

Electron impact total cross sections of CH_x , NH_x and OH radicals *vis-à-vis* their parent molecules

K N Joshipura¹, Minaxi Vinodkumar² and Umesh M Patel¹

¹ Department of Physics, Sardar Patel University, Vallabh Vidyanagar, 388120, India

² VP & RPTP Science College, Vallabh Vidyanagar, 388120, India

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Abstract

Various total cross sections for the impact of electrons on free radicals CH_x , NH_x and OH are calculated at intermediate to high energies. The known ionization data on the parent molecules CH_4 , NH_3 and H_2O are employed to extract total ionization cross sections of the respective radicals using total inelastic cross sections, which we have calculated through a complex optical potential. The results give an *upper bound* of the total ionization cross section in the energy region around 100 eV, and are in suitable harmony with available experimental data at higher energies.

1. Introduction

Cross sections for electron scattering from a variety of molecules as well as radicals are in demand in different fields of the pure and applied sciences (Mason *et al* 1999, Schram 1996, Christophorou 1984). Interest in electron collisions with transient (reactive) radicals such as CH_x ($x = 1, 2, 3$), NH_x ($x = 1, 2$) and OH has grown recently, in view of their important role in developing technological plasma devices. The present paper aims at studying theoretically the electron collision parameters of CH_x , NH_x and OH *vis-à-vis* their parent stable molecules CH_4 , NH_3 and H_2O , respectively. At the impact energies E_i above ionization thresholds (usually around 10–15 eV) considered here, the target–projectile coupling is not strong, but a large number of channels (excitation, ionization, etc) are open. At high energies, since the elastic and the ionization channels dominate, it is meaningful to separate the total (complete) cross section $Q_{\text{tot}}(E_i)$ into total elastic cross section $Q_{\text{el}}(E_i)$ and total inelastic cross section $Q_{\text{inel}}(E_i)$, which includes the total ionization cross section $Q_{\text{ion}}(E_i)$. Extensive theoretical and experimental investigations on electron collisions with CH_4 , NH_3 and H_2O have been reported. Various total cross sections (TCS) of these targets were calculated by Jain and Baluja (1992) and Joshipura (1998). The ionization TCS were measured for various molecules by Rapp and Englander-Golden (1965) and Schram *et al* (1966), for CH_4 by Orient and Srivastava (1987) as well as Tian and Vidal (1998), for NH_3 by Djuric *et al* (1981) and Rao and Srivastava (1992), and for H_2O by Straub *et al* (1998). Different sets of experimental data for the same target are found to be at variance with each other. On the theoretical front, we have successfully examined, at intermediate and high energies, a good number of targets such as NO, CO, O_3 ,

Table 1. Molecular properties (Lide, CRC Handbook 1994).

Target	A–H bond length (a_0)	Ionization energy (eV)
CH	2.12	10.64
CH ₂	2.04	10.40
CH ₃	2.04	9.84
CH ₄	2.05	12.50
NH	1.96	13.49
NH ₂	1.94	11.14
NH ₃	1.91	10.13
OH	1.83	13.17
H ₂ O	1.81	12.6

NO₂ and N₂O (Joshipura and Patel 1996), the reactive targets HF, OH, NH and CH, triatomics H₂S, SO₂ and OCS (Joshipura and Minaxi 1997a, b) and also C₂H₂, C₂H₄, C₂H₆ and CH₃X (X = OH, NH₂ and F) (Joshipura and Minaxi 1999). In these papers Q_{el} and Q_{inel} were obtained by treating the elastic and the cumulative inelastic scattering simultaneously in the complex optical potential formalism. Our results obtained therein on the total (complete) cross sections were in accord with the available experimental data on these molecules. The calculated inelastic TCS Q_{inel} provide an upper limit to the more important quantities Q_{ion} . The two cross sections are quite close to each other at energies around 1000 eV. Based on this fact an alternative approach to calculating Q_{ion} may be developed. A simple theory called the binary-encounter Bethe (BEB) model has been developed by Kim's group (Kim and Rudd 1994, Hwang *et al* 1996, Huo *et al* 2000, Kim 2000) to obtain Q_{ion} for a very large number of molecular targets. This theory together with the one given by Khare *et al* (1999 and references therein) requires certain input data of the target atom or molecule to be obtained separately.

