = \frac{mc}{2\pi e^2 h} Q_{p(W)} \tag{6}$$

The collosional parameter C(W) is given by

$$\ln\frac{C(W)W^2}{4R} = \int_0^{\infty}\frac{\partial f(W,K^2a_\circ^2)}{\partial W}\{\frac{\partial f(W,O)}{\partial W}\}^{-1} d(\ln(K^2a_\circ^2) - \int_{-\infty}^{0}\left[1-\frac{\partial f(W,K^2a_\circ^2)}{\partial W}\left\{\frac{\partial f(W,O)}{\partial W}\right\}.^{-1}\right] d\left[\ln(K^2a_\circ^2)\right] \tag{7}$$

Eq.(5) shows that the factorization of Q(E,*E*) and one factor is the photoionization cross section ,$Q_p(w)$. This clearly demonstrates a connection between high energy photoionization and electron impact ionization in which slow secondaries are produced.

The second domain where W/R and $\mathrm{K}^2 a_0^2$ are large is characterized by the Bethe ridge. Since in the collisions a large amount of energy is transferred from the incident electron to the target electron, such collisions may be regarded as the collision between two free electrons. Such collisions are said to be hard collisions and this problem was investigated quantum mechanically by Moller [23]. According to him for hard collision the ionization cross sections per unit energy range for a one electron atom is given by

$$Q_M(E,\mathcal{E}) = \frac{4\pi a_\circ^2 R^2}{E}\left[\frac{1}{\varepsilon} - \frac{1}{(E-\varepsilon)\varepsilon} + \frac{1}{(E-\epsilon)^2}\right] \tag{8}$$

Where ε is the energy of the secondary electron. It may be noted that $Q_B(E, \varepsilon)$ and $Q_M(E, \varepsilon)$ is given by (5) and (8) are valid for their large value of E and are to be suitably extra ploated to extend their validity for small value of (E> 1).Khare (1969)[17] multiplied (5) and (8) by arbitrary factors $f_1(E, \varepsilon)$ and $f_2(E, \varepsilon)$, respectively, so as to extrapolate them to the low values of E and employed them successfully to investigate ionization of atoms and molecules . It may be noted that factors $f_1(E, \varepsilon)$ was so chosen that it goes to one at large values of E, gives reasonable values of the cross section at smaller values of E and reduces the cross section to zero at the ionization threshold potential. Later Jain Khare(1976)[9&10] formula which may be used successfully throughout the whole energy range ,

$$Q_1((E, \varepsilon) = f_1(E, \varepsilon)\ Q_B(E, \varepsilon) + f_2(E, \varepsilon)\ Q_M(E, \varepsilon) \qquad (9)$$

Khare andMeath (1987) [24]integrate this equation and get

$$Q_M(E, E) = \frac{4\pi a_\circ^2 R^2}{E}\left[\frac{1}{\varepsilon} - \frac{1}{(E-\varepsilon)\varepsilon} + \frac{1}{(E-\epsilon)^2}\right] \qquad (10)$$

And took best available values of $df_1(W,O)/dW$ for the production of different ions as the inputs but assumed C_1 and ε_{01} to be independent of ions and took their values as given by Reike and Prepejchal (1972)[18]and Jain and Khare (1976)[8-9], respectively to obtain dissociative ionization of NH_3,H_2O and H_2S molecules

Gaseous Electron:

Gaseous electron transport is of theoretical and practical importance. A molecule's or an atom's scattering potential and structure may be gleaned from this data. There is a lot of interest in studying electron transport, especially in the low energy region involving sub-ionized and sub-excited electrons, because it has applications in a wide variety of fields, including radiation dosimetry, stopping power calculations, plasma and upper atmospheric physics, and the vast field of gaseous electronics[7-8]. The energy of these electrons is less than the medium's initial electronic excitation potential. These electrons dissipate energy via both elastic and inelastic collisions, with the latter occurring due to vibrational and rotational excitations. It is of main importance in radiation physics to understand the cross sections for the aforementioned processes for different molecules as a function of electron energy. Collision cross sections between electrons and molecules are a useful tool in the investigation of molecular structure in molecular chemistry. It has been shown that these cross sections are also helpful in high-energy molecular gas lasers[9-12].

People are often overexposed to high-energy radiations during radiation treatment. Radiation's impact on damaged cells releases secondary charged particles that ionise the tissue's other atoms.

Additionally, harm is done to living tissues as a result of this prolonged exposure. By limiting both the dosage and duration of exposure to radiation, harm to live tissues may be kept to a minimum. Knowing the ionisation cross sections is necessary for calculating the different parameters needed for this, such as stopping power and energy expanded per ion pair[13-15]. For the creation of energy in today's times of energy problems, fusion is one of the most promising processes. A variety of collosional processes, however, tend to cool the plasma in fusion reactors. That's why it's important to understand the collisional cross sections involved in the different fusion processes.

Conclusion:

There is significant theoretical and practical interest in electron transport in gases. It reveals the fundamentals of scattering potential and molecular structure. In molecular chemistry, electron-molecule collisional cross sections are used to assess a wide range of properties relevant to the study of molecular structure. Fusion is one of the promising process for the generation of energy. However, a number of processes occurring in fusion plasma tend to cool the plasma.

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