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THE ELECTRON-IMPACT IONIZATION CROSS SECTIONS OF H_2O

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Abstract: In present article, the electron-impact ionization cross sections have been calculated by using the modified Khare model and Kim BEB model for water molecule (H_2O) from ionization threshold to 10 MeV. The collision parameters C_{RP} and M^2 also has been calculated. The calculations are compared with available previous experimental data as well as theoretical results. A remarkable agreement is found among the present results, other previous calculations and experimental data.

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Keywords- Water molecule, Collision, Cross section, Electron-impact ionization.

Introduction:

The electron impact ionization cross sections of atoms and molecules are not only important to understand the basic collision mechanism but also in wide range of experimental applications, for example the modelling of semi-conduction manufacturing by plasma processing needs ionization cross sections of molecules used as the ideal gas. The ionization cross sections are also needed in various research areas such as atmospheric physics, astrophysics, radiation physics etc. Water molecule are detected in the atmosphere of planets such as Venus, Uranus, mars, Jupiter, Saturn, Earth and satellites of Jovian planets. Total ionization cross sections are important for modelling of their atmosphere [1-3].

Straub et-al. [4] measured the electron-impact ionization cross sections of water molecule with experimental error 4.5 % from threshold to 1 keV. They have used time of flight mass spectrometer with position sensitive detector. Djuric et-al. [5] have measured ionization cross sections for water molecule with experimental error 7% by using parallel plate ionization chamber from threshold to 80 eV. Rao et-al. [6] have carried out cross sections experimentally from thresholds to 1 keV by utilizing a crossed electron beam and molecular beam collision geometry. Bolorizadeh and Rudd [7] have also reported the total ionization cross sections of water molecule from 20 eV to 2 keV. We have only one experimental data at relativistic energies (0.1-2.7 MeV) those measured by Reike and Prepejchal [8]. They measured the cross sections in term of two collision parameters C_{RP} and M_i^2.

Theory

In 2019, Kumar et-al. [9], have modified Khare-BEB model [10]. They simplified the Bethe cross section of Khare-BEB model. In this modified model, the ionization cross section due to electron impact for j^{th} molecular orbital is given by

$$\sigma_{jT} = \sigma_{jM} + \sigma_{jB} + \sigma_{tj} \qquad (1)$$

Where Mott cross section σ_{jM} is

$$\sigma_{jM} = \frac{AN}{[E+I+U]I} \times \left[1 - \frac{2}{t+1} + \frac{t-1}{2t^2} + \frac{5-t^2}{2(t+1)^2} - \frac{1}{t(t+1)} - \frac{t+1}{t^2}\ln\left(\frac{t+1}{2}\right)\right] \quad (2)$$

where $t = E/I$, $E = \frac{1}{2}mc^2\left[1 - \frac{1}{1+\frac{T}{mc^2}}\right]$ and $A = 4\pi a_0^2 R^2$. The notations U, a_0, I, N, T, m, c and R stand for the average kinetic energy of bound electron, the first Bohr radius, the ionization energy, the occupation number of molecular orbital, the kinetic energy of the incident electron, rest mass of electron, velocity of light and Rydberg energy respectively. The Bethe cross section σ_{jB} is given by

$$\sigma_{jB} = \frac{AN}{2[E+I+U]I}\left[\frac{1}{2}\left(1 - \frac{1}{t^2}\right) - X\right] \quad (3)$$

Where, the term X is given by

$$X = 2ln\left(\sqrt{t} - \sqrt{(t-1)}\right) + \frac{1}{2t^2}\left\{\begin{array}{c} 1 - \frac{1}{2}\left(\frac{t}{t-\sqrt{t(t-1)}}\right)^2 \\ +\frac{1}{2}\left(\frac{t}{t+\sqrt{t(t-1)}}\right) - \left(\frac{t}{t-\sqrt{t(t-1)}}\right) \\ -\frac{3}{4}ln\left(\frac{t+\sqrt{t(t-1)}}{t-\sqrt{t(t-1)}}\right) \end{array}\right\}$$