As regards the radical species, Tarnovsky *et al* (1996, 1997, 1998) reported absolute total ionization cross sections for CD_x, ND_x and OH radicals from threshold to 200 eV. Electron impact total ionization cross sections of CH₂ and CH₃ were first measured by Baiocchi *et al* (1984). The latter data are likely to be on the lower side. Theoretical results of Kim's group include the CH_x radicals. There are no calculations on NH_x and OH radicals, hence presently we estimate the Q_{ion} for all of these targets using a new approach, which can be easily extended to other radicals and molecules. This paper offers extensive results and comparisons of the various total cross sections of the ubiquitous free radicals listed in the title. The molecular properties of these targets are highlighted in table 1 (see also Lide 1994). These properties help us gain an insight into the relative behaviour of the cross sections obtained within the present theoretical approach.

2. Theory and calculations

The e–molecule dynamics is effectively modelled here in terms of a complex local optical potential that can be calculated from the electronic charge density of the target molecule. Consider, as in Joshipura and Patel (1996) and Joshipura and Minaxi (1999), a free radical (or a chemical bond in a molecule) denoted by AH_{*n*}, with *n* the number of H atoms therein. It becomes convenient and useful to write the target charge density ρ_{T} in terms of atomic charge densities ρ_{A} and ρ_{H} as follows:

$$\rho_{\text{T}} = f_{\text{A}}\rho_{\text{A}} + nf_{\text{H}}\rho_{\text{H}} \quad (1)$$

where f_A (f_H) is the modulating factor obtained from the known values of the charge migrated to or from atom A (H), namely q_A (q_H) in the process of covalent bonding. The prescription of equation (1) is better than that given by Bader (1990), i.e.

$$\rho_{AB} = \rho_A + \rho_B \quad (2)$$

for a molecule AB, wherein the bonding or overlap is ignored. The bond charges transferred partially to or from atom A, i.e. q_A in the formation of AH_n , have been tabulated (Bader 1990) in a number of simple cases. In the OH molecule, for example, the charge migrated to the O-atom is $q_A = |-0.585|$, so that the modulating factors in equation (1) are

$$f_A = \frac{N(A) + q_A}{N(A)} \quad (3)$$

and

$$f_H = \frac{N(H) - q_A}{N(H)}. \quad (4)$$

For OH we have $f_A = 1.073$ and $f_H = 0.415$. We employ the factors f_A and f_H in equation (1) so that it integrates to

$$N(T) = N(A) + N(H) \quad (5)$$

where $N(T)$ is the total number of electrons in AH_n , while $N(A)$ and $N(H) = 1$ are the number of electrons for atoms A and H, respectively. We thus obtain the total renormalized charge density of the target AH_n . This charge density is then brought to a single centre at A by employing the standard expansions, as in Gradshetyn and Ryzhik (1980). The charge density $\rho_T(r; R_{A-H})$ determined in this way forms an input to calculate various e- AH_n scattering potentials. Furthermore, the total electron-molecule interaction V is broken up into short- and long-range parts as in our previous work (Joshiyura and Patel 1996), in the following manner:

$$V = V_{SR} + V_{LR} \quad (6)$$

where V_{LR} is the long-range (mainly polarization) potential, for which a dynamic form may be employed. The resulting contribution to the TCS is quite small. For polar molecules the long-range anisotropic dipole potential must be treated separately. The short-range potential in a complex form incorporates various physical effects as follows:

$$V_{SR} = V_{st}(r) + V_{ex}(r, E_i) + iV_{abs}(r, E_i). \quad (7)$$

The first two terms on the right-hand side of equation (7) are the static and the exchange potentials. The absorption potential V_{abs} accounts for the total loss of flux into the open channels of electronic excitation as well as ionization. As in our earlier work we have adopted here a quasi-free non-empirical scattering model of the absorption potential (Staszewska *et al* 1984, Blanco and Garcia 1999), after a slight modification. This absorption potential may be written as

$$V_{abs}(r, E_i) = T_1 + T_2 + T_3. \quad (8)$$

The three terms in equation (8) denote various functions of the target properties such as charge density ρ_T , ionization energy I and an energy parameter Δ , together with the energy of impact E_i . Generally, the parameter Δ is chosen to be equal to the ionization energy of the target atom or molecule. This choice is appropriate for one of the three terms (T_3), which dominate in the valence electron region of the target. The remaining two terms are important in the region of inner shells that are harder to ionize or excite. Hence in this paper we have chosen

