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Bethe collisional parameters for the ionizing collisions of molecules by relativistic electrons

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Abstract : A method based on the first Born approximation which includes relativistic effects, longitudinal as well as transverse interactions of the virtual photons with the molecules but uses only the optical oscillator strengths as its input, has been employed to obtain the Bethe collisional parameters for H_2, N_2, O_2, CO, H_2S, CO_2, NH_3, CS_2 and SF_6 molecules ionized by relativistic electrons. For most of the molecules, our values of the parameters are in good agreement with the experimental data.

Keywords : Ionization, molecules

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Ionization cross sections of atoms and molecules find applications in a number of fields such as upper atmospheric physics, space physics, plasma physics, fusion, laser, radiation physics, mass spectrometry, chemical reactions and even in biological sciences [1]. Hence a large number of investigations for the experimental determination and theoretical evaluation of the ionization cross sections have been carried out. More than twenty years ago Rieke and Prepejchal [2] measured the total ionization cross sections of a number of molecules by electron impact in the energy range 0.1 to 2.7 MeV. They fitted their measured cross sections σ_T to the following relation, extracted from the Bethe theory,

$$\sigma_T = 4\pi\left(\frac{\hbar}{mc}\right)^2\left[M^2\left\{\frac{1}{\beta^2}\ln\left(\frac{\beta^2}{1-\beta^2}\right)-1\right\}+c_{RP}\frac{1}{\beta^2}\right], \qquad (1)$$

where m, $\hbar$ and c are the rest mass of the electron, the Planck's constant divided by 2π and the velocity of light, respectively and $\beta = v/c$, v being the velocity of the projectile,

M^2 and c_{RP} are two Bethe parameters. M^2 can be evaluated with the help of the optical oscillator strength $\frac{df(W, 0)}{dW}$ but the parameter c_{RP} depends on the distribution of the generalized oscillator strengths of the involved transition. Due to non-availability of the generalized oscillator strengths for the ionizing collisions of the molecules, there seems to be no calculation for c_{RP}. In this paper, we propose a new method to calculate the above parameter which uses only optical oscillator strengths as input. We report our calculated values of c_{RP} for a number of molecules namely H_2, N_2, O_2, CO, H_2O, H_2S, CO_2, NH_3, CS_2 and SF_6 ionized by relativistic electrons in the energy range 0.1 to 10^2 MeV.

In the first Born approximation, we have [3]

$$\sigma_T = \sigma_1 + \sigma_t, \tag{2}$$

where σ_1 is the ionization cross section of the molecule due to those virtual photons which have their polarization vectors parallel to $\underline{K}$ (longitudinal interaction) and is given by [3]

$$\sigma_1 = \frac{8\pi a_0^2 R}{mv^2} \int_I^{E_{max}} \int_{\ln (K^2a_0^2)_{min}}^{\ln (K^2a_0^2)_{max}} \frac{R}{W} \frac{df(W, K^2a_0^2)}{dW}$$

$$\times F_{ex}\left(E', K^2a_0^2\right) d\left(\ln K^2a_0^2\right) dW, \tag{3}$$

where a_0 is the first Bohr radius, E' is equal to $\frac{1}{2} mv^2$ and I is the ionization potential. $\frac{df(W, K^2a_0^2)}{dW}$ is the generalized oscillator strength for the energy loss W and momentum transfer $h\underline{K}$. The exchange factor $F_{ex}\left(E', K^2a_0^2\right)$ has been evaluated in the Ochkur approximation. Indistinguishability of the electrons leads to $E_{max} = (E + I) / 2$, E being incident energy. Relativistic expressions for v and $(Ka_0)^2_{max,min}$ are utilised [3].

The cross section σ_t due to those virtual photons which have their polarization vectors perpendicular to $\underline{K}$ (transverse interaction) is significant only at relativistic velocities and in this region, it is given by [3]

$$\sigma_t = \frac{8\pi a_0^2 R}{mv^2} M^2 \left[\ln (1 - \beta^2) + \beta^2\right]. \tag{4}$$

Now we put eq. (4) in eq. (2) and equate the result to eq. (1) to obtain

$$c_{RP} = \frac{E'\sigma_1}{4\pi a_0^2 R} - M^2 \ln \beta^2. \tag{5}$$

It is evident from eq. (5) that to calculate c_{RP}, we require the values of σ_1 which in-turn, requires the distribution of the generalized oscillator strength for its evaluation. In general, the values of the generalized oscillator strengths are not available for molecules. Only for the H_2 molecule, Liu [4] has calculated inelastic scattering factors by using CI wave

functions. Hence, we have adopted an alternative approach. We express the generalized oscillator strengths as a sum of two terms (Mayol and Salvat [5])

$$\frac{df(W,Q)}{dW} = \frac{df(W,0)}{dW}\,\theta(W-Q) + h(Q)\delta(W-Q), \tag{6}$$

where $\theta(W-Q)$ is a step function and $\delta(W-Q)$ is the Dirac delta function, $h(Q)$ is given by

$$h(Q) = \int_I^Q \frac{df(W,0)}{dW}\,dW \tag{7}$$

and $Q = (Ka_0)^2 R$ is the recoil energy.