And cross section due to the transverse interaction is

$$\sigma_{tj} = -\frac{4\pi a_0^2 R}{E} M_j^2[\ln(1-\beta^2) + \beta^2] \quad (4)$$

where β is the ratio of the incident velocity v and the velocity of light c, M_j^2 represents the total dipole matrix squared measured in units of a_0^2 and given by

$$M_j^2 = \int_{I_j}^{E} \frac{R}{w}\frac{df_j(w,0)}{dw}dw \quad (5)$$

Where, $\frac{df_j(w,0)}{dw}$ is the continuum optical oscillator strength (COOS) per unit energy range and given by

$$\frac{df_j(w,0)}{dw} = \frac{NI_j}{w^2} \quad (6)$$

The expression of collision parameter for j[th] molecular orbit C_{jRP} is given by

$$C_{jRP} = \frac{RE}{A}\sum_{j}(\sigma_{jB} + \sigma_{jM}) - {M_j}^2 ln\beta^2 \quad (7)$$

In Kim BEB model [11], the total ionization cross section due to electron impact for j[th] molecular orbital is given by

$$\sigma_T = \frac{AN}{[E+I+U]I}\left[\frac{ln(t)}{2}\left(1 - \frac{1}{t^2}\right) + 1 - \frac{1}{t} - \frac{ln(t)}{t+1}\right] \quad (8)$$

Results and discussion

Equation (1) along with equations (2-4) has been used to evaluate total ionization cross section due to electron impact of molecule. We have calculated the cross sections by using Kim BEB method [11] with adding an extra term, cross section due to the transverse interaction given by equation (4) from threshold to 10MeV to compare our calculations. The collision parameters of molecule are calculated by using equations (5) and (7). The required molecular parameters binding energies I, kinetic energies of bound electrons U and occupation numbers N are taken from reference [12]. In figure (1), the present ionization cross sections along with available previous theoretical as well as experimental results for water molecule are depicted from threshold to 10 keV. Our calculation are in good agreement with the experimental data those measured by Straub et al. [4]. Present cross sections are lower than the experimental results of Rao et-al. [6] by 25% and do not agree. Figure shows a fair agreement between present calculations and experimental results of Bolorizadeh & Rudd [7] and Djuric et al. [5]. Our results and Kim BEB calculation are very close to each other.