$\Delta = I$ in the former case, and $\Delta > I$ in the latter case. This correction effectively reduces the strength of the absorption potential as in the case of Blanco and Garcia (1999). With this we construct V_{abs} as well as the other terms of the short-range potential V_{SR} to determine the complex scattering phase shifts $\delta_l(k)$ by solving the radial Schrödinger equation numerically. Employing standard expressions (Joachain 1983) we then calculate the elastic TCS Q_{el} and the inelastic TCS Q_{inel} such that the total (complete) cross section is determined through

$$Q_{\text{T}}(E_i) = Q_{\text{el}} + Q_{\text{inel}}. \quad (9)$$

To this we must also add the dipole rotational excitation cross section $Q_{\text{rot}}(D, E_i)$ for polar molecules and define the grand total cross section

$$Q_{\text{tot}} = Q_{\text{T}} + Q_{\text{rot}}. \quad (10)$$

Here it is sufficient to calculate Q_{rot} in the first Born approximation. Next we concentrate on Q_{inel} which contains the TCS of ionization together with electronic excitation processes. Theoretically, Q_{inel} is the upper bound of Q_{ion} , but in order to obtain some more information regarding the latter, let us define a ratio

$$R(E_i) = \frac{Q_{\text{ion}}(E_i)}{Q_{\text{inel}}(E_i)} \quad (11)$$

which is less than (but generally close to) 1 and which indicates the relative importance of excitation to discrete versus continuum states. It differs from target to target and cannot be calculated rigorously. For the water molecule Turner *et al* (1982) estimated this ratio theoretically to be about 0.75 for energies above 100 eV. We have noted a trend in this ratio for the molecules CH_4 , NH_3 and H_2O , for which a lot of experimental data exists. Using our calculated Q_{inel} and the measured values of Q_{ion} , the ratio is found to exhibit the following behaviour. For CH_4 ,

$$R(E_i) \cong \begin{cases} 0.7 & \text{at } E_i \cong 100 \text{ eV} \\ 1.0 & \text{for } E_i > 300 \text{ eV.} \end{cases} \quad (12)$$

Above 100 eV, 80% or more of the inelastic cross section comes from the valence electron ionization, in keeping with the observation of Khare *et al* (1999). For NH_3 and H_2O the ratio is

$$R(E_i) \cong \begin{cases} 0.8 & \text{at } E_i \cong 100 \text{ eV} \\ 1.0 & \text{for } E_i \geq 1000 \text{ eV.} \end{cases} \quad (13)$$

In each of these cases the above ratio may be used along with the present values of Q_{inel} to infer Q_{ion} for the respective free radicals.

3. Results, discussions and conclusions

Calculations of various cross sections for the present targets were carried out as discussed in section 2, at electron energies of 20–2000 eV. One may think of obtaining the ratios $R(E_i)$ purely experimentally for the parents CH_4 , NH_3 and H_2O . This requires an experimental measurement of Q_{inel} , which may be extracted through

$$Q_{\text{inel}} = Q_{\text{tot}} - Q_{\text{el}} \quad (14)$$

where both the TCS on the right-hand side should be experimental. We made sample calculations to illustrate this procedure for total e– H_2O inelastic cross sections, and these are

Table 2. Total inelastic cross sections (in 10⁻¹⁶ cm²) of e-H₂O collisions.