The above equations show that in the present approach, the soft collisions (Born-Bethe term) contribute to the ionization only for the recoil energy Q varying from I to W and the contribution of the hard collisions (Mott-Moller term) is only at Bethe ridge *i.e.* $Q = W$. Using Ochkur exchange approximation, putting eqs. (6) and (7) in eq. (3) and integrating over Q we get

$$\sigma_I = \sigma_B + \sigma_M. \tag{8}$$

where σ_B, the Born-Bethe cross section is given by

$$\sigma_B = \frac{4\pi a_0^2 R}{E'}\int_I^{(E+I)/2} \frac{R}{W}\frac{df(W,0)}{dW} \times\left[\ln\left(\frac{W}{Q_{\min}}\right) - \left(\frac{W-Q_{\min}}{E'}\right) + \frac{1}{2E'^2}\left(W^2 - Q_{\min}^2\right)\right]dW \tag{9}$$

with
$$Q_{\min} = \frac{1}{2mc^2}\left\{\sqrt{E(E+2mc^2)} - \sqrt{(E-W)(E-W+2mc^2)}\right\}^2. \tag{10}$$

Similarly, the Moller cross section is given by

$$\sigma_M = \frac{4\pi a_0^2 R^2}{E'}\int_I^{(E+I)/2} h(W)\left(\frac{1}{W^2} - \frac{1}{WE'} + \frac{1}{E'^2}\right)dW, \tag{11}$$

where
$$h(W) = \int_I^W \frac{df(W',0)}{dW'}\,dW'. \tag{12}$$

We have taken the values of the optical oscillator strengths $\frac{df(W,0)}{dW}$ from Brion and Thomson [6], Backx *et al* [7] and Zeiss *et al* [8,9]. Calculations have also been done with $F_{ex}(E', K^2a_0^2) = 1$ *i.e.* neglecting the effect of exchange. In this case E_{max} is equal to E. The present values of M^2 obtained by integrating $\frac{1}{W}\frac{df(W,0)}{dW}$ over W from I to ∞, given in terms of $p = c_{RP}/M^2$ in Table 1, are found to be within 15% of the experimental values of Rieke and Prepejchal [2] for the first eight molecules. Thus, the agreement is quite satisfactory. No experimental values of M^2 for CS_2 and SF_6 molecules seem to be available.

In Table 1, we have also listed the present values of c_{RP} as obtained from eq. (5) with the help of eqs. (8) to (12) for impact energy ranging from 0.1 to 10^2 MeV. At higher impact energies, the values of c_{RP} do not change and hence are not shown. The theoretical

Table 1. Variation of the parameter c_{RP} with the incident energy E and the asymptotic values of the ratio $p = c_{RP}/M^2$ for the ionization of molecules due to electron impact.

	c_{RP}				$(c_{RP})^a_{exp}$	p
Mole/E(MeV)	10^{-1}	10^0	10^1	10^2		
H_2	7.85	7.60	7.56	7.56	8.115	11.00
N_2	35.76	34.56	34.37	34.37	34.84	10.60
O_2	42.85	41.41	41.18	41.18	38.84	10.567
CO	42.18	40.77	40.55	40.55	35.14	10.67
H_2O	30.51	29.49	29.33	29.33	32.26	10.70
H_2S	62.69	60.68	60.37	60.36	42.19	11.11
CO_2	56.00	54.11	53.82	53.81	55.92	10.57
NH_3	38.90	37.62	37.42	37.42	34.86	10.84
CS_2	85.25	82.46	82.03	82.02	-	10.91
SF_6	160.35	154.88	154.03	154.01	-	10.41

[a] shows the experimental values of Rieke and Prepejchal [2] determined from eq. (1) in the energy range 0.1 to 2.7 MeV.

values of c_{RP} at energies higher than 1 MeV are shown to indicate the convergence of the results. The table shows that the present values initially decrease with the increase of the impact energy but attain their asymptotic value at about 1 MeV. It is also noticed that in general, the values of c_{RP} increase with the number of electrons in the molecule and also with its molecular weight. However, isoelectronic molecules like H_2O and NH_3 have quite different values of c_{RP}. The same is found to be true for the isoelectronic molecule N_2 and CO.

A comparison of the present values of c_{RP} at 1 MeV with those obtained by Rieke and Prepejchal [2] shows that for H_2, N_2, O_2, CO, H_2O, CO_2 and NH_3 the two sets of values are in good agreement with each other, the difference between them being less than about 10%. However for H_2S molecule, the difference between the two values is quite large. The reason for this large difference is not understood at present. It may also be noted that σ_T of Rieke and Prepejchal [2] includes contributions of the inner shell also, but the present cross sections exclude them. However, it is expected to be small. For the remaining two molecules CS_2 and SF_6, no other values of c_{RP} seem to be available for comparison. In our energy range, the calculations with $F_{ex}\left(E', K^2a_0^2\right) = 1$ also give the same values of c_{RP}. This is according to the expectation and is in agreement with the experimental observation of Rieke and Prepejchal that the ionization cross sections due to electron and positron impacts are the same.

We conclude with the remark that the theoretical values of c_{RP} for the above molecules are evaluated for the first time. A good agreement between the present and the experimental values of c_{RP} for most of the molecules, shows that the present method which uses only optical oscillator strength as input should be useful in the evaluation of the ionization cross sections of complex target due to electron (positron) impact for incident energies greater than a few times of the ionization potential of the target.

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