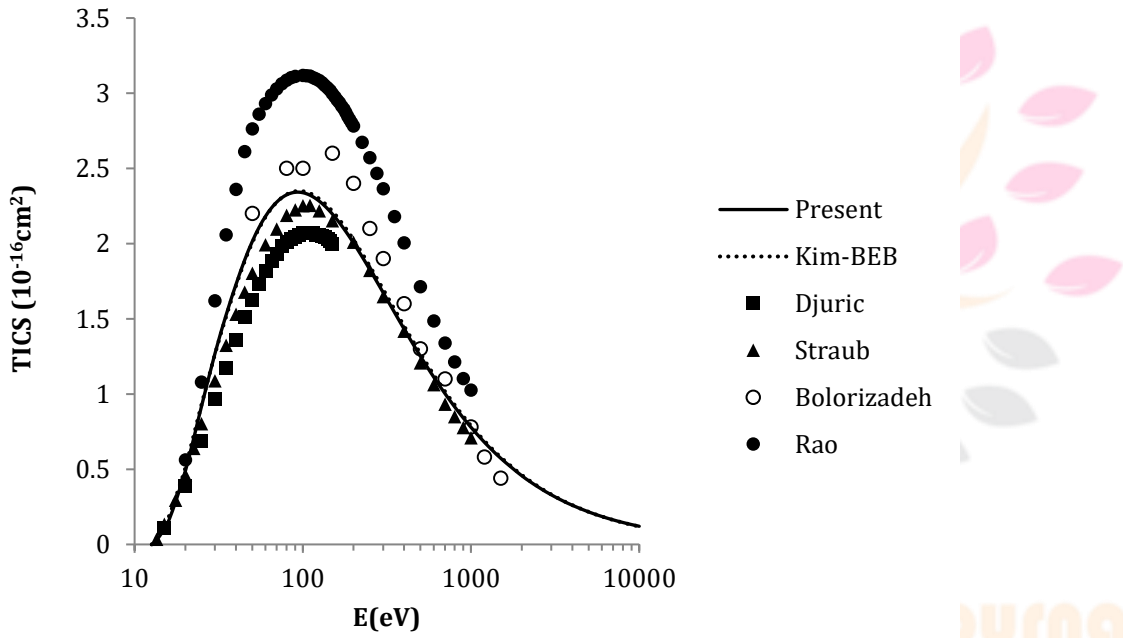

Fig.1 Total ionization cross sections for water molecule in 10^{-16} cm^2. Solid line and dotted line represent present results, and Kim-BEB calculation respectively. Filled rectangles, filled triangles, Open circles and filled circles represent the experimental results of Djuric et al., Straub et al., Bolorizadeh and Rudd and Rao et al. respectively.

The figures (2) show the total ionization cross sections due to electron impact for water molecules respectively. In this figure we have compared the present calculation with the experimental results those measured by Reike and Prepejchal [8].

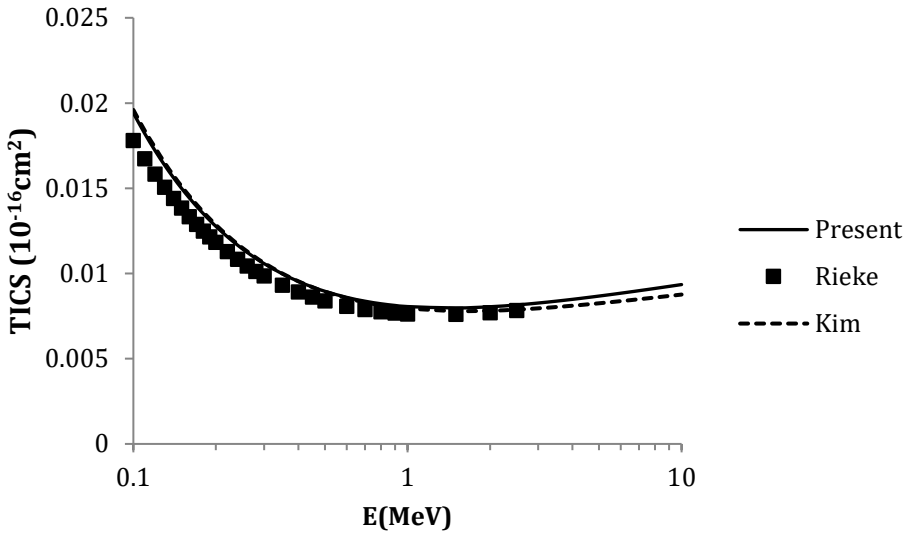

Fig. 2 This figure shows the present total ionization cross sections along with experimental data of Reike and Prepejchal for water molecule in energy range (0.1-10MeV) in 10^{-16} cm^2. Solid line and dotted line represent present results and Kim-BEB calculations respectively.

A good agreement is found between our theoretical results and experimental data. At relativistic impact energies, the ratio of our cross sections and Kim BEB calculations are very close to one.

In table (1), the present theoretical collision parameters along with experimental data are represented.

Molecules	C_{RP}(at 1MeV)	C_{RP}(at 10MeV)	C_{RP}(at 100MeV)	C_{RP}(Exp. Rieke [8])	Present M_j^2	M_j^2 (Exp. Rieke [8])
Water	34.5	34.27	34.27	32.26	3.00	3.24

Table-1 The present calculated values of collision parameter C_{RP} and M_j^2 (in unit of a_0^2) are shown along with the experimental values given by Rieke and Prepejchal. The values of C_{RP} are calculated at incident energies 1, 10 and 100 MeV using equation (7).

On increasing the kinetic energy of incident electron calculated value remains nearly constant, which is according to expectation? The calculated value of C_{RP} is greater that the experimental value by 7.4 %, however present value of dipole matrix squared M_j^2 is lower than the experimental value of Rieke and Prepejchal by 6.2%.

Conclusion:

Khare BEB model is used to calculate the ionization cross sections of water from ionization threshold to 10 MeV. The present cross sections are found in the good agreement with available experimental data over most of incident energy range. The calculated values of parameters are also found in good agreement with the experimental values.

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