Energy (eV)	Present calculations	$Q_{\text{inel}} = Q_{\text{tot}} - Q_{\text{el}}$ (experimental)
30	1.21	0.15 ^b
50	2.17	2.02 ^b
100	2.60 (2.65) ^a	4.21 ^c (2.62) ^d
200	2.12 (2.30) ^a	2.75 ^e
300	1.70	2.06
500	1.22	1.44
700	0.96	1.00
1000	0.73	0.88

^a Theoretical values of Jain (1986).^b Q_{el} of Okamoto *et al* (1993) and Q_{tot} of Sueoka *et al* (1986).^c Q_{el} of Katase *et al* (1986) and Q_{tot} of Zecca *et al* (1987).^d Using the results of Katase *et al* (1986) and Sueoka *et al* (1986).^e This and the rest, as in c above.**Table 3.** The present total ionization cross sections Q_{ion} (10⁻¹⁶ cm²) for various radicals

E_i (eV)	CH	CH ₂	CH ₃	NH	NH ₂	OH
20	0.83	1.20	1.50	0.40	1.05	0.30
30	1.75	2.20	2.40	1.03	2.00	1.00
40	2.47	2.67	3.17	1.60	3.35	1.40
50	2.70	2.91	3.52	1.90	3.71	1.55
60	2.75	3.15	3.80	2.05	3.81	1.70
70	2.82	3.13	3.81	2.12	3.78	1.85
80	2.80	3.05	3.70	2.15	3.70	1.80
100	2.66	2.85	3.38	2.10	3.50	1.78
200	1.95	2.10	2.50	1.55	2.50	1.50
300	1.60	1.76	1.90	1.18	1.91	1.17
400	1.44	1.45	1.65	0.97	1.57	0.98
500	1.30	1.30	1.45	0.82	1.33	0.84
600	1.01	1.07	1.22	0.76	1.16	0.78
700	0.86	—	1.08	0.67	1.03	—
800	0.80	0.92	0.95	0.60	0.92	0.63
900	—	0.85	—	0.57	0.84	0.56
1000	0.66	0.75	0.82	0.52	0.77	0.53
2000	0.35	0.43	0.50	0.32	0.43	0.35

exhibited in table 2. Here the Q_{inel} at and above 100 eV are extracted from the experimental Q_{tot} of Zecca *et al* (1987) and the Q_{el} of Katase *et al* (1986), while below 100 eV the Q_{el} are from Okamoto *et al* (1993) and the Q_{tot} we have used are those measured by Sueoka *et al* (1986). Table 2 compares these ‘experimental’ Q_{inel} with the present theoretical values of Q_{inel} . At 100 eV the Q_{inel} extracted from the same Q_{el} but two different Q_{tot} , namely those of Sueoka *et al* (1986) and Zecca *et al* (1987), differ largely, and are higher than our theoretical results. The theoretical values of Jain (1986) are close to ours (table 2). The two cross sections Q_{tot} and Q_{el} required in equation (14) are usually measured by different groups in different ranges of energy, hence it appears reasonable to use the present theoretical Q_{inel} as obtained in our complex potential calculations, to determine $R(E_i)$ for the concerned parent molecules.

Thus, for the hydrocarbons CH_x ($x = 1, 2, 3$) the present Q_{ion} were obtained from our calculated Q_{inel} by choosing the same ratio $R(E_i)$ as that of the parent CH₄. The choice is appropriate in view of the common central atom (C) and the similarity of covalent bonding

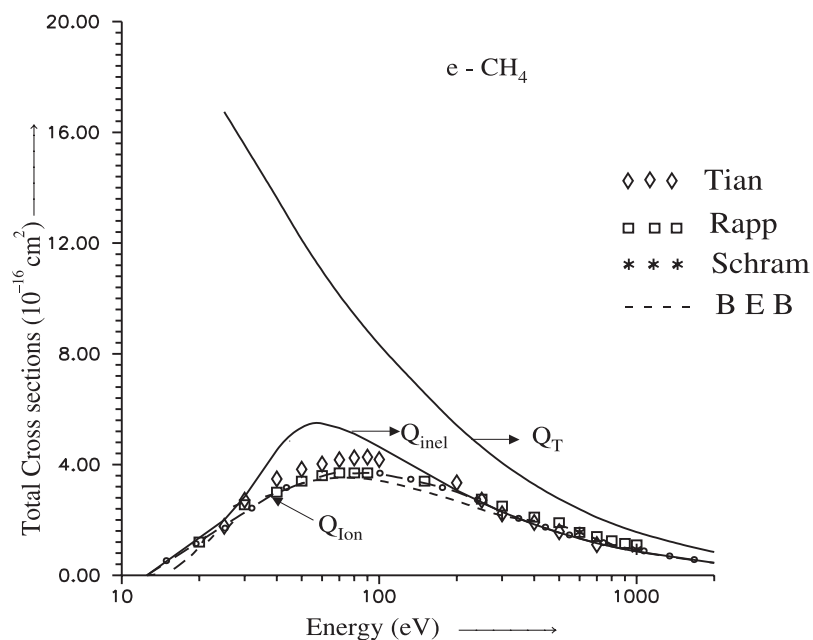


Figure 1. $e\text{-CH}_4$ scattering. Upper curve: —, Q_T , the present total (complete) cross sections; Lower curves: —, present Q_{inel} ; $-\circ-$, present Q_{ion} ; $- - -$, BEB theory. Experimental Q_{ion} data: \diamond , Tian and Vidal (1998); \square , Rapp and Englander-Golden (1965); $*$, Schram *et al* (1966).

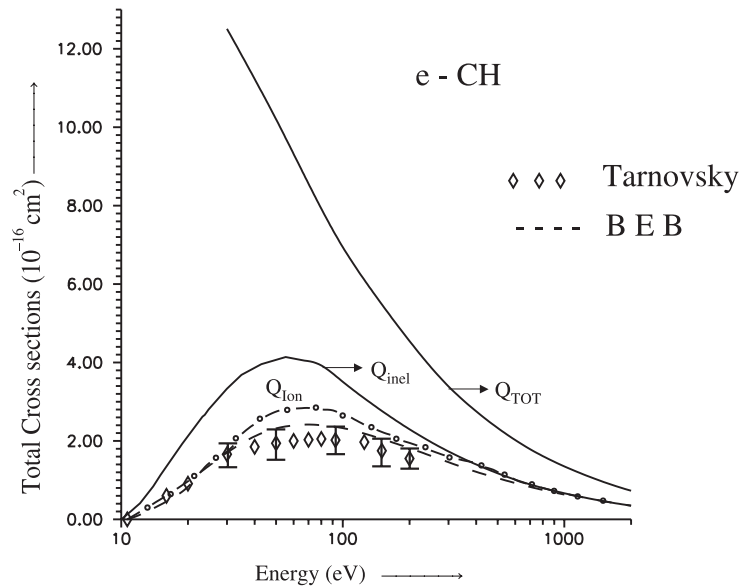


Figure 2. $e\text{-CH}$ scattering. Upper curve: Q_{tot} , the present grand total cross sections. Lower curves: — and $-\circ-$, present results, as in figure 1. $- - -$, BEB theory. Experimental Q_{ion} data: \diamond , Tarnovsky *et al* (1996).

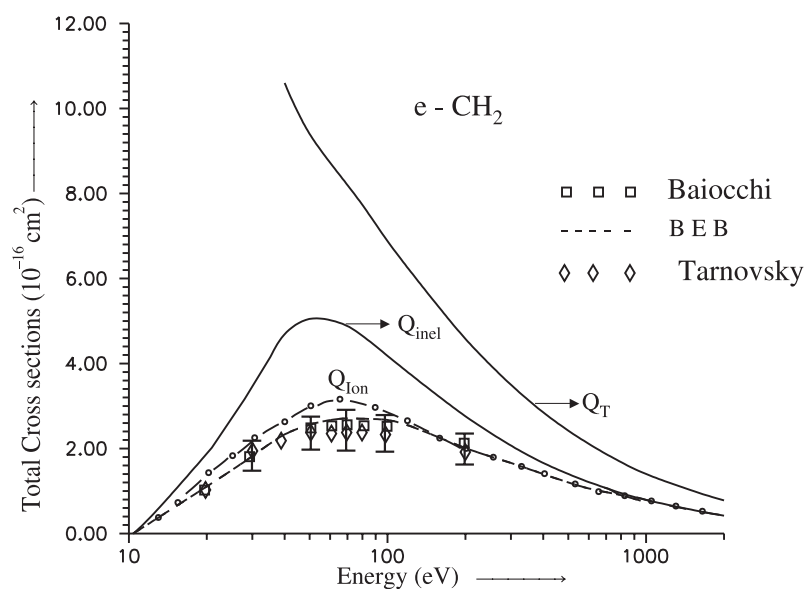


Figure 3. e-CH_2 scattering. Upper curve, —, Q_T , present. Lower curves, same as in figure 1. Experimental Q_{ion} data: \diamond , Tarnovsky *et al* (1996); \square , Baiocchi *et al* (1984).

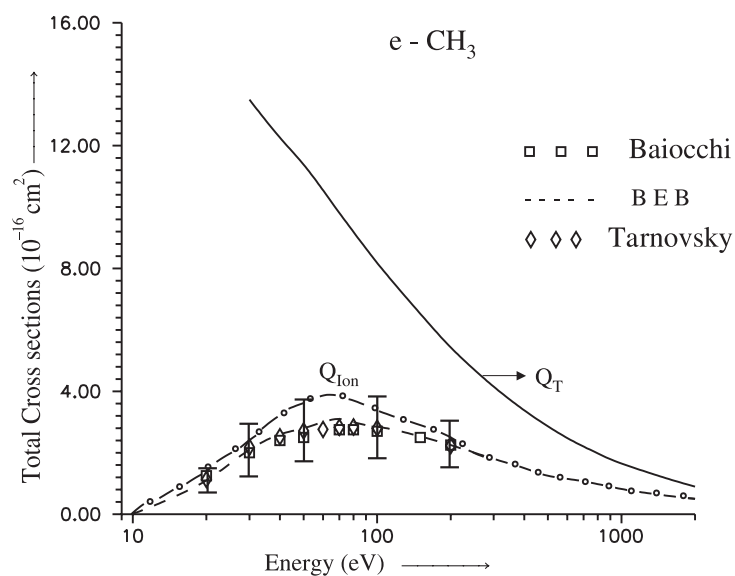


Figure 4. e-CH_3 scattering. Labelling as in figure 3.

among the radicals *vis-à-vis* the parent molecule CH_4 . To calculate the ratio, use was made of our own Q_{inel} together with the Q_{ion} data of Rapp and Englander-Golden (1965). In a similar manner, the ionization TCS of the NH_x ($x = 1, 2$) as well as OH radicals were obtained from our theoretical inelastic TCS by employing the ratios $R(E_i)$ of the parent NH_3 and H_2O , through the Q_{ion} measurements of Rao and Srivastava (1992), and of Straub *et al* (1998), respectively. Table 3 and figures 1–6 represent our results.

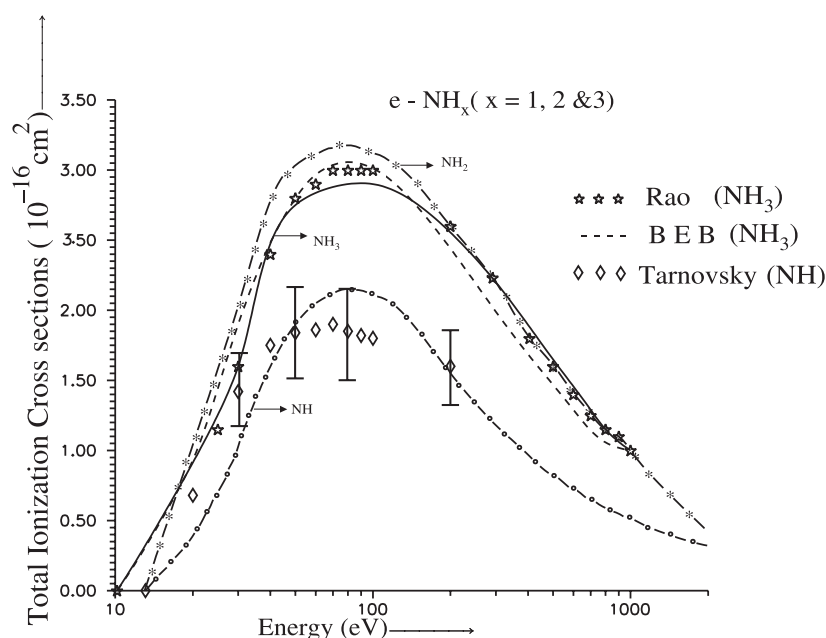


Figure 5. Comparison of the present Q_{ion} for NH_x ($x = 1, 2, 3$) with experiments, $-\circ-$, NH, \diamond , NH, measured Q_{ion} (Tarnovsky *et al* 1997); $- - -$, NH_3 , BEB theory; $—$, NH_3 present; \star , NH_3 , measured data (Rao and Srivastava 1992); $-*-$, NH_2 .

Consider first the present results on $e\text{-CH}_4$ scattering as shown in figure 1. The total (complete) cross sections Q_{T} are seen to be dominated by elastic scattering at intermediate energies, with no dipole rotation in CH_4 . Around 100 eV, the present theoretical Q_{inel} lies above both the experimental data sets, as it should, but as the energy increases our inelastic cross sections and all three measured data exhibited in figure 1, quickly tend to get closer. This behaviour is also observed in the case of C_2H_2 as well as C_2H_6 (Joshipura and Minaxi 1999). The CH_4 ionization results of the BEB model agree very well with the lower set of data, namely that of Rapp and Englander-Golden (1965), in figure 1. In our graphical plots for $e\text{-CH}$ cross sections the Q_{tot} , Q_{el} , Q_{inel} as well as the present Q_{ion} are exhibited as functions of E_i , in figure 2. It is found that low to intermediate energy results in this case are dominated by dipole rotation and elastic scattering. Q_{el} equals Q_{inel} in the peak region of inelastic scattering (see Bransden 1983), i.e. around 70 eV. With increasing energy E_i the inelastic TCS of the CH radical soon approaches its ionization TCS (figure 2), as expected. This appears to be the trend of targets containing the C–H bond. The measurements of Tarnovsky *et al* (1996) are available up to 200 eV. The BEB results lie just above these measurements, and our present Q_{ion} are somewhat higher in the peak region. The experimental values together with both the present and the BEB results tend to merge beyond 400 eV. All the experimental results quoted in our figures 1–6 involve errors of about 17%.

The present results on $e\text{-CH}_2$ and $e\text{-CH}_3$ collisions are depicted in our figures 3 and 4, respectively. Also shown therein are the BEB calculations of Hwang *et al* (1996) as well as the measurements of Tarnovsky *et al* (1996) and Baiocchi *et al* (1984). In the region of maximum Q_{ion} , namely between 50 and 200 eV, both the measured data sets exhibit a flat peak in comparison with both the theories. At these energies the present ionization TCS lie just above (CH_2) or within (CH_3) the experimental error bars. The theoretical values of Hwang

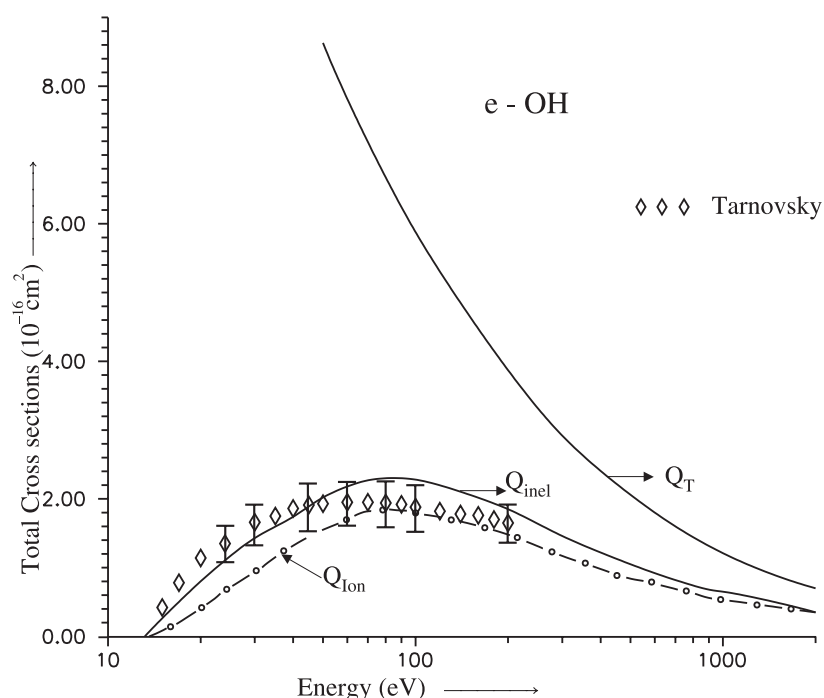


Figure 6. e-OH scattering. Upper and lower curves: present Q_{inel} and Q_{ion} as in figure 1; \diamond , Q_{ion} data (Tarnovsky *et al* 1998).

et al are closer to the measurements, for both CH_2 and CH_3 . The measurements of Baiocchi *et al* (1984) could be a lower bound to the actual ionization TCS since these experiments did not include contributions from C^+ and D^+ ions as mentioned by Tarnovsky *et al* (1996). The present Q_{ion} serve as the corresponding upper bound in the peaking region around 70 eV. The present and the rest of the results tend to merge beyond 200 eV or so. The other features of figures 3 and 4 are similar to those of figure 1.

It is also observed that in the region of maximum values, the ionization cross sections increase slightly along the sequence $\text{CH}-\text{CH}_2-\text{CH}_4-\text{CH}_3$. This is understood in terms of the molecular properties shown in table 1. These properties also affect the peak positions slightly. Towards high energies the Q_{ion} are governed by the total number of electrons and the typical bond lengths in the targets, and hence are close together.

Consider next the free radicals NH_x ($x = 1, 2$) together with NH_3 . For brevity we focus only upon the present Q_{ion} , which have been compared mutually for these targets in figure 5. The ratio $R(E_i)$ in this case is obtained through Q_{ion} of NH_3 , measured by Rao and Srivastava (1992). The trend in NH_x is similar to that of the CH_x species. One notices from figure 5 that among the three targets the NH radical shows the lowest ionization TCS. For reasons of clarity we did not show the data points for NH_2 . For NH_2 and NH_3 the present values are closer, in keeping with the observations of Tarnovsky *et al* (1997). The relative differences in the $\text{NH}-\text{NH}_2-\text{NH}_3$ sequence can be interpreted in terms of the respective ionization energies and the bond lengths, as per table 1. The BEB values available for NH_3 are close to the measured data shown in figure 5. Our Q_{ion} calculations for NH (and NH_2) agree with experimental results within error limits. The BEB results for the radicals NH_x and OH are not available. Finally, our theoretical studies on e-OH scattering are summarized in figure 6. There is a

large contribution from elastic scattering plus rotational excitation at low to medium energies in this case too. It can be seen here that, as compared with our calculated values the Q_{ion} measurements of Tarnovsky *et al* (1998) show a faster rise between the threshold and about 40 eV. Our calculated Q_{ion} matches these measurements in the peak region and beyond. The ionization cross section peaks around 70 eV.

Thus in conclusion we have investigated the ionizing collisions of electrons with the free radicals CH_x , NH_x and OH , at medium to high incident energies. Employing a modified absorption potential we calculated the inelastic TCS Q_{inel} , from which Q_{ion} for each target species were estimated. This approach seems to be reliable since in the present range of energies the single ionization dominates over all the other inelastic processes. The present ionization TCS are seen to be either within the error limits of experimental data or somewhat higher, near 70 eV or so. For targets having an ionization energy of about 10 eV or less, the present theory exceeds other data by nearly 20%. The plus point of this limitation is that our Q_{ion} provide an upper limit of this quantity in the peak region. Therefore, the present approach is worth trying when no experiments are available. At higher energies, the present results are in general accord with other theories and measurements. The relative magnitudes of the cross sections of various target species are explained here in terms of the bond lengths and ionization energies, which are quite well established quantities. The BEB theory which has been applied successfully to a number of targets, rests on the binding energies and the kinetic energies of the target MOs, obtained either experimentally or theoretically. In the present theory the choice of the energy parameter Δ effectively represents the tightly bound inner orbitals, as stated in section 2. Comparative features such as these make the present approach a useful alternative to the existing theories, especially for exotic targets such as the transient radicals for which there is limited or no information available at present. It is of interest now to apply the present method to radicals like SiF , SiF_2 , SiF_3 , OCIO , SiH_x , CF_x , etc, on one hand, and to heavier hydrocarbon molecules, on the other hand.

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